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ABSTRACTS

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling the Behavior of PC/ABS Ternary Blends

Author(s): *A. Francisca Carvalho Alves, *University of Porto*; Bernardo P. Ferreira, *University of Porto*; Francisco M. Andrade Pires, *University of Porto*;

The industrial demand for polymer blends is continuously increasing since it is possible to design the mixture behavior for each specific application. In particular, through the combination of the excellent thermal and mechanical properties of PC and impact properties of ABS, the rubber toughened ternary blend PC/ABS is one of the most successful commercial polymer blends [1]. This blend finds its main applications in the automotive and consumer electronics sectors. Nevertheless, despite the importance of these materials, the relation between their complex heterogeneous microstructure and the overall mechanical properties and fracture mechanisms is not yet fully understood. Several authors have modeled the constitutive behavior of glassy polymers. In particular, Mirkhalaf et al. [2] modified the Eindhoven Glassy Polymer (EGP) model to predict glassy polymers' nonlinear behavior. However, this model does not account for the mechanism of crazing, which is the predominant failure mechanism in brittle polymers. Nevertheless, different techniques to model crazing have also been proposed. Gearing and Anand [3] described the three stages of crazing by using continuum-based models, where deformation by crazing is given as the average response of a Representative Volume Element (RVE) characterizing the craze-microstructure. In the present contribution, an extended version of the Mirkhalaf et al. [2] model is proposed to account for crazing and, hence, allow for a more accurate prediction of glassy polymers' deformation behavior. The extended model's material parameters are calibrated for the PC and ABS materials by conducting uniaxial compression tests at different temperatures. By considering an RVE of PC/ABS blend, here assumed as a heterogeneous two-phase material, first-order hierarchical multiscale analyses based on computational homogenization are conducted. Each phase is modeled with the proposed constitutive model (previously calibrated). The homogenized and experimental results of several tests under different triaxility conditions are then compared for PC/ABS blends with varying mixture ratios. This research is a step forward in the development of a constitutive continuum model for predicting the homogenized thermomechanical behavior of the PC/ABS polymer blend. References [1] Inberg, J. P. F. Fracture of polycarbonate/ABS blends. Universiteit Twente. (2001). [2] Mirkhalaf, S., Andrade Pires, F., and Simoes, R. An elasto-viscoplastic constitutive model for polymers at finite strains: Formulation and computational aspects. Computers & Structures. (2016) 166:60–74. [3] Gearing, B. and Anand, L. On modeling the deformation and fracture response of glassy polymers due to shear-yielding and crazing. International Journal of Solids and Structures. (2004) 41(11-12):3125–3150.

16th U.S. National Congress on Computational Mechanics
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Title: Scale-Senstivite Homogenization Utilizing Deep Neural Networks

Author(s): *Aaron Allred, *University of Colorado Boulder*;

Computational multiscale modeling of heterogeneous material systems requires solving a boundary value problem on the microscale and performing computational homogenization to achieve high fidelity solutions– a task which is often computationally expensive. Alternatives to computational homogenization are often burdened with low fidelity approximations or assumptions derived for periodic microstructures. However, data-driven-based neural networks have emerged as feasible surrogate models in place of numerical and analytical homogenization schemes to describe the constitutive behavior of heterogeneous composite materials. A cornerstone to this idea, Le et al. demonstrated the ability for a neural network to describe the potential function of a nonlinear elastic material [1]. More recent efforts have utilized deep neural networks to predict both the nonlinear plastic response on the macroscale from a macroscopic strain history dataset [2] and the macroscopic elastic tensor from a RVE image using a convolutional neural network [3]. Unfortunately, these surrogate models do not account for the size of the microstructure volume element (MVE) in relation to the macroscale. This effort demonstrates the feasibility of utilizing neural network surrogate models to produce a scale sensitive homogenization scheme by leveraging direct numerical simulation (DNS) snapshot truth data. The incorporation of a DNS snapshot trained surrogate model for homogenization precludes reliance on the separation of scales assumption or other numerical homogenization techniques such as first-order homogenization in which the governing equations are asymptotically expanded to achieve a separation of scales. The MVEs for this task are randomly generated via a Gaussian random process, and the DNS models are subsequently constructed from the MVEs. [1] Le, B. A., Yvonnet, J., and He, Q.-C. “Computational Homogenization of Nonlinear Elastic Materials Using Neural Networks.” International Journal for Numerical Methods in Engineering, Vol. 104, No. 12, 2015, pp. 1061–1084. https://doi.org/10.1002/nme.4953. [2] Logarzo, H. J., Capuano, G., and Rimoli, J. J. “Smart Constitutive Laws: Inelastic Homogenization through Machine Learning.” Computer Methods in Applied Mechanics and Engineering, Vol. 373, 2021, p. 113482. https://doi.org/10.1016/j.cma.2020.113482. [3] Rao, C., and Liu, Y. “Three-Dimensional Convolutional Neural Network (3D-CNN) for Heterogeneous Material Homogenization.” Computational Materials Science, Vol. 184, 2020, p. 109850. https://doi.org/10.1016/j.commatsci.2020.109850.

16th U.S. National Congress on Computational Mechanics
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Title: Simulation of Earthquake-Triggered Landslides and Site Response Using the Material Point Method

Author(s): *Abdelrahman Alsardi, *Virginia Polytechnic Institute and State University*; Alba Yerro, *Virginia Polytechnic Institute and State University*;

Earthquakes catastrophically manifest in strong ground shaking that can lead to large deformations and infrastructure damage. Earthquake-triggered landslides can also be responsible for a significant part of the losses associated with an earthquake (Bird and Bommer, 2004). The current state-of-the-practice, mesh-based and analytical methods, adopt simplified assumptions that restrict their applications to failure initiation, but are unable to predict post-failure deformations and multi-phase interaction. This research proposes the Material Point Method (MPM) that is capable of modeling large strain of history dependent materials for the study and prediction of seismic-induced problems such as landslides. Two types of boundary conditions are proposed: (a) time dependent prescribed velocity approach employed with a moving mesh technique; and (b) tied boundary conditions with a particle domain relocation technique. The first one is employed to prescribe the dynamic shaking on the model while reducing the numerical artifacts due to particle cell crossing. The second one is important to reduce wave reflection on artificial boundaries while allowing for a more accurate simulation of the seismic site response. Firstly, MPM framework is employed to simulate two shaking table laboratory experiments for sand (Hiraoka et al., 2013) and saturated clay (Wartman et al., 2005). Parametric analysis is also conducted with 25 different ground motions to highlight the capabilities of MPM in front of other available techniques (i.e., Finite Elements, Finite Differences and Newmark-type methods). Secondly, a one-dimensional shear wave propagation is simulated and compared to the equivalent-linear iterative approach. The effects of the tied versus fixed boundary conditions and empirical shear modulus degradation curves are parametrically studied. Finally, a centrifuge experiment of level ground shaking is modeled using MPM and an advanced NorSand constitutive approach to validate earthquake site response in saturated sand and pore pressure generation against experimental data. In conclusion, the MPM is presented as a promising tool that is capable of modeling large-strain problems due to seismic loading. References: Bird J.J. & Bommer J.J. (2004). Earthquake losses due to ground failure. Engineering Geology, 75 (2), p. 147-179. Hiraoka, N., Oya, A., Bui, H.H., Rajeev, P. and Fukagawa, R., 2013. Seismic slope failure modelling using the mesh-free SPH method. Int J Geomate, 5(1), pp.660-665. Wartman, J., Seed, R.B. and Bray, J.D., 2005. Shaking table modeling of seismically induced deformations in slopes. Journal of Geotechnical and Geoenvironmental Engineering, 131(5), pp.610-622.

16th U.S. National Congress on Computational Mechanics
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Title: Full Waveform Inversion through a Double-Sweeping Inexact Newton Method

Author(s): *Abdelrahman Elmeliegy Elmeliegy, *North Carolina State University*; Mehran Eslaminia, *Bentley Systems*; Murthy Guddati, *North Carolina State University*;

ABSTRACT Full waveform inversion (FWI), which is widely used in geophysics, reconstructs the unknown material properties given the response at discrete locations at the surface. It is an optimization approach that iteratively estimates the material properties by minimizing the misfit between observed and predicted data. FWI is computationally expensive as it requires the solution of many large-scale forward Helmholtz solves. Large-scale Helmholtz problems with a large number of wavelengths per domain, are notoriously difficult to solve, owing to the oscillatory nature of the solution. Past work on sweeping preconditions (see e.g. [1]) indicates that these problems can be efficiently solved through preconditioners that capture the first arrival as well as the primary reflections. In this effort, we build on this success and adapt the technique in an inexact Newton setting, leading to an efficient FWI methodology. The double-sweeping preconditioner slices the domain into horizontal strips, with each strip interacting with adjacent strips using an interface condition that utilizes the scattering formalism with accurate absorbing boundary conditions [2]. It computes the wavefield starting at the top strip and progressing to the bottom to capture primary arrivals, followed by another sweep in the reverse order to capture the primary reflections that are not captured in the initial sweep. In this work, we utilize the inexact Gauss-Newton approach to perform FWI, where the Hessian vector multiplication is made even more efficient through the (approximate) double-sweeping solver. Through numerical experiments, we show that the convergence of FWI with respect to the number of iterations does not degrade much when the double-sweeping approximation is used. In the end, given that the double-sweeping solver is significantly cheaper than full-wave simulation, the proposed method is several times more efficient than standard FWI. In this talk, we present the complete formulation of the proposed methodology as well as an illustration of its effectiveness to problems of varying complexity ending with the inversion of the Marmousi model from the Geophysics community. REFERENCES [1] Mehran Eslaminia, Murthy N. Guddati, A double-sweeping preconditioner for the Helmholtz equation, J. Comput. Phys., Vol. 314, 2016, 800-823. [2] M.N. Guddati, K.W. Lim, M.A. Zahid, Perfectly Matched Discrete Layers for Unbounded Domain Modeling, "Comput. Methods for Acoustics Prob.", Saxe-Coburg, 2008.

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Title: Stress Fields, Plastic Flow, Contact Friction, and Strain-Induced Phase Transformations in Zr in Traditional and Rotational Diamond Anvils: Coupled Computational and Experimental Approaches

Author(s): *Achyut Dhar, *Iowa State University*; K.K Pandey, *Bhabha Atomic Research Center*; Valery Levitas, *Iowa State University*;

Plasticity and phase transformations (PTs) in materials under high pressure were studied extensively under compression in diamond anvil cell (DAC) and torsion in rotational DAC (RDAC). However, due to very heterogeneous fields of stress and plastic strain tensors and concentration of phases, as well as limited access and measurement possibilities, very limited reliable quantitative information is available [1]. In this work, a coupled computational and experimental framework is proposed to obtain fields of the stress and plastic strain, as well as the concentration of phases throughout the material sample, as well as to calibrate material models. Input from experiments [2] includes variation sample geometry under the load and radial distributions of concentration of phases and radial elastic strain averaged over the sample thickness; variation of lattice parameters of ? and ? phases of Zr under hydrostatic conditions and pressure-dependence of elastic moduli for single and polycrystalline phases. The pressure-dependence of the yield strength of phases was determined. The first level of post-processing of these data was based on a modified Prandtl solution for the stress field, which allowed us to determine the distribution of the shear friction stress at the boundary between sample and anvil and distribution of all stress fields within the sample. Then constitutive model at large elastic and plastic strains and plastic strain-induced PT was developed. The finite element method (FEM) algorithm was developed and used for numerical simulations of a sample's deformational and transformational behavior in DAC and RDAC, including contact interaction between sample and diamonds with variable contact area [3]. A projection gradient-based descent method was applied for the identification of material parameters for plastic flow, contact friction, and strain-induced PT models through minimization of a least-squares functional from experimental data. This approach is applicable for various material systems and PTs.

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Title: Tomography Based Modelling and Design of Next Generation Lithium Ion Battery Electrodes

Author(s): *Adam Boyce, *University College of London*; Emilio Martinez-Paneda, *University College of London*; Xuekun Lu, *University College of London*; Thomas Heenan, *University College of London*; Aaron Wade, *University College of London*; Dan Brett, *University College of London*; Paul Shearing, *University College of London*;

Lithium ion batteries (LIB) span portable electronic devices to electric vehicles, they are ubiquitous in everyday life and play a crucial role in the development of sustainable energy systems. In broad terms, a LIB electrode comprises three discrete phases: the particles where lithium is stored, a porous domain filled with electrolyte where lithium ions are transported, and a conductive additive which provides structural integrity and permits electron flow. Digital twins, i.e. image based models, allow us to develop a greater understanding of these complex multiphase systems whilst providing a platform to optimise and design improved LIB energy storage capabilities. We have used nano and micro X-ray computed tomography to acquire detailed 3D images of the microstructure of a Nickel-Manganese-Cobalt-based LIB electrode. These images form the basis for an experimentally validated physics-based electrochemical model, enabling the prediction of LIB performance. Furthermore, image processing techniques such as morphological operations can be used to make realistic alterations to the original CT image, enabling parametric studies where we may, for example, alter the volume fractions of the phases. The optimisation of battery life cycle is a significant and important challenge which must be overcome in order to provide more sustainable energy storage. Loss in storage life, or capacity is a multifaceted issue driven by, amongst other mechanisms, particle fracture and disintegration. We augment the electrochemical image-based model to predict mechanical swelling of electrode particles which occurs due to lithium insertion. The resultant swelling-induced stresses lead to fracture of the particles and loss in the energy storage and charging capabilities of the electrode over time. Fracture is captured using a physics-based phase field approach allowing complex crack initiation, branching, and propagation to be predicted. The inclusion of particle swelling and fracture within the image-based model facilitates the prediction of various degradation mechanisms such as the delamination of the electrode from its underlying substrate (the current collector), which we compare with experiment. Image based modelling is a powerful technique which facilitates detailed analysis and design of real-life micro- and nanoscale structures, moving beyond the traditional idealised and homogenised modelling frameworks.

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Title: Immersogeometric Analysis of Flow Over Point Cloud Representations of Objects

Author(s): *Aditya Balu, *Iowa State University*; Joel Khristy, *Iowa State University*; Manoj Rajanna, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

We present a novel immersogeometric analysis (IMGA) approach for flow around complex geometries represented using point clouds. Typical CAD models are usually complex and cannot be automatically handled by mesh generation software without manual intervention such as defeaturing, geometry cleanup, and mesh manipulation to solve issues such as missing surfaces, gaps, and mesh overlaps. IMGA overcomes this mesh generation challenge by directly immersing the CAD model into the non-body-fitted background fluid discretization and performing flow analysis. The IMGA method has been successfully applied to simulate both incompressible and compressible fluid flows over CAD models represented using triangles, non-uniform rational B-splines (NURBS), and analytic surfaces [1, 2]. However, performing flow analysis over real-life objects requires reconstructing the CAD model, which could be as tedious as the mesh generation process. Point cloud representation is the direct method for acquiring geometric information in a digital form using LIDAR scanners, optical scanners, or even other passive methods such as multi-view stereo images. In a point cloud representation, the geometry of the object is represented using a set of unstructured points in the Euclidean space with (possible) orientation information in the form of surface normals. The objective of this work is to perform IMGA directly using the point cloud representation of the geometry, thus enabling flow analysis over as-manufactured components. Due to the absence of any topological information in the point cloud, there are no guarantees on the geometric representation to be watertight or 2-manifold, which makes performing the inside-outside test on the background mesh challenging. To address this challenge, we first develop methods for estimating the inside-outside information directly from point clouds. We also compute the Jacobian for the surface integration required for enforcing the Dirichlet boundary conditions necessary for performing the flow analysis. We validate these geometric estimation methods and compare the point cloud IMGA results with those obtained from a CAD model represented using triangles. We finally demonstrate the scalability of our approach by performing immersogeometric analysis on large industrial scale construction machinery represented using a very dense point cloud of more than 4 million points. References: 1. Chenglong Wang, Fei Xu, Ming-Chen Hsu, Adarsh Krishnamurthy; Rapid B-rep model preprocessing for immersogeometric analysis using analytic surfaces, Computer Aided Geometric Design, 52-53:190–204, 2017. 2. Ming-Chen Hsu, Chenglong Wang, Fei Xu, Austin J. Herrema, Adarsh Krishnamurthy; Direct immersogeometric fluid flow analysis using B-rep CAD models, Computer Aided Geometric Design, 43:143–158, 2016.

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Title: A Quasicontinuum Approach for Modeling Fracture and Damage in Polymer Networks: Role of Viscoelastic Properties and Rate Dependent Failure

Author(s): *Ahmed Ghareeb, *University of Illinois at Urbana-Champaign*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*;

Polymer networks constitute the skeleton for many natural and humanmade materials such as biological tissues, rubbers, and gels. The load bearing system of polymer networks could be abstracted as a complex network of non-linearly interacting polymer chains with viscoelastic properties while inter-connected by rate-dependent cross-linkers. Damage and fracture of polymer networks are intrinsically multiscale processes with high dependence on the network microscale topology. However, it is computationally prohibitive to adopt a full discrete approach to capture the local topology effects for large scale samples. In this work, we propose an extension to the adaptive quasicontinuum approach [1] to model polymer networks with viscoelastic properties and rate dependent failure. In regions of high interest, for example near the crack process zone, explicit representation of the polymer chains is retained, whereas away from these imperfections the mechanical response is computationally homogenized to a continuum representation through an energy consistency condition. Dynamic mesh adaptivity enables transition between the discrete and the continuum representations for optimizing both accuracy and computational efficiency. In addition, time adaptivity ensures the time step is adequate for resolving crack propagation accurately. The proposed approach enables accurate modeling of crack initiation and propagation without apriori constraint on the fracture energy while maintaining the influence of large-scale viscoelastic loading in the bulk. We verify the proposed approach against a fully discrete approach to demonstrate its accuracy and efficiency. We further use the method to study the failure patterns and toughness of polymer networks with different viscoelastic and rate-dependent failure properties. [1] Ghareeb, Ahmed, and Elbanna, Ahmed. 2020. “An Adaptive Quasicontinuum Approach for Modeling Fracture in Networked Materials: Application to Modeling of Polymer Networks.” Journal of the Mechanics and Physics of Solids, 137: 103819.

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Title: Modeling Mechanics and Electrochemistry of Ionic Polymer Metal Composites: From Continuum Theories to Finite Element Analysis and Structural Modeling

Author(s): *Alain Boldini, *New York University*; Lorenzo Bardella, *University of Brescia*; Maurizio Porfiri, *New York University*;

Ionic polymer metal composites (IPMCs) are electroactive polymers composed by an ionic polymer between two plated noble metal electrodes. The ionic polymer is a negatively charged porous membrane. A solution with cations saturates the membrane, neutralizing its negative charges and ensuring electroneutrality. A voltage applied across the electrodes disrupts such equilibrium, causing cations' migration within the membrane along with the formation of boundary layers at the interface between the membrane and electrodes. This phenomenon is accompanied by water migration associated with osmotic pressure and by Maxwell stress due to material polarization. These two stresses contribute to the overall eigenstress in the membrane, thereby eliciting macroscopic bending of the IPMC. Despite the vast literature on IPMC modeling, several questions about their mechanics and electrochemistry remain untapped. Finite element (FE) simulations of chemoelectromechanics of IPMCs are scarce, due to the challenges in resolving nanometer-thick boundary layers of charge. Further, whether classical structural models can be utilized to describe IPMC deformations is still unclear. Here, we seek to address these technical gaps through advancements in computational mechanics and structural theories. Building on our group's continuum model of IPMCs [1], we investigate the plane-strain response of a simply supported membrane. We implement a FE model of nonlinear IPMC chemoelectromechanics through a user-defined continuum element in Abaqus, and compare its results against an analytical solution based on matched asymptotic expansions for the electrochemistry and a Saint-Venant solution for the mechanics [2]. We discover a dramatic effect of localized through-the-thickness deformations near the electrodes on membrane's macroscopic bending, thereby challenging the use of low-order structural models. Motivated by this discovery, we establish a new structural model for IPMCs, which extends Euler-Bernoulli beam theory to account for through-the-thickness deformations, computed a-priori from the analytical solution for uniform bending. We demonstrate the accuracy of our model against FE, in the presence of non-uniform bending and metal electrodes. Our work finds application in reduced-order modeling of IPMCs, a critical component of inverse design and optimization. References [1] Cha, Y., & Porfiri, M. (2014). Mechanics and electrochemistry of ionic polymer metal composites. Journal of the Mechanics and Physics of Solids, 71, 156-178. [2] Boldini, A., & Porfiri, M. (2020). Multiaxial deformations of ionic polymer metal composites. International Journal of Engineering Science, 149, 103227. [3] Boldini, A., Bardella, L., & Porfiri, M. (2020). On Structural Theories for Ionic Polymer Metal Composites: Balancing Between Accuracy and Simplicity. Journal of Elasticity, 141(2), 227-272.

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Title: A Total Lagrangian Material Point Method with Non-Local Damage for the Simulation of Solids Subjected to Large Deformation and Damage

Author(s): *Alban de Vaucorbeil, *Deakin University*; Vinh Phu Nguyen, *Monash University*;

The material point method (MPM) has found successful applications in many engineering problems involving large displacement, large deformation, contacts and damage. The standard MPM formulation, which adopts piece-wise linear basis functions, suffers from the so-called cell-crossing instability, low order of convergence and numerical fracture. Modifications have been made to this standard MPM to mitigate these issues: B-spline MPM (BSMPM), the generalized interpolation material point (GIMP) and convected particle domain interpolation (CPDI) all decrease cell-crossing instabilities and increase the order of convergence, but only CPDI effectively suppresses numerical fracture. However, these methods, CPDI in particular, significantly increase the method's implementation and computational complexity. We present a total Lagrangian MPM (TLMPM) that overcomes the issues of the conventional MPM while being more efficient and easier to implement than CPDI. No numerical fracture occurred for simulations involving very large tensile deformation without special treatment such as done in the CPDI and convergence analyses show that the TLMPM shows high order of convergence at both small and large deformation. The model is able to simulate physically based fracture using continuum damage mechanics. However, and similar to FEM, it suffers from damage localization, mesh bias and lack of convergence for the point of damage onset. Non-local damage has been successfully used in FEM to mitigate such problems. We also present how a non-local damage model can be adapted to the TLMPM in particular.

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Title: An Overview of Interface- and Discontinuity-Enriched Finite Element Methods with Emphasis on Topology Optimization

Author(s): *Alejandro Aragón, *Delft University of Technology*; Sanne van den Boom, *Delft University of Technology*; Jian Zhang, *Delft University of Technology*; Dongyu Liu, *Delft University of Technology*; Angelo Simone, *University of Padova*; Fred van Keulen, *Delft University of Technology*;

Alejandro M. Aragón (1), Sanne van den Boom (1), Jian Zhang (1), Dongyu Liu (1), Angelo Simone (2), Fred van Keulen (1) (1) Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Delft, the Netherlands (2) Department of Industrial Engineering, University of Padova, Via Venezia 1, 35131 Padova, Italy Key Words: Enriched FEM, IGFEM/HIFEM/DE-FEM, XFEM/GFEM, weak/strong discontinuities, topology optimization The finite element method (FEM) is the de facto procedure for solving problems in solid mechanics. However, modeling problems with complex/evolving geometries rapidly exposes the main pitfalls of the method: creating finite element (FE) meshes that fit the problem geometry is a tedious and error-prone process. Enriched finite element formulations overcome this issue in an elegant manner by using enrichment functions to decouple problem geometry from the FE discretization. In the case of problems with discontinuities like material interfaces or cracks, enrichment functions recover the accuracy otherwise lost by using a mesh that does not align with the problem's geometry. In interface- and discontinuity- enriched formulations, this is accomplished by adding enriched degrees of freedom along discontinuities. In this presentation we give an overview on interface- and discontinuity-enriched finite element formulations [1–3]. We briefly review ongoing work on material interface, fracture, contact, and immersed boundary (fictitious domain) problems. Then we delve into the use of interface-enriched FEM for level set-based topology optimization. We showcase this new approach for designing phononic crystals (bandgap materials) and for tailoring fracture toughness in brittle materials. References [1] A. M. Aragón, B. Liang, H. Ahmadian, and S. Soghrati. "On the stability and interpolating properties of the Hierarchical Interface-enriched Finite Element Method". In: Computer Methods in Applied Mechanics and Engineering 362 (2020), p. 112671. URL: https://doi.org/10.1016/ j.cma.2019.112671. [2] S. J. van den Boom, J. Zhang, F. van Keulen, and A. M. Aragón. "An interface-enriched generalized finite element method for level set-based topology optimization". In: Structural and Multidisciplinary Optimization 63.1 (2021), pp. 1–20. URL: https://doi.org/10.1007/s00158-020- 02682-5. [3] J. Zhang, S. J. van den Boom, F. van Keulen, and A. M. Aragón. "A stable discontinuity-enriched finite element method for 3-D problems containing weak and strong discontinuities". In: Comput Methods in Appl Mech Eng 355 (2019), pp. 1097–1123.

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Title: Multiscale Global Sensitivity Analysis for Stochastic Chemical Reaction Networks

Author(s): *Alen Alexanderian, *North Carolina State University*; Michael Merritt, *North Carolina State University*; Pierre Gremaud, *North Carolina State University*;

Microscopic models for chemical reaction networks (CRNs) involve to discrete-in-time stochastic systems where the state variables are the numbers of molecules for each of the system species. In addition to intrinsic stochasticity, these systems include rate parameters that are often subject to uncertainty. Global sensitivity analysis (GSA) enables determining rate parameters that are most influential to uncertainty in model output. However, such an analysis is challenging for stochastic models. This is due to the high computational cost of simulating the model and the need to sample the model in a product probability space defined by the product of the probability spaces carrying the parametric uncertainty and intrinsic model stochasticity. On the other hand, it is cheaper to perform GSA on the corresponding mean-field model given by the reaction rate equations (RREs). We propose a multiscale GSA framework for such systems that relates the GSA measures corresponding to RREs to the stochastic GSA measure corresponding to the stochastic system. We will also discuss stochastic models in general and the use of surrogate models for efficiently performing GSA in such systems

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Title: Estimating Approximate Control Variate Weights: with Applications in Importance Sampling and Rare Event Estimation

Author(s): *Alex Gorodetsky, *University of Michigan*; Trung Pham, *University of Michigan*;

The recent growth in multi-fidelity uncertainty quantification has given rise to a large set of variance reduction techniques that leverage information from model ensembles to provide variance reduction for estimates of the statistics of a high-fidelity model. In this talk we describe two contributions: (1) we utilize an ensemble estimator to account for uncertainties in the optimal weights of approximate control variate (ACV) approaches and derive lower bounds on the number of samples required to guarantee variance reduction; and (2) we extend an existing multi-fidelity importance sampling (MFIS) scheme to leverage control variates. As such we make significant progress towards both increasing the practicality of approximate control variates approaches—for instance, by accounting for the effect of pilot samples—and using multi-fidelity approaches more effectively for estimating low-probability events. Numerical results indicate our hybrid MFIS-ACV estimator achieves up to 50% improvement in variance reduction over the existing state-of-the-art. Several simulated examples are shown for computational mechanics systems.

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Title: Entropy Stable Split Forms for the Flux Reconstruction High-Order Method: Three-Dimensional Curvilinear Numerical Validation

Author(s): *Alexander Cicchino, *McGill University*; Siva Nadarajah, *McGill University*;

The flux reconstruction method has gained popularity in the research community as it recovers promising high-order methods through modally filtered correction fields, such as the Discontinuous Galerkin (DG) method, on unstructured grids over complex geometries. Under a class of energy stable flux reconstruction (ESFR) schemes also known as Vincent-Castonguay-Jameson-Huynh (VCJH) schemes [1], the flux reconstruction method allows for larger time-steps than DG while ensuring linear stability on linear elements. Alternatively, for nonlinear problems, split forms emerged as the popular approach proving nonlinear stability for unsteady problems on coarse unstructured grids; albeit only having been proved for the strong form DG scheme and numerically shown for the g_2-lumped Lobatto strong form ESFR scheme for the Euler equations [2, 3]. In this work we show that incorporating split forms with VCJH schemes, alike Ranocha et al. [2] and Abe et al. [3], generally lead to unstable discretizations. We derive a new approach for general, modal, uncollocated ESFR schemes in split forms that ensure energy and entropy stability. This new approach simplifies to VCJH type schemes for linear problems, but for nonlinear problems, it ensures nonlinear stability and the correct orders of convergence. The stability proof is verified with the Taylor-Green Vortex problem on a coarse curvilinear grid, for all uncollocated, modal ESFR schemes, while preserving the correct orders of accuracy. References [1] Vincent, P. E., Castonguay, P., and Jameson, A., “A New Class of High-Order Energy Stable Flux Reconstruction Schemes,” Journal of Scientific Computing, Vol. 47, No. 1, 2011, pp. 50–72. [2] Ranocha, H., Öffner, P., and Sonar, T., "Summation-by-Parts Operators for Correction Procedure via Reconstruction," Journal of Computational Physics, 311, (2016), 299–328. [3] Abe, Y., Morinaka, I., Haga, T., Nonomura, T., Shibata, H., and Miyaji, K. "Stable, Non-Dissipative, and Conservative Vlux-Reconstruction Schemes in Split Forms," Journal of Computational Physics, 353, (2018), 193–227.

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Title: Development of a One-Dimensional CAC Framework to Model Long-Time Shock Wave Propagation

Author(s): *Alexander Davis, *Auburn University*; Vinamra Agrawal, *Auburn University*;

We develop a long-time moving window framework using the Concurrent Atomistic-Continuum (CAC) method to model shock wave propagation and interaction along a one-dimensional monoatomic chain. The moving window formulation follows a propagating shock wave allowing us to model shock propagation much longer than conventional non-equilibrium MD (NEMD) simulations. Additionally, the framework significantly decreases the required domain size and thus reduces the overall computational cost. The method uses CAC to divide the domain into an inner refined region containing the shock wave flanked on either end by coarse-grained regions which incorporate continuum shock conditions. We first perform verification studies to ensure that the system is properly coupled and can reproduce the correct phonon dispersion relation. Next, we update the governing equation to allow waves to pass between the atomistic and coarse-grained regions. Currently, we are implementing a scheme to simultaneously refine the continuum region as well as coarsen the atomistic region at the speed at which the shock wave moves. This will allow us to simulate long-time shock wave propagation and eventually model microstructural shock interactions with dislocations and/or other materials. Such research is necessary because while existing concurrent schemes have been very successful in modeling material defects and their motion, they have not yet been extended to model shock wave propagation through a material.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Uncertainty Quantification of Delamination Failure within Composite Structures using a Submodel Based Multi-Fidelity Approach

Author(s): *Alexander Hanson, *Sandia National Laboratories*;

The use of cohesive zone elements for modeling delamination failure in composites is common; however, the computational cost can be quite high for large composite structures due to the required element size of the cohesive zone elements. Techniques like homogenization can be used to decrease the computational burden, the tradeoff is at the expense of resolving the behavior of the composite plies, which includes delamination failure. If the failure region is known, submodeling can be used to enable the modeling of additional detail required to capture delamination failure within the composite. Driven by a lower fidelity global model, the reduced submodeled region can be modeled at the requisite element size for cohesive zone elements with a lower computational cost. This study explores the use of multi-fidelity uncertainty quantification methods for modeling delamination failure within composites when using a submodeling approach. While, the submodel presents an opportunity to simulate at fidelities and refinement levels that are not realistic at the scale of the entire model, factors like the size of the submodel and the fidelity of the global model can affect the efficiency of the multi-fidelity approach. Several combinations of submodel size and global model fidelities are compared to determine the most effective way to use submodels of composite structures within a multi-fidelity uncertainty quantification study.

16th U.S. National Congress on Computational Mechanics
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Title: A Peridynamic Diffusion Model for Unbounded Problems

Author(s): *Alexander Hermann, *Helmholtz-Zentrum Geesthacht*; Arman Shojaei, *Helmholtz-Zentrum Geesthacht*; Pablo Seleson, *Oak Ridge National Laboratory*; Christian. J Cyron, *Helmholtz-Zentrum Geesthacht*;

Peridynamics (PD) is a recent integral-type nonlocal theory originally introduced as a reformulation of classical continuum mechanics in solids. It has proven to be particularly effective in modeling discontinuous problems such as fracture. The PD formulation was later extended to diffusion, heat conduction and corrosion problem to make use of the advantages of this nonlocal theory in more challenging classes of problems. Particularly, the application to corrosion damage problems has attracted considerable attention in the literature. Chemical or electrochemical reactions may lead to the gradual destruction of a material in a corrosive environment. Modeling these types of problems involves a diffusion process in a coupled electrolyte/metal system with a phase-changing mechanism. The difficulty lies in capturing accurately the evolution of the moving phase boundary. Formulations to do so within the context of classical computational methods such as the finite element method exist but are often computationally expensive. PD models can largely bypass this problem as they can capture the evolution of moving interfaces fairly naturally as part of the solution process. Most of the studies relying on PD published so far are concerned with the solution of bounded domain problems. However, the application of the heat or diffusion equation on (nearly) unbounded domains is of particular interest for many scientific fields such as fluid dynamics, heat conduction, biology, finance and corrosion. In the present study, we propose a novel method of constructing Dirichlet-type absorbing boundary conditions (ABCs) in order to solve the PD diffusion equation on unbounded domains in one, two and three dimensions. To this end, we truncate the unbounded domain at an artificial boundary and impose appropriate ABCs such that the solution on the truncated domain resembles the behavior of the unbounded problem. Similarly to the nonlocal PD formulation, the ABCs are nonlocal and are updated at each time step. As the ABCs are constructed as boundary conditions of Dirichlet-type in the time domain, they neither require Laplace transforms nor special differential operators such as the perfectly matched layer method (PML). Based on a number of benchmark examples we will demonstrate the stability and accuracy of our newly introduced ABCs for long-term simulations. To our best knowledge, it is the first time that a PD model for the solution of a three-dimensional unbounded domains is proposed.

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Title: A New Numerical Approach to Solution of PDEs with Optimal Accuracy on Irregular Domains and Interfaces using Cartesian Meshes. Application to Wave, Heat, Helmholtz, Poisson and Elasticity Equations.

Author(s): *Alexander Idesman, *Texas Tech University*;

A new numerical approach (the optimal local truncation error method (OLTEM)) based on the minimization of the local truncation error is suggested for the solution of partial differential equations. Similar to the finite difference method, the structure and the width of stencil equations are assumed in advance. A discrete system of equations includes regular uniform stencils for internal points and non-uniform stencils for the points close to the boundary. The unknown coefficients of the discrete system are calculated by the minimization of the order of the local truncation error. The main advantages of OLTEM are an optimal high accuracy and the simplicity of the formation of a discrete (semi-discrete) system for irregular domains and interfaces (composite materials). For the regular uniform stencils, the stencil coefficients can be found analytically. For non-uniform cut stencils, the stencil coefficients are numerically calculated by the solution of a small system of linear algebraic equations (20-100 algebraic equations). In contrast to finite elements, a trivial Cartesian mesh (no need in complicated mesh generators) is used with OLTEM. Changing the width of the stencil equations, different high-order numerical techniques can be developed. Currently OLTEM is applied to the solution of the wave, heat, Helmholtz, Poisson and elasticity equations. The theoretical and numerical results show that for the width of the stencil equations similar to that for linear finite elements, OLTEM yields the 4th order of accuracy for the considered scalar PDEs on irregular domains (it is much more accurate compared with the linear and high-order finite elements at the same number of degrees of freedom). E.g., 3-D numerical examples on irregular domains show that at accuracy of 5%, OLTEM reduces the number of degrees of freedom by a factor of greater than 1000 compared to that for linear finite elements with similar stencils. At the computational costs of quadratic finite elements, OLTEM yields the 10th order of accuracy for the time-independent elasticity equations and the 11th order of accuracy for the Poisson equation with complex irregular interfaces. This leads to a huge reduction in computation time for OLTEM at a given accuracy.

16th U.S. National Congress on Computational Mechanics
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Title: Morphometric Characterization of Strength in Porous Media

Author(s): *Alexandre Guevel, *Duke University*; Hadrien Rattez, *Université catholique de Louvain*; Manolis Veveakis, *Duke University*;

To unravel the origin of porous media’s response to degradation processes, we propose here a compromise between microscopic and macroscopic modeling. Namely, we link the macroscopic flow stress with the adequate descriptors of the microstructure, called morphometers. To model the exact microstructure, we use phase-field modeling, which tracks the interfaces between grains and pores, under mechanical loading. A morphometric strength law is inferred from numerical simulations on 2D synthetic tunable microstructures, which provide a sufficiently large and representative ensemble of data. We thereupon find an exponential dependence between the strength and the morphometers, chosen as the three first Minkowski functionals of the microstructures, i.e. the porosity, the surface area and the mean curvature, as per Hadwiger's theorem. This law is verified with real microstructures of geomaterials and biomaterials. This framework paves the way for predicting the behavior of porous media with the minimal amount of data possible and in particular, minimizing the use of destructive tests.

16th U.S. National Congress on Computational Mechanics
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Title: Physics-Informed Nonlocal Closure Schemes for Turbulent Flows

Author(s): *Alexis-Tzianni Charalampopoulos, *Massachusetts Institute of Technology*; Themistoklis Sapsis, *Massachusetts Institute of Technology*;

In this work we demonstrate the ability of deep neural network architectures to act as closure models for a number of different systems in fluid dynamics. We employ machine-learning ideas to formulate, physics informed, spatiotemporally nonlocal closure schemes for turbulent, possibly multi-phase, fluid flows found in engineering and geophysical settings. The generic framework of the systems we focus on includes a linear part, external forcing and a bi-linear, energy-preserving operator. For such systems, we aim to answer how can we use the governing equations and data sets to formulate physics-informed, data-driven closures that will provide coarse-grained evolution equations for uncertainty quantification (UQ). To that end, as regularly done in UQ, we model the state of the system by its mean and a fixed orthonormal basis., thus deriving the equations for the covariance matrix and mean state of the system. For the statistics of this low-order model, we incorporate machine learning (ML), in the form of recurrent deep neural networks and spatio-temporal convolutions to device a closure scheme. Enforcing the appropriate energy constraints, a consequence of the nature of the quadratic operator, during the training of our closure schemes, improves the performance of the resulted closures but also stabilizes the coarse-grained equations in cases that are other- wise numerically unstable. Finally, we test our approach on turbulent multiphase flows and quasigeostrophic flows in the ocean and atmosphere. Our data-informed closure scheme is then applied on coarse-scale resolu- tions of the problems and compared to fine-scale direct numerical simulations. The numerical tests showcase both that no numerical instabilities occur, a crucial property in chaotic dynamical systems, but also very good agreement between our ML-enhanced predictions and Monte-Carlo (MC) simulations.

16th U.S. National Congress on Computational Mechanics
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Title: Spline Gauss Quadrature Rules for Refined Isogeometric Discretizations

Author(s): *Ali Hashemian, *Basque Center for Applied Mathematics*; Michael Barton, *Basque Center for Applied Mathematics*; David Pardo, *University of the Basque Country*;

We propose the use of spline Gauss quadrature rules [1] for refined isogeometric analysis (rIGA) [2]. The main idea is to benefit from cost improvements associated with both system integration and faster system solution. When using rIGA discretization, we subdivide the computational domain into macroelements separated by zero-continuity basis functions, which decrease the matrix connectivity. Thus, considering an optimal macroelement size, rIGA solves the linear systems asymptotically up to O(p^2) times faster than maximum-continuity IGA (the improvement is approximately of O(p) for small domains). Additionally, continuity reduction of basis functions adds more degrees of freedom and improves the approximation quality of our discretization. When constructing system matrices element-wise using polynomial Gauss quadrature rule, the system integration cost increases approximately by O(n^d*p^d) for large domains where n and p are the number of elements and polynomial degree in each direction, respectively, while d is the space dimension. The spline Gauss quadrature rule suggests using an optimal number of quadrature points over the macroelements. Thus, considering a fixed macroelements size, we have an improvement of up to two times in 2D and three times in 3D for "sequential" system integration (the improvement factor depends on the continuity of space and number of quadrature we use for different domains). The main advantage of using this macroelement-wise integration is that we can integrate over macroelements in "parallel" and save more computational time in system construction. As a practical case study, we consider the structural analysis of freeform shells based on Reissner–Mindlin shell theory [3]. This is a multi-field problem where each node has five field variables. The main challenge in dealing with this problem is that we need to increase the polynomial degree of B-spline bases to at least three or four to avoid the so-called locking phenomenon. Having a fine mesh on a complex freeform geometry with a high polynomial degree increases both the integration and solution costs, which improve significantly with the proposed method. References: [1] M. Barton, V.M. Calo. "Optimal quadrature rules for odd-degree spline spaces and their application to tensor-product-based isogeometric analysis". Comput. Methods Appl. Mech. Engrg. 305(2016)217–240. [2] D. Garcia, D. Pardo, L. Dalcin, M. Paszynski, N. Collier, V.M. Calo. "The value of continuity: Refined isogeometric analysis and fast direct solvers". Comput. Methods Appl. Mech. Engrg. 316(2017)586–605. [3] A.H. Niemi, J. Pitkäranta. Bilinear finite elements for shells: Isoparametric quadrilaterals. Int. J. Numer. Methods Engrg. 75(2008)212–240.

16th U.S. National Congress on Computational Mechanics
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Title: Snapshots Construction Using In Situ Visualization Tools for Data-Driven Reduced Order Modeling

Author(s): Gabriel Barros, *Universidade Federal do Rio de Janeiro*; Malu Grave, *Universidade Federal do Rio de Janeiro*; Jose Camata, *Universidade Federal de Juiz de Fora*; *Alvaro Coutinho, *Universidade Federal do Rio de Janeiro*;

The interest in snapshots-based surrogate models has been growing in the past decades. These methods often rely on the construction of a basis containing coherent structures existent in data to generate surrogate models able to predict, extrapolate, interpolate or reconstruct solutions for time-critical or many-query applications. In the present study, we introduce a strategy to create snapshots from images generated by in situ visualization tools [1]. The extraction of features existent in these images reduces the I/O pressure in the offline phase of reduced-order modeling. It enables using snapshots-based methods on simulations using adaptive mesh refinement and coarsening (AMR/C), where the outputs have different dimensions and topology. We illustrate our strategy with two examples: a 2D lock-exchange gravity current [1] and a 3D bubble rising problem [2]. The high-fidelity data is generated using the parallel finite element library libMesh, and the adaptor for the in-situ visualization infrastructure of ParaView Catalyst [1] provides the images. The high-fidelity simulations run in parallel in an HPC machine and the offline phase on a workstation. We consider Dynamic Mode Decomposition (DMD) [3] as our method of choice to generate surrogate models from snapshots. We compare DMD results in terms of accuracy and efficiency on both reconstruction and short-time predictions on the solutions obtained through this procedure and note that they are in good agreement with the original solutions. We also show that the results in terms of relevant quantities of interest for each simulation, such as front position, bubble center of mass, and bubble sphericity, are also in good agreement with the simulation solutions. [1] JJ Camata, V. Silva, P Valduriez, M Mattoso, ALGA Coutinho, In situ visualization and data analysis for turbidity currents simulation. Computers & Geosciences, (2018) 110(C), 23-31. [2] M Grave, JJ Camata, ALGA Coutinho. "A new convected level-set method for gas bubble dynamics." Computers & Fluids 209 (2020): 104667. [3] SL Brunton, JN Kutz, Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control, Cambridge University Press, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Shock-Capturing for High-Order Compact Schemes via Boundary Variation Diminishing Approach and its Applications

Author(s): *Amareshwara Sainadh Chamarthi, *Technion - Israel Institute of Technology*; Jonathan Hoffmann, *Technion - Israel Institute of Technology*; Omri Argov, *Technion - Israel Institute of Technology*; Steven Frankel, *Technion - Israel Institute of Technology*;

This paper presents a novel shock-capturing approach for compact schemes (compact reconstruction and a novel compact gradient finite volume) via boundary variation diminishing (BVD) methodology. In our approach, we combine a non-dissipative central or a compact upwind interpolation and a fifth-order monotonicity preserving scheme (MP5) through the BVD algorithm. BVD method chooses the highest order possible interpolation in the smooth regions, and for the discontinuities, the algorithm selects the monotone scheme. Several numerical test cases are carried out to verify the proposed schemes' capability for single and multicomponent inviscid and viscous flows. The approach is further extended for complex geometries via immersed boundary method to facilitate simulations for practical applications.

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Title: Experimental and Modeling Characterization of Amorphous/Crystalline Metal Composite Interface Mechanical Behavior by Nanoindentation

Author(s): *Amir Abdelmawla, *Iowa State University*; Thanh Phan, *Iowa State University*; Liming Xiong, *Iowa State University*; Ashraf Bastawros, *Iowa State University*;

Amorphous/crystalline metallic composites (A/C-MCs) have sparked widespread research owing to their unique properties and potential applications. However, the mechanisms responsible for the co-deformation of crystalline (C-) and amorphous (A-) phases have not been fully understood yet. Here we study the plastic flow in A/C-MCs under indentation loads using experimental nanoindentation and molecular dynamic (MD) simulations with the aim of quantifying how the nanoscale amorphous/crystalline interface (ACI) mediates the plastic flow in such materials. The spatial atomic structure near the ACI is characterized for six different compositions of crystalline/amorphous (Cu/CuxZr100-x, x = 20 – 64 %). The atomic-level deformation processes in both C- and A- phases nearby the ACI are investigated in details, and are correlated with the material's constitutive behavior, i.e., the force-displacement curve, at the microscale. Several major findings are: (i) a gradient in the population of geometrically unfavorable motifs structures (GUM) exists near the ACI, giving rise to residual shear stress distribution near ACI; (ii) the GUM population gradient is modulated by the chemical composition; (iii) the atomistic scale short and medium range order gives rise to an ACI-induced transition zone with a thickness at a level of ~8 nm; (iv) the ACIs enable a co-deformation of the A- and C-phases through "stiffening" the soft phases but "softening" the stiff phases in A/C-MCs; (v) deformation within the A- shows diffused deformation pattern with the increase in the GUMs fraction; (vi) the carefully designed indentation experiment and simulation provides full quantification of the strong coupling between dislocations and shear transformation zones (STZs), when plasticity flows across the ACI. In details, STZs can be activated when the dislocation-mediated plasticity flows from the C- to the A-phase, and vice versa, dislocations are nucleated when the STZ-mediated plasticity flows from the A- to the C-phase; and (vii) the nanoscale MD-simulation-predicted mechanisms can be mapped to the "pop-in" or "excursion" events on the force-displacement curves extracted from microscale indentation experiments at different spatial distance from the ACI, although there is a length scale gap in between. These findings may be used to advance the understanding of the deformation behavior of A/C -MCs, and in turn, to provide a support for designing such materials with unprecedented properties from the bottom up.

16th U.S. National Congress on Computational Mechanics
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Title: Dynamical Modeling and Control of Fluid-Structure Interaction: From High-Fidelity to Data-Driven Computing

Author(s): *Amir Chizfahm, *University of British Columbia*; Rajeev Jaiman, *University of British Columbia*;

Advances in high-performance computing (HPC) have empowered us to perform large-scale simulations for millions of variables in coupled fluid-structure systems involving complex geometries and multiphase flows. These high-fidelity simulations via nonlinear partial differential equations (PDE) have been providing invaluable physical insight for the development of new design and devices in aerospace and marine/offshore engineering. Despite efficient numerical methods and powerful supercomputers, the state-of-the-art computational fluid dynamics (CFD) and coupled fluid-structure simulations are somewhat inefficient hence less attractive with regard to the design optimization, parameter space exploration and the development of control and monitoring strategies for aerospace and offshore structures. The primary focus of this study is to develop efficient reduced-order models for the physical modeling of fluid-structure systems. A series of canonical academic test cases will be covered to elucidate the integration of standard CFD with model reduction and deep learning techniques for the prediction of vortex-induced loads and motion effects. Some efforts on the iterative optimization and feedback active control of unsteady wake flow and vortex-induced vibration will be demonstrated. The proposed hybrid high-fidelity CFD with data-driven computing framework is precisely aligned with the current aerospace/marine industry needs on structural life prediction, diagnosis and monitoring via digital twin.

16th U.S. National Congress on Computational Mechanics
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Title: Subgrid Surface Connectivity for Shallow Water Equations

Author(s): *Amirhiseub Begmohammadi, *University of Notre Dame*; Damrongsak Wirasaet, *University of Notre Dame*; Diogo Bolster, *University of Notre Dame*; Andrew Kennedy, *University of Notre Dame*; Joel Dietrich, *North Carolina State University*;

Subgrid models based on upscaled forms of the 2D shallow water equations that account for unresolved topography use coarse grids for computational efficiency. Although excessively coarse grids can reduce the computational cost, it can lead to artificial cross flows between disconnected areas separated by physical barriers that are much smaller than the grid size. In this study, a simple approach is proposed based on introducing additional degrees of freedom through nested cloning the coarse grids (a clone is a group of areas with connected flow path in each grid cell) and an overflow formula to handle the subgrid barriers according to flow conditions. The algorithm accommodates both the removal of the artificial cross flows and the possibility the subgrid barriers being inundated during an extreme event. Numerical results from a series of idealized and more realistic test cases shows substantial improvements of the proposed algorithm over existing methodologies.

16th U.S. National Congress on Computational Mechanics
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Title: Convolution Finite Element Method

Author(s): *Amirhossein Amiri-Hezaveh, *University of Illinois at Urbana-Champaign*; Arif Masud, *University of Illinois at Urbana-Champaign*; Martin Ostoja-Starzewski, *University of Illinois at Urbana-Champaign*;

Several methods have been developed to solve initial boundary value problems with FEM. These approaches basically fall into two main categories: (i) space-time decoupled approaches and (ii) space-time coupled approaches. The solution is assumed as the product of functions of spatial and time variables in the first category. Subsequently, governing equations are reduced into a set of time-wise ODEs, typically solved by explicit/implicit time integration methods. On the other hand, the resulting coupled integral forms in the second category are typically dealt with the space-time FEM: time variable is mainly treated similar to spatial ones, leading to the simultaneous discretization of time and spatial variables. Continuous Galerkin (CG) and discontinuous Galerkin (DG) are the two main methods employed in the space-time FEM. While both the CG and DG are capable of approximating the solution accurately, the continuity of fields, in the earlier, may enforce algebraic equations that are computationally intense. The latter seems to be efficient as the solution is considered on the level of elements, where the space-wise and or time-wise continuity of fields are weakly met. In the present study, a new solution procedure stemming from Gurtin's alternative field equations is introduced. The technique lies in the second category. The resulting algorithm for elastodynamics, however, becomes similar to the time integration method. Since the technique is based on a weak formulation closely related to variational principles involving the convolution product, it is called the 'convolution finite element method.' Although the algorithm is versatile enough to solve some other physical processes, we herein mainly focus on linear elastodynamics. To illustrate this point, in numerical results, we briefly consider the mass-spring-damper problem, a prototype of structural dynamics, and highlight its applicability to computational elastodynamics. We finally show that the present approach inherits the following desirable characteristics in the case of elastodynamics: 1) it is versatile to gain higher-order accuracy for any given time interval. 2) it has the potential of detaching the spurious part of the response similar to algorithmic damping methods 3) it does not require time-space discretization 4) it is computationally justifiable if compared to other methods.

16th U.S. National Congress on Computational Mechanics
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Title: Hybrid Physics-Based and Data-Driven Modeling of Near-Wall Blood Flow with Physics-Informed Neural Networks

Author(s): *Amirhossein Arzani, *Northern Arizona University*; Jian-Xun Wang, *University of Notre Dame*; Roshan M Dsouza, *University of Wisconsin-Milwaukee*;

Near-wall blood flow and wall shear stress (WSS) regulate cardiovascular disease, yet they are challenging to quantify with high fidelity. Computational fluid dynamics (CFD) models can leverage high-performance computing to enable high-resolution and accurate quantification of WSS. However, these models suffer from uncertainty in parameters and boundary conditions. On the other hand, direct experimental measurement in-vivo could reduce uncertainty, however, these measurements typically do not meet the spatial resolution requirement in calculating WSS and struggle to accurately quantify near-wall flow. Physics-informed neural networks (PINN) provide a flexible machine learning framework to integrate mathematical equations with measurement data. Herein, we demonstrate how PINN could be used to improve WSS quantification in diseased arterial flows. Specifically, we assume we do not have any knowledge of the inlet boundary condition and incoming flow. We demonstrate that with very few measurement points collected even away from the vessel wall, we could use PINN to compute WSS with very high accuracy. We also show an interesting scenario where PINN does not correctly recover the inlet boundary condition but is still able to reconstruct WSS in the region of interest. We demonstrate examples in idealized stenosis and aneurysm models and discuss the implications of our model in transforming near-wall hemodynamics modeling.

16th U.S. National Congress on Computational Mechanics
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Title: A Multi-Resolution Approach to Hydraulic Fracture Simulations

Author(s): *Andre Costa, *Duke University*; John Dolbow, *Duke University*; Randall Settgast, *Lawrence Livermore National Laboratory*; Tao Jin, *University of Ottawa*; Matteo Cusini, *Lawrence Livermore National Laboratory*;

We describe a new methodology to enable the simulation of hydraulic fracture problems. The approach is applied to problems in which flow through porous media is coupled with crack growth, including flow in the aperture. Our approach attempts to couple the bulk physics with crack growth through the use of separate domains that correspond to coarse and fine scales. At the coarse scale the crack geometry is assumed relatively fixed, while the fine scale is employed to capture detailed processes in the vicinity of crack tips. This is effected by instantiating local domains on the fly and transferring the mechanical drivers for the crack evolution from the coarse scale to the fine scale. At the coarse scale, fields are discretized within the GEOSX framework using a mix of finite volume and finite element methods, including embedded discontinuity techniques. At the fine scale, a diffuse representation of the crack geometry is employed to facilitate the simulation of complex crack evolution. Examples from standard benchmark problems are provided to illustrate the efficacy of the proposed approach.

16th U.S. National Congress on Computational Mechanics
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Title: Adaptive Virtual Element Methods for Simulations of Flow in Fractured Media

Author(s): *Andrea Borio, *Politecnico di Torino*; Stefano Scialò, *Politecnico di Torino*; Fabio Vicini, *Politecnico di Torino*; Stefano Berrone, *Politecnico di Torino*; Alessandro D'Auria, *Politecnico di Torino*;

We present novel strategies based on Virtual Elements (VEM) to perform simulations of flows in Discrete Fracture Matrix models. The flexibility of generalized polygonal meshes that can be handled by VEM, even allowing aligned edges and aligned faces, is a very useful tool for mesh generation. The presented strategies rely on a fast mesh generation process and on suitable refinement techniques designed for generalized polytopal meshes, that are used to adapt the mesh according to a posteriori error estimates, in order to reduce the number of degrees of freedom used to obtain high quality solutions. REFERENCES [1] Stefano Berrone, Andrea Borio, Alessandro D'Auria, Refinement strategies for polygonal meshes applied to adaptive VEM discretization, Finite Elements in Analysis and Design, Volume 186, 2021, 103502, ISSN 0168-874X, https://doi.org/10.1016/j.finel.2020.103502.
(https://www.sciencedirect.com/science/article/pii/S0168874X20301827)

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Title: Two-Dimensional Elastic Fracture Analysis with the Extended Virtual Element Method

Author(s): *Andrea Chiozzi, *University of Ferrara*; Gianmarco Manzini, *Los Alamos National Laboratory*; N. Sukumar, *University of California, Davis*; Elena Benvenuti, *University of Ferrara*;

First proposed in [1], the virtual element method (VEM) is a stabilized Galerkin scheme stemming from mimetic finite differences. The VEM allows for very general polygonal meshes, and does not require the explicit knowledge of the shape functions within the problem domain. For this reason, such functions are dubbed virtual. Instead, the discrete counterpart of the continuum formulation of the problem is defined by means of a suitable projection of the virtual shape functions onto a polynomial space, which allows the decomposition of the bilinear form into a consistent part, reproducing the polynomial space, and a correction term guaranteeing stability. Inspired by the features of the extended finite element method (X-FEM) [2], we proposed an extended virtual element method (X-VEM) for the Laplace problem with singular or discontinuous solutions [3]. In the present contribution, we devise an X-VEM for two-dimensional elastic fracture problems, in which we extend the standard virtual element space with the product of vector-valued virtual nodal shape functions and suitable enrichment fields. We define an extended projection operator that maps functions in the extended virtual element space onto a set spanned by the space of linear polynomials augmented with the enrichment fields. For the crack tip singularity, we choose, as enrichments, the mode I and mode II displacements fields. For crack discontinuities, we adopt the approach of Hansbo and Hansbo [4]. Once the element projection matrix has been computed, consistency and stabilization matrices are obtained as in standard VEM. We present several numerical examples in 2D elastic fracture to assess convergence and accuracy of the proposed method for both quadrilateral and general polygonal meshes. [1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L.D. Marini and A. Russo, Basic principles of virtual element methods. Math. Models Methods Appl. Sci., 23, 199-214, 2013. [2] N. Moës, J. Dolbow and T. Belytschko, A finite element method for crack growth without remeshing. Int. J. Numer. Methods Engrg., 46, 131-150, 1999. [3] E. Benvenuti, A. Chiozzi, G. Manzini and N. Sukumar, Extended virtual element method for the Laplace problem with singularities and discontinuities. Comput. Methods Appl. Mech. Engrg., 356, 571-597, 2019. [4] A. Hansbo and P. Hansbo, A Finite Element method for the simulation of strong and weak discontinuities in elasticity. Comput. Methods Appl. Mech. Engrg., 193, 3523-3540, 2004.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Exploiting the Piezoelectric Effect for Energy Harvesting - A Finite Element System Simulation Approach

Author(s): *Andreas Hegendörfer, *University of Erlangen-Nuremberg*; Julia Mergheim, *University of Erlangen-Nuremberg*;

A piezoelectric vibration-based energy harvester (PVEH) is composed of an electromechanical structure along with an energy extraction circuit. The objective of such a device is converting otherwise unused mechanical energy to electrical energy to power e.g. wireless sensors. The piezoelectric effect, used as the energy conversion principle, describes the appearance of electrical voltage when the piezoelectric material is mechanically deformed and vice versa. In an energy harvesting application the electromechanical structure and the electrical circuit have an influence on each other. This necessitates the accurate modeling of both parts and their interactions [1]. However, until now all finite element (FE) based methods reported in literature, which are not coupled to a circuit simulation software, are limited to linear circuit elements and passive electrical interfaces. The FE based methods, which are combined with an external circuit simulation tool, consider only linear electromechanical structures or the coupling between the electromechanical structure simulation and the electric circuit simulation is not very efficient. To overcome the mentioned drawbacks of existing FE methods for PVEH we developed a FE based approach, which can simulate nonlinear behavior of electromechanical structures as well as nonlinear and active electric circuits [2]. The influence of the circuit on the electromechanical structure is considered via the vector of external forces and an implicit time integration scheme is applied. The proposed method allows for consistent and efficient simulations of the complete possibly nonlinear PVEH using only one software tool. After explaining the working principle of a PVEH the presentation begins with a brief overview of various principle simulation techniques for PVEHs, in which the advantages and disadvantages of each method are discussed. Furthermore, our method is presented and embedded in the overview of the available simulation methods for PVEHs. Exploiting the capabilities of our method an application example considering a PVEH with nonlinear electromechanical structure as well as nonlinear electronic circuitry is given. REFERENCES [1] Gedeon D and Rupitsch SJ (2018) Finite element based system simulation for piezoelectric vibration energy harvesting devices. Journal of Intelligent Material Systems and Structures 29(7): 1333-1347. [2] Hegendoerfer A and Mergheim J Nonlinear finite element system simulation of piezoelectric vibration based energy harvesters. In preparation.

16th U.S. National Congress on Computational Mechanics
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Title: An Efficient Approach to Solve the System of Equations of Hypercomplex Finite Element Methods Using a Block Forward Substitution Scheme

Author(s): *Andres M. Aguirre-Mesa, *The University of Texas at San Antonio*; Manuel J. Garcia-Ruiz, *Angelo State University*; Mauricio Aristizabal, *Universidad EAFIT*; David Wagner, *NASA Langley Research Center*; Daniel Ramirez-Tamayo, *The University of Texas at San Antonio*; Arturo Montoya, *The University of Texas at San Antonio*; Harry Millwater, *The University of Texas at San Antonio*;

The hypercomplex finite element method (ZFEM) uses hypercomplex algebras to perform higher-order FEM based sensitivity analysis [1, 2]. When the analyst applies a perturbation to one or multiple imaginary axes of an input variable, the hypercomplex algebra differentiates all dependent variables. Then, ZFEM obtains the original problem's sensitivities from the imaginary parts of the hypercomplex solution vector. Hypercomplex operations are not supported by standard linear algebra libraries, such as LAPACK or SuperLU, nor by commercial FEM programs, such as Abaqus. The hypercomplex FEM system can be rewritten as an equivalent real-valued system of equations, based on the Cauchy-Riemann matrix form of hypercomplex numbers. However, this approach considerably increases the solution time with respect to the original FEM system. Due to this deficiency, the block forward substitution method (BFS) was developed. The new method splits the hypercomplex system of equations into multiple real-valued systems, whose system matrix is the real-valued FEM stiffness matrix, and whose solution vectors are the real and imaginary parts of the hypercomplex system. BFS factors the stiffness matrix once to solve the original FEM problem. Then, it solves the remaining systems as alternative right-hand sides of the original FEM system. The new method generalizes the semi-analytical complex-variable method [3] for higher-order sensitivity analysis. The methodology is applicable to multicomplex, hyperdual and quaternion algebras. BFS reduces the solution time of hypercomplex FEM systems to a fraction of the time used by the Cauchy-Riemann matrix approach. The methodology was implemented on Abaqus through user element subroutines. [1] A. Voorhees, H. Millwater and R. Bagley, "Complex variable methods for shape sensitivity of finite element models," Finite Elements in Analysis and Design, vol. 47, pp. 1146-1156, 2011. [2] J. E. Garza and H. R. Millwater, "Sensitivity Analysis in Structural Dynamics using the ZFEM Complex Variable Finite Element Method," in 54th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, 2013. [3] Jin, W., Dennis, B. H., & Wang, B. P. (2010). Improved sensitivity analysis using a complex variable semi-analytical method. Structural and Multidisciplinary Optimization, 41(3), 433-439.

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Title: Active Importance Sampling for Efficient Surrogate Modeling of Unit Operations in the Biochemical Conversion Process

Author(s): *Andrew Glaws, *National Renewable Energy Laboratory*; Hariswaran Sitaraman, *National Renewable Energy Laboratory*; Jonathan Stickel, *National Renewable Energy Laboratory*; Ethan Young, *National Renewable Energy Laboratory*;

Surrogate models for expensive physics-based models expend an upfront cost in order to enable a range of outer-loop studies, e.g., optimization and uncertainty quantification, that require multiple model evaluations. Dimension reductions methods, such as active subspaces and sufficient dimension reduction, can reduce this upfront cost of constructing the surrogate by building the model only along directions in the input parameter space that significantly impact the output of interest. In practice, identifying these directions and building the surrogate require sampling the original full-dimensional design space. However, this process can result in wasted model evaluations that do not effectively explore the variations in the outputs. In this work, we propose an active importance sampling scheme that emphasizes sampling the parameter space along directions that have the greatest impact on the output. This is an iterative approach that alternates between updating the active subspace and generating new samples. New samples are drawn uniformly along the active directions and conditionally in the inactive directions. Global metrics with respect to the original input density function are preserved using an importance sampling reweighting. We apply this method to the design of surrogate models for expensive unit operations within a virtual engineering (VE) workflow for the low-temperature conversion of biomass. This workflow includes multiple biochemical computational fluids dynamics (CFD) models, including a bubble column bioreactor and enzymatic hydrolysis, that can take on the order of hours to days to run and depend on multiple input parameters. The implementation of cheap surrogate models can enable optimization, sensitivity analysis, and uncertainty quantification of the full VE workflow.

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Title: Maximization of the Expected Information Gain of Experiments Using Stochastic Gradient Descent.

Author(s): *André Carlon, *King Abdullah University of Science and Technology*; Ben M. Dia, *King Fahd University of Petroleuma nd Minerals*; Luis Espath, *RWTH Aachen University*; Rafael H. Lopez, *Federal University of Santa Carina*; Raúl Tempone, *RWTH Aachen University*;

In Bayesian optimal experimental design, through mathematical modeling of experiments, one seeks experimental designs for optimal acquisition of information for Bayesian inference of model parameters of interest. One measure of the quality of an experiment is the Expected Information Gain (EIG), the mutual information between observations and the model parameters of interest. Here, we apply the stochastic gradient descent method (SGD) to find the model design parameters that maximize the EIG. To reduce the cost of estimating the gradients of the EIG, we employ a Laplace approximation of the posterior and a Laplace-based importance sampling for the estimation of the evidence. Under certain regularity assumptions about the EIG with respect to both the design parameters and the parameters of interest, our approach converges to local maxima of the EIG. To validate our methodology, we apply SGD for the optimization of benchmark experiments.

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Title: Physics-Informed Deep Learning for Solving a Magnetostatic Problem

Author(s): *Andrés Beltrán-Pulido, *Purdue University*; Ilias Bilionis, *Purdue University*; Dionysios Aliprantis, *Purdue University*;

In a trend towards sustainable electrification, designing robust electromagnetic devices is required for high-performance applications. As part of the design process, it is customary to utilize partial differential equations, derived from Maxwell's equations, to model the governing physics of these devices. The parameter space is often high-dimensional in these models, requiring several parameters to describe geometric features, material characteristics, and operating point conditions. As a consequence of the high-dimensionality, finding the magnetic field solution using the finite element method becomes intractable as the computational cost increases exponentially. The emerging physics-informed deep learning framework is a state-of-the-art approach that seeks to alleviate the curse of dimensionality. This paradigm has shown promising results in multiple engineering applications. However, Maxwell's equation applications, and in particular electromagnetic devices, have been barely explored under this framework. Therefore, our objective is to investigate the physics-informed deep learning framework's capability for solving a two-dimensional magnetostatic problem with multiple parameters. Here, we consider a magnetically linear square-core inductor. Our approach is as follows. We systematically investigate the impact of the different elements that are part of the training process. Specifically, we explore the magnetic field solution's parameterization, the sampling strategy, the optimization algorithm, and the loss function. We use the Euclidean norm to assess the solutions' accuracy by comparing the predicted magnetic field solution with the solution obtained from a finite element model. The studies suggest that the standard physics-informed deep learning technics do not perform properly in this particular magnetostatic problem. We identify that some of the causes of poor performance are: localized features in the solution, high-contrast permeability among materials, and the relatively complex inductor's geometry. Therefore, we propose a methodology to overcome these issues, where we embed information about the square-core inductor in the training process. Besides, we provided some suggestions on how we could extend our approach to other problems. Also, we solve an uncertainty propagation problem.

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Title: Mechanical Properties of Scar Tissue of Hip Capsule Ligament for Different Implant Materials after a Total Hip Arthroplasty.

Author(s): *Angelina Avgeri, *University Paris Diderot*; Bertrand Cinquin, *ENS Paris-Saclay, University Paris Saclay*; Laurent Sedel, *University Paris Diderot*; Pascal Bizot, *University Paris Diderot*; Elisa Budyn, *ENS Paris- Saclay, University Paris Saclay*;

Total hip arthroplasty is a surgical procedure in which the hip joint is replaced by artificial materials (implants) in order to restore its function. In this study, the morphological and mechanical properties of hip capsule ligament scar tissues that formed around implants composed of either polymer and metal or ceramic on ceramic are compared to native tissues removed during an initial total hip arthroplasty. The patients' age and sex are provided. Immuno-histological analyses of the samples using Hematoxylin and Eosin, Masson's trichrome and collagen I staining revealed different hierarchical structures of the tissues over three scales: the fiber (macroscale), the fascicle (mesoscale) and the tissue scale (macroscale). At the tissue scale, micro-tensile tests were performed on millimetric samples, first assuming that the tissue is a homogeneous transverse isotropic continuum with collagen fibers aligned to the tensile direction. Their non-linear elastic responses were identified by either an exponential law or an Ogden third-order constitutive model. The tissues exhibited different behaviors depending on the implant material they had grown around. First and second Piola-Krichhoff stresses and normal and Green-Lagrange strains were calculated to build the constitutive laws at the macro and micro scales. The cells formed ligaments composed of fascicles containing wavy fibers of varying densities and aligned with the main in vivo loading main direction observed under confocal microscopy. At the fiber scale, a patient-specific micro-scale finite element model was created based on measured morphological parameters such as the amplitude and period of the fiber motives. The FEM unit cell included single or multiple fiber combinations immersed in a matrix composed of a mixture of fibers in ground substance. The Ogden constitutive models for both fiber and matrix were identified. Three regimes of loading were determined at the tissue scale and applied at the boundary of the microscale model. The microscopic stress and strain fields were calculated and compared for the three different FEM models for the different tissue types. The experimental curves in the macroscale were plotted along with the corresponding stress- strain responses of the microscale. REFERENCES [1] L. Sedel, Clin. Orthop. Relat., 473:3803-3805, 2015. [2] R.P. Pitto, M. Garland, L. Sedel, Clin. Orthop. Relat., 473(12):3790-3795, 2015.

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Title: An Approach to the Simulation of the Behaviour of Interfaces between the Layers of TRISO Coated Particle Nuclear Fuel with Peridynamics

Author(s): *Angelo Battistini, *Imperial College London*; Thomas Haynes, *Imperial College London*; Mark Wenman, *Imperial College London*;

Trisostructural (TRISO) coated particle fuel is a concept for accident resistant nuclear fuel, one of the most important components of generation IV high temperature reactors (HTR). The HTR reactor is one design currently under development in the UK with several state and private funded projects, including U-Battery. The main safety objective of a well-designed fuel particle is the ability to prevent the release of fission products throughout its operation and most of its remaining life. Due to the working conditions of the fuel in current HTR designs, TRISO coating consists of four layers of materials with different purposes. Firstly, a graphite buffer layer that accommodates most of the fission fragments generated in the Uranium dioxide (UO2) kernel. Then, an inner pyrolytic carbon (PyC) layer to prevent oxidation of the outer layers due to UO2 degradation. Next, a silicon carbide (SiC) layer, acting as the main barrier against fission product release due to internal pressurisation and thermal expansion. Finally, an outer pyrolytic carbon layer to protect the SiC layer from erosion. The cited materials are known for their temperature tolerance, but they are also brittle, which could result in the formation and propagation of cracks even if their stress limits are not reached during reactor transients. In addition, this design incurs the challenge of using materials with different thermo-mechanical properties in proximity or bonded, which may lead to crack propagation through different layers of the materials, essentially eliminating the benefit of a multilayer design. This issue is of fundamental importance in the safety assessment of TRISO particles, and current finite element (FE) models are not able to reproduce the aleatory nature of crack generation and propagation through materials or interfaces. For this reason, a non-local bond-based peridynamics approach implemented in the commercial FE code Abaqus is being updated to model the behaviour of the interface between the layers of the TRISO particle. Sensitivity analyses of single material uniaxial tensile tests and thermal expansion with respect to mesh resolution have been performed, using finite element modelling and analytical solutions as benchmarks for the peridynamics models. A set of tensile and expansion tests of a 2D bi-material strip has been carried out, to ascertain the fundamental behaviour of interfaces, between different materials, modelled using peridynamics. The results of this work will form the basis for future developments of a complete TRISO peridynamics model.

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Title: Regularity Theory for Nonlocal Space-Time Master Equations

Author(s): *Animesh Biswas, *University of Nebraska-Lincoln*; Marta De-Leon Contrears, *University of Reading*; Pablo Stinga, *Iowa State University*;

We analyze regularity estimates for solutions to nonlocal space time equations driven by fractional powers of parabolic operators in divergence form. These equations are fundamental in semi-permeable membrane problems, biological invasion models and they also appear as generalized Master equations. We develop a parabolic method of semigroups that allows us to prove a local extension problem characterization for these nonlocal problems. As a consequence, we obtain interior and boundary Harnack inequalities and sharp interior and global parabolic Schauder estimates for solutions. For the latter, we also prove a characterization of the correct intermediate parabolic Holder spaces in the spirit of Sergio Campanato.

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Title: Strongly Imposed and Entropy-Stable No-Slip Wall Boundary Condition

Author(s): *Anita Gjesteland, *University of Bergen*; Magnus Svärd, *University of Bergen*;

In the context of well-posedness of PDEs, it is well-known that the boundary conditions play an important role. First, for the continuous problem, the correct number and type of conditions must be chosen. Second, they must be implemented stably. When going from the continuous to the (semi-)discrete setting, a number of choices of implementation techniques for the boundary conditions appear. A popular and robust technique is the SAT, which sets the boundary conditions weakly [1,2]. Another popular method is the so-called injection method, that imposes them strongly by overwriting the boundary nodes with the boundary values after each time step. The injection method is intuitive and simple, and is therefore appealing. We propose a numerical scheme for the compressible Navier-Stokes equations that imposes the no-slip condition for the velocities using the injection method and a Neumann condition for the temperature using the SAT technique. The equations are discretised in space by a second-order finite difference SBP operator. By utilising the energy method and the notion of entropy, we demonstrate that the scheme is both linearly and non-linearly stable. Numerical simulations for the second-order scheme are performed to demonstrate our findings, in addition to simulations of a fourth-order scheme that is linearly stable. [1]: M. Parsani, M. H. Carpenter, and E. J. Nielsen. Entropy stable wall boundary conditions for the three-dimensional compressible Navier-Stokes equations. Journal of Computational Physics, 292:88-113, 2015. [2]: L. Dalcin, D. Rojas, S. Zampini, D. C. Del Rey Fernández, M. H. Carpenter, and M. Parsani. Conservative and entropy stable solid wall boundary conditions for the compressible Navier-Stokes equations: Adiabatic wall and heat entropy transfer. Journal of Computational Physics, 397:108775, 2019.

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Title: A Goal Oriented Hp Adaptive DPG Scheme

Author(s): *Ankit Chakraborty, *RWTH Aachen University*; Ajay Rangarajan, *RWTH Aachen University*; Georg May, *Von Karman Institute for Fluid Dynamics*;

In many industrial and academic applications, certain quantities of interest, such as flux across a specific boundary or solution in a particular sub-domain, are subject of more interest than the solution variable over the whole domain. In these cases, adapting the mesh for resolving the governing PDE's solution features may result in an unwanted increase in the number of degrees of freedom involved. In this context, goal-oriented mesh adaptation techniques have been a critical development for producing meshes that only focus on resolving the target functional. In these adaptations, the element size distribution is often computed by solving a compatible dual problem, but this can be complemented by selecting a correct local polynomial order for approximating the primal variables. In terms of meshing techniques, it has been already shown that metric-based mesh generation can produce anisotropic meshes having substantial advantages while resolving anisotropic flow features such as sharp boundary layers and shocks [1]. In this work, we will present a goal-oriented metric-based mesh adaptation scheme where we employ the recently proposed DPG-star scheme [2] for solving the compatible dual problem and an associated a posteriori error estimate for size distribution. Also, we solve certain local problems and utilize the well-established energy norm error estimator [3] to obtain an appropriate polynomial order of approximation for the primal variables and anisotropy of the elements in the mesh. To this end, we propose an adaptation scheme that aims at producing optimal approximation spaces in terms of shape, size, and polynomial distribution of elements to resolve the target functional at a given cost. References: [1] Ajay Rangarajan and Aravind Balan and Georg May, Mesh optimization for discontinuous Galerkin methods using a continuous mesh model. AIAA Journal (2018)10:4060–4073 [2] Leszek Demkowicz and Jay Gopalakrishnan and Brendan Keith, The DPG-star method. Computers & Mathematics with Applications. (2020)11:3092 - 3116 [3] Leszek Demkowicz and Jay Gopalakrishnan, A Class of Discontinuous Petrov-Galerkin Methods II. Optimal Test Functions. Numerical Methods for Partial Differential Equations. (2011)27:70–105

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Title: Efficient Lattice Green Function Method for Atomistic/Continuum Coupling

Author(s): *Ankit Gupta, *École polytechnique fédérale de Lausanne*; Max Hodapp, *Skolkovo Institute of Science and Technology*; William Curtin, *École polytechnique fédérale de Lausanne*;

The lattice Green function method (LGFM)~[1] is the discrete counterpart of the continuum boundary element method (BEM) and is a natural approach for solving intrinsically discrete solid mechanics problems such as atomistic-continuum coupling. Coupled atomistic-continuum problems involve two sets of surfaces: (i) interior atoms that are coupled to an embedded atomistic domain and (ii) exterior atoms where external boundary conditions are applied. Typically, the number of interior surface atoms is very small compared to the number of exterior surface atoms. An efficient approximate method is presented for controlled coarse graining of the outer boundary degrees of freedom. This greatly reduces the number of degrees of freedom and the size of the dense Green's function matrices while preserving high accuracy. The new coarse graining method is demonstrated on various example problems to show the reductions in computational costs versus relative error of the approximate solution with respect to exact reference solutions. Traditionally, LGFs are computed up to some cutoff radius, beyond which a transition to the continuum Green's function (CGF) is made. This transition creates spurious forces near the transition region, leading to producing non-negligible errors in the solution. This has not been previously recognized. We will discuss the origins of these extra forces and remedies to reduce them with specific examples. [1] M.~Hodapp, G.~Anciaux, and W.~Curtin. \newblock~Lattice green function methods for atomistic/continuum coupling: {Theory} and data-sparse implementation. Comput. Methods Appl. Mech. Eng., 348:1039--1075, May 2019.

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Title: High-Order HDG Formulations for Compressible, Incompressible and Weakly Compressible Flows

Author(s): *Antonio Huerta, *Universitat Politècnica de Catalunya*; Matteo Giacomini, *Universitat Politècnica de Catalunya*;

The development of robust high-order solvers capable of accurately simulating flows in different regimes currently represents a major challenge in the field of computational fluid dynamics. The Hybridizable Discontinuous Galerkin (HDG) method offers several appealing properties in this context, including a natural framework to stabilise convection phenomena, a stable discretization using equal order approximations for all variables, optimal convergence of the stress tensor and robustness in the incompressible limit [1]. This talk reviews some recent advances concerning HDG approximations of flow problems across different regimes, spanning compressible, incompressible and weakly compressible flows. In the context of inviscid and viscous laminar compressible flows, the treatment of convective fluxes by means of positivity-preserving Riemann solvers is explored. The HDG method with HLL-type Riemann solvers provides robust approximations for different flow regimes, outperforming traditional hybrid discretizations with Roe and Lax-Friedrichs fluxes in supersonic cases and in the approximation of viscous boundary layers, respectively [2]. The coupling of HDG with high-order time integrators is then discussed in the framework of viscous laminar incompressible Navier-Stokes flows. Singly diagonally implicit Runge Kutta and Rosenbrock-type methods are proposed to devise robust time marching schemes for differential algebraic equations with effective time step control strategies. Finally, an HDG formulation for weakly compressible viscous flows is coupled with a continuous Galerkin formulation for nonlinear elastic structures via Nitsche's method to devise a multiphysics solver for fluid-structure interaction problems [3]. [1] M. Giacomini, R. Sevilla and A. Huerta. Tutorial on Hybridizable Discontinuous Galerkin (HDG) Formulation for Incompressible Flow Problems. In: Modeling in Engineering Using Innovative Numerical Methods for Solids and Fluids, L. De Lorenzis and A. Düster (eds.), CISM, 599:163-201, Springer (2020). [2] J. Vila-Pérez, M. Giacomini, R. Sevilla and A. Huerta. Hybridisable discontinuous Galerkin formulation of compressible flows. Archives of Computational Methods in Engineering, to appear. doi.org/10.1007/s11831-020-09508-z [3] A. La Spina, M. Kronbichler, M. Giacomini, W.A. Wall and A. Huerta. A weakly compressible hybridizable discontinuous Galerkin formulation for fluid-structure interaction problems. Computer Methods in Applied Mechanics and Engineering, 372:113392 (2020).

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Title: Development of a Stable and Conserving Time-Integration Framework for Mortar-Based Contact Dynamics

Author(s): *António Manuel Couto Carneiro, *University of Porto*; Rodrigo Pinto Carvalho, *University of Porto*; Francisco Manuel Andrade Pires, *University of Porto*;

Modelling contact interaction between deformable bodies is a central challenge in engineering, as it operates as the medium for energy exchanges. From a phenomenological perspective, the characterisation of interfacial mechanics is very elaborate, due to its complex multiscale and multi-physics nature. From the numerical and computational standpoint, contact is at is core associated with generally nonsmooth laws and constraints, thus leading to several complications in the mathematical and numerical treatment of this class of problems. This contribution focuses on a numerical framework towards a conserving and robust time integration scheme, applicable to nonlinear solid mechanics equations at large strains, incorporating contact interaction within the dual mortar contact algorithm. Three scenarios will be analysed. Firstly, considering just the equilibrium problem of a single body without the presence of contact interactions, a stable and asymptotically conserving time integration of the structural equations is formulated and implemented, based on the so-called energy-momentum methods. Second, the stabilization of the Lagrange Multipliers oscillations over time—resulting from the coupling between the differential equations in time and the algebraic contact constraints—is tackled by means of a singular mass matrix computed via non-standard quadrature formulas, extending upon recent endeavours on the topic. Last, the investigation addresses the energy and momentum conservation in the general setting incorporating the contact nonlinearities, by employing discrete versions of the persistency condition along the normal contact direction. The numerical behaviour and conserving properties of the individual contributions and also the complete time-integration scheme are demonstrated and validated through several numerical applications. References [1] Kuhl D, Ramm E. Generalized Energy–Momentum Method for non-linear adaptive shell dynamics. Computer Methods in Applied Mechanics and Engineering. 1999 Aug 1;178(3):343–66. [2] Hager C, Hüeber S, Wohlmuth BI. A stable energy-conserving approach for frictional contact problems based on quadrature formulas. International Journal for Numerical Methods in Engineering. 2008;73(2):205–25. [3] Laursen TA, Love GR. Improved implicit integrators for transient impact problems—geometric admissibility within the conserving framework. International Journal for Numerical Methods in Engineering. 2002;53(2):245–74.

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Title: 3-D Modeling of Multi-Stage Hydraulic Fracturing from a Borehole within a GFEM Framework

Author(s): Nathan Shauer, *University of Illinois at Urbana-Champaign*; *Armando Duarte, *University of Illinois at Urbana-Champaign*;

Hydraulic Fracturing is the process in which a fracture propagates through the injection of pressurized fluid in its cavity. This process is widely used in the oil and gas industry to increase reservoir permeability which leads to high rates of both injection and production. Hydraulic fractures are often created in a multi-stage process which leads to complex fracture geometries due to interactions and fractures realignment with the preferential propagation direction. The fracture shape, and consequently pressure drop, varies significantly between fracture clusters. As a result, the majority of the gas and oil production comes from only 20 to 30% of the clusters. Computational methods able to predict the near-wellbore tortuosity and pressure drop can play a key role in improving the performance of multistage fracturing. This presentation reports on recent advances of an adaptive Generalized Finite Element Method (GFEM) for the simulation of multiple 3-D non-planar hydraulic fracture propagation near a wellbore. This method is particularly appealing for the discretization of the fractures since it does not require the finite element mesh to fit fracture faces. Additionally, analytical asymptotic solutions are used to enrich the fracture fronts, which increases the accuracy of the approximation. Several wellbore and fracture configurations are investigated to demonstrate the non-intuitive propagation behavior in these near-wellbore conditions and the robustness of the proposed GFEM methodology. They show that even a fairly small misalignment between the wellbore and the minimum in-situ stress leads to fracture geometries that are vastly different from those predicted by simulations that assume fracture planarity – a simplification often adopted in the simulation of hydraulic fractures propagation.

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Title: Stochastic Deep Learning Parameterization of Ocean Momentum Forcing

Author(s): *Arthur Guillaumin, *New York University*; Laure Zanna, *New York University*;

Despite the use of supercomputers, coupled climate ensemble simulations that span multi-centuries cannot routinely be run at a high-enough spatial resolution to resolve mesoscale (10-100km horizontal scale) ocean dynamics. Standard parameterizations representing unresolved mesoscale dynamics can still lead to biases and to under-dispersive ensemble simulations. Recently, a few studies have considered the use of Deep Learning tools to parameterize subgrid ocean dynamics in highly idealized models. Here, we present results on the use of Deep Learning to infer the subgrid forcing using data from a global 1/10-degree state-of-the-art coupled climate model, namely CM2.6 simulations. We successfully train a Convolutional Neural Network for the subgrid ocean momentum forcing using resolved surface velocities. The novelty of our approach is to learn a stochastic Deep Learning representation of the subgrid momentum forcing: rather than predicting a single number using a standard Mean Square Error loss function, we predict the two moments of a Gaussian distribution. Our offline tests show that our learnt parameterization generalizes well to the global oceans, and to a climate with increased CO2 levels, without further training. We present preliminary results on an online implementation of our parameterization in a Shallow Water Model. While stochastic parameterizations are in use in atmospheric modeling, most proposed Deep Learning parameterizations have been purely deterministic so far. Our work demonstrates the potential of combining Deep Learning tools with a probabilistic understanding of uncertainty in parameterizing non-resolved dynamics. In the future, we expect stochastic deep learning will help reduce biases in climate models and lead to more reliable ensemble predictions.

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Title: Bayesian Calibration of Interatomic Potential Models for Binary Alloys

Author(s): *Arun Hegde, *Sandia National Laboratories*; Elan Weiss, *The Ohio State University*; Wolfgang Windl, *The Ohio State University*; Habib Najm, *Sandia National Laboratories*; Cosmin Safta, *Sandia National Laboratories*;

Developing reliable interatomic potential models with quantified predictive accuracy is critical to the successful application of molecular dynamics (MD) simulations. These potentials are typically derived from empirical considerations and contain unknown parameters that must be properly fit before use. It is standard practice that this fitting is performed through comparison with a more expensive first-principles method, e.g., density functional theory (DFT). In this work, we cast the problem of calibrating such potentials in a Bayesian statistical setting [1]. Here, probabilistic assertions about the parameters, model error, and other uncertainties are updated by including a training set of DFT-simulated data. The result is a posterior distribution over the aforementioned items, which can then be propagated forward to quantify predictive uncertainties. We apply these techniques to investigate various potential model forms based on the RAMPAGE framework for complex alloy systems [2]. The potentials are used with the LAMMPS MD simulation software to predict relevant physical quantities of interest – lattice parameters, mixing enthalpies, and elastic constants. As a case study, we examine Au-Cu binary alloys over a wide range of compositions and use the above techniques to suggest avenues for model improvement. The reliability of this approach hinges on adequately exploring the posterior distribution. This is typically accomplished using Markov Chain Monte Carlo (MCMC) sampling algorithms, which entails very many runs of the LAMMPS code. To alleviate this computational burden, we develop a strategy in which low-order polynomial surrogates are constructed over an initial trust-region, which is then sequentially adapted as guided by MCMC. The resulting Bayesian posteriors are used to assess the quality of the proposed interatomic potentials through comparison with the higher accuracy DFT information. Moreover, we investigate different techniques for computing the Bayes evidence for model selection and demonstrate its utility in comparing among multiple proposed interatomic potential models. [1] Sargsyan, K., H. N. Najm, and R. Ghanem. "On the statistical calibration of physical models." International Journal of Chemical Kinetics 47.4 (2015): 246-276. [2] L. Ward, A. Agrawal, K. M. Flores, and W. Windl. "Rapid production of accurate embedded-atom method potentials for metal alloys." arXiv preprint arXiv:1209.0619 (2012).

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Title: Data?Driven Super?Parameterization Using Deep Learning: Experimentation With Multiscale Lorenz 96 Systems and Transfer Learning

Author(s): *Ashesh Chattopadhyay, *Rice University*; Adam Subel, *Rice University*; Pedram Hassanzadeh, *Rice Univeristy*;

To make weather and climate models computationally affordable, small?scale processes are usually represented in terms of the large?scale, explicitly resolved processes using physics?based/semi?empirical parameterization schemes. Another approach, computationally more demanding but often more accurate, is super?parameterization (SP). SP involves integrating the equations of small?scale processes on high?resolution grids embedded within the low?resolution grid of large?scale processes. Recently, studies have used machine learning (ML) to develop data?driven parameterization (DD?P) schemes. Here, we propose a new approach, data?driven SP (DD?SP), in which the equations of the small?scale processes are integrated data?drivenly (thus inexpensively) using ML methods such as recurrent neural networks. Employing multiscale Lorenz 96 systems as the testbed, we compare the cost and accuracy (in terms of both short?term prediction and long?term statistics) of parameterized low?resolution (PLR) SP, DD?P, and DD?SP models. We show that with the same computational cost, DD?SP substantially outperforms PLR and is more accurate than DD?P, particularly when scale separation is lacking. DD?SP is much cheaper than SP, yet its accuracy is the same in reproducing long?term statistics (climate prediction) and often comparable in short?term forecasting (weather prediction). We also investigate generalization: when models trained on data from one system are applied to a more chaotic system, we find that models often do not generalize, particularly when short?term prediction accuracies are examined. However, we show that transfer learning, which involves re?training the data?driven model with a small amount of data from the new system, significantly improves generalization. Potential applications of DD?SP and transfer learning in climate/weather modeling are discussed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A 3-D Computational Homogenization Scheme For Multi-Scale Simulations Of Fluid-Saturated Porous Media

Author(s): *Ashkan Almasi, *University of Connecticut*; Tim Ricken, *University of Stuttgart*; David M. Pierce, *University of Connecticut*;

The theory of porous media (TPM) plays an important role in many diverse areas of engineering, particularly including the biomechanics of soft tissues (e.g. liver, brain, and cartilage) [1]. The remarkable macro-mechanics of soft tissues derives from the complex micro-mechanics of their constituents, e.g. proteoglycans, collagens, and electrolytic fluid, and their interactions. To facilitate mechanistic understanding and improved analyses (e.g. of experimental results) of the multi-scale mechanics of soft tissues we aimed to establish a computational framework specific to fluid-saturated, fibrous soft tissues and engineered materials. We can apply experiments to quantify mechanical properties and biology of tissues, and imaging to estimate tissue structure and even strains; however, only computational models can estimate intra-tissue stresses in human joints and tissues during daily activities because the required in vivo experiments are impossible or unsafe. Here we established a multi-scale framework within FEBio (University of Utah) to perform finite element discretizations of boundary value problems (BVPs) on both macro and micro scales to facilitate studies of fluid-saturated porous media. We combined the TPM and the FE2-method (i.e. the TPM2 method) to solve 3-D, two-scale, non-linear, coupled, and time-dependent BVPs for materials with porous microstructures. To solve the multiscale BVPs we first provide the microscopic representative volume elements (RVEs) with macroscopic quantities as boundary conditions (BCs). These BCs must comply with Hill-Mandel homogeneity conditions [2]. The microscopic RVEs must then provide the first Piola-Kirchhoff stress tensors back to the macroscale model at each integration point. We considered both isotropic, homogeneous RVEs and those with inclusions, the latter with relatively stiff and impermeable inclusions. To validate our implementation we compared our numerical results from simulations in 3-D plane strain to those obtained by Bartel et al. in 2-D [2,3]. Emerging multi-scale FE2 methods (FE analyses augmented to derive the material behaviors from a distribution of finer scale FE analyses) are ideally suited to bridge the joint, tissue, and intra-tissue scales, but have not yet been applied to multi-phase, fibrous materials. We will leverage our TPM2 framework, e.g. to establish how physical activity propagates micro-damage in the collagen network of cartilage in vivo. References [1] R. De Boer, Springer, 2012. [2] F. Bartel et al., PAMM, 15:447-448, 2015. [3] F. Bartel et al., PAMM, 17:577-578, 2017.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: 2D and 3D Microstructure Reconstruction using a Transfer Learning Approach and Structure-Property Studies

Author(s): *Ashwini Gupta, *Johns Hopkins University*; Anindya Bhaduri, *Johns Hopkins University*; Lori Graham-Brady, *Johns Hopkins University*;

Computational analysis, modeling, and structure-property prediction of many phenomena in materials require a three-dimensional (3D) microstructure sample that embodies the salient features of the material system under study. Deep learning approaches, in particular convolutional neural networks, are particularly well-suited to process microstructures image data and study structure-property links. A short-range-correlation (SRC) model is introduced in the framework of transfer-learning based approach to reconstruct random heterogeneous materials. We integrate information about the statistical descriptors such as n-point correlation functions within a deep neural network framework, for example, by including them in the overall objective function. This helps us achieve significant computational efficiency in simulating microstructures that retain the critically important physical properties of the original microstructure. We further modify the cost function to include correlations along the depth to reconstruct a 3D microstructure. Numerical examples for the reconstruction of 2-D and 3-D bi-phase porous ceramic material demonstrate the efficiency of the proposed methodology. We further analyse the algorithm's capacity to capture the variability of various material properties with respect to those of the target microstructure by performing a detailed finite element analysis (FEA) of the reconstructed microstructures to calculate effective elastic modulus, thermal conductivity, and hydraulic conductivity. This study finds its use in generating a high-resolution microstructure from low-resolution micrographs, reconstructing 3D microstructures from 2D/3D images, generation of massive datasets of material systems with targeted properties, and microstructure induced uncertainty quantification and propagation.

16th U.S. National Congress on Computational Mechanics
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Title: On the Behavior of Entropy-Stable Schemes in the Low Mach Regime

Author(s): *Ayoub Gouasmi, *Universities Space Research Association / NASA Ames Research Center*; Scott M. Murman, *NASA Ames Research Center*; Karthik Duraisamy, *University of Michigan*;

A well-known issue with upwind-type schemes developed for compressible flows is that their performance degrades (stiffness and accuracy) in the low Mach number regime [1], most notably in the incompressible limit, despite the fact that the incompressible Euler equations are a particular occurrence of the more general compressible Euler equations. Entropy-Stable (ES) schemes [2], which showed promise in under-resolved compressible turbulent flow calculations, suffer from the same issues, in part because they typically use upwind-type dissipation operators. In this work, we build upon previous studies, such as that of [1], to investigate the behavior of ES schemes in the low Mach number regime. We focus on the accuracy degradation problem and its mitigation using flux-preconditioning techniques. We demonstrate, analytically and numerically, that these techniques are compatible with entropy-stability. We provide arguments explaining the accuracy issues and their mitigation. We also consider the acoustic limit and follow up on recent work [3]. [1] Turkel, E. : Preconditioning Techniques in Computational Fluid Dynamics, Annu. Rev. Fluid Mech., 31 pp. 385-416, 1999. [2] E. Tadmor, E. : Entropy stability theory for difference approximations of nonlinear conservation laws and related time dependent problems, Acta Numerica 12 (2003) 451-512. [3] Bruel, P., Delmas, S., Jung, J., and Perrier, V. : A low Mach correction able to deal with low Mach acoustics, J. Comput. Phys., 378 pp. 723-759, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Isogeometric Analysis of Cahn-Hilliard Phase Field-Based Binary-Fluid-Structure Interaction Based on an ALE Variational Formulation

Author(s): *Babak Sayyid Hosseini, *Technical University of Dortmund*; Stefan Turek, *Technical University of Dortmund*; Matthias Möller, *Delft University of Technology*;

Current work presents a computational model and simulation technique capable of capturing the complex physics behind the intriguing phenomena of Elasto-capillarity. Elasto-capillarity refers to the ability of capillary forces or surface tensions to deform elastic solids through a complex interplay between the energy of the surfaces (interfaces) and the elastic strain energy in the solid bulk. The described configuration gives rise to a three-phase system featuring a fluid-fluid interface (for instance the interface of a liquid and an ambient fluid such as air) and two additional interfaces separating the elastic solid from the first and second fluids. This setup is encountered in the wetting of soft substrates which is an emerging young field of research with many potential applications in biomechanics and micro- and nanotechnology. The two-phase flow problems considered, are immiscible two-component incompressible flow problems which we address with a Cahn-Hilliard phase field-based two-phase flow model through the Navier-Stokes-Cahn-Hilliard (NSCH) equations. Our computational model for the FSI subproblem is based on a hyperelastic material model for the solid. When modeling the coupled dynamics of FSI, one is confronted with the dilemma that the fluid model is naturally based on an Eulerian perspective while it is very natural to express the solid problem in Lagrangian formulation. The monolithic approach we take, uses a fully coupled Arbitrary Lagrangian--Eulerian (ALE) variational formulation of the FSI problem and applies Galerkin-based Isogeometric Analysis for the discretization of the partial differential equations involved. This approach solves the difficulty of a common variational description and facilitates a consistent Galerkin discretization of the FSI problem. Besides, the monolithic approach avoids any instability issues that are associated with partitioned FSI approaches when the fluid and solid densities approach each other. The BFSI computational model presented, is obtained through the combination of the above described phase field-based two-phase flow and the monolithic fluid-structure interaction models and yields a very robust and powerful method for the simulation of elasto-capillary fluid-structure interaction problems. In addition, we also show that it may also be used for the modeling of FSI with free surfaces, involving totally or partially submerged solids. Our BFSI model may be classified as quasi monolithic as we employ a two-step solution algorithm, where in the first step we solve the pure Cahn-Hilliard phase field problem and use its results in a second step in which the binary-fluid-flow, the solid deformation and the mesh regularization problems are solved monolithically.

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Title: An Accelerated Hybrid Data-Driven/Model-Based Approach for Poroelasticity Problems with Multi-Fidelity Multi-Physics Data

Author(s): *Bahador Bahmani, *Columbia University*; WaiChing Sun, *Columbia University*;

We present a hybrid model/model-free data-driven approach to solve poroelasticity problems. Extending the data-driven modeling framework originated from \citet{kirchdoerfer2016data}, we introduce one model-free and two hybrid model-based/data-driven formulations capable of simulating the coupled diffusion-deformation of fluid-infiltrating porous media with different amounts of available data. To improve the efficiency of the model-free data search, we introduce a distance-minimized algorithm accelerated by a k-dimensional tree search. To handle the different fidelities of the solid elasticity and fluid hydraulic constitutive responses, we introduce a hybridized model in which either the solid and the fluid solver can switch from a model-based to a model-free approach depending on the availability and the properties of the data. Numerical experiments are designed to verify the implementation and compare the performance of the proposed model to other alternatives.

16th U.S. National Congress on Computational Mechanics
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Title: Improvements to Dual Weighted Residual Error Estimation and Adaptation for Asymptotically Consistent FEM Discretizations

Author(s): *Ben L. S. Couchman, *Massachusetts Institute of Technology*; David L. Darmofal, *Massachusetts Institute of Technology*; Steven R. Allmaras, *Massachusetts Institute of Technology*; Marshall C. Galbraith, *Massachusetts Institute of Technology*;

When solving fluid dynamic problems characterized by strong shocks or other under-resolved features, higher-order finite element methods require stabilization operators (such as artificial diffusion) to prevent non-physical oscillation in the solution variables. It is common for these stabilization operators to be asymptotically consistent. The presence of an asymptotically consistent contribution must be accounted for in residual-based error estimates. In this work, we show that some common forms of the dual weighted residual (DWR) error estimate vanish (as element size decreases) at a rate faster than the true error. That is, in these situations the effectivity of the DWR does not converge to one. We introduce a localizable correction to the DWR, which correctly accounts for the asymptotically consistent contribution to the residual. To assess the efficacy of the corrected DWR, we compare the performance of an output-based grid adaptation algorithm when using both the corrected and uncorrected forms of the DWR. Comparisons are made for fluid dynamic, shock dominated problems, using higher-order finite element methods with artificial diffusion.

16th U.S. National Congress on Computational Mechanics
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Title: A Coupled Fluid-Particle Solver for Active Suspensions

Author(s): *Benjamin Deußen, *Technical University Darmstadt*; Florian Kummer, *Technical University Darmstadt*; Martin Oberlack, *Technical University Darmstadt*;

An active suspension consist of a fluid, usually Newtonian, and a large number of embedded active particles. The latter term describes rigid objects which exert a force onto the surrounding fluid and, hence, propel themselves through the suspension. Such conglomerates can be found in nature or as designed objects. For example, flocks of birds, swarming fish and bacteria colonies can be described as active suspensions. Our work is focused on microscopic active particles, e.g. colonies of Escherichia coli. We discuss the challenges resulting from the highly viscous environment of the active particles and present first results. Our model is based on the Janus approach for active particles. On one half of the particle surface an active tangential stress together with a slip boundary condition is applied and a no-slip boundary condition on the other half [1]. The fluid is modelled by the Navier-Stokes equations. The solution for the flow field is approximated with with a high-order discontinous Galerkin solver, which is part of the BoSSS-framework [2]. Newton-Euler equations are used to describe the translational and rotational motion of the particles. Collisions between multiple particles are represented with a momentum conservation model. An iteration scheme generates the coupling between the fluid and the particles. We present results for near field interactions within an active suspension using a model system of two particles. Furthermore, we present statistical data for large systems with N>1000 particles obtained with the presented solver. [1] Saintillan, D. and Shelley, M.J. Active suspensions and their nonlinear models. C. R. Physique (2013) 14:497-517 [2] Kummer, F., Weber, J. and Smuda, M. BoSSS: a package for multigrid extended discontinuous Galerkin methods. Computers & Mathematics with Applications (2020) 81:237-257

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Analysis of Non-Normal Systems

Author(s): *Benjamin Herrmann, *University of Washington*; Peter J. Baddoo, *Imperial College London*; Richard Semaan, *Technical University of Braunschweig*; Steven L. Brunton, *University of Washington*; Beverley J. McKeon, *California Institute of Technology*;

Many fluid flows behave as selective amplifiers of external disturbances –where most perturbations are damped out, a few favored excitation patterns lead to largely amplified responses. Resolvent analysis is a technique to identify these most-responsive forcings along with the corresponding most-amplified responses, based on the governing equations of the system. Interest in the method has continued to grow during the past decade due to its potential to reveal structures in turbulent flows, and to guide sensor/actuator placement for flow control applications. However, resolvent analysis requires access to high-fidelity numerical solvers to produce the linearized dynamics operator. In this talk, I present the development of a purely data-driven algorithm to perform resolvent analysis to obtain the forcing and response modes of a linear system, without recourse to its governing equations, but instead based on snapshots of its transient evolution. The formulation of the method follows from two established facts: 1) dynamic mode decomposition can approximate eigenvalues and eigenvectors of the underlying operator governing the evolution of a system from measurement data, and 2) a projection of the resolvent operator onto an invariant subspace can be built from this learned eigendecomposition. I demonstrate the method on numerical data of the linearized complex Ginzburg--Landau equation and of three-dimensional transitional channel flow, and discuss data requirements. The ability to perform resolvent analysis in a completely equation-free and adjoint-free manner will play a significant role in lowering the barrier of entry to resolvent research and applications. Even with partial measurements and a limited dataset, experimental applications of data-driven resolvent analysis will enable learning high-gain input-output pairs of modes to provide valuable –and otherwise unavailable– information to guide controller design in non-normal systems.

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Title: Computational Modeling of Visco-Elasto-Capillary Phenomena of Soft Polymeric Solids

Author(s): *Berkin Dortdivanlioglu, *The University of Texas at Austin*; Ali Javili, *Bilkent University*;

To date, the mechanics of interfaces of soft solids, e.g., polymeric gels, remain elusive. In particular, the mechanical properties of the bulk gel can differ from its boundary due to the fundamental role of surface tension and lower-dimensional energetics at length scales of nanometers to millimeters. From a theoretical perspective, classical continuum mechanics is size-independent and hence lacks a physical length-scale. A characteristic length scale and size-dependent material response can be captured in continuum models by accounting for the energetic competition between the bulk gel and its boundary. This energetic competition is referred to as the elasto-capillary effect, and plays an important role in cavitation, soft composites, wetting on soft substrates, adhesive failure, and pattern formations such as beading, creasing, and wrinkling. A fundamental challenge in understanding the behaviors of soft materials at small scales is elucidating the nonlinear effects due to complex surface stresses, e.g., including viscous effects. Extending the well-established surface elasticity theory [1], surface viscoelasticity can capture the size-dependent dissipation of soft polymeric gels. In this contribution, we endow both surface and bulk gel with their own energy and derive the equations governing the response of a polymeric gel undergoing large viscoelastic deformations along with fluid transport. As a result, surface and bulk can show distinctive mechanical, diffusional, and other multiphysical behaviors. The couplings between surface and bulk and the couplings between different fields can lead to a wide range of interesting properties, yet to be explored. The key focus of this presentation is to develop a computational framework modeling viscoelastic materials with surface viscoelasticity using the geometrically exact isogeometric finite element technique and to study nonlinear bulk-boundary coupling effects on the overall deformation behaviors. We show that surface viscoelasticity enriches the nonlinearities in creep and relaxation behaviors of the coupled structure and further introduces characteristic length and time scales as well as time-dependent surface tension into the problem. The proposed methodology provides a robust computational foundation to elucidate visco-elasto-capillary deformations at soft gels [2]. [1] Gurtin, M. E. & Ian Murdoch, A. A continuum theory of elastic material surfaces. Arch. Rational Mech. Anal. 57, 291–323 (1975). [2] Dortdivanlioglu, B. & Javili, A. Boundary viscoelasticity theory at finite deformations and computational implementation using isogeometric analysis. Computer Methods in Applied Mechanics and Engineering 374, 113579 (2021).

16th U.S. National Congress on Computational Mechanics
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Title: A Octree Based LES Framework for Exploring the Impact of Vegetation on Thermal Response of the Building Environment

Author(s): *Boshun Gao, *Iowa State University*; Kendrick Tan, *Iowa State University*; Breanna Marmur, *Iowa State University*; Jan Thompson, *Iowa State University*; Yuyu Zhou, *Iowa State University*; Ulrike Passe, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

Due to climate changes, households that did not have air conditioning are more susceptible to heat events that may lead to fatal consequences. It is generally accepted that vegetation can positively moderate these heat events. Despite this, there are very few studies done on the cooling effect of vegetation on near-building environment. Here, we numerically study the effect of a variation in the tree count and placement on its nearby environment for a low-income neighborhood in the city of Des-Moines, Iowa. We use a large-eddy simulation (LES) type simulation – based on the variational multiscale method – deployed on a massively parallel octree based framework that greatly simplifies mesh generation. We incorporate an experimentally calibrated evapo-transpirational (ET) vegetation model, along with remotely measured weather data, available data on vegetation (i.e. a tree inventory), and GIS data of the neighborhood construction. In general, an increased tree count led to a decrease in the average heat transfer between the building and its nearby environment. We explore how tree placement reduces the local flow parameters (such as the Re and Gr), which can lead to a reduction in heat flux when combined.

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Title: On the Equations of Equilibrium for Asymmetric Tiltedlipid Bilayers

Author(s): *Brett Hendrickson, *University of California, Berkeley*; Milad Shirani, *University of California, Berkeley*; David Steigmann, *University of California, Berkeley*;

Multiple ad-hoc two-dimensional models of the mechanics of tilted bilayers have been published in the membrane biophysics literature. In this work, we present a model derived from three-dimensional liquid crystal theory in which each of the two bilayers possesses its own independent director field. We then consider a special case of a tilted plane lipid bilayer.

16th U.S. National Congress on Computational Mechanics
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Title: Coupling Methods for Multiphysics Modelling of Enhanced Geothermal Systems

Author(s): *Bruce Gee, *University of Waterloo*; Robert Gracie, *University of Waterloo*;

In an enhanced geothermal system (EGS), hydraulic fracturing is used to increase the permeability of a hot dry rock mass. Cold fluid is then injected through the fractures to extract heat for power generation and direct heating. EGS wells have access to vast reserves of energy but are susceptible to short-circuiting due to the phenomena of flow channeling. Flow channeling is a positive multiphysics feedback loop which redirects cold fluid away from hot areas of the rock mass, causing the production temperature of an EGS to decrease over time and reducing the viability of the system as an energy source. Flow channeling only occurs when considering the coupled thermo-hydro-mechanical behaviour of the system, but few models capture the general behaviour of the system in which an initially dispersed flow patterns decays into a short-circuited configuration. Existing work on enhanced geothermal systems have relied upon sequentially or loosely-coupled models to capture the interaction between multiphysics processes. In this paper, we present the development of the first monolithic thermo-hydro-mechanical finite element model for EGS problems [1]. The model considers the coupling between deformation and temperature of the rock mass along with fluid pressure and temperature within the fracture planes. We consider and address the numerical issues that arise from this system, such as advection stabilization and spurious oscillations. The fully-coupled model is compared with sequential and loosely-coupled solution schemes on the merits of accuracy, efficiency, stability, and rates of convergence. The model has been applied to a three-dimensional rock mass with interconnected two-dimensional crack planes. Several different multiscale short-circuiting mechanisms are observed and described, and the implications of the modelling for true rock masses is discussed. [1] B. Gee and R. Gracie, “Comparison of fully-coupled and sequential solution methodologies for enhanced geothermal systems” Computer Methods in Applied Mechanics and Engineering, vol. 373, p. 113554, 2021.

16th U.S. National Congress on Computational Mechanics
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Title: Implementation of Local Boundary Conditions in Nonlocal Wave Propagation

Author(s): *Burak Aksoylu, *Texas A&M University–San Antonio*;

We give an overview of local boundary conditions (BC) in nonlocal problems as presented in [1]. We explain methodically how to construct forcing functions to enforce local BC and their relationship to initial values. We elaborate in great detail how to implement BC when a collocation method is utilized. We put a special emphasis on how to implement the local Neumann BC. In particular, a critical interpolation strategy is employed to find the appropriate value of the forcing function from its derivative. We present numerical results and computed displacement and strain fields with local Dirichlet and Neumann BC. [1] Burak Aksoylu George A. Gazonas, On Nonlocal Problems with Inhomogeneous Local Boundary Conditions, Journal of Peridynamics and Nonlocal Modeling (2020) 2:1-25, https://doi.org/10.1007/s42102-019-00022-w

16th U.S. National Congress on Computational Mechanics
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Title: A Versatile Computational Framework For Scalar Transport In Cardiovascular Simulations

Author(s): Sabrina Lynch, *University of Michigan*; Christopher Arthurs, *King's College London*; Nitesh Nama, *University of Michigan*; Onkar Sahni, *Rensselaer Polytechnic Institute*; *C. Alberto Figueroa, *University of Michigan*;

Simulation of cardiovascular reaction-advection-diffusion (RAD) problems offers significant numerical challenges such as highly advective flows (with Péclet (Pe) numbers up to 107) and flow reversal at outlet boundaries. Historically, little attention has been given to identification of appropriate outflow boundary conditions that preserve the accuracy of the solution. Lastly, there is currently a pressing need for a flexible computational framework that enables simple prototyping of arbitrary RAD models coupled with cardiovascular flows to enable simulation of complex biochemical interactions between scalar species. The overarching aim of this work is to address these issues by developing a set of computational tools to study 3D, transient cardiovascular RAD transport. Herein, we present a stabilized finite element (FE) framework [1] that incorporates four salient features: (i) backflow stabilization for Neumann outlet boundaries; (ii) a consistent flux boundary condition that minimally disturbs the local physics of the problem; (iii) a front-capturing stabilization to regularize solutions in high Pe numbers; and (iv) a flexible Python-interface for rapid prototyping of arbitrary RAD models. Key Words: Python, Reaction-Advection-Diffusion, Staggered, Stabilized Finite Elements References [1] Lynch, SR, Nama, N, Xu, Z, Arthurs, CJ, Sahni, O, Figueroa, CA. Numerical considerations for advection?diffusion problems in cardiovascular hemodynamics. Int J Numer Meth Biomed Engng. 2020; 36:e3378.

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Title: Near-Melt Material Model Calibrations for Stainless Steel 304L – Leveraging Experimental Data to Improve Residual Stress Predictions Induced by Welds and Additive Manufacturing

Author(s): *Carl Herriott, *Sandia National Laboratories*; Scott Smith, *Sandia National Laboratories*; Lauren Beghini, *Sandia National Laboratories*; Kyle Karlson, *Sandia National Laboratories*; Chris San Marchi, *Sandia National Laboratories*; Zahra Ghanbari, *Sandia National Laboratories*; Coleman Alleman, *Sandia National Laboratories*; Michael Stender, *Sandia National Laboratories*;

Residual stress predictions for welding and additive manufacturing are strictly contingent upon accurate descriptions of the material behavior at near-melt temperatures. However, due to limited data availability and testing challenges, previous material model fits were only calibrated in the forging temperature regime, around 900 Celsius, and thus are not sensitive to near-melt behavior. The lack of calibrations for near-melt temperatures calls into question the reliability of lifetime estimates of critical mechanical parts and systems. Using a Gleeble® thermomechanical simulator and additively manufactured stainless steel (SS) 304L bars, uniaxial tension experiments were conducted at temperatures and strain-rates expected for an electron beam weld. Both force-displacement data and video of necking profiles were obtained. Using the collected data, an internal calibration package, MatCal, and multi-physics simulation workflows, high fidelity calibrations and simulations were conducted and compared to equivalent simulations using legacy SS 304L calibrations. Results will be presented that show to obtain accurate and numerically stable process simulations, improvements of legacy calibrations for SS 304L with near-melt experimental data is essential. Legacy material parameter sets calibrated to forging temperatures for SS 304L are first compared to the high-temperature Gleeble® experimental data and are shown to over-predict the yield strength and failure displacements by factors larger than two. Upon incorporation of the high temperature force-displacement curves into the calibration, notable improvements are seen in the replicate Gleeble® simulation results in addition to the higher resolution stress profiles for a fully coupled electro-thermal-mechanical weld simulation. However, a comparison of the initial predicted necking profiles to the measured necking profiles for the same experiments results in substantial departures – suggesting that the calibrations inaccurately predict the transverse deformations. Lastly, all of the collected experimental data is incorporated into the calibration and shown to improve necking profile predictions while reducing the accuracy of the predicted force-displacement curves. These outcomes further motivate the need to: consider other model forms at near-melt temperatures, expand the present experimental testing suite, and develop a clear methodology to respectively weight the importance of force-displacement and necking profiles on calibration outcomes.

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Title: Spectral Analysis of Isogeometric Discretizations of Eigenvalue Problems

Author(s): Sven-Erik Ekstrom, *Uppsala University*; *Carlo Garoni, *University of Rome Tor Vergata*; Thomas J. R. Hughes, *The University of Texas at Austin*; Carla Manni, *University of Rome Tor Vergata*; Francesca Pelosi, *University of Rome Tor Vergata*; Alessandro Reali, *University of Pavia*; Hendrik Speleers, *University of Rome Tor Vergata*; Stafano Serra-Capizzano, *Università degli studi dell'Insubria*;

We focus on the numerical solution of one-dimensional second-order differential eigenvalue problems by isogeometric analysis (IgA) discretization methods. Through a kind of spectral analysis known as generalized locally Toeplitz (GLT) analysis [1], we are able to provide an a priori prediction of the global distribution of the numerical eigenvalues by means of a function called spectral symbol [2]. The spectral symbol allows, for instance, to predict the existence of p-k optical branches in the numerical spectrum, where p is the degree and k the smoothness of the considered IgA basis functions. This proves in particular that the IgA paradigm based on maximal smoothness basis functions does not suffer from the optical branches pathology, contrary to more traditional finite element approaches. Generalizations of the GLT analysis to multidimensional eigenvalues problems and more advanced IgA techniques such as box spline IgA [3] are also discussed. REFERENCES [1] Garoni C., Serra-Capizzano S. Generalized Locally Toeplitz Sequences: Theory and Applications (Volume I). Springer (2017). [2] Garoni C., Speleers H., Ekstrom S.-E., Reali A., Serra-Capizzano S., Hughes T.J.R. Symbol-Based Analysis of Finite Element and Isogeometric B-Spline Discretizations of Eigenvalue Problems: Exposition and Review. Arch. Comput. Methods Engrg. (2019). [3] Garoni C., Manni C., Pelosi F., Speleers H. Spectral Analysis of Matrices arising from IgA based on Box Splines. In preparation.

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Title: Piecewise Chebyshevian Splines for Isogeometric Analysis

Author(s): *Carolina Beccari, *University of Bologna*; Marie-Laurence Mazure, *Université Grenoble-Alpes*;

Rational B-splines (NURBS) are the crucial CAD tools on which isogeometric analysis methods were initially based, with a view to build exact geometric models. From this point of view, it was then shown that generalized B-splines can sometimes advantageously replace NURBS (see [2] and associated literature). Now, NURBS as well as generalized B-splines are few examples in the very large class of piecewise Chebyshevian refinable B-spline bases. Such bases exist in spaces of splines with pieces taken from different Chebyshevian spaces provided that the connection conditions between consecutive pieces are of a certain type, characterised in [3]. It is well known that the parameters inherently attached to Chebyshevian spaces can be efficiently used to modify/improve the solutions to classical problems. It is well known too that piecewise Chebyshevian refinable B-spline bases satisfy fundamental properties similar to polynomial B-splines. Moreover, they permit the exact representation of a very large variety of geometric models. These reasons explain why they have already proved to be useful in many domains (e.g., design, interpolation, approximation, multiresolution analysis). These reasons also make them natural candidates to build general isogeometric analysis methods. This is the subject of the present talk. The Chebyshev section-spaces being suggested according to the partial differential equations to be solved, the difficult and crucial question to answer upstream is: how to choose their associated parameters to ensure the existence of corresponding refinable B-spline bases? Fortunately, in [1] the theoretical characterisation obtained in [3] could be translated into an efficient numerical test which can be understood as a black box to be used before starting the IgA methods themselves. This test both answers the existence question and, if applicable, yields an evaluation routine for the B-spline bases. The talk presents the class of Chebyshevian refinable B-splines along with the associated numerical test, and it illustrates their relevancy for isogeometric analysis through a few examples. [1] Beccari, C., Casciola, G., Mazure, M-L.: Design or not design? A numerical characterisation for piecewise Chebyshevian splines. Numer. Algorithms 81, 1–31 (2019). [2] Manni, C., Pelosi, F., Sampoli, M.L.: Generalized B-splines as a tool in isogeometric analysis. Comput. Methods Applied. Mech. Engrg. 200, 867–881 (2011). [3] Mazure, M.-L.: How to build all Chebyshevian spline spaces good for geometric design? Numer. Math. 119, 517–556 (2011).

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Chicago, IL, July 25-29. 2021

Title: The AFRL AM Modeling Challenge: Predicting Micromechanical Fields in AM IN625 Using an FFT-Based Method with Direct Input from a 3D Microstructural Image

Author(s): *Carter Cocke, *The University of Utah*; Anthony Rollett, *Carnegie Mellon University*; Ricardo Lebensohn, *Los Alamos National Laboratory*; Ashley Spear, *The University of Utah*;

The efficacy of an elasto-viscoplastic fast Fourier transform (EVPFFT) code was assessed based on blind predictions of micromechanical fields in a sample of IN625 produced with additive manufacturing (AM) and experimentally characterized with high-energy x-ray diffraction microscopy (HEDM) during an in-situ tensile test. These blind predictions were made in the context of the AFRL AM Modeling Challenge Series. Challenge 4 in the Series required predictions of grain-averaged elastic strain tensors for 28 target grains at six specific loading states given a 3D microstructural image, initial elastic strains of target grains, and macroscopic stress-strain response. Among all participants, the EVPFFT-based submission presented in this work achieved the lowest total error in comparison to experimental results. The agreement between the model predictions and experimental data was excellent in the elastic regime but steadily worsened with plastic strain accumulation, similar to that report by Tari, et al. [1]. During post-submission investigation, several EVPFFT models were created and tested using no additional information beyond what was initially provided for the challenge. A material parameter optimization scheme was utilized to match the macroscopic material response more accurately, thus reducing over- and underprediction of specific strain components in the target grains compared to the submitted model. The residual elastic strain field was incorporated into multiple models, and the total error of each model was reduced by at least 20% compared to the submitted model. Using methods presented by Pokharel and Lebensohn [2], the residual elastic strain field was incorporated through eigenstrains calculated with an Eshelby approximation, which further improved the model predictions, especially in the plastic regime. The methods described in [2] were enhanced to calculate the eigenstrain field using an ellipsoidal grain shape assumption rather than using the assumption of spherical grains. This method resulted in the best model performance with a total error reduction of over 25% compared to the submitted model, with the additional benefit that no empirical correctional term described in [2] was necessary. The numerical Eshelby approximation scheme has since been implemented in DREAM.3D, an open-source microstructural dataset software, to make the method more accessible. Lessons learned for predicting full-field micromechanical response using the EVPFFT modeling method will be discussed, especially in the context of AM metals. [1] Vahid Tari, et al. Act. Mat. (2018). https://doi.org/10.1016/j.actamat.2018.05.036 [2] Reeju Pokharel and Ricardo A. Lebensohn. Scr. Mat. (2017). https://doi.org/10.1016/j.scriptamat.2017.01.025

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Title: Low-Dimensional Mapping Strategies for Enhancing Multifidelity Uncertainty Quantification of Cardiovascular Models

Author(s): *Casey Fleeter, *Stanford University*; Gianluca Geraci, *Sandia National Laboratories*; Daniele Schiavazzi, *University of Notre Dame*; Andrew Kahn, *University of California, San Diego*; Alison Marsden, *Stanford University*;

Cardiovascular models derived from patient-specific anatomy inherently contain multiple sources of uncertainty, rendering deterministic simulations less than ideal for clinically relevant applications. By incorporating our models in a stochastic framework, we can propagate uncertainties to simulation outputs, providing statistics on model predictions. Although computational methods for analyzing numerical models continue to advance, standard approaches are hindered by large random input spaces and the high computational cost of realistic three-dimensional simulations. Previous work showed the benefit of employing multifidelity estimators to reduce the variability seen in the expected values of output quantities of interest. Multilevel-multifidelity (MLMF) estimators resulted in several orders of magnitude cost savings when compared to traditional methods [1]. These improvements are attributable to offloading cost by solving computationally inexpensive low-fidelity models. However, as the MLMF framework relies on strong correlations between our high- and low-fidelity models, which often requires an identical parametrization of the inputs, current methods are constrained to specific low-fidelity formulations. Introducing low-dimensional mapping strategies for sampling allows us to improve the accuracy for quantities captured only approximately in low-fidelity models, such as wall shear stress, by improving correlations. Additionally, by mapping our uncertain parameters to a shared input subspace, we can leverage models characterized by a dissimilar parameterization, and thus explore uncertainties in three-dimensional parameters which are not present in low-fidelity models. Active subspace [2] methods with gradient approximation via least squares can be employed to yield one-dimensional subspaces. For higher dimensional subspaces, adaptive basis methods offer an alternative strategy, as recently demonstrated in [3]. By combining these mapping methods for sampling with the uncertainty quantification algorithms explored in previous work, we can further accelerate and reduce the variance in our estimators. These methods are compared and validated in patient-specific models of diseased pulmonary and coronary artery anatomies to show the improved performance. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. [1] Fleeter, C.M., Geraci, G., Schiavazzi, D.E., Kahn, A.M., and Marsden, A.L., Multilevel and multifidelity uncertainty quantification for cardiovascular hemodynamics, CMAME, 2020 [2] Geraci, G., and Eldred, M.S., Leveraging Intrinsic Principal Directions for Multifidelity Uncertainty Quantification, SAND2018-10817, 2018. [3] Zeng, X., Geraci, G., Gorodetsky, A.A., Eldred, M.S., Jakeman, J.D., Ghanem, Roger, Uncertainty Quantification with Multifidelity Strategies based on Models with Dissimilar Parameterizations, WCCM-CCOMAS Congress 2020.

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Title: C^1 Hierarchical Splines on Multi-Patch Geometries for Isogeometric Analysis

Author(s): *Cesare Bracco, *University of Florence*; Carlotta Giannelli, *University of Florence*; Mario Kapl, *University of Carinthia*; Rafael Vázquez, *École polytechnique fédérale de Lausanne*;

Locally refinable spline spaces are successfully used in Isogeometric Analysis (IgA) to construct adaptive schemes for solving PDEs. In particular, efficient methods with optimal convergence rates can be obtained by employing hierarchical splines (see, e.g., [1] for an overview). Since multi-patch geometries and C^1-continuous splines give and advantage in IgA to handle high-order problems over complex domains, a current research direction is investigating the construction of smooth tensor-product spaces on domains composed of several patches (see, e.g., [3]). Our goal is to combine these techniques with the hierarchical framework: we will show how to obtain locally refinable C^1-continuous spline spaces on multi-patch domains starting from the results obtained for the basic two-patch case [2] and the tensor-product construction [3]. A selection of numerical examples will be presented. [1] Bracco, C., Buffa, A., Giannelli, C., and Vázquez R., Adaptive isogeometric methods with hierarchical splines: an overview, Discret. Contin. Dyn. S. 39 (2019), 241-261. [2] Bracco, C., Giannelli, C., Kapl, M. and Vázquez R., Isogeometric analysis with C^1 hierarchical functions on planar two-patch geometries, Comput. Math. Appl. 80 (2020), 2358-2562. [3] Kapl, M., Sangalli G. and Takacs, T., An isogeometric C^1 subspace on unstructured multi-patch planar domains, Comput. Aided Design 69 (2019), 55-75.

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Title: Integrated Shape and Topology Optimization of Compliant Mechanism with Stress Constraints Using Embedding Domain Discretization Method

Author(s): *Chaitanya Dev, *University of Erlangen-Nuremberg*; Gabriel Stankiewicz, *University of Erlangen-Nuremberg*; Paul Steinmann, *University of Erlangen-Nuremberg*;

In the present study, we combine shape and topology optimization to generate a compliant mechanism subjected to stress constraint. By combining the two approaches we obtain an exact surface representation of the compliant mechanism. In our study, we use topology optimization to obtain a layout of the compliant mechanism. Then we use shape optimization and impose an additional stress constraint to obtain a mechanism without hinges. The density variables distributed using topology optimization allows us to have an optimal mechanism layout achieving the best system performance. The node variables, updated using the shape sensitivity, enables us to improve stress-based local performance around the hinges. Thus, we attempt to amalgamate the advantages of both topology and shape optimization methods to obtain an optimal mechanism. As noted in [1], consideration of local stress constraint remains a challenge in the design of the compliant mechanism. Further, in [2] it is noted that the issue of point flexures in compliant mechanisms remains unresolved. In our approach, we tackle this problem by considering the local stress constraint in a shape optimization framework. The sequential topology and shape optimization with the consideration of stress constraint in the shape optimization phase is the novelty of the present work. This allows us to get the best of both techniques: (1) consideration of the topology optimization techniques to obtain the mechanism layout, (2) use of the shape optimization techniques to consider local stress constraint. [1] Duysinx, P., Van Miegroet, L., Lemaire, E., Brüls, O. and Bruyneel, M., 2008. Topology and generalized shape optimization: Why stress constraints are so important?. International Journal for Simulation and Multidisciplinary Design Optimization, 2(4), pp.253-258. [2] Deepak, S.R., Dinesh, M., Sahu, D.K. and Ananthasuresh, G.K., 2009. A comparative study of the formulations and benchmark problems for the topology optimization of compliant mechanisms. Journal of Mechanisms and Robotics, 1(1).

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Title: Bayesian Inference via Conditional Generative Adversarial Networks

Author(s): *Chengyang Huang, *University of Michigan*; Xun Huan, *University of Michigan*;

The characterization of uncertainty is highly important for parameter estimation in engineering and science applications when only sparse and noisy measurements are available. The Bayesian inference paradigm, built upon the axioms of probability, presents a mathematically principled framework to quantify and update the uncertainty surrounding these estimates, conditioned on new information and data. Solving the Bayesian inference problem typically entails generating samples from the posterior distribution using Markov Chain Monte Carlo (MCMC)algorithms, which are computationally intensive especially with expensive forward models that describe complex physical systems, and become prohibitive when online speed (e.g., real-time)requirements are present. We thus take a different approach that avoids MCMC altogether, and aim to directly build a generative model for condition distributions of the parameter conditioned under different possible measurement outcomes. In particular, we train a conditional generative adversarial network (cGAN) offline, and pass into it (i.e., condition on) the measurement value encountered during online usage to achieve fast posterior sampling. We note that only one cGAN needs to be trained, which can then be used for repeated Bayesian inference under different posterior scenarios, and extremely useful for optimal experimental design. We demonstrate our method on algebraic test problems as well as a chemical combustion example for learning kinetic parameters.

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Title: High-Order Large-Eddy Simulations of a Ducted Wind Turbine

Author(s): *Chi Ding, *Clarkson University*; Bin Zhang, *Clarkson University*; Chunlei Liang, *Clarkson University*; Kenneth Visser, *Clarkson University*; Guangming Yao, *Clarkson University*;

A high-order flux reconstruction method coupled with a sliding mesh was applied to analyze the performance of a ducted wind turbine at a Reynolds number of 2.5E+6. To investigate the impact of the duct, computations for a ducted wind turbine and the corresponding open rotor turbine are performed for a range of tip speed ratios from 3.0 to 6.0. It is shown that the ducted turbine obtains a higher thrust and power output than the open rotor due to the increased mass flow rate in the rotor plane. To evaluate the effects of the yawed flow, simulations are also performed for the turbine under different yaw angles. The load distribution of the blades and the velocity field are analyzed and will be presented. The results demonstrate that the ducted wind turbine can maintain its power output for a larger range of yaw angles than its bare counterpart.

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Title: A Fractional Model for Anomalous Diffusion with Increased Variability

Author(s): Marta D'Elia, *Sandia National Laboratories*; *Christian Glusa, *Sandia National Laboratories*;

Fractional equations have become the model of choice in several applications where heterogeneities at the microstructure result in anomalous diffusive behavior at the macroscale. In this work we introduce a new fractional operator characterized by a doubly-variable fractional order and possibly truncated interactions. Under certain conditions on the model parameters and on the regularity of the fractional order we show that the corresponding Poisson problem is well-posed. We also introduce a finite element discretization and describe an efficient implementation of the finite-element matrix assembly in the case of piecewise constant fractional order. Through several numerical tests, we illustrate the improved descriptive power of this new operator across media interfaces. Furthermore, we present one-dimensional and two-dimensional h-convergence results that show that the variable-order model has the same convergence behavior as the constant-order model.

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Title: Adaptive Spacetime Meshing in 3D x Time for Causal Spacetime Discontinuous Galerkin Solvers

Author(s): *Christian Howard, *University of Illinois at Urbana-Champaign*; Amit Madhukar, *University of Illinois at Urbana-Champaign*; Robert Haber, *University of Illinois at Urbana-Champaign*; Jeff Erickson, *University of Illinois at Urbana-Champaign*; Reza Abedi, *The University of Tennessee Space Institute*;

Causal Spacetime Discontinuous Galerkin (cSDG) methods, sometimes called Tent-Pitching methods, are highly effective hyperbolic system solvers. They construct unstructured and asynchronous spacetime meshes that satisfy a so-called causality constraint that localizes the spacetime solution to small clusters of spacetime elements called patches so that the solution in any patch depends only on solutions in adjacent previously solved patches as well as prescribed initial or boundary data. This structure supports patch-by-patch direct solvers. Moreover, localized patch solutions and adaptive meshing operations can execute at a common patch-level granularity [1]. The spacetime mesh is constructed incrementally by advancing an asynchronous space-like front mesh through the spacetime analysis domain. Each incremental advance sweeps out a spacetime patch which is immediately solved and tested against adaptive error indicators. We discard any patch that fails the accuracy test and locally refine the front mesh to generate more refinement the next time the front advances. Other adaptive operations execute in spacetime within specialized patches. This strategy provides fine-grained adaptive meshing capable of tracking fast solution features, such as dynamic crack nucleation, extension and branching [2]. Production adaptive cSDG implementations have previously been limited to 2D x time due to the substantial jump in complexity of adaptive operations in 3D x time. The causality constraint and an associated progress constraint make adaptive refinement particularly challenging. This presentation introduces the first complete suite of adaptive cSDG operations in 3D x time and demonstrates their use in production simulations, including a parallel–adaptive example featuring dynamic probabilistic load and data balancing. [1] R. Abedi, S.–H. Cheng, J. Erickson, Y. Fan, M. Garland, D. Guoy, R. Haber, J. Sullivan, S. Thite and Y. Zhou. Spacetime meshing with adaptive refinement and coarsening, in 20th Ann Symp Comp Geometry, New York, USA, June 8–11 (2004), pp 300–309. [2] R. Abedi, R. B. Haber and P. L. Clarke. Effect of random defects on dynamic fracture in quasi-brittle materials, Int J Fract 208 (2017), pp 241–268.

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Title: Bayesian Deep Learning for Partial Differential Equation Parameter Recovery Using Sparse and Noisy Data

Author(s): *Christophe Bonneville, *Cornell University*; Christopher Earls, *Cornell University*;

Machine learning (ML) has gained tremendous popularity in the past decade. In the particular field of computational mechanics and engineering, physics-informed ML (or scientific ML) is now emerging as a hybrid research discipline at the intersection between purely statistical models and traditional mechanistic simulation methods like finite elements for both forward and inverse problems (Raissi et. al. [1]). One caveat of scientific ML however is its need for large amounts of (clean) data, in order to recover full system responses or underlying physical models. Bayesian methods have emerged as a promising approach to overcome these challenges as they are typically less sensitive to the vagaries of sparsity and noise, as compared with their frequentist counterparts. In this conference presentation, we propose to use Bayesian neural networks (BNN) [2] in order to: 1) Recover the full system states from sparse and noisy measurements (e.g. temperature throughout a domain, displacements in an elastic solid, etc.). We use Hamiltonian Monte-Carlo to sample the posterior distribution of a deep and dense BNN, while showing that it is possible to accurately capture physics of varying complexity without overfitting; unlike standards Deep neural networks. 2) Recover the parameters in the underlying partial differential equation (PDE) governing the physical system. Using the trained BNN as a surrogate of the system response, we take advantage of auto-differentiation tools in modern ML libraries to generate datasets of derivatives potentially comprising the latent PDE of the observed system. We build on the approach outlined by Rudy et. al. [3], and perform a linear-regression between the successive derivatives to recover the original PDE parameters. In our work, we go further by taking advantage of the confidence intervals on the BNN outputs and introduce a weighted least-squared loss function to discard the influence of highly uncertain derivatives, which allows for more accurate parameters recovery. We demonstrate our approach on a handful of example applied to physics and mechanics. References [1] Raissi, M., Perdikaris, P., Karniadakis, G.E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics 378 (2019): 686-707 [2] Neal, R. M., Bayesian Learning for Neural Networks, Ph.D Thesis, Dpt. Of Computer Science, University of Toronto (1994) [3] Rudy, S.H., Brunton, S.L, Proctor, J.L., Kutz, J.N. Data-driven discovery of partial differential equations, Science Advances 3-4 (2017)

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Title: A Probabilistic Artificial Neural Network for a Robust Identification of the Random Apparent Elasticity Tensor Field at Mesoscale

Author(s): *Christophe Desceliers, *Université Gustave Eiffel*; Florent Pled, *Université Gustave Eiffel*;

For many materials, the microstructure is complex and highly heterogenous. An efficient approach for constructing the model of such materials consists in modeling their apparent elasticity properties at mesoscale by a tensor-valued random field. Nevertheless, an important challenge is related to the identification of the hyperparameters of such a probabilistic mesoscopic model with limited experimental measurements. An efficient methodology has been recently proposed] to address this statistical inverse problem, which consists in solving a multiscale and multi-objective optimization problem with limited experimental information at both macroscale and mesoscale. In this work, we propose to train an artificial neural network in using in silico data generated by a multiscale computational model and a probabilistic mesoscopic model of the random material, for which the output layer corresponds to the values of the hyperparameters and the input layer corresponds to the values of three scalars characterizing the spatial fluctuations of the strain tensor experimentally measured at mesoscale and the six algebraically independent components of the effective elasticity tensor at macroscale. Nevertheless, training an artificial neural network with such in silico data usually fails to solve the statistical inverse problem. That is why a training dataset is constructed by processing the input data as the conditional mean values of the experimental features given the values of the hyperparameters to be identified. Then, a probabilistic model of such processed inputs is introduced given the experimental features. Consequently, for any given experimental feature obtained at both macroscale and mesoscales, we finally designed a stochastic artificial neural network that quantifies the uncertainties on the optimal values of the hyperparameters given experimental features.

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Title: A Process-Based Modeling Approach for Fused Filament Fabrication

Author(s): *Christopher Bock, *University of Maine*; Brett Ellis, *University of Maine*; Massoud Rais-Rohani, *University of Maine*;

Thermal gradients introduced in Fused Filament Fabrication (FFF) additive manufacturing cause residual stresses that can lead to inter-bead delamination and warpage, more so in thin-walled parts. Traditional voxel-based finite element (FE) approaches are plagued with fine discretization requirements and an inability to characterize inter-bead geometry and process-dependent inter-bead properties. This research seeks to address these shortcomings via a process-dependent extrusion-path FE approach that explicitly models the deposition and amalgamation of beads and removal of the part from the print bed. The proposed approach models FFF processes via two sequential simulations. First, a process model simulates temperature distributions throughout a part given a toolpath, process settings (e.g., deposition temperature, bead profile, print-head speed, and build plate temperature), and material properties (e.g., heat capacity, temperature-dependent thermal expansion, and temperature-dependent mechanical properties) assuming conductive, convective, and radiative heat transfer. The temperature field is utilized to calculate mechanical deformations and residual stresses via an assumed anisotropic temperature-dependent plasticity model. Second, a service model simulates deformations and stresses after removal of the part from the print bed and application of any pertinent mechanical tractions or boundary conditions the part would be subject to in service. Twelve polylactic acid (PLA) parts were manufactured and tested within a fractional factorial design of experiment (DOE) to validate the numerical approach. All parts utilized a right-cylindrical shell geometry having a 1-mm sidewall thickness and open surfaces on the top and bottom faces. The DOE considered four factors: nozzle temperature [190 – 230 °C], layer height [0.1 – 0.2 mm], outer diameter [40 – 50 mm], and number of layers [30 – 50 layers]. Preliminary dimensional results indicate numerical simulations agree within approximately 20% of the experimental values. In addition to the direct comparison of results, a comparison between the response of the model and experiments with respect to the various factors was completed. This work is significant in that a novel toolpath and manufacturing process driven modeling approach is developed and validated. The resulting simulation approach will allow researchers to quantify process-dependent warpage and residual stresses, while offering an avenue to quantifying process-dependent inter-bead strengths required to estimate process-induced delamination. Furthermore, the approach is anticipated to improve the prediction of process-structure-property-performance relations and design of FFF parts.

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Title: Modeling Impace of Combined Statistical and Discretization Error for Ergodic Chaotic Systems

Author(s): *Cory Frontin, *Massachusetts Institute of Technology*; David Darmofal, *Massachusetts Institute of Technology*;

The simulation of chaotic, ergodic systems involves the competing effects of statistical and discretization induced errors. In this work, we develop a error model that includes both discretization error and statistical error in approximations of long-term mean outputs of interest of ergodic chaotic ODEs. Using this model, we derive relationships between error and the total cost of simulating a chaotic system in a parallel computing environment, in which statistical error can be mitigated by either temporal averaging over a longer sampling period or by ensemble averaging over multiple independent instances computed in parallel. We demonstrate the validity of the model when applied to the Lorenz equations. Finally, we consider the implications of these findings for the discretization of chaotic systems using adaptive and higher-order methods and approaches for identifying the model at lower cost, as well as generalization of these findings to chaotic PDE systems.

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Title: Numerical Modeling of Rail Ballast Settlement

Author(s): *Craig Foster, *University of Illinois at Chicago*; Shubhankar Kulkarni, *Gamma Technologies*;

Track settlement is a major issue in the rail industry. Differential settlement, especially around stiffness transitions such as bridge approaches, is particularly an ongoing problem. Differential settlement can increase forces on the wheels [1] decrease ride quality, create the need for frequent maintenance, and, if left unchecked, become a danger to rail passengers. In this investigation, we perform a coupled finite element and multibody analysis of the dynamic settlement of ballast, subballast, and subgrade due to passing vehicles. The multibody model takes as inputs modal values of the linearized stiffness of the rail and substructure. The mode shapes can be truncated such that only the nodes involved directly in the multibody calculations are needed [2]. A suspended wheelset representing the train forces is run along the track. The forces generated on the rails from the multibody model are reconstructed in the finite element model, which models the ballast with a 3-invariant visco-plasticity model [3]. Permanent settlements are periodically updated and run through the multibody algorithm. As the substructures settles, forces at the transition increase, accelerating settlement. [1] A.I. El-Ghandour and C.D. Foster “Coupled finite element and multibody systems dynamics modelling for the investigation of the bridge approach problem” Journal of Rail and Rapid Transit, 2019. DOI: 10.1177./0954409719828599 [2] A.I. El-Ghandour, M.B. Hamper, and C.D. Foster. “Coupled Finite Element and Multibody Dynamics Systems Modeling of a 3D railroad system”. Journal of Rail and Rapid Transit, Vol. 230 No. 1, 2016, 283-294. DOI: 10.1177/0954409714539942 [3] M.H. Motamedi and C.D. Foster “An improved implicit numerical integration of a non-associated, three- invariant cap plasticity model with mixed isotropic-kinematic hardening for geomaterials.” International Journal of Numerical and Analytical Methods in Geomechanics. Vol 39, 2015, 1853-1883. DOI: 10.1002/nag.2372

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Title: Data-Driven and Topological Design of Structural Metamaterials for Fracture Resistance

Author(s): *Daicong Da, *Northwestern University*; Liwei Wang, *Northwestern University*; Yu-chin Chan, *Northwestern University*; Wei Chen, *Northwestern University*;

Abstract Overcoming the conflict between toughness and strength is a major challenge in the design of material microstructures. Data science as the fourth paradigm provides novel and diverse opportunities for materials design attaining exceptional mechanical properties. From both single- and multi-scale perspectives, this work aims to improve toughness and strength of structural brittle materials through precisely controlling the stress and combining topological optimization (TO) with data-driven techniques. First, mixed TO is developed to maximize the strain energy under displacement loading, while a maximum threshold is imposed on the local stress as a constraint [1]. Fracture response is tailored and compared between optimized structural materials by setting the threshold and adopting the phase field modeling method. Secondly, we propose a data-driven design framework for fracture resistance of the metamaterials with aperiodic microstructures. A deep neural network model consisting of a variational autoencoder (VAE) and a regressor for property prediction is trained to allow complex designs [2]. The latent space of the constructed VAE enables easy manipulation between different types of microstructures and generates new ones with tailored material properties. Thereafter, it is integrated in a topology-like distribution optimization for each component of the effective elasticity matrix. Finally, the targeted unit cells from the database are assembled into the macroscopic global structure to achieve the optimal distribution of the material properties. Consistency between different unit cells is guaranteed via a graph-based optimization method. We show the fracture resistance of porous structures can be significantly enhanced by the present method [3]. References: [1] D. Da. "Tailoring fracture properties of brittle structural materials." (Under review). [2] L. Wang, Y.C. Chan, F. Ahmed, Z. Liu, P. Zhu, and W. Chen. "Deep generative modeling for mechanistic-based learning and design of metamaterial systems." Computer Methods in Applied Mechanics and Engineering 372 (2020): 113377. [3] D. Da, L. Wang, Y.C. Chan, W. Chen. "Data-driven and topological design of structural metamaterials for fracture resistance." (in preparation).

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Title: A 3D Agent-Based Model to Explore DIPG Cells Invasion in Different-Stiffness Matrices

Author(s): *Daniel Camacho-Gómez, *Universidad de Zaragoza*; José Manuel García-Aznar, *Universidad de Zaragoza*; María José Gómez-Benito, *Universidad de Zaragoza*;

Diffuse intrinsic pontine glioma (DIPG) constitutes 15-20% of all childhood brain tumors, and it is the main cause of death in children with brain tumors. Tumor resection is not feasible and their delicate anatomical location makes biopsies rarely performed. Recently, autopsy protocols were implemented to obtain tumor material within a brief post mortem interval, and mouse models were also developed. This has allowed the characterization of primary cell cultures [1,2]. The most important hallmark of DIPG is its extreme infiltrative diffuse phenotype. They exhibit a more solid core and an invasive front. The invasive front is composed of single cells and by groups of cells. Moreover, they show that DIPG cells formed large, highly diffusive cell aggregates with many branches, and an increase in matrix stiffness produces a dense aggregate of cells. Here, we develop a 3D agent-based model to study the invasiveness of DIPG cells in different-stiffness extracellular matrices (ECM). Agent-based models have been widely used to study cell and tumor growth [3]. On the one hand, our model provides a mathematical model for cell proliferation. On the other hand, we consider cells' mechanical interactions based on pairwise potential functions and the interaction with the ECM by means of a friction coefficient that represents the dynamic viscosity of the matrix. Moreover, we introduce an active migration force to replicate the infiltrative diffuse characteristic of DIPG cells. Thus, we show that an increase in matrix rigidity reduces the migration capability of cells and therefore hinders cell invasiveness. In a low-stiffness matrix, the matrix does not oppose much resistance to cells' movement. Consequently, the active migration force makes cells invade adjacent areas. Hence, a central core and an invasive front of cells are formed. When the matrix rigidity is high, the matrix opposes to cells' movement. This limitation of cells' movement produces a solid core with no invasive front. [1] Caretti, V., et al. 2010. Monitoring of Tumor Growth and Post-Irradiation Recurrence in a Diffuse Intrinsic Pontine Glioma Mouse Model. Brain Pathology, 21(4), pp.441-451. [2] Wang, C., et al. 2020. A comparative study of brain tumor cells from different age and anatomical locations using 3D biomimetic hydrogels. Acta Biomaterialia, 116, pp.201-208. [3] Van Liedekerke, P., Palm, M., Jagiella, N. and Drasdo, D., 2015. Simulating tissue mechanics with agent-based models: concepts, perspectives and some novel results. Computational Particle Mechanics, 2(4), pp.401-444.

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Title: An Enriched Finite Element Method for Stiff Interfaces

Author(s): Amir Latifaghili, *University of Technology Sydney*; Milad Bybordiani, *The University of Sydney*; Emre Erkmen, *Concordia University*; *Daniel Dias-da-Costa, *The University of Sydney*;

Fracture leading to material failure is relevant in many applications found in engineering, medicine, and geology. Significant effort has been devoted to understand the phenomenon and develop rigorous tools for simulation/design purposes. One major step in the development of modelling techniques was the introduction of the eXtended/generalized finite element method (XFEM/GFEM), where strong discontinuities are not constrained to the mesh. XFEM/GFEM has proven to provide significant efficiency, as well as relative ease of implementation. Yet, there have been a number of difficulties and limitations that deserved attention, such as ill-conditioned systems and inaccurate local solutions around the crack path. The present work revisits the long-standing problem of traction oscillations found in discontinuities and proposes a strategy to fully overcome them. Since oscillations are in nature related to coupling found with standard shape functions of the elements for certain discontinuity arrangements, the subdomains partitioned by the discontinuity are here enriched with special shape functions to avoid over enrichment. The implementation is derived within the variational form that eliminates the need for blending elements. The performance was studied using element and structural examples with significantly stiff cracks in the domain. Further assessment was conducted in a range of crack propagation problems, including mixed-mode fracture of concrete beams and a peel test. Excellent agreement was found with experimental/numerical data, in terms of force-displacement and traction profile over the discontinuity. Results were shown to be objective with respect to the mesh and penalty stiffness.

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Title: Least-Squares and DPG Approximation of Eigenvalue Problems

Author(s): Linda Alzaben, *King Abdullah University of Science and Technology*; Fleurianne Bertrand, *University of Twente*; *Daniele Boffi, *King Abdullah University of Science and Technology*; Henrik Schneider, *Humboldt Universität zu Berlin*;

In this talk we consider the numerical approximation of eigenvalue problems arising from elliptic partial differential equations. We discuss, in particular, schemes based on least-squares finite element and DPG methods. The study of the spectrum of discrete operators is essential for several applications. First of all a careful modal analysis is important by itself when dealing with models involving oscillatory phenomena, such as vibrations of structures or acoustic problems; then the knowledge of the spectrum is crucial when dealing with transient problems. Our investigation started with the least-squares finite element approximation of the Laplace eigenproblem by using various formulations, including FOSLS and LL* [1]. The analysis is then extended to linear elasticity, for which a two- and a three-formulation are considered [2]. Finally, we considered the DPG approximation of the Laplace eigenproblem, but taking into account the primal and the ultra-weak formulations [3]. We provide optimal a priori and a posteriori error analysis. Some numerical simulation confirm the good behavior of the discrete spectrum which provides a good approximation of the exact solution. In this talk we will focus on the numerical implementation and on the outcome of the numerical results, discussing how to interpret them in order to confirm the theoretical investigations. [1] F. Bertrand and D. Boffi. First order least-squares formulations for eigenvalue problems. IMA Journal of Numerical Analysis, to appear. arXiv:2002.08145 [math.NA] [2] F. Bertrand and D. Boffi. Least-squares for linear elasticity eigenvalue problem. Computers and Mathematics with Applications, to appear. arXiv:2003.00449 [math.NA] [3] F. Bertrand, D. Boffi, and H. Schneider. DPG approximation of eigenvalue problems. Submitted. arXiv:2012.06623 [math.NA]

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Title: A Discrete Exact Grad-Curl-Div Complex on Generic Polyhedral Meshes. Part 1: Algebraic Properties

Author(s): *Daniele Di Pietro, *Université de Montpellier*; Jérôme Droniou, *Monash University*;

Certain physical or engineering models are represented by partial differential equations whose well-posedness strongly relies on particular properties of the underlying differential operators. A relevant example of such properties is the de Rham complex, which states (on topologically trivial domains) some equality relations between images and kernels of the gradient, curl and divergence operators; relevant PDEs whose analysis relies on these properties are, e.g., Navier-Stokes and electromagnetic models. Designing stable and convergent numerical methods requires to reproduce, at the discrete level, these properties of the differential operators. In the context of Finite Elements, this has led to the Finite Element Exterior Calculus theory [1]. The methods covered by this theory are, however, limited to meshes with specific element topology (most usually, these elements must be hexahedra or tetrahedra). In this talk, we will present a novel discrete approximation of the de Rham complex that applies to meshes with generic polyhedral elements and can achieve any order of accuracy [2,3]. This discrete de Rham (DDR) method relies on polynomial unknowns on suitable geometric entities (vertices, edges, faces, and elements, depending on the space in the complex and on the chosen degree of accuracy), and on fully discrete versions of the gradient, curl and divergence operators acting between these spaces. Our focus will be on presenting the principles of the DDR method, as well as its algebraic properties: exactness, polynomial consistency, and commutation properties between interpolators and discrete differential operators. References: [1] D. Arnold. Finite Element Exterior Calculus. SIAM, 2018. doi: 10.1137/1.9781611975543. [2] D. A. Di Pietro and J. Droniou. "An arbitrary-order discrete de Rham complex on polyhedral meshes. Part I: Exactness and Poincaré inequalities". Submitted, 2021. https://hal.archives-ouvertes.fr/hal-03103526 [3] D. A. Di Pietro and J. Droniou. "An arbitrary-order discrete de Rham complex on polyhedral meshes. Part II: Consistency.". Submitted, 2021. https://hal.archives-ouvertes.fr/hal-03103535

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Title: Sparsifying Priors for Bayesian Uncertainty Quantification in Model Discovery

Author(s): Seth Hirsh, *University of Washington*; *David Barajas-Solano, *Pacific Northwest National Laboratory*; J. Nathan Kutz, *University of Washington*;

We propose a probabilistic model discovery method for identifying ordinary differential equations (ODEs) governing the dynamics of observed multivariate data. Our method is based on the "sparse identification of nonlinear dynamics" (SINDy) framework, in which target ODE models are expressed as a sparse linear combinations of prespecified candidate functions. Promoting parsimony through sparsity in SINDy leads to interpretable models that generalize well to unknown data. Instead of targeting point estimates of the SINDy (linear combination) coefficients, in this work we estimate these coefficients via sparse Bayesian inference. The resulting method, UQ-SINDy, quantifies not only the uncertainty in the values of the SINDy coefficients due to observation errors and limited data, but also the probability of inclusion of each candidate function in the linear combination. UQ-SINDy promotes robustness against observation noise and limited data, interpretability (in terms of model selection and inclusion probabilities), and generalization capacity for out-of-sample forecast. We perform sparse inference in UQ-SINDy employing Markov Chain Monte Carlo, and we explore two sparsifying priors: The spike-and-slab prior, and the regularized horseshoe prior. We apply UQ-SINDy to synthetic nonlinear datasets from a Lotka-Volterra model and a nonlinear oscillator, and to a real world dataset of lynx and hare populations. We find that UQ-SINDy is able to discover accurate and meaningful models even in the presence of noise and sparse samples.

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Title: Using First-Principles Calculations to Predict the Mechanical Properties of Transmuting Tungsten Under First Wall Fusion Power-Plant Conditions

Author(s): *David Cereceda, *Villanova University*; Yichen Qian, *Villanova University*; Mark Gilbert, *Culham Centre For fusion Energy*; Lucile Dezerald, *Universite de Lorraine*;

Tungsten (W) and tungsten alloys are being considered as leading candidates for structural and functional materials in future fusion energy devices. The most attractive properties of tungsten for the design of magnetic and inertial fusion energy reactors are its high melting point, high thermal conductivity, low sputtering yield and low long-term disposal radioactive footprint. Yet, despite these relevant features, tungsten also presents a very low fracture toughness, mostly associated with inter-granular failure and bulk plasticity, which limits its applications. Significant neutron-induced transmutation happens in these tungsten components during nuclear fusion reactions, creating transmutant elements including Re, Os and Ta. Density functional theory (DFT) calculations that allow the calculation of defect and solute energetics are critical to better understand the behavior and evolution of tungsten-based materials in a fusion energy environment. In this study, we perform DFT calculations to predict elastic and plastic mechanical properties (such as bulk modulus, shear modulus, ductility, etc.) on a variety of W-X compositions that result when pure tungsten is exposed to the EU-DEMO fusion first wall conditions for ten years.

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Title: Element-Local Approach to Error Estimation Using Machine Learning

Author(s): *David Del Rey Fernandez, *NASA Langley Research Center*; Romit Maulik, *Argonne National Laboratory*;

In engineering and science, simulation efficiency and reliability are tightly coupled with the mesh used to discretize the governing equations. Often, the construction of high-quality meshes for well-understood problems requires significant time investment by domain knowledge experts, while for new problems a trial-and-error approach is necessary. A viable alternative is to use mathematics to drive an iterative mesh adaptation process whereby, starting from a coarse mesh, a final optimized mesh is achieved. In the context of steady problems, both feature- and adjoint-based mesh adaptation are routinely used; indeed, the latter has emerged as the primary tool to obtain optimal meshes for the approximation of functionals. In either case, however, the cumulative cost of the primal solve on multiple meshes represents a significant computational expense. In the context of transient problems, the state of the art resides in feature-based adaptive mesh refinement technologies. However, these approaches result in suboptimal meshes when functionals are of interest. While adjoint-based approaches could be used for nonchaotic or regularized transient problems, their computational costs and memory requirements make them infeasible for large simulations. Our long-term goal is in the development of a scientific machine learning (SciML) framework that accelerates this optimization procedure by significantly reducing (or entirely removing) the number of mesh adaptation steps required to reach the optimized mesh. In this talk, we discuss preliminary developments in support of this goal. Specifically, we discuss the construction of SciML algorithms for error estimation that are based on local element-wise information and compare them against standard polynomial error-based approaches for predicting on the same set of information.

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Title: Comparison between a Continuum and a Discrete Damage Model to Study the Sub-Ply Failure Mechanism of a Unidirectional Carbon Fiber Composite

Author(s): *David Garoz Gomez, *IMDEA Materials Institute*; Mark Flores, *Air Force Research Laboratory*; David Mollenhauer, *Air Force Research Laboratory*; Carlos Gonzalez, *IMDEA Materials Institute*;

The sub-ply failure mechanism of a fiber-reinforced composite laminate occurs when there are fiber-matrix debonding and matrix cracking inside the ply. These two initial damage modes affect the damage progression through the ply and, therefore, the final failure of the whole laminate. Nowadays, the final failure of composite laminates represents a challenge to engineers who design structural parts based on composite materials to reduce the overall weight without losing mechanical properties. In this work, the sub-ply failure mechanism has been studied using the multiscale simulation strategy for the case of a realistic micro-pillar specimen under compression of a unidirectional carbon fiber composite. Then, a Finite Element model represents the real geometry of the micro-pillar obtained from the microscope. The model describes the sub-ply failure under the specified compression load based on the mechanical properties of the constituents, fiber and matrix as well as their interface. Therefore, a transversely isotropic model describes the behavior of the carbon fibers. A cohesive damage law represents the interface fiber-matrix. Finally, an isotropic elastic model with damage behavior describes the matrix. Two different damage models for the matrix have been proposed, a continuum damage model and a discrete damage model. Although both models use equivalent material parameters, the main difference is that the discrete damage model represents the crack orientation in the matrix. In addition, experimental tests in the micro-pillar specimen of carbon fiber composites under compression are compared with the results of the multiscale simulations using the two different damage models, continuum and discrete. The compared results are the fracture behavior, the sequence of the damage, and the homogenized behavior under the compressive load. Keywords: sub-ply failure, multiscale simulations, micro-scale, fiber-reinforced composite, continuum damage model, discrete damage model.

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Title: Efficient Numerical Quadrature for Unfitted Finite Element Methods: Perspectives and New Techniques

Author(s): *David Gunderman, *University of Colorado Boulder*; Kenneth Weiss, *Lawrence Livermore National Laboratory*; John A. Evans, *University of Colorado Boulder*;

Unfitted finite element methods (FEM) are attractive because they couple geometric modelling and numerical analysis; however, some numerical algorithms become far more difficult to formulate robustly and efficiently in the case of unfitted methods. For example, in classical FEM integration over high-order or rational parametric tetrahedra, hexahedra, prisms, and other finite element zoo shapes can be performed efficiently using optimized, polynomially-exact quadrature rules mapped parametrically from those shapes' parent spaces. In the case of unfitted FEM, these classical quadrature methods default to low accuracies within cut elements, because integrands are discontinuous across unfitted boundaries or interfaces, negating the benefits of polynomially-exact quadrature rules. Quadrature errors in cut cells can dominate overall solution error, prevent optimal convergence rates, and ultimately drive-up computational costs. This motivates the formulation of novel high-accuracy quadrature schemes for cut cell geometries, spawning a variety of novel algorithms for each novel paradigm. Saye's method relies on iterative dimension-reduction of an integral using the implicit function theorem, but only handles integration over regions bounded by hypercubes and implicit-defined boundaries/interfaces. Fries and Omerovic also studied the problem for implicit geometries by remeshing the implicitly defined surfaces or volumes. Recently, Marussig has introduced a method which integrates over trimmed B-spline surfaces while retaining advantages associated with weighted quadrature. Finally, moment-fitting techniques have been used by Sukumar to develop high-accuracy integration rules for arbitrary polyhedral cells, including those with curved polynomial-parametric faces. In this talk, I will give a brief overview of the theory and methods of integration over cut cells. Then, I will introduce some novel iterative dimension-reduction techniques for integration which use Stokes theorem, matrix implicitization, numerical antidifferentiation, and other methods to achieve high-order convergence to correct integrals over cut cells without meshing. These methods can be used to integrate over a wide variety of shapes, including arbitrary geometries formed as Booleans (intersections, unions, and differences) of classical finite element zoo shapes such as intersections between surface meshes and background meshes that often appear in unfitted finite element methods. The primary goal of this research is to improve efficiency of the underlying numerical algorithms so that optimal convergence rates can be achieved. We present results which compare our novel algorithms to state-of-the-art algorithms in the literature and show higher-convergence and better accuracy on a variety of geometries. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Title: Uncertainty Quantification of Electro-Poration Ablation Effect in Liver Cancer

Author(s): *Davide Baroli, *RWTH Aachen University*; Karen Veroy-Grepl, *Eindhoven University of Technology / RWTH Aachen University*; Tan Zhipeng, *RWTH Aachen University*;

A recent promising non-thermal technique for treatment of metastasis cancer is electroporation. The prediction of the tumor-ablation is highly influenced by the positioning of cancer and conductivity of the tissue, whose measurement is affected by uncertainty and noise. In this talk, we consider a Gaussian emulator that serves a surrogate model to speedup the forward modeling and identify the statistical calibration of the prediction. Further, we investigate the use of optimal sampling strategy to increase accuracy of surrogate emulator, that serves as tool for optimization routines for online treatment planning algorithms and Bayesian inverse problem. This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 818473) and ITN-MSCA-ElectroPros. References: Aycock, K.N. and Davalos, R.V., 2019. Irreversible electroporation: background, theory, and review of recent developments in clinical oncology. Bioelectricity, 1(4), pp.214-234. Gardner, Jacob R., Geoff Pleiss, David Bindel, Kilian Q. Weinberger, and Andrew Gordon Wilson. " GPyTorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration." In NeurIPS (2018).

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Title: Dynamically and Geometrically Conservative Fully-Discrete Stabilized Finite Element Methods for Conservation Laws on Moving Domains With Controllable Numerical Dissipation

Author(s): *DeAnna Gilchrist, *University of Colorado Boulder*; John Evans, *University of Colorado Boulder*;

In this talk, we introduce a new fully-discrete stabilized finite element method for compressible flows on moving domains that is (i) dynamically conservative (that is, it admits discrete balance laws for mass, momentum, and energy), (ii) geometrically conservative (that is, it preserves constant flow states), and (iii) endowed with controllable numerical dissipation. To arrive at this method, we first discretize the compressible Navier-Stokes equations on a moving domain in space using an Arbitrary Lagrangian Eulerian (ALE) Streamline-Upwind Petrov-Galerkin (SUPG) finite element method and residual-based shock capturing. We then discretize both the resulting semi-discrete system of equations as well as an accompanying geometric conservation law in time using a slight modification of the generalized-alpha method. We prove that this approach yields a dynamically and geometrically conservative method if conservative, primitive, or entropy variables are employed. By contrast, we show dynamic conservation is lost if one does not separately discretize the geometric conservation law in time. Finally, we illustrate the efficacy of the new fully-discrete stabilized finite element method with a collection of numerical experiments spanning subsonic, transonic, and supersonic flows.

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Title: Biomembranes Undergo Complex, Non-Axisymmetric Deformations Governed by Kirchhoff-Love Kinematics and Revealed by a Three-Dimensional Computational Framework

Author(s): *Debabrata Auddya, *University of Wisconsin-Madison*; Xiaoxuan Zhang, *University of Michigan*; Rahul Gulati, *University of Wisconsin-Madison*; Ritvik Vasan, *University of California, San Diego*; Padmini Rangamani, *University of California, San Diego*; Krishna Garikipati, *University of Michigan*; Shiva Rudraraju, *University of Wisconsin-Madison*;

Membranes play a central role in cell biology driving many essential processes such as cell locomotion, filopodial protrusion, vesicle trafficking, wound repair, etc. As such they undergo significant morphological changes in the form of deformation, fission and constriction. Traditional modeling of these biological membrane phenomena has relied on axisymmetric assumptions, there-by eliminating the possibility of capturing lower symmetry (and potentially lower energy) kinematic modes. In this work, we present an isogeometric analysis based, finite-strain Kirchhoff-Love thin-shell implementation and its applications to various biomembrane problems. Specifically, we consider three classical, yet non-trivial, membrane deformation problems: formation of tubular shapes and their lateral constriction, generation of membrane footprint using Piezo1 protein and budding of membranes by protein coats during endocytosis. We model the evolution of deformation and mechanical instabilities in various membrane geometries, study the suitability of Helfrich-like material models, and determine the boundary conditions needed to induce preferred deformation modes. Interesting insights into non-axisymmetric modes that lower energy barriers will be discussed. Further, extensions of this framework to problems involving mechano-chemistry on membranes will also be presented.

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Title: Effect of Particle Shapes on Bulk Behavior Using Peridynamics-Based Discrete Element Method

Author(s): *Debdeep Bhattacharya, *Louisiana State University*; Lipton Robert, *Louisiana State University*;

We study the effect of individual particle shapes on the mechanical response of the bulk. The intra-particle force is modeled using peridynamics, and inter-particle repulsive, friction, and damping forces are incorporated when the particles are close by. A simplified model for particle-wall interaction is also introduced to improve the simulation speed of large particle beds. Peridynamic theory provides us access to the force and deformation fields on and within the grain boundaries, while a damage model allows fractures to emerge naturally due to progressive bond-failure. The collisions between arbitrarily shaped (in particular, non-convex) grains are detected dynamically to allow large displacements and breakage. We observer complex contacts between grains in 2D and 3D that lead to particle jamming, rotation, and sliding, as well as particle damage such as attrition, spallation, and fracture that affect the bulk behavior. This work is a part of a MURI project for predicting and controlling the response of particulate systems through grain-scale engineering.

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Title: Elastodynamics of Sandwich Beams Using a Mixed Layer-Wise Formulation and Least-Squares Space-Time Finite Element Method

Author(s): *Devin Burns, *Virginia Polytechnic Institute and State University*; Romesh Batra, *Virginia Polytechnic Institute and State University*;

As composite materials have become more ubiquitous in structural applications, the need to understand and accurately predict their transient behavior in complex loading environments has increased. The challenges include satisfying displacement and traction continuity conditions at layer interfaces, identifying when and where the structure fails first, and satisfying boundary conditions. We analyze transient response of a sandwich beam undergoing plane stress deformations under shock loads by using a least-squares space-time finite element method (FEM), Hooke's law for transversely anisotropic materials, and a mixed layer-wise formulation of the governing equations in which the transverse stresses, velocities and in-plane normal strain at a point are taken as unknowns. Displacements are computed by integrating the velocity solutions with respect to time using a Legendre-Gauss-Lobatto (LGL) integration rule. The sum of residuals in the governing equations, the initial conditions and the boundary conditions on all surfaces is minimized using the least squares method. These equations are integrated in space and time using an LGL rule, which results in a system of coupled linear algebraic equations for the unknowns. Thus, the method is implicit and unconditionally stable. The software has been verified by using the method of manufactured solutions, and the convergence of the numerical solution with respect to the time-step size and the spatial discretization has been studied. Results for sandwich beams with varied face sheet-core stiffness ratios, aspect ratios, and boundary conditions are presented and compared with those found by using the commercial FE software, ABAQUS. For thick clamped and cantilever sandwich beams (L/h = 5), the proposed method produces results that agree to within 1.26% and 0.149% for the beam's maximum kinetic and strain energies, respectively, with the solution of the linear elasticity theory equations found using ABAQUS. Continuity conditions at layer interfaces and bounding surfaces are very well satisfied in a least-squares sense. References: [1] F. Moleiro et al., "Layerwise mixed least-squares finite element models for static and free vibration analysis of multilayered composite plates", Composite Structures, 92, 2328-2338, 2010. [2] Brent C. Bell, Karan S. Surana, "A space-time coupled p-version least squares finite element formulation for unsteady two-dimensional Navier-Stokes equations", International Journal for Numerical Methods in Engineering, 39, 2593-2618, 1996.

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Title: Using Hierarchical Bayesian Calibration with Diverse Experimental Data to Parameterize the PTW Strength Model for Ti-6Al-4V Alloys

Author(s): *Devin Francom, *Los Alamos National Laboratory*; David Walters, *Los Alamos National Laboratory*; Sky Sjue, *Los Alamos National Laboratory*; JeeYeon Plohr, *Los Alamos National Laboratory*; Ayan Biswas, *Los Alamos National Laboratory*; Darby Luscher, *Los Alamos National Laboratory*;

The Preston-Tonks-Wallace strength model is intended to reasonably represent the flow stress of a material covering several orders of magnitude of strain-rates and temperatures. Calibration of the PTW model parameters is usually more successful when multiple experiments cover the full range of conditions expected during the application of the model. Often, multiple experiment types are required (e.g., quasistatic, Hopkinson bar, Taylor cylinder, flyer plates) to deform materials through a large array of strain, strain-rate, and temperature conditions. We have leveraged Bayesian statistics along with emulation techniques to perform joint calibrations of the PTW model for a range Ti-6Al-4V alloys covering multiple experiment types. Our Bayesian approach implements a hierarchical structure [1] which allows for each experiment to have different parameter vectors which are shrunk towards a common vector of parameters. This enables flexibility in selecting appropriate parameters which operate best at the physical conditions expected to be encountered by the model during particular applications. This technique provides a measure of uncertainty for the common vector of parameters as well as individual parameters sets unique to each experiment which are influenced by the global set of experiments. The significance of these uncertainty ranges is demonstrated by simulating the deformation of a narrow conical Ti-6Al-4V specimen impacting a rigid anvil, similar to a Taylor cylinder. In this test case, a characteristic strain, strain-rate, and temperature were determined to generate a distribution of probable parameter sets, and ranked based on the computed flow stress produced by the PTW model at the input conditions. Multiple simulations (shown in parentheses) of the conical horn taken around the 5th (4), 50th (3), and 95th (4) quantiles of ranked list of flow stresses show significant differences in the deformed shape of the specimen at the different quantile selections. Each draw of parameters around a specific quantile of flow stress produced significantly different vectors of PTW parameters, but still resulted in similar final deformation patterns clustered around each quantile group. [1] Fugate, M., Williams, B., Higdon, D., Hanson, K. M., Gattiker, J., Chen, S.-R., and Unal, C. (2005), “Hierarchical Bayesian Analysis and the Preston-Tonks-Wallace Model,” Los Alamos National Laboratory Technical Report LA-UR-05-3935.

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Title: Physics Informed Generative Models for Morphology Reconstruction

Author(s): *Dhruv Gamdha, *Iowa State University*; Augusto Menezes-Savaris, *Iowa State University*; Kumar Saurabh, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

There has been an unmet need for the design of new material to address the pressing problems of the current century. Characterizing the material microstructure or morphology can help advance the material design by understanding the functional property relation. Morphology reconstruction of a material is a complicated process, mainly because of the vast number of possibilities in which the material can be arranged. Subsequently the time for microstructure reconstruction increases exponentially with the size of microstructure. In this work, we plan to address the morphology reconstruction problem using generative adversarial networks (GAN) in conjunction with recently developed fast virtual instrumentation for pRSoXS (polarized Resonant Soft X-ray Scattering) measurement. The availability of the fast forward simulator enables us to encode the physics pRSoXS measurement during the training process. The overall inverse problem can be stated as: given a pRSoXS scattering pattern I(q) and associated measurements such as anisotropy A(q), identify the most plausible 3D morphology (characterized as a set of voxels with each voxel having a volume fraction and crystallinity orientation information) whose (virtual) characterization matches with that of the measured data. The overall training can be performed in a data-free manner which makes this approach very powerful. Once, the generator of the GAN generates a 3D microstructure of the polycrystalline material, it will be sent to the virtual instrument to obtain the resultant scattering pattern. This resultant scattering pattern will serve as feedback to the network. Once the network is trained, we will be able to extensively explore the whole morphology space to isolate promising compositions that predict the given scattering pattern and respects the explicitly enforced physical invariances. This will also enable fast querying and visual exploration of trends. The automated and adaptive sampling provided by the physics-aware machine learning algorithms will allow us to minimize the number of experiments while maximizing the configuration space explored.

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Title: Shape Dynamics of a Red Blood Cell in Microcirculation

Author(s): *Dhwanit Agarwal, *The University of Texas at Austin*; George Biros, *The University of Texas at Austin*;

We use numerical simulations to study the dynamics of red blood cells (RBCs) in unconfined and confined Poiseuille flow. Previous numerical studies with 3D vesicles have indicated that the slipper shape observed in experiments at high capillary number can be attributed to the bistability due to the interplay of wall push and outward migration tendency at higher viscosity contrasts. In this paper, we study this outward migration and bistability using numerical simulations for 3D capsules and provide phase diagrams of RBC dynamics with and without viscosity contrast in both confined and unconfined Poiseuille flow. Our results agree (both quantitatively and qualitatively) with the experiments where both slipper and croissant shapes are observed at high capillary numbers. To our knowledge, this is the first study that provides phase diagrams for 3D capsules with experimentally relevant initial conditions (initial shape, viscosity contrast and initial stress) in unconfined flow and confined Poiseuille flow.

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Title: Electro-Chemo-Mechanics of Two-Dimensional Materials-Based Energy Storage Systems

Author(s): *Dibakar Datta, *New Jersey Institute of Technology*;

Despite advances in energy storage, the development of new batteries with high energy density, power density, and life cycle remains elusive. Two-dimensional materials (2DM) such as graphene, transition metal dichalcogenides (TMD), MXenes, and their heterostructures are among the most promising energy materials for radically advanced batteries. Electro-chemo-mechanics, the coupling of mechanics and electrochemistry, plays a crucial role in designing these systems. This talk addresses two important computational aspects of 2DM-based batteries – (i) 2DM-based anode materials and (ii) 2DM as van der Waals (vdW) slippery interface. The conventional anode materials have several problems, such as low gravimetric capacity and high-volume expansion. Our First-Principal modeling shows that topologically modified 2DM can be designed for stable high-capacity anode materials for ion batteries. Several electro-chemo-mechanical challenges such as trapping of adatoms at the defect sites, diffusion-induced stress, and mechanical degradation at defect sites during intercalation/deintercalation are discussed. The second part of the talk discusses the interface between anode and current-collector (e.g., silicon anode and copper current-collector in Li-ion battery). Our computational study reveals the reduction of interfacial stress between the anode and graphene-coated current collector. Therefore, we recommend using the graphene layer over the current collector as a vdW slippery surface. Experimental findings are in good agreement with our computational results.

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Title: Topology Optimization Design of Blood Flow Devices Considering a Hemolysis Model

Author(s): *Diego Hayashi Alonso, *Polytechnic School of the University of São Paulo*; Emílio Carlos Nelli Silva, *Polytechnic School of the University of São Paulo*;

Topology optimization has been studied for designing fluid flow devices in the past years, including channels, valves and pumps, and also taking non-Newtonian fluid flows, such as blood, into account. In the design of blood flow devices, the importance of the quantification and minimization of the blood damage (given mainly by hemolysis) may be highlighted. However, up to now, hemolysis has been minimized in an indirect manner in topology optimization, such as by considering shear stress (or even energy dissipation) as the objective function while aiming to indirectly minimize hemolysis. This approach may possibly give a general idea of where there may or may not be hemolysis, but the actual hemolysis distribution can not be easily correlated. This means that a more direct measure may be better in the evaluation of hemolysis. The direct way to consider hemolysis is from the hemolysis index, which is computed from a differential equation model (a “hemolysis model”). In this work, the hemolysis index obtained from a hemolysis model is included in the topology optimization formulation. With the aim of illustrating this approach, the design of a 2D swirl flow device, which consists of axisymmetric fluid flow with or without rotation around an axis, is considered. One example that is relevant for blood flow devices is the design of blood pumps, which has been previously evaluated in topology optimization for indirectly reducing hemolysis. More specifically concerning pump design for 2D swirl flow, the design of a Tesla-type blood pump is considered. A Tesla-type pump is a type of fluid flow device that is bladeless, and whose pumping effect is governed by the boundary layer effect. This principle of operation may induce less blood damage. While including the hemolysis index, the topology optimization is also formulated including the relative energy dissipation (for indirectly maximizing efficiency). The fluid is modeled through a non-Newtonian fluid model, while the fluid flow is solved from the finite element method. The solid material being used to block the fluid flow is the “Brinkman-Forchheimer model”, and an additional penalization is considered for the non-Newtonian viscosity. The optimization problem solution is obtained through IPOPT (Interior Point Optimization algorithm).

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Title: Thermal Finite Element Analysis of an Intraocular Display Prosthesis for Corneal Blindness

Author(s): *Dipika Gongal, *University of Illinois at Chicago*; Siddhant Thakur, *Arthrex Inc.*; Ashaya Panse, *University of Illinois at Chicago*; John Stark, *University of Illinois at Chicago*; Charles Yu, *Stanford University*; Craig Foster, *University of Illinois at Chicago*;

Corneal opacity is the fourth leading cause of blindness worldwide. Corneal transplants can restore vision, but sometimes fail, and a shortage of donor corneas often leads to long wait times. Artificial corneas are sometimes effective, but are easily infected and can have other complications. A recently proposed intraocular projection device [1,2] is a potential alternative treatment with great promise. An externally mounted camera records an image, which is transmitted to a projector inside the eye. The projector, in turn, displays an image onto the retina. The projector is surgically implanted in the eye after removing the lens, and saline replaces the aqueous humor. As with all electronic devices, the projector generates heat which must be dissipated from the eye. Federal and international guidelines state that living tissues should experience a temperature increase of no more than 2 degrees Centigrade. A thermal finite element analysis of the eye is performed to determine the power the device can produce and not overheat the tissue. Heat dissipation in the eye due to blood perfusion and convection heat flow on the heat dissipation is studied. The implant when placed 1.95 mm away from the retina can safely operate at 100 mW without increasing the eye tissue temperature above 2 degrees Centigrade. The power budget established helps to design and develop the electronic intraocular devices.

16th U.S. National Congress on Computational Mechanics
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Title: Improved Plasticity and Damage Models by Symbolic Regression of Microscale Finite Element Simulations

Author(s): *Donovan Birky, *The University of Utah*; Jacob Zamora, *The University of Utah*; John Emery, *Sandia National Laboratories*; Coleman Alleman, *Sandia National Laboratories*; Brian Lester, *Sandia National Laboratories*; Geoffrey Bomarito, *NASA Langley Research Center*; Jacob Hochhalter, *The University of Utah*;

Currently, the engineering community relies heavily on existing empirical data sets and phenomenological constitutive models to inform decisions regarding structural performance. Engineering constitutive models that capture component-scale plasticity and damage, such as Gurson-Tvergaard-Needleman (GTN) and Cocks-Ashby, have become engrained in engineering software for three categorical reasons: 1) they are flexible in the sense that they can be calibrated to a variety of use cases; 2) they are interpretable in the sense that they can be understood, provide insight, and are defensible based on physics and mechanics concepts; 3) they are computationally tractable, especially when compared to higher-fidelity microscale models. However, after decades of application, it is understood that these engineering constitutive models are limited in their accuracy and validity due in part to their basis on idealized microstructural configurations (e.g. structured configurations of spherical voids). As an alternative, machine learning methods promise to enable significant improvements in accuracy, but trials to date have largely focused on black-box methods that, while improving accuracy, do not inherently provide the necessary level of interpretability, defensibility, and opportunity for insight at which their purely mechanics-based predecessors excelled. We discuss here an ML-based methodology whereby more accurate constitutive models and their parameters can be evolved in a manner that maintains interpretability and defensibility. Specifically, genetic programming with symbolic regression (GPSR) is employed to generate constitutive models, trained by higher-fidelity microscale simulation results, which produces symbolic expressions (as with GTN or Cocks-Ashby). Training data for the GPSR algorithm is generated by extracting homogenized results of finite element models with explicitly-represented heterogeneities (i.e. voids), producing load traces along the (homogenized) macroscale yield surface. First, we present the results of a verification study whereby the ability of GPSR to discover existing models is tested by enforcing in the training simulations the same idealizations made by GTN. We then systematically relax the inherent GTN assumptions individually to discover additional terms to enable accurate models for the more complex reality, while maintaining interpretability and defensibility.

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Title: Accelerating Lagrangian Hydrodynamics Simulation with Space-time Reduced Order Models

Author(s): *Dylan Copeland, *Lawrence Livermore National Laboratory*; Kevin Huynh, *Lawrence Livermore National Laboratory*; Siu Wun Cheung, *Lawrence Livermore National Laboratory*; Youngsoo Choi, *Lawrence Livermore National Laboratory*;

Although many model reduction schemes have been developed to reduce the computational cost of simulations while minimizing the error introduced in the reduction process, there are challenges in advection-dominated problems such as sharp gradients, moving shock fronts, and turbulence, which hinder those model reduction schemes from being practical. In this talk, we will present a space-time reduced order model for Lagrangian hydrodynamics simulation, with which we will demonstrate both good accuracy and speed-up for several advection-dominated problems, e.g., Sedov blast, Gresho vortices, Taylor-Green, and triple-point problems. Lagrangian hydrodynamics is formulated as a nonlinear problem, which requires a proper hyper-reduction technique. We apply the over-sampling DEIM approach to reduce the complexity due to the nonlinear terms.

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Title: Multi-Scale Modeling of Dislocation Dynamics

Author(s): *Eduardo Barros de Moraes, *Michigan State University*; Mohsen Zayernouri, *Michigan State University*;

Reliable design of engineering components requires a deep understanding of the underlying stochastic evolution of defects inherently present in a material's micro-structure. The presence of vacancies, dislocations, voids and cracks affect the mechanical behavior across multiple length and time-scales, demanding robust and efficient coupling frameworks between the scales, leading to consistent propagation of numerous sources of uncertainty from atomistic to eventually aging continuum mechanics. We developed a multi-scale framework for stochastic modeling of dislocation dynamics in crystals, where a stochastic graph surrogate model is infused with data from high-fidelity atomistic simulations. The framework provides an efficient propagation of material parameters and uncertainties across the scales, incorporating stochastic effects of lower scales into the collective behavior of defects propagated to the continuum.

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Title: Mollified Finite Element Approximants of Arbitrary Order and Smoothness

Author(s): *Eky Febrianto, *University of Cambridge*; Michael Ortiz, *California Institute of Technology*; Fehmi Cirak, *University of Cambridge*;

The approximation properties of the finite element method can often be substantially improved by choosing smooth high-order basis functions. It is extremely difficult to devise such basis functions for partitions consisting of arbitrarily shaped polytopes. We propose the mollified basis functions of arbitrary order and smoothness for partitions consisting of convex polytopes. On each polytope an independent local polynomial approximant of arbitrary order is assumed. The basis functions are defined as the convolutions of the local approximants with a mollifier. The mollifier is chosen to be smooth, to have a compact support and a unit volume. The approximation properties of the obtained basis functions are governed by the local polynomial approximation order and mollifier smoothness. The convolution integrals are evaluated numerically first by computing the boolean intersection between the mollifier and the polytope and then applying the divergence theorem to reduce the dimension of the integrals. The support of a basis function is given as the Minkowski sum of the respective polytope and the mollifier. The breakpoints of the basis functions, i.e. locations with non-infinite smoothness, are not necessarily aligned with polytope boundaries. Furthermore, the basis functions are not boundary interpolating so that we apply boundary conditions with the non-symmetric Nitsche method as in immersed/embedded finite elements. The presented numerical examples confirm the optimal convergence of the proposed approximation scheme for Poisson and elasticity problems.

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Title: Interplay between Regional and Loading Based Variability in Aortic Aneurysm Tissue Mechanics

Author(s): Miriam Nightingale, *University of Calgary*; Taisiya Sigaeva, *University of Waterloo*; Michael Baran Scott, *Northwestern University*; Samaneh Sattari, *University of Calgary*; Julio Garcia, *University of Calgary*; Jehangir Appoo, *University of Calgary*; Chris Malaisrie, *Northwestern University*; Patrick McCarthy, *Northwestern University*; Michael Markl, *Northwestern University*; Paul Fedak, *University of Calgary*; Alexander Barker, *University of Colorado Anschutz*; *Elena Di Martino, *University of Calgary*;

Aortic biomechanics are largely a product of alterations in elastin and collagen. In ascending aneurysmal tissue there is localized remodeling resulting in dilatation and mechanical weakening. We postulate that inter-patient variability confounds the ability to measure regional variability of biomechanics behavior, and both effects must be considered. In our first project, three regional specimens (anterior, greater curvature, posterior) from 14 patients were each tested on a biaxial testing device and the resulting stress-strain response was fitted to a four-parameter Fung constitutive model. Results show the ability for population average models to fit individual tissue behaviour is dependent on inter-patient and regional effects. When patient variability was statistically accounted for , the greater curvature region appeared stiffer than the other regions. This heterogeneity could be a consequence of localized altered loading conditions such as elevated wall shear stress (WSS). In our next project, mechanical properties were compared across region and between levels of wall shear stress. Preoperative 4D flow MRI of the thoracic aorta was performed in 24 patients undergoing elective prophylactic aortic surgery. The WSS (normal vs high) was calculated based on an age-matched healthy atlas [1]. A low and high strain modulus (LTM and HTM) was determined from planar biaxial testing of 84 tissue samples taken from the mid-ascending aorta (anterior, posterior, or greater curvature). LTM in the circumference direction was found to produce a trend (P=0.058) with WSS, being higher in regions of elevated WSS when accounting for patient variability. While no regional or WSS differences were found in the axial direction. HTM in each direction was found to be significantly higher in the greater curvature region versus anterior (P=0.005, circumference and P=0.001, axial) and the posterior region in the axial direction (P=0.022). Elastin is thought to dominate aortic tissue behavior during lower loading conditions (LTM response) while collagen remains crimped. As the collagen engages and straightens as stress increase, it becomes the dominant tissue component at high loads (HTM response). Wall shear stress has been previously linked to elastin fragmentation. These results may indicate early collagen engagement as the elastin is depleted. To confirm these results, further research will focus on collagen content, cross-linking, and type as it related to mechanical properties.
[1] van Ooij, P, et al., A methodology to detect abnormal relative wall shear stress on the full surface of the thoracic aorta using four-dimensional flow MRI. Magn Reson Med, 2015. 73(3): p. 1216-27

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Title: Thermodynamics-Informed Neural Networks

Author(s): Quercus Hernandez, *Universidad de Zaragoza*; Beatriz Moya, *Universidad de Zaragoza*; Alberto Badias, *Universidad de Zaragoza*; David González, *Universidad de Zaragoza*; Francisco Chinesta, *Arts et Métiers ParisTech*; *Elias Cueto, *Universidad de Zaragoza*;

We present thermodynamics-informed neural networks (TINN), a method for the machine learning of physical phenomena that guarantees the satisfaction, by construction, of the principles of thermodynamics. The method is based on the employ of sparse autoencoders, on one hand, that ensure the proper identification of the intrinsic dimensionality of data, while guaranteeing the use of a minimal number of degrees of freedom. On the other hand, the proposed method enforces a metriplectic structure on the learned data. This ensures the compliance to the principles of thermodynamics (conservation of energy, growth of entropy) for both conservative and dissipative phenomena. Examples will be show that demonstrate the performance of the proposed method. In particular, it is worth mentioning that we have observed that, the more physics knowledge is added to the learning process, the less data is necessary and the more accurate predictions will result. This is in line with other works in the field. References [1] Structure-preserving neural networks. Q. Hernandez, A. Badias, D. Gonzalez, F. Chinesta, E. Cueto. Journal of Computational Physics, Volume 426, 2021, 109950. [2] Deep learning of thermodynamics-aware reduced-order models from data. Quercus Hernandez, Alberto Badias, David Gonzalez, Francisco Chinesta, Elias Cueto. Submitted, arXiv:2007.03758, 2020. [3] Maier, A.K., Syben, C., Stimpel, B. et al. Learning with known operators reduces maximum error bounds. Nat Mach Intell 1, 373–380 (2019). https://doi.org/10.1038/s42256-019-0077-5

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Title: Fluid-Structure Interaction (FSI) Resolution for Cerebral Aneurysm Behaviour.

Author(s): *Elie Hachem, *Mines ParisTech - CFL - CEMEF*; Ramy Nemer, *Mines ParisTech - CFL - CEMEF*; Thomas Foliard, *Mines ParisTech - CFL - CEMEF*; Aurelien Larcher, *Mines ParisTech - CFL - CEMEF*;

Key Words: Variational Multi-Scale Method, Solid Modeling, Blood Modelling, Finite Elements, electrodynamics, arbitrary geometry, biomechanics. Fluid-Structure Interaction (FSI) applications are of interest in a wide array of engineering applications, and in particular, biomechanical systems such as blood flow, heart valve, and cerebral aneurysm…. For the latter case, the accurate prediction of rupture should be assessed to choose the appropriate treatment. When in contact with blood, the aneurysm exhibits deformation that may become critical, based on the pressure of its surrounding, and due to the inevitable interaction between both sides. The rupture risk in aneurysms is usually evaluated using hemodynamics[1]. Accurate and precise modeling of such biomechanical system can serve as an important tool for the diagnostics. For the aforementioned reasons, we conducted FSI simulations for cerebral aneurysm. An Adaptive Immersed Mesh (AIM) method for FSI using finite elements was utilized. AIM incorporates the independent results of a time accurate solid dynamics solver[3] onto a fully Eulerian Monolithic framework. This is done using by immersing the solid mesh, onto the fluid-solid mesh, using the Level-set method. The Navier--Stokes equations are solved for the fluid[2], with the appropriate blood rheology. Hyperelastic solid dynamics equations are solved for the solid, which can handle both compressible and incompressible material. The Variational Multi Scale (VMS) stabilization method is used for both methods. It helps stabilize the advection dominated regime for the fluid flow, and damp out spurious pressure oscillations for the solid problem. 3D results are presented to show the accuracy and robustness of the hybrid method in assessing the behavior of a cerebral aneurysm. REFERENCES [1] Cho, K. C., Yang, H., Kim, J. J., Oh, J. H., & Kim, Y. B. (2020). Prediction of rupture risk in cerebral aneurysms by comparing clinical cases with fluid–structure interaction analyses. Scientific reports, 10(1), 1-8. [2] E. Hachem, B. Rivaux, T. Kloczko, H. Digonnet, and T. Coupez, Stabilized finite element method for incompressible flows with high Reynolds number. Journal of Computational Physics, Vol. 229, pp. 8643-8665, 2010. [3] R. Nemer, A. Larcher, T. Coupez, E. Hachem. (2021). Stabilized finite element method for incompressible solid dynamics using an updated Lagrangian formulation. arXiv: 2101.07057 [math.NA] (2021) (available at http://arxiv.org/abs/2101.07057).

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Title: Tracking and Quantifying Human Bone Formation in a Bone-on-Chip

Author(s): Rachel Sagar, *University College of London*; Bertrand Cinquin, *Pierre Gilles de Genes Institute*; Christine Chappard, *University of Paris*; Pascale Guillot, *University College of London*; *Elisa Budyn, *ENS Paris-Saclay*;

Studying bone formation in vitro is challenging. New bone is formed in defects by mesenchymal stem cells (MSCs) that differentiate into osteoblasts and osteocytes. Native bone is a physiologically relevant 3D environment for bone cells. We used a bone-on-chip composed of multiple decellularized bone pieces recellularized with either human primary adult MSCs or foetal osteoblast progenitors to become stem cell derived osteocytes (SCDOs) and form new bone. The systems showed multi-level spatial reorganization of the cells, the collagen fibers and the bone pieces. The systems were cultured up to 26 months and mechanically stimulated in either 3-point bending or compression to mimic exercise and characterize the tissue. In situ immuno-histology by confocal microscopy confirmed MSCs differentiation and their calcium response to mechanical stimulation. Image-based Finite Element Models of the cells and tissues created numerical twins to quantified relevant stress fields inside growing bone. Both adult and foetal cells differentiated into osteocytes displaying E11 and sclerostin between 30 to 547 days. The cells adapted their cytoplasmic calcium response to the expected in vivo mechanical load and organized in layers of alternating orientations of 45o. Adult cells formed large quantity of mineralized tissue with a stiffness of 4 GPa at 109 days while foetal cells tend to form smaller quantity of highly mineralized bone leading to a stiffness of the native and neoformed bone mix of 21 GPa at 126 days. FTIR confirmed different levels of mineralization and protein secretion. Systems composed of multiple bones spatially reorganized as in vivo. Foetal cells produced highly mineralized and fatty tissue. Adult cells assembled multiple bone samples to rebuild a Haversian system. Our bone-on-chip provided a 3D environment to study cell differentiation, mechanobiology and analyse bone formation with respect to parameters such as mechanical stimulation or cell age.

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Title: Physics-Aware Deep-Learning-Based Proxy for Petroleum Reservoir Simulation Models

Author(s): *Emilio Coutinho, *Texas A&M University*; Eduardo Gildin, *Texas A&M University*;

In this talk, we extend our Physics-aware machine learning (ML) framework of [1] to 3D models and assess its potential use as a replacement to a computationally expensive reservoir (multiphase flow in porous media flow) simulation. Physics-aware machine learning (ML) techniques have been used to endow proxy models with features closely related to the ones encountered in nature; examples span from material balance to conservation laws. We developed a hybrid-based approach that incorporates physical constraints (physics-based) and yet is driven by input/output data (data-driven), leading to fast, reliable, and interpretable reservoir simulation models [1]. A deep-neural network (DNN) architecture is used to predict the state variables evolution after training an autoencoder coupled with a control system approach along with the addition of some physical components (Loss functions) to the neural network training procedure. By doing this, it is possible to estimate the evolution in time of both the state and output variables simultaneously. Such a non-intrusive data-driven method does not need to have access to the reservoir simulation internal structure, so it can be easily applied to commercial reservoir simulators. To make the framework general for 3D reservoir models, we changed the structure of the DNNs, by replacing the 2D convolutional and transpose convolutional layers to their 3D counterparts. The application of the Embed to Control and Observe method to a realist reservoir model is presented here. A 3D reservoir model with oil and water phases, 5 producers, and 4 injectors wells was used to test the proxy performance. The results show that our model can be used to replace the reservoir simulator in a control optimization framework. [1] E.J.R. Coutinho, E. Gildin, and M.J. Dall'Aqua, Physics-aware Deep-learning-based Proxy Reservoir Simulation Model Equipped with State and Well Output Prediction. Accepted to be published at the SPE Reservoir Simulation Conference. March 1-3, 2021. Texas, USA.

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Title: Combining Iterative Solvers with Randomization for Efficient Nonlinear Structural Optimization

Author(s): *Eric de Sturler, *Virginia Polytechnic Institute and State University*;

Many structural optimization problems require the repeated computation or approximation of a block quadratic form that depends nonlinearly on a large number of parameters. This quadratic form involves the inverse of the system matrix of a very large finite element model evaluated for hundreds of right hand sides; see, for example, [1]. Hence, the optimization would require, in principle, the solution of many large linear systems in each optimization step, leading to overwhelming computational cost. We can reduce this cost drastically using randomization [1,2,3]. Further reductions are possible by combining randomization with iterative solvers [2]. As randomization leads inherently to estimations, there is no need to solve linear systems accurately, making iterative solvers even more appropriate. In addition, attaining sufficiently accurate estimates involves a complex combination of the number of samples as well as the accuracy with which to solve the linear system for each sample, which leads to dynamic choices in the nonlinear optimization and linear solves. This presentation addresses important new questions in the efficient solution of expensive nonlinear structural optimization problems combining randomization with iterative solvers for optimal efficiency. [1] X.S. Zhang, E. de Sturler, G.H. Paulino, Stochastic Sampling for Deterministic Structural Topology Optimization with Many Load Cases: Density-based and Ground Structure Approaches, Computer Methods in Applied Mechanics and Engineering, 325 (2017), 463 – 487. [2] X.S. Zhang, E. de Sturler, A. Shapiro, Topology Optimization with Many Right-Hand Sides Using a Mirror Descent Stochastic Approximation – Reduction from Many to a Single Sample, Journal of Applied Mechanics, 87 (2020), 051005. [3] S.S. Aslan, E. de Sturler, M.E. Kilmer, Randomized Approach to Nonlinear Inversion Combining Random and Optimized Simultaneous Sources and Detectors, SIAM Journal on Scientific Computing, 41 (2019), B229 – B249.

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Title: Scaled Boundary Cubature Scheme for Numerical Integration over Planar Regions with Affine and Curved Boundaries

Author(s): *Eric B. Chin, *Lawrence Livermore National Laboratory*; N. Sukumar, *University of California, Davis*;

This talk introduces the scaled boundary cubature (SBC) scheme for accurate and efficient integration of functions over polygons and two-dimensional regions bounded by parametric curves [1]. Over two-dimensional domains, the SBC method reduces integration over a region bounded by m curves to integration over m regions, where each region is bounded by two line segments and a curve. With counterclockwise orientation of the boundary curves, the scheme is applicable to convex and nonconvex domains. Additionally, for star-convex domains, a tensor-product cubature rule with positive weights and integration points in the interior of the domain is obtained. If the integrand is homogeneous, we show that this new method reduces to the homogeneous numerical integration scheme [2]; however, the SBC scheme is more versatile since it is equally applicable to both homogeneous and non-homogeneous functions. We also introduce several methods which work with the SBC scheme for smoothing integrands with point singularities and near-singularities. When these methods are combined, highly efficient integration of weakly-singular functions is realized. Furthermore, we discuss the applicability of the SBC scheme to three dimensional domains, such as polyhedra and curved solids. The SBC method is applied to several benchmark problems, which reveal its broad applicability and superior performance (in terms of time to generate a rule and accuracy per cubature point) when compared to existing methods of integration. References [1] E.B. Chin, N. Sukumar, Scaled boundary cubature scheme for numerical integration over planar regions with affine and curved boundaries, Computer Methods in Applied Mechanics and Engineering (in review). [2] E.B. Chin, J.B. Lasserre, N. Sukumar, Numerical integration of homogeneous functions on convex and nonconvex polygons and polyhedra, Computational Mechanics 56 (6) (2015) 967-981.

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Title: Paper Straw Development by Virtual Modelling, Physical Testing Combined with Virtual Testing

Author(s): *Eskil Andreasson, *Tetra Pak*; Tommy Lindström, *Tetra Pak*;

Paperboard material characterization and paperboard mechanics have been an active research field for at least 30 years in the Academia and Industry. A large number of research projects and scientific publications have been finalized during the last decades within the area. Fundamental understanding of the governing material behaviour has been established by performing a large set of experimental test campaigns. However, many challenges are still identified when trying to transfer the material properties i.e. “reality” of paperboard mechanics into constitutive material models. Recent development and new experimental techniques have enhanced the capabilities to further visualize and identify the local material deformation mechanisms and intrinsic material mechanical behaviour, such as Digital Image Correlation (DIC), In-situ testing, and X-ray Computerized Tomography (XCT). In this work we discuss the potential, feasibility, and benefit of combining advanced experimental material characterization techniques with sophisticated numerical simulations (FEM+CFD). The application in focus for this presentation is the ongoing product development of paper based drinking straws, i.e. Paper Straws (https://www.tetrapak.com/about-tetra-pak/news-and-events/newsarchive/first-carton-packaging-company-to-launch-paper-straws) in the Packaging Industry addressing the sustainability transformation. Computer simulation models is today used to aid the decision support in Industry. With the help of a few use cases, we will present a novel method to capture the paperboard physics and mechanics in a realistic and reliable way. The framework presented here is an extension of the work presented in [1] and takes variable circumstances such as different moisture, temperature, and strain rates dependency into account. Moreover, non-linear material response, anisotropic material behaviour, asymmetric tensile/compressional behaviour, large deformation and damage/fracture mechanics are identified effects needed in the application simulations. Therefore, all these aforementioned functionalities are all included in the virtual material model. The paperboard constitutive material model is written as a user subroutine in FORTRAN based on the total deformation concept and available for the commercial Finite Element solver AbaqusTM. This methodology is selected to make the iterations very robust, more efficient, and faster compared to the existing available material models. Moreover, the material model should be simple to calibrate and use for the application engineers. Reliable material data used for virtual simulation of the Paper Straw manufacturing, use and disposal is extracted from experimental mechanical material characterization and calibration of the paperboard materials. [1] Borgqvist E., Lindström T. et al., (2014), Distortional hardening plasticity model for paperboard, International Journal of Solids and Structures, Volume 51, ScienceDirect https://doi.org/10.1016/j.ijsolstr.2014.03.013.

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Title: A Mechanics-Informed, Data-Driven Approach to Material Modeling and Application to Multiscale Problems

Author(s): *Faisal As'ad, *Stanford University*; Philip Avery, *Stanford University*; Charbel Farhat, *Stanford University*;

A mechanics-informed, data-driven approach to learning a constitutive law for complex materials from stress-strain data is proposed. The approach features a robust and accurate method for training a regression-based, surrogate model capable of capturing highly nonlinear stress-strain mappings while preserving some principles that are important to computational mechanics. In this sense, the proposed approach is a structure-preserving approach for constructing a data-driven model that features both the form-agnostic advantage of purely phenomenological data-driven regressions and the physical soundness of mechanistic models. The proposed training procedure is equally compatible with both numerical and experimental stress-strain data. As such, it is also suitable for accelerating multiscale computational frameworks such as those based on the concept of a locally attached microstructure. In the setting of a regression Artificial Neural Network (ANN), the proposed methodology supplements a typical loss function with mechanics-informed terms and therefore provides the two following benefits. First, the space of mappings between a set of training strains and stresses that can be learned by an ANN is in general larger than that of physically permissible or energy-stable material laws: thus, the proposed approach constrains this mapping space with physics-based restrictions. Second, embedding a priori a knowledge of mechanics into the training of an ANN favors the learning of the structure of a constitutive relation rather than the overfitting to the training data: hence, the proposed approach reduces a surrogate model's sensitivity to noise and promotes its robustness to inputs outside of the training domain. In this lecture, the context is set to that of constructing a computationally affordable, data-driven, and yet structure-preserving surrogate model for accelerating the dynamic analysis of a structural system made of a highly heterogeneous material by computational homogenization of the micro-structure. Indeed, it was recently shown that the computational tractability of a homogenization framework based on the concept of a locally attached microstructure benefits significantly from a computationally inexpensive functional mapping between, for example, the macro-scale in-plane Lagrange-Green strains and the Second Piola-Kirchoff stresses: therefore, it is a natural fit for the proposed mechanics-informed surrogate modeling. Specifically, various physics-based constraints for a loss function will be discussed. A method for training a form-agnostic ANN for a plane-stress material model that enforces isotropy, hyper elasticity, and energy-stability will be presented and illustrated with the nonlinear, dynamic, multiscale simulation of the supersonic inflation of an atmospheric aerodynamic decelerator system including a parachute canopy made of a woven fabric.

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Title: Double-Phase-Field Modeling of Mixed-Mode Fracture in Rocks

Author(s): *Fan Fei, *The University of Hong Kong*; Jinhyun Choo, *The University of Hong Kong*;

Phase-field modeling has been increasingly applied to the numerical simulation of rock fracture. So far, almost all phase-field models used for rock fracture simulation have treated rocks as purely brittle materials. However, it is well known that rocks are indeed quasi-brittle materials characterized by gradual softening. Further, cracking in rocks often manifest a combination of tensile (mode I) and shear (II) fractures, of which the shear fractures involve marked friction. Yet no phase-field model has been able to capture the combination of cohesive tensile and frictional shear fractures in rocks. Here we present a novel approach – double-phase-field modeling – that makes use of two different phase fields to describe cohesive tensile fracture and frictional shear fracture. We will discuss how the two phase-fields are rigorously combined considering the contact condition of the material point and an energy-based criterion for mixed-mode fracture. Through qualitative and quantitative validation against experimental data on mixed-mode fracture in rocks, we demonstrate two standout features of the double-phase-field model: (1) it allows for direct use of material strengths measured from experiments, (2) it can simulate and distinguish between tensile and shear fractures without complex algorithms.

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Title: Convergent approximations to Global Minima of Integral Functionals Using Polynomial Optimization and Finite Element Methods

Author(s): *Federico Fuentes, *Cornell University*; Giovanni Fantuzzi, *Imperial College London*;

Computation of minima of nonlinear integral functionals (e.g. strain energy) is typically done by using a variation of Newton's method or a gradient descent method on the Euler-Lagrange PDEs associated to the functional. However, these procedures only guarantee finding an approximation to a local minimum, but say nothing of whether the solution is a global minimum of the functional, which often is the goal. Finding an algorithm that provably converges to a global minimum is a classical and fundamental challenge in many fields, including nonlinear elasticity, fluid mechanics, pattern formation and PDE analysis. In this work, we combine the fields of sparse polynomial optimization and finite element (FE) methods to present such an algorithm. The techniques include exploiting properties of sparse sum-of-squares (SOS) relaxations and Gamma convergence to prove convergence to a global minimum of a functional with a polynomial integrand as the mesh is refined and the moment-SOS relaxation order is raised. We present numerical examples which result in excellent approximations to the global minima of different nonlinear functionals, including the pattern-forming Swift-Hohenberg free energy in two spatial dimensions, even when one uses sparse SOS relaxations that are computationally cheaper, but lack convergence guarantees. Finally, we will outline remaining theoretical and practical challenges to extending FE-SOS methods to PDE-constrained optimization.

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Title: A Statistical Finite Element Method (statFEM) for Coherent Synthesis of Observation Data and Model Predictions

Author(s): *Fehmi Cirak, *University of Cambridge and The Alan Turing Institute*; Eky Febrianto, *University of Cambridge and The Alan Turing Institute*; Mark Girolami, *University of Cambridge and The Alan Turing Institute*;

The increased availability of observation data from engineering systems in operation poses the question of how to incorporate this data into finite element models. To this end, we propose a novel statistical construction of the finite element method that provides the means of synthesising measurement data and finite element models. The Bayesian statistical framework is adopted to treat all the uncertainties present in the data, the mathematical model and its finite element discretisation. From the outset, we postulate a statistical generating model which additively decomposes data into a finite element, a model misspecification and a noise component. Each of the components may be uncertain and is considered as a random variable with a respective prior probability density. The prior of the finite element component is given by a conventional stochastic forward problem. The prior probabilities of the model misspecification and measurement noise, without loss of generality, are assumed to have a zero-mean and a known covariance structure. Our proposed statistical model is hierarchical in the sense that each of the three random components may depend on one or more non-observable random hyperparameters with their own corresponding probability densities. We use Bayes rule to infer the posterior densities of the three random components and the hyperparameters from their known prior densities and a data dependent likelihood function. Because of the hierarchical structure of our statistical model, Bayes rule is applied on three different levels in turn. On level one, we determine the posterior densities of the finite element component and the true system response using the prior finite element density given by the forward problem and the data likelihood. In this step, approximating the prior finite element density with a multivariate Gaussian distribution allows us to obtain a closed-form expression for the posterior. On the next level, we infer the hyperparameter posterior densities from their respective priors and the marginal likelihood of the first inference problem. These posteriors are sampled numerically using the Markov chain Monte Carlo (MCMC) method. Finally, on level three we use Bayes rule to choose the most suitable finite element model in light of the observed data by computing the respective model posteriors. We demonstrate the application and versatility of statFEM with one and two-dimensional examples.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Strength-Induced Hybrid Local/Nonlocal Continuum Mechanics Modeling of Fractures in Brittle Materials

Author(s): *Fei Han, *Dalian University of Technology*; Gilles Lubineau, *King Abdullah University of Science and Technology*;

A hybrid classical continuum mechanics and peridynamics model is proposed for brittle fractures [1], in which the peridynamics is activated according to a strength criterion. The proposed model can simulate fracture progress, including elastic deformation, crack nucleation, and propagation. The classical continuum mechanics and peridynamics are coupled into a closed equation system, and an adaptive approach is developed to solve it. The approach initially applies the classical continuum mechanics through the entire structure for its mechanical behaviors. Once the stress state reaches the strength of the material at a point, the peridynamics adaptively starts to work in the vicinity of that point to simulate the crack nucleation and propagation further. Two-dimensional numerical examples illustrate that this hybrid modeling approach can achieve successful fracture simulations of complex structures. Besides, a formula of the peridynamic horizon is proposed in this work, which is derived by considering the size of a fracture process zone that links material strength with fracture toughness. [1] Y. Wang, F. Han, G. Lubineau, Strength-induced peridynamic modeling and simulation of fractures in brittle materials, Computer Methods in Applied Mechanics and Engineering 374 (2021) 113558.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Painless Goal-Oriented hp-Adaptive Strategy for Indefinite Problems

Author(s): *Felipe Caro, *Basque Center for Applied Mathematics*; Vincent Darrigrand, *CNRS-IRIT*; Elisabete Alberdi, *University of the Basque Country*;

Felipe V. Caro*, Vincent Darrigrand†, Elisabete Alberdi Celaya††, and David Pardo††† *Basque Center for Applied Mathematics (BCAM) University of the Basque Country (UPV-EHU) e-mail: msc.felipe.caro@gmail.com † CNRS-IRIT email: vincent.darrigrand@gmail.com †† University of the Basque Country (UPV-EHU) email: elisabete.alberdi@ehu.eus ††† University of the Basque Country (UPV-EHU) Basque Center for Applied Mathematics (BCAM) Ikerbasque, Basque Foundation for Science email: dzubiaur@gmail.com ABSTRACT In 2017, Zander et al. [7] introduced a multi-level hierarchical data-structure that enables refinement and coarsening procedures. Based on this data-structure, Darrigrand et al. [2] proposed an automatic hp-adaptive algorithm for symmetric and positive definite (SPD) problems. It is based on performing global refinements followed by a selection of optimal unrefinements. This algorithm marks the basis functions with the lowest contributions to the energy of the solution and removes them. However, in many engineering applications, the global energy of the problem may be a quantity of limited relevance. This motivated the design of goal-oriented adaptive finite element methods (see e.g. [1,4-6]). They intend to approximate a particular Quantity of Interest (QoI) using an error estimator based on the solution of the adjoint problem to guide the refinements. In this context, Darrigrand et al. [3] proposed an alternative dual operator for representing the error in the QoI. In this presentation, we extend the aforementioned work [2] to non-SPD problems in the framework of hp goal-oriented adaptivity. To do so, we evaluate the contribution to the energy in the alternative dual operator proposed by Darrigrand et al. [3]. We solve both, the direct and the adjoint problem using the bilinear form associated with the direct problem. As a result, we obtain a hp-adaptive algorithm for SPD and non-SPD problems in the context of goal-oriented adaptivity. In this framework, we test and analyze our algorithm on two-dimensional (2D) Laplace, Helmholtz, and convection-dominated problems. We are also extending this adaptive algorithm to deal with multiphysics problems possibly involving H1, H(curl), H(div), and L2 spaces. We also describe the main features and limitations of the proposed method. In particular, our algorithm is robust and simple to implement; therefore, it is suitable for industrial applications. REFERENCES [1] Becker, R., & Rannacher, R. (1996). Weighted a posteriori error control in FE methods. IWR. [2] Darrigrand, V., Rodríguez?Rozas, Á., Muga, I., Pardo, D., Romkes, A., & Prudhomme, S. (2018). Goal?oriented adaptivity using unconventional error representations for the multidimensional Helmholtz equation. International Journal for Numerical Methods in Engineering, 113(1), 22-42. [3] Darrigrand, V., Pardo, D., Chaumont-Frelet, T., Gómez-Revuelto, I., & Garcia-Castillo, L. E. (2020). A painless automatic hp-adaptive strategy for elliptic problems. Finite Elements in Analysis and Design, 178, 103424. [4] Oden, J. T., & Prudhomme, S. (2001). Goal-oriented error estimation and adaptivity for the finite element method. Computers & mathematics with applications, 41(5-6), 735-756. [5] Prudhomme, S., & Oden, J. T. (1999). On goal-oriented error estimation for elliptic problems: application to the control of pointwise errors. Computer Methods in Applied Mechanics and Engineering, 176(1-4), 313-331. [6] Rannacher, R., & Suttmeier, F. T. (1998). A posteriori error control in finite element methods via duality techniques: Application to perfect plasticity. Computational mechanics, 21(2), 123-133. [7] Zander, N. D. (2017). Multi-level hp-FEM: dynamically changing high-order mesh refinement with arbitrary hanging nodes (Doctoral dissertation, Technische Universität München).

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Title: U-Net Based Neural Network for Singularity Tracing of Quadrilateral Mesh

Author(s): *Flavien Boussuge, *French Alternative Energies and Atomic Energy Commission*;

It is essential for the generation of structured multi-block quadrilateral (quad) meshes to extract a network of singularity interior boundaries which divides an initial 2D shape into macro quadrilateral domains. Existing methods are typically based on topological and geometrical transformation and can be sensitive to small features on the boundaries, to the mesh size or particular boundary edge configurations [1]. In this presentation, we introduce a pixel-based U-Net deep learning approach for direct extraction of singularity interior boundaries of a 2D shape. This work is inspired by the success of Convolutional Neural Networks (CNNs) regarding shape segmentation and skeleton extraction from real images [2]. The proposed research work uses a U-Net segmentation neural network which is trained to output a pixel-wise mask in the shape of the predicted interior boundaries of the quadrilateral decomposition of an input 2D shape. The dataset used to train the network contains squared shapes with multiple holes and their corresponding pixel-wise masks. Different convolutional layers of different sizes are used to propagate the feature extraction of a singularity mask. The advantage of a U-net architecture is its ability to obtain general information of the image combining localisation and contextual information. To evaluate the effectiveness and limitations of the approach, we generate different artificial datasets of quad-block images and masks which are used to train and test the model. Different training scenarios are considered to understand the influence of the dataset content and to evaluate the generalisation of the approach on unseen 2D shapes. [1] C. G. Armstrong, H. J. Fogg, C. M. Tierney, and T. T. Robinson, “Common Themes in Multi-block Structured Quad/Hex Mesh Generation,” Procedia Eng., vol. 124, pp. 70– 82, 2015. [2] O. Panichev and A. Voloshyna, “U-net based convolutional neural network for skeleton extraction,” in Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition Workshops, 2019, p. 0.

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Title: Least Squares and DPG Approximation of Eigenvalues

Author(s): *Fleurianne Bertrand, *University of Twente*; Daniele Boffi, *King Abdullah University of Science and Technology*; Henrik Schneider, *Humboldt Universität zu Berlin*;

In this talk, the discontinuous Petrov–Galerkin and the Least-Squares approximations of the Laplace eigenvalue problem will be discussed. Convergence together with a priori error estimates will be presented, as well as two possible error estimators and the corresponding a posteriori error analysis. The theoretical results will be confirmed numerically.

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Title: Topology Optimization of Support Structures for a Layer by Layer Simulation with Plasticity

Author(s): *Florian Dugast, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

The use of additive manufacturing to create complex parts at an industrial scale is very appealing but face many challenges. Two main issues are the amount of residual stresses that can be generated by the laser powder bed process and the need of support structures to deal with overhangs. A topology optimization method is used to generate such support structures so they can also help to decrease the magnitude of residual stresses inside the part. Different works have been published on this topic but either by using a one shot approach (Cheng et al., 2019) or by dealing only with elastic cases (Takezawa et al., 2020). The idea of this contribution is to use topology optimization for a layer by layer simulation within the elastoplasticity framework for the model to be more realistic. The plasticity model is computed with the finite element method and considers bi-linear hardening and the von Mises criterion. The thermal load is based on the inherent strain model rather than coming from a detailed simulation so the forward problem can be relatively cheap to compute. Also a matrix-free conjugate gradient is implemented on Graphics Processing Card (GPU) to further increase the efficiency of the computation for the forward and adjoint problems. The optimization objective is to minimize the p-norm stress in the computational domain subject to a volume constraint and the material distribution is represented by a density approach combined with a lattice structure. A comparison of the optimized result is performed against a one shot method and an elastic case for the same initial configuration, so one can conclude on the influence on these different levels of simplications on the final design. The optimized geometry is then printed so one can evaluate the ability of the support structures to reduce build failures. REFERENCES Cheng, L., Liang, X., Bai, J., Chen, Q., Lemon, J., & To, A. (2019). On utilizing topology optimization to design support structure to prevent residual stress induced build failure in laser powder bed metal additive manufacturing. Additive Manufacturing, 27(March), 290–304. https://doi.org/10.1016/j.addma.2019.03.001 Takezawa, A., To, A. C., Chen, Q., Liang, X., Dugast, F., Zhang, X., & Kitamura, M. (2020). Sensitivity analysis and lattice density optimization for sequential inherent strain method used in additive manufacturing process. Computer Methods in Applied Mechanics and Engineering, 370, 113231. https://doi.org/10.1016/j.cma.2020.113231

16th U.S. National Congress on Computational Mechanics
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Title: Perspectives in Peridynamics: Mathematical Constructs and Computations

Author(s): *Florin Bobaru, *University of Nebraska-Lincoln*;

Prof. Oden's influence on the origin, establishment, and future evolution of the Computational Mechanics field cannot be overstated. The "Big Three" (Oden, Hughes, and Belytschko) have sowed and nurtured the seed of the "Big Tree" of Computational Mechanics. From placing solid mathematical foundations to numerical methods used to simulate engineering-relevant physical phenomena, to landmark textbooks and leading our flagship CMAME journal, Prof. Oden has directly or indirectly inspired generations of researchers and engineers near and far. In this talk I will survey several important aspects of peridynamic modeling of fracture, diffusion, and corrosion. I will show how the integral approach for representing damage and other discontinuous phenomena can lead to surprisingly accurate simulations of physical realities. I will also discuss some recent analytical solutions of nonlocal models generated by peridynamics as well as a puzzling discovery: obtaining exact solutions of a local problem using approximate solutions of corresponding nonlocal ones. I will conclude with a brief overview of some recent progress on fast convolution-based methods for efficiently computing peridynamic models with billions of discretization nodes. This work in is collaboration with Prof. Ziguang Chen (Huazhong University of Science and Technology), Siavash Jafarzadeh (UNL), Jiangming Zhao (UNL), and Prof. Adam Larios (UNL Math). References [1] S. Jafarzadeh, L. Wang, A. Larios, F. Bobaru, "A fast convolution-based method for peridynamic transient diffusion in arbitrary domains", Computer Methods in Applied Mechanics and Engineering, 375, 113633, (2021). [2] Z. Chen, S. Jafarzadeh, J. Zhao, F. Bobaru, "A coupled mechano-chemical peridynamic model for pit-to-crack transition in stress-corrosion cracking", Journal of the Mechanics and Physics of Solids, 146, 104203, (2021) [3] S. Jafarzadeh, A. Larios, F. Bobaru, "Efficient Solutions for Nonlocal Diffusion Problems Via Boundary-Adapted Spectral Methods", Journal of Peridynamics and Nonlocal Modeling, 2: 85-110 (2020).

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Title: Material Hybrid Descriptions Combining Physics Based and Data-Driven Models

Author(s): *Francisco Chinesta, *Arts et Métiers ParisTech*; Elias Cueto, *Universidad de Zaragoza*; Victor Champaney, *Arts et Métiers ParisTech*; Jean Louis Duval, *ESI Group*;

The hybrid framework that we propose around the modelling and simulation of materials concerns different levels of and functionalities: i) Fast and reliable calibration procedures applied to state-of-the-art constitutive equations, where the problem can be formulated as a problem of parametric inference. By constructing parametric coupons and the associated parametric solutions corresponding to “any” coupon geometry, “any” virtual test (loading) and “any” material expressible from a constitutive template. ii) The gap between the best calibrated model predictions and the measurements reveals an amount of intrinsic “ignorance”, sometimes of epistemic nature. In these circumstances MHL looks for reducing the ignorance by constructing on-the-fly a data-driven model based on the application of physics-aware artificial intelligence on the deviation data. These physics-aware modeling methodologies enables fulfilling fundamental principles. iii) When combining the just referred functionalities, physics-based and data-driven, a hybrid material description results. iii) Extracting knowledge from data. The first step consists of determining from collected data the intrinsic dimensionality of its behaviors (manifold learning), identifying useless parameters, informing on the existence of hidden parameters (internal or state variables), helping to identify the parameters that acts in a combined manner. iv) Variability is addressed by constructing probabilistic material descriptions (constitutive equation), and the uncertainty propagated by using probabilistic models. v) Data compression using sparse sensing allows to reduce the acquisition rate, improve the testing machine resolution. v) Numerical microscope. The use of space-separated representation (e.g. in-plane-out-of-plane) allows zoom-in in order to exacerbate mechanical confinement effects, and localized behaviors. The possibility of solving 3D problems with the computational complexity of 2D problems allows de construction of a new kind of enriched shell representations. vii) In some circumstances, the description of rich microstructures as well as highly fluctuating data series face the difficulty of choosing the parameters for their complete and concise description (at a given scale and with a given purpose) as well as the metric of analysis, the Euclidian proving often inadequate. New techniques based on the topology of data, with the inherent invariance properties that topology provides, are disrupting data processing, time series and images analyses. TDA – topological data analysis – based on homology persistence has been successfully applied. The persistence images perfectly describe static or time-evolving microstructures.

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Title: Multigrid Poisson Solvers Using Super-Resolved Interpolation

Author(s): *Francisco Holguin, *Los Alamos National Laboratory*; Sidharth GS, *Los Alamos National Laboratory*; Gavin Portwood, *Lawrence Livermore National Laboratory*;

The multigrid algorithm is an efficient numerical technique used for solving a variety of elliptic partial differential equations. The method recursively damps residuals at different scales, accelerating the convergence of standard iterative methods. They are therefore widely employed in engineering computations. Two important components of the multigrid algorithm are prolongation (or interpolation) and restriction operators. These operators involve projection of the residuals and corrections between fine and coarse grids. Common prolongation operators include trilinear or spline based interpolants. For grids where upscaling factors are large i.e. O(10x), the prolongation operator can lend itself to a more accurate data-driven treatment with ML super-resolution. Super-resolution is commonly used in ML literature to increase the resolution of photographic images. On this idea, we propose a novel plug-n-play integration of a super resolution generative adversarial network (GAN) within the multigrid prolongation operator. Paired with a self-consistent restriction operator, we develop a solver to accelerate solution to Poisson equations. The specific problem that we train the GAN on, are pressure Poisson sources encountered in Navier-Stokes solutions to multiscale turbulent flowfields. The pressure-Poisson-solve is a critical step in incompressible fluid solvers to ensure mass-conservation. In the present work, we address the learning of homogeneous flow datasets but since the GAN operates on local windows with ghost layers, our technique readily applies to inhomogeneous flows as well. We employ a 2 level multigrid solver with a net 16x resolution coarsening using the GAN architectures of Ledig(2017). Our results show that the residual drops faster with GAN prolongation in comparison to commonly used bivariate spline interpolation. We continue to test the implementation on new datasets for generalizability of the solver, and stress-test the scaling of the solver with fixed lowest possible resolution and fixed upscaling factors. Our principal contribution to the field is a non-intrusive setup where the prolongation operator is learnt from the nature of the PDE and its solutions. Our work fits an ML component seamlessly into an efficient PDE numerical algorithm and accelerates the solver to a fixed level of accuracy. We foresee scalable computations with our method as the architecture super-resolves domain-decomposed sectors of the discretization. Ledig et al. "Photo-realistic single image super-resolution using a generative adversarial network." In Proceedings of the IEEE conference on computer vision and pattern recognition, 2017

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Title: Finding Flows of a Navier-Stokes Fluid through Quantum Computing

Author(s): *Frank Gaitan, *University of Maryland, College Park*;

There is great interest in using quantum computers to efficiently simulate a quantum system's dynamics as existing classical computers cannot do this. Little attention, however, has been given to quantum simulation of a classical nonlinear continuum system such as a viscous fluid even though this too is hard for classical computers. Such fluids obey the Navier-Stokes nonlinear partial differential equations, whose solution is essential to the aerospace industry, weather-forecasting, plasma magnetohydrodynamics, and astrophysics. Here we describe a recently introduced quantum algorithm for solving the Navier-Stokes equations [1]. The algorithm was tested by using it to find the steady-state inviscid, compressible flow through a convergent-divergent nozzle when a shockwave is (is not) present. We find excellent agreement between numerical simulation results and the exact solution, including shockwave capture when present. Finally, we compare the quantum algorithm's computational cost to deterministic and random classical algorithms and show that a significant speed-up is possible. This new work opens up a large new application area for quantum computing with substantial economic impact, including the trillion-dollar aerospace industry, weather-forecasting, and engineered-plasma technologies. [1] F. Gaitan, "Finding flows of a Navier-Stokes fluid through quantum computing", npj Quantum Inf. 6, 61 (2020); https://doi.org/10.1038/s41534-020-00291-0

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Title: Machine Learning Driven Contouring of High-Frequency Four-Dimensional Cardiac Ultrasound Data

Author(s): *Frederick Damen, *Purdue University*; David Newton, *Purdue University*; Guang Lin, *Purdue University*; Craig Goergen, *Purdue University*;

Automatic boundary detection of 4D ultrasound (4DUS) cardiac data is a promising yet challenging application at the intersection of machine learning and medicine. Using recently developed murine 4DUS cardiac imaging data, we demonstrate here a set of three machine learning models that predict left ventricular wall kinematics along both the endo- and epi-cardial boundaries. Each model is fundamentally built on three key features: 1) the projection of raw US data to a lower-dimensional subspace, 2) a smoothing spline basis across time, and 3) a strategic parameterization of the left ventricular boundaries. Model 1 is constructed such that boundary predictions are based on individual short-axis images, regardless of their relative position in the ventricle. Model 2 simultaneously incorporates parallel short-axis image data into its predictions. Model 3 builds on the multi-slice approach of model 2 but assists predictions with a single ground-truth position at end-diastole. To assess the performance of each model, Monte Carlo cross-validation was used to assess the performance of each model on unseen data. For predicting the radial distance of the endocardium, models 1, 2, and 3 yielded average R2 values of 0.41, 0.49, and 0.71, respectively. Monte Carlo simulations of the endocardial wall showed significantly closer predictions when using model 2 versus model 1 at a rate of 48.67% and using model 3 versus model 2 at a rate of 83.50%. These findings suggest that a machine learning approach where multi-slice data is simultaneously used as input and predictions are aided by a single user input yields the most robust performance. Subsequently, we applied these models to 4DUS data from wild-type mice (n=71) and two murine models of cardiac hypertrophy (i.e. CPT2M-/- (n=41) and Nkx2-5183P/+ (n=24)) to explore how computed metrics of global function and regional strain compare between ground-truth and predicted boundaries. We observed negligible deviations from ground-truth when using predicted boundaries alone, except for early diastolic strain rate which was consistently underestimated, providing confidence for the use of such machine learning models for rapid and reliable assessments of murine cardiac function. To our knowledge, this is the first application of machine learning to murine left ventricular 4DUS data. Future work will strengthen model performance with advanced machine learning techniques, extend applicability to different cardiac disease models, and translate analysis methods to clinical 4D ultrasound data.

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Title: Dynamic Mode Decomposition for AMR/C Fluid Flow Simulations

Author(s): *Gabriel F. Barros, *Universidade Federal do Rio de Janeiro*; Malú Grave, *Universidade Federal do Rio de Janeiro*; Alex Viguerie, *Gran Sasso Science Institute*; Alessandro Reali, *University of Pavia*; Alvaro L. G. A. Coutinho, *Universidade Federal do Rio de Janeiro*;

Dynamic Mode Decomposition (DMD) [1] is a powerful data-driven method used to extract spatio-temporal coherent structures that dictate a given dynamical system. The method consists of stacking collected temporal snapshots into a matrix and mapping the nonlinear dynamics using a linear operator. The standard procedure considers that snapshots possess the same dimensionality for all the observable data. In this work, we evaluate DMD's capability to extract spatio-temporal coherent structures from adaptive mesh refinement and coarsening simulations (AMR/C). The adapted mesh solutions are projected into a reference mesh to generate snapshots with the same dimensions. We illustrate the procedure with two examples using different simulation softwares supporting AMR/C: a 2D lock-exchange gravity current [2] in FEniCS and a 3D bubble rising problem [3] in libMesh. We evaluate the DMD accuracy and efficiency for these cases on the reconstruction of the signal and the extrapolation in time (short-time future estimates) using solution snapshots from fixed and projected AMR/C meshes. We observe that signal reconstruction and extrapolation with data from projected AMR/C meshes are in good agreement with those from snapshots computed with fine fixed meshes. We also show that relevant quantities of interest for each simulation, such as front position, bubble center of mass, and bubble sphericity, are well captured by the projected AMR/C meshes snapshots. [1] S.L. Brunton, J.N. Kutz, Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control, Cambridge University Press, 2019. [2] J.J. Camata, V. Silva, P. Valduriez, M. Mattoso, A.L.G.A. Coutinho, In situ visualization and data analysis for turbidity currents simulation. Computers & Geosciences, (2018) 110(C), 23-31. [3] M. Grave, J.J. Camata, A.L.G.A. Coutinho. A new convected level-set method for gas bubble dynamics. Computers & Fluids 209 (2020): 104667.

16th U.S. National Congress on Computational Mechanics
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Title: Evaluating Vaginal Creep Using Extension-Inflation Testing

Author(s): *Gabrielle Clark-Patterson, *Tulane University*; Raffaella De Vita, *Virginia Polytechnic Institute and State University*; Kristin Miller, *Tulane University*;

The vagina is a viscoelastic fibromuscular organ that plays a role in supporting the female pelvic organs. Failure in pelvic support leads to the descent of the pelvic organs into the vagina known as pelvic organ prolapse (POP). The underlying mechanisms that contribute to POP are unknown, however, changes in viscoelasticity are reported. Most studies evaluate vaginal viscoelasticity under a single load. The vagina, however, is subjected to dynamic multiaxial loading. It is unknown how varied multiaxial loading conditions affects vaginal viscoelastic response. Extension-inflation (E-I) protocols evaluated viscoelastic creep in colon [2] under various loading conditions by pressure. Further, we recently quantified the elastic mechanical properties of the murine vagina using E-I protocols [1]. This suggest that E-I protocols may be advantageous to evaluate vaginal creep. Therefore, the objective was to develop experimental methods using E-I protocols to quantify creep in the murine vagina as a function of pressure, and then to identify a mathematical relationship that describes vaginal creep. It is hypothesized that creep strain and rate increase with increased pressure. Female C57BL6 x 129SvEv mice (n=7; 3-6 months) vaginas were explanted and secured within a E-I device (IACUC approved). The physiologic length was identified followed by preconditioning and equilibration. At the physiologic length, pressure increased to a target pressure of 5, 7, 10, or 15 mmHg. Pressure held constant for 100 seconds and the laser micrometer optically tracked the outer diameter. Pressure was then removed for 1000 seconds of recovery, and the protocol was repeated at the remaining randomly allocated pressures. Peleg's equation linearized the nonlinear creep data, and a linear regression determined Peleg's constants to quantify the rate of creep [3]. A One-way ANOVA evaluated the effect of pressure on the creep rate and strain, with Tukey post-hoc test when necessary (p<0.05). Pressure significantly (p=0.03) affected creep strain at 100 seconds. Creep strain increased (p=0.04) under 15 compared to 5 mmHg of pressure. Peleg's method described vaginal creep reasonably well (=0.94 0.02).The vagina displayed a similar creep response to the medial collateral ligament, where higher loads significantly increased creep strain. Quantifying vaginal viscoelastic properties is critical for identifying the structural processes that contribute to POP.
1. Robison et. al., J Biomech Eng, 2017. 2. Carniel et. al., Proc Inst Mech Eng, 2015. 3. Peleg, Mater Sci Eng, 1979.

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Title: An Adaptive Multi-Fidelity Ensemble Kalman Filter Using Hyperreduced ROMs

Author(s): *Geoff Donoghue, *University of Toronto*; Masa Yano, *University of Toronto*;

We present an adaptive framework for the rigorous uncertainty quantification of stochastic time-dependent hyperbolic and convection-dominated partial differential equations that controls both spatial and stochastic discretization errors while quantifying aleatoric uncertainty by assimilating experimental data. This algorithm is particularly applicable to conservation laws in aerodynamics that exhibit strong nonlinearities, widely ranging scales, and non-Gaussian probability distributions. This work presents analysis yielding error bounds for mean and covariance estimates in the presence of numerical and input uncertainty and uses these bounds to inform an adaptive algorithm to efficiently provide robust and complete uncertainty quantification. The formulation comprises the following technical components: (i) an ensemble Kalman filter to tractably handle high-dimensional strongly-nonlinear data assimilation problems; (ii) multi-fidelity forecast models constructed on-the-fly, informed by \textit{a posteriori} error estimates; (iii) hyperreduction for the reduced order model, based on the empirical quadrature procedure, using discontinuous Galerkin methods; and (iv) \textit{a priori} error estimates that quantify the impact of both numerical discretization and statistical sampling error. We show that the efficient construction of the reduced order model, the rigorous control of numerical errors, and the judicious selection of adaptation procedures enables the rapid and reliable uncertainty quantification for practical nonlinear dynamical systems. Lastly, we demonstrate the effectiveness of our framework for engineering relevant aerodynamics problems with synthetic data taken from pressure taps along an airfoil to accurately estimate drag in the presence of uncertain flow conditions, and demonstrate the speedup of multi-level estimation with hyperreduction in comparison with naive assimilation methods.

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Title: MXMC: Generalized Multi-Model Monte Carlo Simulation for Uncertainty Propagation

Author(s): *Geoffrey Bomarito, *NASA Langley Research Center*; James Warner, *NASA Langley Research Center*; Patrick Leser, *NASA Langley Research Center*; William Leser, *NASA Langley Research Center*; Luke Morrill, *NASA Langley Research Center*;

This work focuses on the development of a general capability for computing the statistics of outputs from an expensive, high-fidelity model by leveraging faster, low-fidelity models for speedup. For instance, the low-fidelity models could arise from coarsened discretizations in space/time (e.g., Multilevel Monte Carlo - MLMC), or from general data-driven or reduced order models (e.g., Multifidelity Monte Carlo - MFMC). Given a fixed computational budget and a collection of models of varying cost/accuracy, the goal is to determine a sample allocation strategy that results in an estimator with optimal variance reduction. The foundation of the proposed approach is recent work on the approximate control variate (ACV) framework that unified and improved upon traditional MLMC-based/MFMC methods [1, 2]. The numerical optimization problem for optimal sample allocation required by the ACV method is revisited here in an effort to provide more robust schemes that yield improved estimator performance. An open-source Python library for general multi-model uncertainty propagation is introduced that allows a user to easily and efficiently search for an optimal sample allocation and then seamlessly compare its performance to existing methods. The necessity of such model comparisons and the utility of a Python library are illustrated through a systematic study that identifies the domains in which each sample allocation strategy provides best variance reduction. [1] Gorodetsky, A.A., et al. Journal of Computational Physics (2020) [2] Bomarito, G.F., et al. arXiv:2012.02750

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Title: An Energy-Based Coupling Approach to Interface Problems in Nonlocal Diffusion

Author(s): *Giacomo Capodaglio, *Los Alamos National Laboratory*; Marta D'Elia, *Sandia National Laboratories*; Pavel Bochev, *Sandia National Laboratories*; Max Gunzburger, *Florida State University*;

I will present recent results on the nonlocal modeling of interface problems in the context of nonlocal diffusion. First, I will lay out the mathematical foundation of the problem, which is based on a minimization of the nonlocal energy of the system. Such an approach provides a useful mean to identify transmission conditions leading to a well-posed interface problem. A theoretical study of local limits of the nonlocal weak form shows that under certain sufficient conditions on the kernel function of the nonlocal operator the classical weak formulation is recovered, guaranteeing physical consistency. Next, I will discuss the approximation of the nonlocal interface problem using the finite element method, and present several numerical results that support the theoretical predictions obtained analytically. More specifically, I will consider 1D examples to show that the proposed discretized nonlocal interface models achieve the appropriate order of convergence expected from the finite element method. Furthermore, results on numerical convergence to the local limits will also be reported, with a specific focus on the behavior of the nonlocal solution at the interface. Finally, I will discuss other relevant work on nonlocal interfaces arising in a domain decomposition setting, and discuss future research directions.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Formulation and Stability Analysis of Unstructured Spacetime Discontinuous Galerkin Method for Hyperbolic and Parabolic Partial Differential Equations

Author(s): *Giang Huynh, *The University of Tennessee Space Institute*; Reza Abedi, *The University of Tennessee Space Institute*; Robert Haber, *University of Illinois at Urbana-Champaign*;

The causal Spacetime Discontinuous Galerkin (cSDG) method [1,2] can be used directly to solve hyperbolic problems. It has proven very effective in this role due to its local conservation properties, linear computational complexity, powerful adaptive meshing capabilities, and other favorable properties. The localization of the cSDG method is related to a causality constraint that requires all boundary facets of the patch (a collection of elements that are solved simultaneously) be space-like. This limits the time advance of the vertices in the space-like front to be proportional to element size and the reciprocal of the wave speed. For a simple parabolic equation such as the Fourier heat equation, the stability limit of an explicit method is proportional to the square of element size and the reciprocal of the diffusion coefficient. We demonstrate that the cSDG method can directly be used to solve a parabolic PDE when a stability limit similar to the aforementioned condition is enforced in determining the time advances of the vertices. Spectral stability method is used to derive the stability limit of the DG method for the solution of parabolic PDEs. This analysis is done both for one patch of elements and a global domain. The von Neumann method is also used to derive the numerical dispersion relation for both hyperbolic and parabolic PDEs. This analysis determines the rate at which dissipation and dispersion errors tend to zero for different polynomial orders in spacetime as the element size goes to zero. The stability limit determined by von Neumann analysis is compared to those derived based on the spectral stability method. For both hyperbolic and parabolic cases, the effect of the choice of target value on stability limit will be discussed. Moreover, we discuss how the stability limit of a damped hyperbolic equation is related to those of an undamped hyperbolic and a parabolic PDE. Finally, we compare the numerical results of hyperbolic and parabolic Fourier heat conduction models for a problem solved by the spacetime DG method. References: [1] R. Abedi, B. Petracovici, and R.B. Haber, “A space-time discontinuous Galerkin method for linearized elastodynamics with element-wise momentum balance”, Computer Methods in Applied Mechanics and Engineering, 195:3247-3273, 2006. [2] R. Abedi, S.H. Chung, J. Erickson, Y. Fan, M. Garland, D. Guoy, R.B Haber, J.M. Sullivan, S. Thite, and Y. Zhou. "Spacetime meshing with adaptive refinement and coarsening." In Proceedings of the twentieth annual symposium on Computational geometry, 300-309. 2004

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multifidelity UQ Sampling for Stochastic Simulations

Author(s): *Gianluca Geraci, *Sandia National Laboratories*; Laura Swiler, *Sandia National Laboratories*; Bert Debusschere, *Sandia National Laboratories*;

Multifidelity (MF) sampling estimators are emerging as an effective tool for performing Uncertainty Quantification (UQ) of high-fidelity and computationally expensive models. Despite the recent advancements in developing efficient estimators, e.g. Multilevel BLUE [1] and ACV [2], virtually no attention has been devoted to understand how MF UQ estimators perform in the presence of intrinsic stochasticity in both the high and lower fidelity models. Stochastic solvers are widespread in computational engineering applications, e.g. radiation transport, turbulent simulations etc. The challenge in performing UQ for stochastic solvers is that the Quantities of Interest (QoIs) need to be obtained by, for instance, averaging time signals or replicas corresponding to each nominal realization of the random input space. The effect of the averaging procedure is twofold. First, by averaging multiple replicas the statistics of the stochastic solvers are better resolved and the noise contribution to the estimator variance is reduced. Second, the computational cost of the UQ workflow increases linearly with the number of replicas. In the MF UQ context, an additional effect needs to be considered. The reduction in the noise contribution to the models' response translates in a larger correlation among models, which, if correctly managed, could potentially result in a larger efficiency for the estimator. In this contribution, we plan to rigorously explore all these issues from a MF UQ perspective. In particular, we plan to identify the dependence of the statistics, e.g. correlation, with respect to the number of replicas of the stochastic solver and use this knowledge to formulate an augmented MF sample allocation optimization problem that includes the number of replicas in addition to the standard variables, like number of high- and low-fidelity evaluations. We plan to present a comprehensive set of numerical results based on both verification test problems and computer networks applications based on [3]. [1] Gorodetsky, A.A., Geraci, G., Eldred, M.S., and Jakeman, J.D., A Generalized Approximate Control Variate Framework for Multifidelity Uncertainty Quantification, J. Comput. Phys., 408:109257, 2020. [2] Schaden D., Ullmann, E., "On Multilevel Best Linear Unbiased Estimators", SIAM/ASA Journal on Uncertainty Quantification, Vol. 8, No. 2, pp. 601-635, 2020. [3] Geraci, G., Crussell J., Swiler, L., Debusschere, B., Exploration of multifidelity UQ sampling strategies for computer network applications, Accepted for publication, International Journal of Uncertainty Quantification, 2021. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physiology-Enhanced Data Analytics for a Personalized Approach to Disease Diagnosis and Management

Author(s): *Giovanna Guidoboni, *University of Missouri*; Alon Harris, *Icahn School of Medicine at Mount Sinai*; James Keller, *University of Missouri*; Marjorie Skubic, *University of Missouri*;

Disease diagnosis and management can be based on numerous and diverse physiological variables, spanning from cardiovascular to biochemical signals. Integrating these diverse data in a physiologically-meaningful way is very challenging, yet crucial to provide reliable information on the status of the patient. To address this issue, we have developed a novel method for physiology-enhanced data analytics that combines physiology-based mathematical models with machine learning and artificial intelligence. In this presentation, we will describe how we have successfully utilized this method to monitor the cardiovascular status via noninvasive sensors and to assess the relevance of vascular factors in glaucoma patients.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Wave Propagation in Peridynamics

Author(s): *Giuseppe Fanizza, *University of Lisbon*;

We present a rigorous study regarding the propagation of waves in a non-local model of elasticity. In particular, already in the one-dimensional propagation, it emerges that a dispersive behavior occurs and the dispersion relation, reflecting the non-locality property, is characterized by interaction range of the non-local inner forces. It turns out that dispersive effects are unavoidable and sublinear at scales smaller than the interaction length, whereas the waves at larger scales do not experience any dispersive behavior. We also discuss the conserved quantities for the proposed peridynamics model and show numerical examples about the wave propagation in the nonlinear case.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Comparing the Thermodynamically Consistent and Boussinesq Approaches for the Simulation of Buoyancy Flows

Author(s): *Guillermo Hauke, *EINA*; Jorge Lanzarote, *REPSOL*;

Two stabilized methods for the simulation of buoyant low speed flows are presented and compared. The formulations are based on the unified approach for compressible and incompressible flows [1], which solves monolithically the continuity, momentum and total energy equations. The first strategy uses the Boussinesq approximation to account for the temperature driven forces. This method models the thermal terms in the momentum equation through a temperature-dependent nonlinear source term. It is known that the Boussinesq approximation poses numerical challenges for high Rayleigh numbers, which manifest in slow or lack of convergence. The second approach introduces variable density thermodynamics of the liquid or gas without any artificial buoyancy terms, thus, without introducing any approximate models into the Navier-Stokes equations. Furthermore, this formulation holds for flows driven by high temperature differences and it is thermodynamically consistent. Various benchmarks [2] will be used to illustrate the performance and advantages of each approach. [1] G. Hauke, T.J.R. Hughes, “A Unified Approach to Compressible and Incompressible Flows,” Computer Methods in Applied Mechanics and Engineering, v. 113, p. 389-396, 1994. [2] G. de Vahl Davis, “Natural Convection of Air in a Square Cavity: a Bench Mark Numerical Solution,” International Journal for Numerical Methods in Fluids, v. 3, p. 249-264, 1983.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Accurate Crack Path Prediction in Mixed-Mode Cohesive Fracture using Virtual Element Method

Author(s): *Habeun Choi, *Yonsei University*; Heng Chi, *Siemens Corporate Technology*; Kyoungsoo Park, *Yonsei University*;

(Abstract) To predict an accurate crack path and describe the cohesive fracture behavior under mixed-mode condition, the present study proposes an element splitting scheme in conjunction with the virtual element method (VEM) and the cohesive zone modeling (CZM). Based on the element splitting scheme with the domain integral, mesh bias and dependency issues are successfully eliminated in the cohesive surface element approach (Choi and Park, 2019). In addition, arbitrarily shaped polygonal elements, generated during the element split process, are consistently handled using VEM. For the accurate approximation of a stress field around a crack tip region to evaluate the crack propagation direction, simple and effective stress recovery methods are utilized (Chi et al., 2019; Choi and Park, 2019). Then, a cohesive surface element is adaptively inserted along the direction of an external crack initiation criterion. To consistently handle mesh modification events, i.e., element splitting, the topology-based data structure (TopS) is utilized, which gives adjacent information of topological entities (Celes et al., 2005). The proposed computational framework is verified and validated by illustrating mixed-mode fracture examples such as four-point shear test and L-shaped beam peeling test. (References) H. Choi, and K. Park, 2019, Removing mesh bias in mixed-mode cohesive fracture simulation with stress recovery and domain integral, International Journal for Numerical Methods in Engineering 120(9), 1047-1070. H. Chi, L. Beirão da Veiga, and G.H. Paulino, 2019, A simple and effective gradient recovery scheme and a posteriori error estimator for the Virtual Element Method (VEM). Computer Methods in Applied Mechanics and Engineering, 347, 21-58. W. Celes, G.H. Paulino, and R. Espinha, 2005, A compact adjacency?based topological data structure for finite element mesh representation. International Journal for Numerical Methods in Engineering, 64(11), 1529-1556.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Physics-Constrained Machine Learning Approach to Solving Heat Transfer Equations on Chip

Author(s): *Haiyang He, *Ansys Inc.*; Jay Pathak, *Ansys Inc.*; Norman Chang, *Ansys Inc.*; Rishikesh Ranade, *Ansys Inc.*; Amir Maleki, *Ansys Inc.*; Priya Kasimbeg, *Ansys Inc.*; Stephen Pan, *Ansys Inc.*; Jimin Wen, *Ansys Inc.*; David Geb, *Ansys Inc.*;

Solving heat transfer equations on chip becomes very critical in the upcoming 5G and AI chip-package-systems. However, batches of simulations have to be performed for data driven machine learning models. Data driven methods are data hungry, to address this issue, Physics Informed Neural Networks (PINN) have been proposed. However, conventional PINN models solve one fixed heat equation at a time, and the models have to be retrained for heat equations with different source terms. Additionally, issues related to multi-objective optimization have to be resolved while using PINN to minimize the PDE residual, satisfy boundary conditions and fit the observed data etc. Therefore, this paper investigates an unsupervised learning approach for solving heat transfer equations on chip without using solution data and generalizing the trained network for predicting solutions for heat equations with unseen source terms. Specifically, a hybrid framework of Auto Encoder (AE) and Image Gradient (IG) based network is designed. The AE is used to encode different source terms of the heat equations. The IG based network implements a second order central difference algorithm for structured grids and minimizes the PDE residual. The effectiveness of the designed network is evaluated by solving heat equations for various test cases. It is proved that with limited number of source terms to train the AE network, the framework can not only solve the given heat transfer problems with a single training process, but also make reasonable predictions for unseen cases (heat equations with new source terms) without retraining.

16th U.S. National Congress on Computational Mechanics
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Title: A Computational Model of Myocardial Perfusion: Roles of Myogenic and Metabolic Responses in Coronary Autoregulation

Author(s): *Hamidreza Gharahi, *University of Michigan*; Johnathan Tune, *University of North Texas*; C. Alberto Figueroa, *University of Michigan*; Daniel Beard, *University of Michigan*;

Coronary blood flow is tightly regulated to ensure that myocardial oxygen delivery meets the metabolic demand (myocardial oxygen consumption, MVO2). This regulation is manifested in a wide range of physiological processes such as autoregulation, in which perturbations in coronary perfusion pressure (CPP) are met with commensurate changes in microvascular resistance to maintain a constant coronary blood flow at a given level of MVO2. Myocardial perfusion—particularly to the inner layers of the myocardium—occurs primarily during diastole. During systole the contracting myocardium exerts a constricting pressure on the vessels of myocardium, tending to impede systolic blood flow. Because the developed pressure is greatest in the innermost layer of the myocardium, this layer is most vulnerable to ischemia. Despite the critical nature of the coronary circulation, our understanding of its regulation remains largely limited due to the complex and multi-scale nature of the interacting mechanisms that govern myocardial perfusion. In this study, we analyze a set of experimental data on coronary pressure, flow, and myocardial oxygen delivery using a multi-scale computational model that represents the interrelationship between prominent mechanisms of coronary autoregulation: myogenic, metabolic, and autonomic control mechanisms. Experimental data are from in vivo measurements of dynamic changes in distal coronary perfusion pressure and oxygen uptake following rapid occlusion of the left-anterior descending coronary artery. Experiments were performed in open-chest swine in the absence and presence of hemodilution, with and without infusion of dobutamine [1]. A lumped parameter model of myocardial perfusion [2] is used to account for transmural hemodynamic variations (subendocardial, mid-wall, and subepicardial layers) and to quantify vascular tone in each layer. A model of autoregulation is used to describe the blood flow regulation with input stimuli from myogenic, metabolic, and autonomic control mechanisms. Overall, this multi-scale model provides a unique framework to test multiple competing hypotheses regarding the underlying mechanisms in coronary autoregulation. The developed model is used to investigate the degree to which hypothesized regulatory mechanisms, including a previously proposed ATP-mediated metabolic feedback pathway [3], are able to reproduce the experimental observations. [1] A. M. Kiel et al. Basic Res. Cardiol., 113:33 (2018). [2] J. P. Mynard & J. J. Smolich. Am. J. Physiol. Heart Circ. Physiol., 311 (2016), H11–H23 [3] R. K. Pradhan et al., Am. J. Physiol. Heart Circ. Physiol., 310 (2016), H1683–H1694

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Parametrically Robust Model Reduction via Enrichment with Locally Supported Basis Functions

Author(s): *Han Gao, *University of Notre Dame*; Matthew Zahr, *University of Notre Dame*;

High-fidelity numerical simulations of complex phenomena play an important role in the design and optimization of engineering systems and exploration of unknown physics. Despite significant advancements in computational science over the past several decades, such simulations remain computationally expensive. Reduced-order models (ROMs) can dramatically reduce the computational cost of a dynamical system simulation while retaining a high-degree of accuracy by constraining the dynamics to evolve in a low-dimensional subspace learned through training. However, a major limitation of ROMs is their lack of parametric robustness away from training parameters. In this work, we present a novel approach to model reduction of partial differential equations that is a hybrid between projection-based model reduction and finite element methods. The method employs a trial space as the span of a small number of data-driven basis functions with global support (as in model reduction), which are supplemented with polynomial functions with local support (as in finite element methods). The global basis functions are used to endow the method with a high degree of accuracy at a small computational cost in the non-parametric setting, while the local basis functions are used to enrich the approximation to achieve parametric robustness. Several numerical examples are provided to demonstrate the parametric robustness and speedup potential of the method.

16th U.S. National Congress on Computational Mechanics
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Title: Stochastic Fatigue Model Identification for Welded Joints Based on Structural Experimental Data

Author(s): *Han Guo, *Université de Technologie de Compiègne*; Pierre Feissel, *Université de Technologie de Compiègne*; Frédéric Druesne, *Université de Technologie de Compiègne*; Nikolaos Limnios, *Université de Technologie de Compiègne*; Salim Bouzebda, *Université de Technologie de Compiègne*; Alain Patigniez, *Renault*; Stephane Bouyaux, *Renault*;

The fatigue is an important failure reason for mechanical structures, including the automotive components, where the welded joints are critical locations. In an industrial framework, the validation of a design is always done through a combination of experiments and numerical simulations. To perform the finite element simulation of the fatigue behavior of automotive components, the knowledge of the welding joints fatigue behavior is required. The latter can be described by S-N curves and their associated dispersions [1], that are the properties to be identified. However, the identification of such a stochastic model from standard homogeneous specimen tests is not straight forward for welded joints. Our study aims at developing an identification strategy based on data collected from real mechanical tests on automotive components. Due to the heterogeneity of the mechanical fields, we proposed an inverse approach based on the minimization of an objective function to be defined [2]. Our methodology is based on the comparison of experiments on structural components with their simulation: - The experimental fatigue life data for every welded joint of a given component comes from the observation of cracks by dye penetrant inspection which interrupts the structural test. The fatigue life is interval censored because the inspections are not performed in real-time; - The stochastic model of the experiment is built under two main assumptions: (1) the deterministic numerical model is reliable, (2) the effect of uncertainty sources is grouped on the S-N curve. The finite element simulation is based on elastic assumption. The S-N curve is thus described through a stochastic model; - The identification methodology aims at characterizing the stochastic parameters of the S-N curve by minimizing the distance between the computation results and the experimental fatigue life. Furthermore, some studies have been done to understand the individual performance of different objective functions. As application, the method was firstly applied on synthetic data and then on the real experimental data and gives accurate results. Finally, the uncertainty is propagated to the calculation of finite element fatigue life. [1] C. Li, S. Wu, J. Zhang, L. Xie, Y. Zhang, Determination of the fatigue psn curves–a critical review and improved backward statistical inference method, International Journal of Fatigue 139 (2020) 105789. [2] B. V. Rosi?, A. Ku?erová, J. S`ykora, O. Pajonk, A. Litvinenko, H. G. Matthies, Parameter identification in a probabilistic setting, Engineering Structures 50 (2013) 179–196.

16th U.S. National Congress on Computational Mechanics
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Title: Stationary Dislocation at Stress Much Lower than the Peierls Stress

Author(s): *Hao Chen, *East China University of Science and Technology*; Valery Levitas, *Iowa State University*; Liming Xiong, *Iowa State University*; Xiancheng Zhang, *East China University of Science and Technology*;

As the intrinsic lattice resistance to a dislocation motion, the Peierls stress is the minimum stress required to start the motion of a static straight dislocation at zero temperature. Here we found that the Peierls stress should be exceeded for starting the motion of a dislocation, but not to maintain its stationary motion. The stationary motion of shuffle screw and 60^{o} dislocations in silicon when the applied shear, ?_{ap}, is much below the static Peierls stress, ?_p^{max}, is proved and quantified through a series of molecular dynamics (MD) simulations at 1 K and 300 K, and also by solving the continuum-level equation of motion, which uses the atomistic information as inputs. The concept of a dynamic Peierls stress, ?_p^d, below which a stationary motion can never be possible, is built upon a firm atomistic foundation. In MD simulations at 1 K, the dynamic Peierls stress is found to be 0.33 GPa for a shuffle screw dislocation and 0.21 GPa for a shuffle 60^o dislocation, versus ?_p^max of 1.71 GPa and 1.46GPa, respectively. The critical velocity v_0^c (?_ap) above which a dislocation can maintain a stationary motion at ?_p^d<?_{ap}<?_{ap}^{max} is found. The velocity dependence of the dissipation stress associated with the dislocation motion is then characterized and informed into the equation of motion of dislocation at the continuum level. A stationary dislocation motion below ?_p^{max} is attributed to: (i) the periodic lattice resistance smaller than ?_p^{max} almost everywhere; and (ii) the change of a dislocation’s kinetic energy, which acts in a way equivalent to reducing ?_p^{max}. The results obtained here open up the possibilities of a dynamic intensification of a plastic flow and defects accumulations, and consequently, the strain-induced phase transformations. Similar approaches can be applicable to partial dislocations, twin and phase interfaces.

16th U.S. National Congress on Computational Mechanics
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Title: Reverse Shape Compensation via a Gradient-Based Moving Particle Optimization Method for Elastoplastic Problems

Author(s): *Hao Deng, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

Reverse shape compensation is widely used in additive manufacturing to offset the displacement distortion caused by various sources, such as volumetric shrinkage, thermal cooling, etc. Also, reverse shape compensation is also an effective tool for the Q3 four-dimensional (4D) printing techniques, shape memory polymers (SMPs), or 3D self-assemble structures to achieve a desired geometry shape under environmental stimuli such as electricity, temperature, gravity, etc. In this paper, a gradient-based moving particle optimization method for reverse shape compensation is proposed to achieve a desired geometry shape under a given stimulus. The geometry is described by discrete particles, where the radius basis kernel function is used to realize a mapping from particle to density field, and finite element analysis is used to compute the deformation under the external stimulus. The optimization problem is formulated in detail, and the method of moving asymptotes (MMA) is implemented to update the location of discrete particles based on sensitivity information. In this work, shape deformation due to thermal expansion based on elastoplastic material model is considered. The objective of the problem is then to find the initial shape so that the deformed shape under thermal expansion is close to the desired geometry shape. A shape interpolation method based on artificial neural network (ANN) is proposed to reconstruct the accurate geometric prototype. The computational framework for reverse shape compensation described in this paper has the potential to be extended to consider linear and non-linear deformation induced by other external stimuli.

16th U.S. National Congress on Computational Mechanics
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Title: Insights from In-Silico Models of Atherosclerosis and the Role of Leukocytes and Biomechanics

Author(s): *Heather Hayenga, *The University of Texas at Dallas*; Rita Bhui, *The University of Texas at Dallas*; John Yoo, *The University of Texas at Dallas*; Jeremy Warren, *The University of Texas at Dallas*; Maziyar Keshavarzian, *The University of Texas at Dallas*; Clark Meyer, *The University of Texas at Dallas*;

Atherosclerosis and other cardiovascular diseases remain the primary cause of death in the world. Although a lot of research has elucidated the events involved in leukocyte adhesion and extravasation into the artery wall, a comprehensive mechanobiological model to capture these spatiotemporal events and predict the growth and remodeling of an atherosclerotic artery is still lacking. Artery hemodynamics, solid mechanics and biological heterogeneity all play a role in the remodeling process. In this talk I will present a computational multiscale model of leukocyte extravasation and plaque evolution in the left anterior descending (LAD) coronary artery. The model integrates cellular behaviors via agent-based modeling (ABM) and hemodynamic effects via computational fluid dynamics (CFD). In this computational framework, the ABM implements the diffusion kinetics of key biological proteins to predict chemotactic driven leukocyte migration into and within the artery wall. The ABM also considers wall shear stress (WSS) dependent leukocyte extravasation and compensatory arterial remodeling obeying Glagov's phenomenon. Using finite element methods (i.e. FEBio), recent efforts have incorporated solid mechanical properties of patient-specific coronary arteries, reconstructed from IVUS-virtual histology. Together using the model we can begin to understand the details of how an atherosclerotic artery remodels and the underlying causes. Specifically the number of leukocytes entering the artery wall increase monotonically with time, yet not at a constant rate. Interestingly at periodic plaque shapes the WSS changes rapidly resulting in a sudden increase in leukocyte extravasation. This observation suggests that certain plaques will give rise to rapid plaque growth rates if left untreated. Understanding the evolving solid mechanics informs the remodeling process as well as the acute likelihood of arterial rupture. Overall this multi-scale and multi-physics approach appropriately captures and integrates the spatiotemporal events occurring at the cellular level in order to predict leukocyte transmigration and plaque evolution. This model holds potential as a stepping stone to a fuller understanding of the atherosclerosis process and prognosis.

16th U.S. National Congress on Computational Mechanics
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Title: Floating Isogeometric Analysis (FLIGA) for Simulations with Extreme Deformations

Author(s): *Helge Christopher Hille, *ETH Zurich*; Siddhant Kumar, *Delft University of Technology*; Laura De Lorenzis, *ETH Zurich*;

Isogeometric analysis (IGA) has been widely successful in addressing some shortcomings of classical finite elements. Unfortunately, like finite elements, isogeometric discretizations fail in simulations featuring extreme deformations due to severe mesh distortions. Remedial techniques such as adaptive remeshing and arbitrary Lagrangian-Eulerian formulations address the issue to some extent but are computationally expensive and complex. On the contrary, classical meshless methods give up the notion of a mesh altogether but exhibit well-known instabilities in updated-Lagrangian or Eulerian simulations, particularly in the solid mechanics context. Here we propose a new strategy, which we term floating IGA or FLIGA. This strategy preserves the benefits of Lagrangian IGA (over finite elements and meshless methods) while enabling an adaptive and seamless update of connectivities as the mesh evolves during large deformation simulations. We depart from the classical subdivision of the parametric space in Bézier elements according to the classical tensor-product structure. In one of the parametric directions (which we term characteristic direction) we release the element structure. This uncouples the approximants along different directions which can be exploited for their deformation-dependent evolution in the parametric domain. Besides its Lagrangian character and remedy of mesh distortion, the proposed technique unifies several other advantages. Firstly, compared to many remeshing algorithms, the construction rules of the updated meshes are simple and their application does not incur significant computational effort. Secondly, unlike in material point methods, the mesh is tailored to the evolving physical boundary and keeps the weak-Kronecker delta property, allowing for simplified treatment of boundary conditions. Finally, compared to certain meshfree methods, the construction of approximants is very robust, does not require any adaptive parameter control and results in a consistent approximation of desired spline order. We demonstrate the performance of the method on benchmark simulations such as Taylor-Couette flow and apply it to extrusion-based additive manufacturing with (prototypical) Newtonian fluids as well as viscoelastic fluids.

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Title: Frequency Response Control of Composite Rubber Structures Using Energy-Based Topology Optimization

Author(s): *Hiroya Hoshiba, *Nagoya University*; Junji Kato, *Nagoya University*;

This study aims to develop a topology optimization method to control the frequency response of composite rubber structures. The topology optimization problem and sensitivity analysis algorithms are formulated based on the rheological viscoelastic model and dynamic finite element analysis. In this formulation, several objective functions are defined as related to storage and loss energy of the entire structure, corresponding to storage elastic modulus, loss elastic modulus, and loss tangent, respectively. By maximizing or minimizing these objective functions under a prescribed vibration load, the mechanical frequency characteristics of composite rubber structures are controlled. In this presentation, the detailed formulation and numerical examples will be shown to discuss the physical validity and the engineering usefulness of this method.

16th U.S. National Congress on Computational Mechanics
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Title: Extending the Subset of Analysis-Suitable T-Splines: Various Extraordinary Points Per Face

Author(s): Xiaodong Wei, *École polytechnique fédérale de Lausanne*; Xin Li, *University of Science and Technology of China*; Kuanren Qian, *Carnegie Mellon University*; Thomas J.R. Hughes, *The University of Texas at Austin*; Yongjie Jessica Zhang, *Carnegie Mellon University*; *Hugo Casquero, *University of Michigan-Dearborn*;

Analysis-suitable T-splines (AST-splines) are a promising candidate to achieve a seamless integration between the design and the analysis of thin-walled structures in industrial settings. In this work, we generalize AST-splines to allow multiple extraordinary points within the same face. This generalization drastically increases the flexibility to build geometries using AST-splines; e.g., much coarser meshes can be generated to represent a certain geometry. The AST-spline spaces detailed in this work have C^1 inter-element continuity near extraordinary points and C^2 inter-element continuity elsewhere. We mathematically show that AST-splines with multiple extraordinary points per face are linearly independent and their polynomial basis functions form a non-negative partition of unity. We numerically show that AST-splines with multiple extraordinary points per face lead to optimal convergence rates for second- and fourth-order linear elliptic problems. To illustrate a possible isogeometric framework that is already available, we design the B-pillar and the side outer panel of a car using T-splines with the commercial software Autodesk Fusion360, import the control nets into our in-house code to build AST-splines, and import the Bezier extraction information into the commercial software LS-DYNA to solve eigenvalue problems. The results are compared with conventional finite elements. Good agreement is found, but conventional finite elements require significantly more degrees of freedom to reach a converged solution than AST-splines.

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Title: Causal Random Computational Nonlinear Dynamical Model in the Framework of Viscoelasticity in Finite Displacement with Modeling Uncertainties

Author(s): *Ibrahim Benslim, *Léonard de Vinci Pôle Universitaire, Research Center*; Mohamed Guerich, *Léonard de Vinci Pôle Universitaire, Research Center*; Evangeline Capiez-Lernout, *Université Gustave Eiffel*; Christophe Desceliers, *Université Gustave Eiffel*;

It is well known that computational nonlinear dynamical models are very sensitive to uncertainties. In the framework of the robust design, it is therefore important to quantify the level of uncertainties on the solution of a given computational nonlinear dynamical model. A very efficient approach consists in modeling the uncertainties by the theory of the probability and to construct a probabilistic model for the sources of uncertainties. Among the different sources of uncertainties, some of them are related to the values of the parameters of the computational nonlinear dynamical model and those that are related to the modeling. Modeling uncertainties can be modelled by replacing the matrix-valued representations of the nonlinear operators by random matrix-valued representations. It has been shown in recent works that, in the case of linear viscoelasticity, that special attention should be given to the probabilistic model of the random stiffness and damping matrix-valued operators because they are statistically dependent through a set of compatibility equations, imposed by the causality principle. This system of equations involves Hilbert transforms when the formulation of the problem is rewritten in the frequency domain. A previous methodology has been already developed for the modeling uncertainties in computational linear dynamical models within the framework of the linear viscoelasticity in the frequency domain. In this work, this methodology is extended to the modeling uncertainties in computational nonlinear dynamical models within the framework of viscoelasticity in finite displacement in the time domain. The following steps will be presented (1) the construction of an ad hoc probabilistic model for the matrix-valued representation of the nonlinear operators of the problem that are not statistically independent in order to be compliant with the principle of causality, (2) a numerical application that illustrates the gap between two random computational nonlinear dynamical models to quantify the modeling uncertainties and when their probabilistic models takes into account the principle of causality or not.

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Chicago, IL, July 25-29. 2021

Title: Stabilized Finite Element Formulation for Phase-Field Fracture in Soft Materials

Author(s): *Ida Ang, *Cornell University*; Bin Li, *Guangdong Technion--Israel Institute of Technology*; Nikolaos Bouklas, *Cornell University*;

The formulation of the regularized approximation of brittle fracture in incompressible materials, where cracks are represented by a phase-field variable, can exhibit severe volumetric locking issues near the incompressible limit. At that limit, traditional mixed displacement and pressure formulations coupled with the damage field can lead to the development of a “pressure bubble”, applied as a traction boundary condition on the newly created fracture surface. To circumvent this unphysical feature, we present a mixed formulation, in which we introduce a damage dependent relaxation of the incompressibility constraint to account for crack opening or microcrack growth. We utilize a combination of a pure Lagrangian formulation for enforcing incompressibility in the undamaged material and a perturbed Lagrangian formulation for the damaged material to diminish the effects of residual pressure fields on the diffused crack faces. A stabilization technique, formerly utilized for the Stokes flow and incompressible linear/finite elasticity, based on the residuals of the Euler-Lagrange equations multiplied with a differential operator acting on the weight space, and evaluated elementwise is utilized. The stabilization of the mixed finite element method allows for linear interpolation of all field variables that is beneficial to large simulations. This formulation is implemented in FEniCS using a Newton based nonlinear solver and the variational inequality solver distributed in the PETSc/TAO library for hyperelastic and damage sub-problem respectively. For benchmarking, we consider a plane-stress hyperelastic model under uniaxial tension and compare the simulation to the analytical solutions for the asymptotic deformation fields around the crack tip confirming that the phase-field fracture approximation captures well the asymptotic response. Additionally, we investigate problems for crack nucleation, initiation and propagation in full three-dimensional simulations.

16th U.S. National Congress on Computational Mechanics
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Title: A Posteriori Error Estimation via Equilibrated Stress Reconstruction for Unilateral Contact Problems

Author(s): *Ilaria Fontana, *Université de Montpellier / EDF Lab Paris-Saclay*; Daniele Di Pietro, *Université de Montpellier*; Kyrylo Kazymyrenko, *EDF Lab Paris-Saclay*;

Engineering teams often use finite element numerical simulations to study large hydraulic structures. In particular, the models for concrete dams have to be capable to take into account the non-linear behavior of discontinuities which strongly depends on the presence of contact. In this presentation we focus on the unilateral contact problem without friction, in which the contact is mathematically represented by some inequalities on the involved boundary part. In literature different numerical methods are proposed, notably penalty methods, mixed methods and Nitsche-based methods. We consider the latter since it allows to treat contact boundary conditions in a weak sense with a consistent formulation and without the introduction of additional unknowns such as Lagrange multipliers. For this problem we show a posteriori error estimation based on an equilibrated stress reconstruction. This equilibrated stress is used to compute some local and global estimators which separate the different components of the computational error. In particular, the local estimators show how the error is distributed over the mesh and, as a consequence, provide a method to refine the mesh in an adaptive way. Moreover, based on the properties of these estimator, we can define local or global stopping criteria for the linearization solver and for the adjustment of some parameters. We also propose a practical way to obtain an equilibrated, H(div)-conforming, weakly symmetric stress reconstruction via local problems defined on patches around the vertices of the mesh using the Arnold-Falk-Winther mixed element space. Finally, we present some simulations in which we adaptively refine the coarse initial mesh using the distribution of the local estimators and obtaining a better convergence order of the error.

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Title: Collagen Density Regulates Tumour Spheroid Growth through Cell Motility

Author(s): *Inês G. Gonçalves, *Universidad de Zaragoza*; Jose Manuel García-Aznar, *Universidad de Zaragoza*;

Recently, several studies have revealed an interplay between the mechanical properties of the cellular microenvironment and the emergent cell behaviour. For instance, experimental studies conducted with 3D scaffolds, such as hydrogels composed of collagen, have been helpful to improve the understanding of the role of the extracellular matrix (ECM) on cellular processes. However, it is still unclear how matrix density regulates tumour growth. On the one hand, it is well established that matrices of higher density may suppress growth by exerting compressive forces on cells. On the other hand, experimental studies have also shown that matrices with higher density tend to limit cell movement due to steric hindrance. In turn, this situation promotes individual cell migration in matrices composed of lower collagen concentrations, which can subsequently affect the tumour's size. In this work, we aim to define the role of matrix density on tumour growth through an agent-based computational framework. We have used previously published experimental data, [1], to characterize the general dynamics of individual cellular movement, accounting for the mechanical properties of the ECM. Specifically, the premise of this previous work was to seed individual cancer cells in collagen matrices of varying concentrations and to assess how the collagen density modulates cell behaviour. The experimental results suggest that tumour spheroid growth is enhanced in high-density matrices, through the inhibition of individual cell motility. To simulate these experiments, we have extended the open-source PhysiCell modelling framework (version 1.7.1) [2], and we have introduced the effect of drag forces imposed by the ECM by taking into account the dynamic viscosity of the collagen matrices, as previously characterized through rheology assays in [3]. Moreover, we have defined cell-generated forces using the data in [2], which enabled us to better capture the heterogeneity in cell movement. Overall, our results show that our model successfully replicates the experimental results. In fact, we have been able to qualitatively describe how an increase in matrix density leads to smaller cell velocity values and how this, in turn, suppresses the invasion of single cells, producing cell clusters of larger areas. In contrast, lower density values enable cell migration, resulting in sparser and smaller tumours. References: 1. Plou et al, Sci Rep, 8(1):12723, 2018. 2. Ghaffarizadeh et al, PLoS Comput. Biol, 4(2):e1005991. 2018. 3. Valero et al, PloS One, 3(4):e0195820. 2018 Acknowledgements: This work was supported by the PRIMAGE project (no: 826494).

16th U.S. National Congress on Computational Mechanics
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Title: A Variational Multiscale Immersed Reproducing Kernel Particle Method for Fluid-Structure Interaction in Blast Events

Author(s): *J. S. Chen, *University of California, San Diego*; Tsung-Hui (Alex) Huang, *National Tsing Hua University*;

In blast events, strong shock waves with air-structure interaction lead to severe damage and fragmentation for structure. The complex phenomena in fluid-solid coupled systems pose considerable difficulties to conventional mesh-based numerical methods. In this work, an immersed Reproducing Kernel Particle Method (RKPM) framework is developed for modeling fluid-structure interaction (FSI) problems in the shock regime. A variational multiscale approach is employed for the proposed immersed framework, termed the variational multiscale immersed method (VMIM). The fine-scale solutions represent the residual of the coarse-scale equations, and the embedment of the fine-scale solutions results in a stabilized Petrov-Galerkin formulation, leading to increased accuracy and enhanced stability in the coarse-scale solutions. The proposed VMIM also exhibits a better convergence rate than the conventional immersed method with comparable efficiency [1]. It allows an effective body-unfitted spatial discretization for the fluid/solid domains, suitable for problems involving complex geometry. RKPM also naturally avoids computational challenges associated with low-quality meshes, allows efficient adaptive refinement, and provides flexible control of continuity and locality in numerical approximations [2]. A shock-enhanced meshfree algorithm is employed to ensure the enforcement of essential shock physics and control the Gibbs phenomenon due to the shocks, where a Riemann-enriched smoothed flux divergence is introduced under the stabilized conforming nodal integration (SCNI) framework. Besides, a flux splitting approach is employed to avoid advection-induced instabilities in fluid modeling, and the Monotonic Upstream Scheme for Conservation Laws (MUSCL)-type oscillation limiter is employed to avoid over and undershooting at the shock front and to capture moving discontinuities with minimal diffusion [3]. The proposed shock-enhanced immersed framework for FSI is applied to the blast event modeling. Reference [1] T. H. Huang, J. S. Chen, M. R. Tupek, J. J. Koester, F. N. Beckwith and E. H. Fang, A Variational Multiscale Immersed Meshfree Method for Heterogeneous Material Problems, Computational Mechanics, In press, 2021. [2] J. S. Chen, M. Hillman and S.-W. Chi, Meshfree methods: progress made after 20 years. Journal of Engineering Mechanics, 143(4), 04017001, 2017. [3] T. H. Huang, J. S. Chen, H. Wei, M. J. Roth, J. Sherburn, J. E. Bishop, M. R. Tupek and E. H. Fang, A MUSCL-SCNI approach for meshfree modeling of shock waves in fluids. Computational Particle Mechanics, 7(2), 329-350, 2020.

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Title: Minimum-Residual Scalable Multigrid Solver for High-Frequency Wave Propagation

Author(s): *Jacob Badger, *The University of Texas at Austin*; Leszek Demkowicz, *The University of Texas at Austin*;

Multigrid solvers are known to provide near-optimal performance when applied to problems with elliptic operators; however application to wave propagation remains challenging due to the indefinite nature of the operator. Minimum-residual discretization produces positive definite discretization of indefinite operators, so one natural approach is to apply multigrid to the 'ellipticized' minimum residual system. In this work we consider a multigrid method with discontinuous Petrov-Galerkin methodology with optimal test functions (DPG-MG) [Petrides, S. and Demkowicz, L. An adaptive multigrid solver for DPG methods with applications in linear acoustics and electromagnetics. arXiv:2010.06793 (2020)] applied to high-frequency wave propagation problems. In particular we observe that the uniform coarsening techniques known to be optimal for multigrid applied to elliptic operators are not optimal for multigrid applied to the 'ellipticized' wave propagation problem. Instead, adaptive refinements lead to a series of non-uniform refinements that 'sweep' in the direction of propagation. Use of this 'sweeping' refinement strategy in the DPG-MG solver has been observed to produce robust, near-linear scaling for high-frequency wave propagation problems but these observations are not currently explained by theoretical results. This work presents numerical studies on convergence and interpolation estimates to motivate future theoretical development on non-uniformly coarsened multigrid applied to wave propagation.

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Title: On the Equivalence Between the Multiplicative Hyper-Elasto-Plasticity and the Additive Hypo-Elasto-Plasticity Based on the Modified Kinetic Logarithmic Stress Rate

Author(s): *Jacob Fish, *Columbia University*; Yang Jiao, *General Electric*;

We critically examine a half a century old idea of decomposing the rate of deformation into elastic and plastic parts. We show that even the most recent additive variant based on the logarithmic rate is inconsistent with the notion of elasticity in so-called unloading stress ratchetting obstacle test while the earlier corotational variants based on the Jaumann and Green–Naghdi rates are well known not to be integrable. We then propose a stress-dependent so-called kinetic logarithmic stress rate that is both integrable and passes the unloading stress ratchetting obstacle test. We also demonstrate that the additive hypo-elasto-plasticity model based on the proposed kinetic logarithmic rate is weakly invariant under isochoric reference change for simple materials in the sense of Noll. In two theorems we then prove and subsequently demonstrate in several numerical examples involving homogeneous deformation that for isotropic materials, hyper-elasto-plasticity models based on the multiplicative decomposition of the deformation gradient coincide with an additive hypo-elasto-plasticity model that employs the spin tensor based on the kinetic logarithmic rate. References: Y. Jiao and J. Fish. Is the framework based on the additive decomposition of rate of deformation and objective stress rates passé? Computer Methods in Applied Mechanics and Engineering, Vol. 327, pp. 196–225, 2017 Y. Jiao and J. Fish. On the equivalence between the multiplicative hyper-elasto-plasticity and the additive hypo-elasto-plasticity based on the modified kinetic logarithm stress rate. Computer Methods in Applied Mechanics and Engineering, Vol. 340, pp. 824-863, 2018.

16th U.S. National Congress on Computational Mechanics
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Title: Extracellular Matrix Density Modulates Jamming-Unjamming Transitions in Breast Cancer Spheroids

Author(s): *Jacopo Ferruzzi, *The University of Texas at Dallas*; Wenying Kang, *Harvard T.H. Chan School of Public Health*; Catalina-Paula Spatarelu, *Dartmouth College*; Yu Long Han, *Massachusetts Institute of Technology*; Yasha Sharma, *Harvard T.H. Chan School of Public Health*; Stephan Koehler, *Harvard T.H. Chan School of Public Health*; Jennifer Mitchel, *Harvard T.H. Chan School of Public Health*; James Butler, *Harvard T.H. Chan School of Public Health*; Darren Roblyer, *Boston University*; Muhammad Zaman, *Boston University*; Jin-Ah Park, *Harvard T.H. Chan School of Public Health*; Ming Guo, *Massachusetts Institute of Technology*; Zi Chen, *Dartmouth College*; Adrian Pegoraro, *University of Ottawa*; Jeffrey Fredberg, *Harvard T.H. Chan School of Public Health*;

The early malignant tumor invades surrounding extracellular matrix (ECM) in a manner that depends upon material properties of constituent cells and ECM. Cancer cells are known to invade as single cells or as multicellular collectives, though a physical picture accounting for both modalities of cell migration is currently lacking. Recent work using classical two-dimensional (2D) cultures of breast cancer cells established that cells of increasing invasive potential transition from a non-migratory and solid-like phase (jammed) to a highly migratory and fluid-like phase (unjammed). Here we sought to address whether such phase transitions are involved in three-dimensional (3D) cancer invasion and, if so, to define the role played by the ECM. As a simplified model of an invasive carcinoma, we first used MCF-10A micro-spheroids embedded within an interpenetrating network of Matrigel and Alginate. By quantifying cell shape and migratory dynamics, we found that cells near the spheroid core are nearly jammed while cells at the invasive front are unjammed. To assess the generality of these results, we examined invasion patterns and jamming / unjamming signatures in macro-spheroids embedded in collagen hydrogels of various densities. Depending upon cell type (MCF-10A vs. MDA-MB-231) and ECM density (1 to 4 mg/ml collagen), cancer cells within the spheroid display a variety of spatially heterogeneous collective behaviors, including a jammed solid-like phase and progressively unjammed liquid-like and gas-like phases. At a critical collagen density, unjammed cancer cells at the spheroid periphery transition in an almost switch-like fashion between gas-like single cell invasion and liquid-like collective invasion. In the case of MDA-MB-231 spheroids, we find that when ECM density is 2 mg/ml or smaller single cells scatter from the spheroid in the form of discrete gas-like particles, but when ECM density is 3 mg/ml or greater these cells flow collectively in continuous fluid-like invasive branches. By combining high resolution microscopy, confined compression testing, and continuum biphasic modeling, we show that such phase transitions are modulated by collagen fiber density. Finally, an agent-based model of cell migration suggests that the spheroid mass can transition between multiple material phases in a manner that is superficially similar to common inanimate multiphasic systems at thermodynamic equilibrium, but here arising in living cellular systems, all of which are displaced far from thermodynamic equilibrium. We conclude that non-equilibrium phase separation based upon jamming dynamics may provide a new physical picture to describe cellular migratory dynamics within and invasion from a tumor.

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Title: Anderson Acceleration for the Staggered Solution of Phase-Field Models for Fracture in Poroelastic Media

Author(s): *Jakub Both, *University of Bergen*; Erlend Storvik, *University of Bergen*; Michael Sargado, *Technical University of Denmark*; Jan Nordbotten, *University of Bergen*; Florin Radu, *University of Bergen*;

Fluid flow in fractured, deformable porous media is of high relevance in applications ranging from geological to industrial applications as, e.g., geothermal energy. In particular, hydraulic fracturing takes a major role in the stimulation and operation of enhanced geothermal systems. Flow in deformable porous media is commonly described by the quasi-static Biot equations for poroelastic media. Furthermore, a popular approach for modeling brittle fracture is to use phase-field models. Instead of resolving fractures as sharp entities, they are smeared out and represented by an additional variable, characterized by an additional model equation. In this work, we consider a fully coupled model, coupling fluid flow, deformation, and fracturing via phase-fields. For both, poroelasticity models as well as phase-field models, staggered solution schemes are widely used [1]. In particular, for coupled poroelasticity models, they serve as basis for efficient and flexible solver technology, whereas for phase-field models staggered schemes are often employed due to their increased robustness compared to monolithic schemes. However, for the latter staggered schemes may become quite slow in situations of brutal fracturing.To mitigate this issue, we propose an acceleration strategy combining overrelaxation and Anderson acceleration [2], previously developed for merely elastic media [3]. In this work, we extend the previous efforts and propose a staggered scheme for the coupled model for hydraulic fracture in poroelastic media and enhance its convergence by a similar acceleration strategy. The efficiency and robustness of the approach will be analyzed based on numerical examples. [1] Both JW, Borregales M, Nordbotten JM, Kumar K, Radu FA. Robust fixed stress splitting for Biot’s equations in heterogeneous media. Applied Mathematics Letters. 2017 Jun 1;68:101-8. [2] Both JW, Kumar K, Nordbotten JM, Radu FA. Anderson accelerated fixed-stress splitting schemes for consolidation of unsaturated porous media. Computers & Mathematics with Applications. 2019 Mar 15;77(6):1479-502. [3] Storvik E, Both JW, Sargado JM, Nordbotten JM, Radu FA. An accelerated staggered scheme for phase-field modeling of brittle fracture. arXiv preprint arXiv:2008.11787. 2020 Aug 26.

16th U.S. National Congress on Computational Mechanics
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Title: Neural Autoencoders for Discretization-Independent Modeling of Continuous Fields

Author(s): *James Duvall, *University of Michigan*; Shaowu Pan, *University of Michigan*; Karthik Duraisamy, *University of Michigan*;

We develop a learning architecture to construct reduced models by processing solutions of partial differential equations on meshes with different discretizations and topologies, including geometrical variations. Most model reduction and machine learning techniques are discretization dependent as they rely on use of data with a fixed spatial structure. Following recent advances in computer graphics, the weights and biases of the trained network are viewed as an implicit representation of the geometry. The framework consists of encoder and parameter networks which lift spatial features to latent spaces, and a decoder network which maps from the latent spaces to field predictions. The encoder network operates in a pointwise, mesh-independent fashion. The framework is demonstrated to predict aerodynamic flow fields around airfoil and vehicle shapes including parametric and non-parametric variations.

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Title: Multidimensional Galerkin-POD for Uncertainty Quantification of PDE Solutions with Random Parameters

Author(s): Peter Benner, *Max Planck Institute for Dynamics of Complex Technical Systems*; *Jan Heiland, *Max Planck Institute for Dynamics of Complex Technical Systems*;

Already a single forward simulation of a PDE model in three spatial dimensions can be demanding in terms of memory requirements and computational effort. To quantify uncertainties in the solution that are induced by random changes in model parameters, either many sample simulations are needed (as in Monte-Carlo methods and its variants) or additional model dimensions have to be introduced (as in Galerkin-type approaches). In any case, the complexity may easily exceed reasonable computational resources so that the use model reduction techniques is mandatory. The Galerkin-type approach of polynomial chaos expansion (PCE) bases on a (truncated) expansion of the uncertainty component in the solutions. In this PCE model, every uncertainty component adds one dimension to be discretized. It has been observed that the resulting multidimensional problem can be well approximated in a tensorized space. Although a tensorized representation is in fact a complexity reduction, the overall number of unknowns will still be the product of all dimensions of the single dimensions. In this talk, we report on our recent work [1] on using Galerkin POD for tensorized bases to reduce the single dimensions optimally with respect to multidimensional snapshot data. We will introduce the relevant generalizing point of view of POD that we have successfully applied for optimal control of deterministic PDEs and show its extension to combined Finite Elements and PCE discretization, and how it efficiently enables Uncertainty Quantification of a 3D convection-diffusion process. [1]: Benner, Heiland (2020): Space and Chaos-Expansion Galerkin POD Low-order Discretization of PDEs for Uncertainty Quantification. arxiv:2009.01055

16th U.S. National Congress on Computational Mechanics
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Title: Physics Informed Machine Learning For Turbulence Model Uncertainty Estimation

Author(s): *Jan Felix Heyse, *Stanford University*; Aashwin Ananda Mishra, *Stanford University*; Gianluca Iaccarino, *Stanford University*;

Turbulence models represent the workhorse for academic and industrial studies involving real life manifestations of fluid turbulence. However, due to the simplifications inherent in their formulation, such turbulence models have a high degree of epistemic uncertainty associated with their predictions. Estimating this model form uncertainty is a critical and long standing problem in turbulence modeling and engineering design. The direct application of machine learning to estimate turbulence model uncertainties ignores physics based domain knowledge and may even lead to unphysical results. Hence, a framework is used that utilizes data driven algorithms in conjunction with physics based constraints to generate reliable uncertainty estimates for turbulence models while ensuring that the solutions are physically permissible. Random forest Machine Learning models are trained on different datasets and embedded in a Computational Fluid Dynamics solver. They are applied to complex problems to test efficacy and study generalization on new cases.

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Constitutive Laws: Three Dimensional Homogenization for Finite-Strain Hyperelasticity

Author(s): *Jan Niklas Fuhg, *Cornell University*; Michele Marino, *University of Rome Tor Vergata*; Nikolaos Bouklas, *Cornell University*;

In hyperelastic continuum mechanical problems, constitutive equations generally represent a relationship between strains (input) and stresses (output) attained at each material point of a continuum body. The predictive capabilities of numerical simulations are significantly influenced by the accuracy of the constitutive models and strategies to increase their effectiveness are a major open topic in the field. One promising advancement are computational multiscale models (e.g. numerical homogenization, domain decomposition) which are based on the definition of numerical models with a detailed description of material microstructure as well as on the consistent mapping of microstructural mechanical properties to the macroscale on the basis of numerical simulations conducted at the microscale. These methods provide an unprecedented insight to material-mechanistic details, but are associated with high computational costs and numerical complexities. Data-driven approaches have the potential to efficiently predict the effective responses of lower scales and therefore, avoid explicit simulations of the microscale problem at each Gauss point at run time. The presented work aims to offer a general framework utilizable for finite strain three dimensional hyperelastic problems. However, there are several open issues in context of finite strain mechanics which are discussed in this talk. First and foremost, the load-dependent strain input range, i.e. training region, is a priori not known for a general structural mechanics problem. Therefore an adaptive enlargement of the datasets needs to be envisioned in order to ensure the applicability of the metamodel in general finite element simulations. Secondly, compared to small strain mechanics the degree of nonlinearities is considerably higher which generally requires a possibly exhaustive number of high-fidelity simulations. Hence, effective placement schemes of samples, in context of available computational resources, need to be discussed. Lastly, favorably trained models should aim to achieve similar (quadratic) convergence behavior in the utilized bisection method as the original simulation and therefore need to provide considerable accuracy when fitting the material tangent. In context of these problems different machine learning techniques are compared including (scalable) Gaussian process regression as well as neural networks and the trained models are tested on three-dimensional structural benchmark problems with different microscale complexities using the finite-element method.

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Title: Data-Driven Inverse Design of Truss Lattices with Tunable Anisotropy

Author(s): *Jan-Hendrik Bastek, *ETH Zurich*; Siddhant Kumar, *Delft University of Technology*; Dennis M. Kochmann, *ETH Zurich*;

Advances in additive manufacturing have established periodic trusses as a popular choice for creating metamaterials with tailored properties and functionality, required e.g., for topology optimization or wave dispersion. This success is mainly due to the freedom to freely tune the underlying unit cell (UC) architecture (i.e., its topology and geometry), which determines the macroscopic behavior of the truss. While effective properties such as the stiffness of a given UC can be efficiently computed with the finite element method, the inverse problem – i.e., the identification of a UC matching a desired homogenized stiffness, cannot directly be solved with the same techniques. We propose a data-driven inverse model based on a combination of deep neural networks (DNNs) with enforced physical constraints to bypass this challenge. A dataset comprising one million different UC architectures and including the corresponding homogenized constitutive tensors was generated to train the DNNs. Generated UC architectures differ both in qualitative and quantitative features (i.e., in their structural topology and geometry) to cover a large class of anisotropic mechanical responses. To obtain a finite and systematic catalog of different topologies, we seek inspiration from existing descriptors of trusses. Results show that our inverse model accurately identifies UC architectures matching previously unseen stiffness responses while also being orders of magnitude more efficient than traditional optimization frameworks. We furthermore extend the generative ability of our model by introducing a stochastic variational sampling for potential topologies, such that different UCs matching a required stiffness response are proposed, effectively giving the designer more freedom in choosing the appropriate UC. We conclude the study by presenting a strategy to functionally grade between any predicted architectures in a large structure, without encountering discontinuous topologies or other issues typically arising in periodic topologies. This demonstrates the direct applicability of this framework to design trusses with controlled anisotropy.

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Title: Learning stochastic closure models for multiscale nonlinear dynamics

Author(s): *Jared Callaaham, *University of Washington*; Georgios Rigas, *Imperial College London*; Jean-Christophe Loiseau, *Arts et Métiers ParisTech*; Steven Brunton, *University of Washington*;

Many systems of practical and basic research interest are characterized by strongly nonlinear dynamics across a wide range of scales. Typically, the dominant behavior is determined by the largest (slow) scales, although the effects of the smaller (fast) scales must be accounted for in order to accurately resolve quantities of interest. For fluid dynamics applications, this perspective motivates a variety of closure models based on estimating an appropriate eddy viscosity to approximate small-scale energy dissipation. Projection-based reduced-order models face a similar challenge, as heavily truncated models are often unstable due to under-resolution of the viscous scales. Recent work has demonstrated the efficacy of data-driven model reduction for deterministic systems (e.g. laminar flows). Here we discuss the extension of this approach to systems that are effectively stochastic (e.g. high Reynolds number turbulence), drawing from methods developed in climate modeling and nonequilibrium statistical mechanics. We identify low-dimensional models which approximate the evolution of large-scale structures with simple nonlinear dynamics driven by random forcing from unobserved degrees of freedom. We demonstrate that this method can effectively learn stochastic models of complex fluid flows, including both experimental and numerical examples.

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Title: Iterative Global-Local Algorithm for Coupling 3D Solid and Shell Models

Author(s): *Javier Avecillas Leon, *University of Illinois at Urbana-Champaign*; Haoyang Li, *University of Illinois at Urbana-Champaign*; Armando Duarte, *University of Illinois at Urbana-Champaign*;

This paper presents the numerical results of a non-intrusive coupling algorithm used to solve fine-scale phenomena on structural-scale models. The global model that captures the structural response is solved with commercial finite element software using dimensionally reduced models (DRM) such as plates and shells. The fine-scale phenomena such as geometry details, local nonlinear behavior, or cracks are simulated with the Generalized Finite Element Method with global-local enrichments (GFEMgl). Coupling both methodologies with an iterative global-local (IGL) algorithm enables capturing of localized 3D effects while keeping the computational efficiency of the structural model [1]. However, without an adequate acceleration technique, the IGL algorithm may require many iterations or diverge. Therefore, the robustness of an acceleration algorithm based on dynamic relaxation is investigated for various shell configurations. The accuracy of the IGL-GFEMgl is compared against a reference solution provided by a Direct Generalized Finite Element Analysis. The results show that the proposed framework is able to capture the structural-scale response as well as 3D localized stress concentration and singularities. References: [1] Li, Haoyang (2020). A multiscale computational framework for the simulation of local features in large structures. Doctoral dissertation, University of Illinois at Urbana-Champaign. Available at: http://hdl.handle.net/2142/108335

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Title: Explicit Time Stepping for SUPG Stabilized Finite Element Methods

Author(s): *Jay Appleton, *Clarkson University*; Brian Helenbrook, *Clarkson University*;

In this work we present an explicit time stepping scheme for an advection dominated, one-dimensional convection diffusion equation with SUPG stabilization. Explicit time stepping of finite elements offers an efficient approach to advancing the approximate solution of a partial differential equation in time, but it requires the inversion of a mass matrix at each time step. For diffusion dominated problems, the popular p-degree nodal Gauss-Lobatto-Legendre (GLL) finite element method trivializes the inversion by means of an approximate diagonal mass matrix evaluated under numerical integration. In the advection dominated case the GLL finite element method requires the use of a stabilization technique to mitigate instability driven oscillations. However, the use of a stabilization term destroys the diagonality of the GLL mass matrix. This results in an increase of computation costs and a general decrease in performance. In previous works we defined pseudo-mass matrices to be any other matrix acting in place of the standard mass matrix. We then developed accurate pseudo-mass matrix methods for explicit time-stepping of continuous triangular finite elements methods. Building off of those works, we develop a one-dimensional, SUPG stabilized, pseudo-mass matrix approach to the advection dominated convection diffusion problem. The result is a high order, continuous finite element that is appropriate for computationally inexpensive, and accurate, explicit time stepping. We will present the necessary concepts and the desired accuracy constraints, discuss the construction of the pseudo-mass matrix, illustrate the resultant inversion scheme, and then present some computational results.

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Title: Structure-Aware Taylor Schemes for Propagating Hyperbolic Solutions Through Tents

Author(s): *Jay Gopalakrishnan, *Portland State University*; Joachim Schöberl, *TU Wien*; Dow Drake, *Portland State University*; Christoph Wintersteiger, *TU Wien*;

We consider numerical methods based on an unstructured partitioning of a spacetime domain into tent-shaped regions that respect causality. Provided that an approximate solution is available at the tent bottom, the equation can be locally evolved up to the top of the tent. By mapping tents to a domain which is a tensor product of a spatial domain with a time interval, it is possible to construct a fully explicit scheme that advances the solution through unstructured meshes. Arguing that solving the hyperbolic system on the mapped domain requires a specialized time stepping scheme, we proceed to develop the SAT (Structure-Aware Taylor) scheme. We will show its suitability for simulating linear wave phenomena. Elements of a theory we have constructed will be presented, together with a number of open issues surrounding what we currently know about the stability of such schemes.

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Title: Robust Invariant Domain Preserving Approximation of the Compressible Navier-Stokes Equations

Author(s): *Jean-Luc Guermond, *Texas A&M University*;

The objective of this talk is to present a fully-discrete approximation technique for the compressible Navier-Stokes equations. The method is implicit-explicit, second-order accurate in time and space, and guaranteed to be invariant domain preserving. The restriction on the time-step size is the standard hyperbolic CFL condition. One key originality of the method is that it is guaranteed to be conservative and invariant domain preserving under the standard hyperbolic CFL condition. This is a joint work with M. Maier, B. Popov and I. Tomas.

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Title: A XFEM - Cohesive Zone Model Coupled Approach for 3D Numerical Modeling of Ductile Failure

Author(s): *Jean-Philippe Crété, *Quartz/SUPMECA*; Konstantinos Nikolakopoulos, *Institut Clément Ader/ISAE-SUPAERO*; Patrice Longère, *Institut Clément Ader/ISAE-SUPAERO*;

Ductile fracture is a complex process which, when treated under the sole framework of local continuous damage mechanics using the standard finite element method, leads to pathological mesh dependence of the numerical results. The objective of this work is to present an original unified three-dimensional methodology capable of faithfully reproducing in a commercial code the successive steps leading to the ductile failure of metallic structures while ensuring the mesh objectivity of the numerical results. Ductile failure is generally the consequence of (i) more or less diffuse damage induced by the germination and growth of micro-cavities, (ii) localization of the damage / strain in a narrow band, and (iii) the formation and propagation of macro-cracks. In the present approach, to describe the diffuse damage (i), the material is supposed to obey the microporous plasticity GTN model. In the third step (iii), the kinematic consequences of crack opening are described by the extended finite element method (XFEM) [1]. The intermediate localization step (ii), which is the most complex to reproduce from a physical and numerical point of view, is described here via a cohesive zone model (CZM) in the framework of the XFEM [2]. The CZM makes it possible to describe the progressive degradation of the mechanical properties of the material within the localization band, induced by the coalescence of the micro-cavities and ultimately leading to the appearance of the macro-crack. The model is implemented as a user routine (UEL) in the commercial calculation code Abaqus. Its performances are evaluated by three-dimensional numerical simulations of specimens subjected to various loading cases. The proposed methodology is mesh objective and capable of correctly reproducing the inclination of the fracture surfaces. In particular, the "cup and cone" rupture in the case of an axisymmetric tensile test specimen is well reproduced numerically [3]. [1] J.P. Crété, P. Longère and J.M. Cadou, “Numerical modelling of crack propagation in ductile materials combining the GTN model and X-FEM”, Computer Methods in Applied Mechanics and Engineering, vol. 275, pp. 204-233, 2014. [2] J. Wolf, P. Longère, J.M. Cadou and J.P. Crété, “Numerical modeling of strain localization in engineering ductile materials combining cohesive models and X-FEM”, International Journal of Mechanics and Materials in Design, vol. 14, no. 2, pp. 177-193, 2018. [3] K. Nikolakopoulos, J.P. Crété and P. Longère, “Progressive failure of ductile metals: Description via a three-dimensional coupled CZM-XFEM based approach”, Engineering Fracture Mechanics, vol. 243, 2021.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analysis of Structural Components Subjected to Blast Loads Using blastFoam

Author(s): *Jeff Heylmun, *Synthetik Applied Technologies*; Robert Browning, *Synthetik Applied Technologies*; Tim Brewer, *Synthetik Applied Technologies*; Peter Vonk, *Synthetik Applied Technologies*;

As terrorism and accidental explosions continue to pose serious threats, both government and private sector agencies continue to need robust methods for assessing structures subjected to blast loading. This is frequently vital to ensure the survival of occupants and/or irreplaceable or dangerous contents. While performing physical experiments is often still necessary, in most cases it is unrealistic to test all possible threat scenarios, especially for full scale buildings. Thus, numerical modeling and simulation has become a mainstay of the protective design community for assessing complex threats and the subsequent structural response. This has led to the broad adoption of using computational fluid dynamics (CFD) to evaluate the threat environments and then either applying these loads directly to numerical models of the structure or coupling the CFD model to the structural model via fluid-structure-interaction (FSI) methods. Here, we present simulation results of the structural response of several structural components subjected to blast loading simulated using the open-source CFD code blastFoam. In addition to being open-source and freely available, blastFoam is also attractive due to its being built upon the well-established OpenFOAM library. It is also very flexible in terms of mesh generation and case setup, and offers features such as automatic mesh refinement and dynamic load balancing. In the current approach, blastFoam was used to model the detonation and propagation of blast waves throughout the domain. Prior to this, blastFoam has primarily been used solely to simulating blast wave interaction with static, non-deforming geometries. Recent developments in the code, however, now make it possible to account for structural deformation, thus permitting FSI between blast waves and the surrounding structures. This new capability is currently being evaluated and compared with existing data. References Heylmun, J., Vonk, P., Browning, R. S., and Brewer, T. (2020). blastFoam theory and user guide: Version 4.0.0. Synthetik Applied Technologies, LLC. OpenCFD Ltd., 2018. OpenFOAM - The Open Source CFD Toolbox - User’s Guide, 2nd ed. United Kingdom.

16th U.S. National Congress on Computational Mechanics
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Title: Iterative Simulation-Based Techniques for Control of Laser Powder Bed Fusion Additive Manufacturing

Author(s): *Jeff Irwin, *Autodesk, Inc*; Qian Wang, *The Pennsylvania State University*; Pan Michaleris, *Autodesk, Inc*; Abdalla Nassar, *The Pennsylvania State University*; Yong Ren, *The Pennsylvania State University*; Christopher Stutzman, *The Pennsylvania State University*;

One of the challenges for process control of laser powder bed fusion additive manufacturing lies in thermal control. Excessively low laser power may lead to incomplete melting, while too high laser power can lead to keyholing, increasing the porosity of parts. Although tools like process maps can help find optimal energy densities, no generic material-independent and geometry-independent simulation-based method exists to modulate process parameters in order to control local thermal-related defects. Considering a thermal finite-element model from our prior work, a secant-based iterative method is proposed and implemented in this work to control the simulated laser power to attain a constant melt-pool size. Several experimental samples of Inconel 625 are designed and built with the EOSINT M280 system, and cross-sectioned to evaluate the effectiveness of the iterative simulation-based controller of laser power. Cross-sectional area statistics are collected near laser turnarounds, where the melt pool is most dynamic. The iterative simulation-based controller reduces the variation of melt pool size by between 13.4 % and 48.8 % compared to applying constant laser power for all configurations. With the extra iterations from the secant method, the controlled simulations take roughly 2.3 times longer than the simulations under constant laser power.

16th U.S. National Congress on Computational Mechanics
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Title: Accurate and Efficient Partitioned Approaches for Conjugate Heat Transfer

Author(s): *Jeffrey Banks, *Rensselaer Polytechnic Institute*;

This talk will discuss the development and analysis of accurate and robust partitioned solvers for conjugate heat transfer (CHT) problems. CHT is a critical component of many important physical systems, for example thermal exchange between ocean and atmosphere in the global climate system, and accurate robust treatment of these coupled systems has been a numerical challenge. The approach advocated here treats the governing temperature equations in different material domains using implicit time-stepping, while the interface coupling is explicit. The new approach, called the CHAMP scheme (Conjugate Heat transfer Advanced Multi-domain Partitioned), is based on a discretization of the interface coupling conditions using a generalized Robin (mixed) condition. The weights in the Robin condition are determined from the optimization of a condition derived from a local stability analysis of the coupling scheme. The interface treatment combines ideas from optimized-Schwarz methods for domain-decomposition problems together with the interface jump conditions and additional compatibility jump conditions derived from the governing equations. Both second- and fourth-order accurate schemes are considered. Time permitting, results coupling the new CHT capability with high-order accurate incompressible flow solvers will also be discussed.

16th U.S. National Congress on Computational Mechanics
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Title: Nonlinear Strategies for Recovering Governing Equations from Noisy Data

Author(s): Alexandre Cortiella, *University of Colorado Boulder*; Hee-Sun Choi, *University of Colorado Boulder*; *Jeffrey Hokanson, *University of Colorado Boulder*; Alireza Doostan, *University of Colorado Boulder*;

In modern science and engineering, coupled systems of non-linear ordinary differential equations are frequently employed to represent a dynamical system of interest. However, in some applications the underlying governing equations of the system are either unknown or not fully understood. One approach to constructing models of such system is to rely on experimental measurements of the states to select an optimal instance from a set of parametric models. In doing so, difficulties arise when the amount of data is limited or when the data is corrupted with noise. This work will consider both a priori and simultaneous denoising and recovery strategies designed to mitigate the impact of noise on the stability and accuracy of the numerical procedures used to construct a model. To this end we will rely on advanced machine learning representations that enable non-linear approximation. Several non-linear ODE models will be used to illustrate various aspects of the proposed strategies.

16th U.S. National Congress on Computational Mechanics
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Title: Mechanical Consequences of Structural Heterogeneity in Healing Myocardial Scar

Author(s): Laura Caggiano, *University of Virginia*; *Jeffrey Holmes, *The University of Alabama at Birmingham*;

Introduction: Following a myocardial infarction (heart attack), damaged heart muscle is replaced by collagenous scar. The mechanical properties of post-infarction scar are critically important to clinical outcomes, and modifying those properties holds therapeutic promise. Scar mechanical properties are determined primarily by the density and alignment of collagen fibers, which varies widely in different experimental models and exhibits spatial heterogeneity. In some scars, many highly aligned pockets of collagen fibers extending 100-200 microns differ in orientation, so that the overall population of fibers is isotropically distributed [1]. While much is known about scar mechanics and structure at the whole-tissue level, the impact of spatial heterogeneity within the scar has received less attention. Methods and Results: We developed and tested a polynomial strain energy function for myocardial scar that incorporates measured fiber distributions through a structure tensor and modified invariant proposed by Holzapfel [2]. We compared our constitutive law to other strain energy functions that have been employed or proposed for myocardial scar and showed that our polynomial-structural formulation provided the best fits to mechanical test data from post-infarction scars with the least variation in fitted parameters. Then, we implemented our constitutive law in FEBio through a custom plugin and simulated controlled-displacement mechanical tests to explore the impact of measured spatial variations in collagen density and collagen orientation on deformation in individual 6-week rat infarct scars. We compared predicted heterogeneity in deformation to the actual heterogeneity we measured by speckle tracking during testing of those same scars on a CellScale BioTester. We found that incorporating regional variability in collagen alignment in our simulations could account for most of the experimentally observed variability in regional stretch. Variations in collagen density – while present in our samples – appeared to play a minor role in determining regional mechanics. Discussion: This work introduces a structure-based constitutive law that appears to capture post-infarction mechanics well, and an FEBio plugin to facilitate finite-element simulations of scar mechanics. Our work suggests that spatial heterogeneity in collagen alignment produces substantial heterogeneity in deformation during mechanical loading. The functional consequences of this heterogeneity for global phenomena such as infarct rupture [3] warrant further study, as do the mechanisms that determine the scale of the observed structural variations. References: [1] Richardson and Holmes, Biophys J, 110(10):2266-77, 2016; [2] Holzapfel et al., J R Soc Interface 12(106):20150188, 2015; [3] Korenzuk et al., J Biomech 141(9):0910151-9, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Variational Bayesian Inference for Convolutional Neural Networks in Precision Health Balance Training

Author(s): *Jeremiah Hauth, *University of Michigan*; Steven Teguhlaksana, *University of Michigan*; Jamie Ferris, *University of Michigan*; Kathleen Sienko, *University of Michigan*; Xun Huan, *University of Michigan*;

Deep neural networks (DNNs) are a powerful tool for automating expert assessment tasks in the fields of medicine and physical therapy, and can substantially reduce the workload of trained technicians. In this work, we use convolutional neural networks in a novel application of assessing balance potential for older adults and adults with inner ear disorders. However, DNNs often fail to sufficiently (or at all) convey appropriate uncertainty information, which is critical to both medical professionals and patients alike. We quantify uncertainty in DNN models by performing Bayesian inference for their weight parameters, i.e., creating Bayesian neural networks. With parameter dimension often reaching hundreds of thousands for DNNs, we conduct approximate inference using algorithms such as Flipout mean-field variational inference (MFVI) and Stein variational gradient descent (SVGD). Prior distributions for the DNN weights also tend to be very abstract, and at times arbitrary. We illustrate that priors on DNN parameters can in fact be used to create intuitive prior predictions while also inducing prediction-enhancing regularization. Furthermore, a hierarchical Bayesian framework is also demonstrated in which the model can learn the quality of data and carefully weigh the impact of the data on modifying the prior. We use these techniques to conduct Bayesian inference on a number of model architectures and conduct model selection based on the quality of their respective uncertainties. Ideally, high quality uncertainty quantification would reward high uncertainty when model predictions are poor and reward low uncertainty when predictions are good, rather than only rewarding low uncertainty across all predictions regardless of prediction quality. This work presents important steps toward automated evaluation of physical therapy exercises and notably includes uncertainty estimates that could be very valuable for future progression plans.

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Title: A Discrete Exact Grad-Curl-Div Complex on Generic Polyhedral Meshes. Part 2: Analytical Properties

Author(s): Daniele Antonio Di Pietro, *Université de Montpellier*; *Jerome Droniou, *Monash University*;

This talk focuses on the analytical properties of the discrete de Rham (DDR) complex introduced in the companion presentation "A discrete exact grad-curl-div complex on generic polyhedral meshes. Part 1: algebraic properties". The algebraic properties of the DDR complex ensure that, for each given polyhedral mesh, a scheme designed using the discrete spaces and operators in this complex has a unique solution, without the need for artificial stabilisations or projection procedures. The convergence, as the mesh size tends to zero, of the solution to such a scheme however requires further properties, to ensure the uniform stability of the scheme with respect to the mesh size and its convergence towards the correct solution. We will present a whole range of analytical properties, for all the space and operators in the DDR complex, that provide all the tools required for establishing optimal error estimates. Poincaré inequalities for the discrete gradient, curl and divergence ensure the uniform boundedness of the discrete solution. The consistency properties, which enable the proof of optimal error estimates in discrete energy norm, concern the primal consistency of the operators (and potentials) on each space in the sequence, but also adjoint consistency properties, which are essential when a formal integration by parts is used to write the weak formulation of the model (and thus the scheme). We will use a magnetostatics model to demonstrate how these properties lead to straightforward error estimates, and we will present numerical tests to illustrate these estimates. References: [1] D. Arnold. Finite Element Exterior Calculus. SIAM, 2018. doi: 10.1137/1.9781611975543. [2] D. A. Di Pietro and J. Droniou. "An arbitrary-order discrete de Rham complex on polyhedral meshes. Part I: Exactness and Poincaré inequalities". Submitted, 2021. https://hal.archives-ouvertes.fr/hal-03103526 [3] D. A. Di Pietro and J. Droniou. "An arbitrary-order discrete de Rham complex on polyhedral meshes. Part II: Consistency.". Submitted, 2021. https://hal.archives-ouvertes.fr/hal-03103535

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Title: Entropy Stable Reduced Order Modeling of Nonlinear Conservation Laws

Author(s): *Jesse Chan, *Rice University*;

Reduced order models of nonlinear conservation laws in fluid dynamics do not typically inherit stability properties of the full order model. We introduce projection-based hyper-reduced models of nonlinear conservation laws based on a "flux differencing approach". The resulting reduced models are conservative and (for physical solutions) inherit a semi-discrete entropy inequality independently of the approximation space and choice of parameters.

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Title: Learning Nonlocal Constitutive Models with Neural Networks

Author(s): *Jiequn Han, *Princeton University*; Xu-Hui Zhou, *Virginia Polytechnic Institute and State University*; Heng Xiao, *Virginia Polytechnic Institute and State University*;

Constitutive and closure models play important roles in computational mechanics and computational physics in general. Classical constitutive models for solid and fluid materials are typically local, algebraic equations or flow rules describing the dependence of stress on the local strain and/or strain-rate. Closure models such as those describing Reynolds stress in turbulent flows and laminar–turbulent transition can involve transport PDEs (partial differential equations). Such models play similar roles to constitutive relations, but they are often more challenging to develop and calibrate as they describe nonlocal mappings and often contain many submodels. Inspired by the structure of the exact solutions to linear transport PDEs, we propose a neural network representing a region-to-point mapping to describe such nonlocal constitutive models. The range of nonlocal dependence and the convolution structure are derived from the formal solution to transport equations. The neural network-based nonlocal constitutive model is trained with data. Numerical experiments demonstrate the predictive capability of the proposed method. Moreover, the proposed network learned the embedded submodel without using data from that level, thanks to its interpretable mathematical structure, which makes it a promising alternative to traditional nonlocal constitutive models.

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Title: The Crushing and Cutting Effects of Drill Bit Cutter on Deep Well Rock Based on Peridynamics

Author(s): *Jingkai Chen, *China University of Petroleum (East China)*; Zhangcong Huang, *China University of Petroleum (East China)*; Hualin Liao, *China University of Petroleum (East China)*; Yanting Zhang, *China University of Petroleum (East China)*;

During the drilling operation, the bit rotates and vibrates under certain weight on bit and penetrates into the target formation. The cutting and crushing effects of drill bit dominate the crack propagation of rock, but this process is complex depending on the types of rocks and the types of drill bit. In this research, a two-dimensional peridynamic model is proposed to analyze the crack propagation of formation rock subjected to bit cutter. Endowed by the advantages of peridynamics on modeling crack involved problems, this research utilizes peridynamics theory to analyze the rock crack behavior subjected to bit cutter. First, the state-based peridynamic constitutive relation and the bond break criterion are reformulated and calibrated considering the plasticity of the rock under high pressure high temperature downhole condition. Then, the nonlocal contact algorithm is proposed to model the relation between the cutter and the rock. After rebuilding the constitutive equation and the bond break criterion, the rock cracking process subjected to the crushing and cutting effect of drill bit cutter is simulated. The influences of different drilling conditions on the rock crack mechanism are analyzed, including the pure rotary cutting, the pure percussion cutting, the hybrid cutting and etc. Further, the influence of the cutter's parameter on the rock crack behaviors is discussed, including the cutting angle, the cutting depth, the cutting velocity and etc. The proposed model takes advantages of the peridynamics on solving discontinuity involved problems and successfully captures the damage propagation of rock without remeshing process. This research casts light on the detailed mechanism of high-speed drilling techniques.

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Title: Modeling Loading and Fragmentation in Compacted Granular Systems

Author(s): *Joel Clemmer, *Sandia National Laboratories*; Dan Bolintineanu, *Sandia National Laboratories*; Jeremy Lechman, *Sandia National Laboratories*;

Hard particle jamming in the limit of zero pressure is well studied in granular physics, but many applications are far from this limit. As pressure increases, rearrangement is no longer the only mechanism for densification as grains will deform and eventually fracture. The breakdown of granular matter, or comminution, produces irregular shapes and sizes and affects macroscopic properties including rheology. We explore the compaction of brittle granular systems using bonded discrete element simulations. Each grain is composed of many smaller, fundamental particles which are connected by a network of breakable bonds. This allows grains to crack and fragment. During loading, we monitor both the evolution of macroscopic properties (e.g. stress and porosity) as well as the evolution of grain size distributions. We explore how compaction depends on strain rate and material properties. Finally, the pressure at which single grains fail is identified and compared to theory. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

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Title: Modeling Active and Passive Periaortic Interactions Using the Inverse Finite Element Method with in vivo DENSE-MRI data

Author(s): *Johane Bracamonte, *Virginia Commonwealth University*; John Wilson, *Virginia Commonwealth University*; Joao Soares, *Virginia Commonwealth University*;

Displacement Encoding with Stimulated Echoes Magnetic Resonance Imaging (DENSE-MRI) is a technique that quantifies regional cardiovascular kinematics non-invasively. Applied to the aorta, this technique has shown that its in vivo deformation is axially and circumferentially heterogeneous [1]. Perivascular support and tethering are likely relevant factors in vascular mechanics and one of the possible causes of deformational heterogeneity [2]. Furthermore, the thoracic aorta is actively pushed by the movement of the heart throughout the cardiac cycle. This active interaction is an external source of mechanical energy usually neglected in the analysis of aortic mechanics. We propose a generalized approach to model the effect of active and passive interactions with perivascular structures on the in vivo function of the aorta while maintaining a low computational expense. Periaortic interactions are modeled as a heterogeneous Elastic Foundation Boundary Condition (EFBC). This is implemented in the Finite Element model as a collection of unidimensional springs attached to the adventitial surface and a movable opposite end. In this quasi-static model, a luminal pressure-pulse inflates the aortic wall against an EFBC of uniform stiffness. Then, the EFBC is displaced to further compress or relax the springs, generating a heterogeneous-adventitial load distribution. An optimization algorithm iterates over the material constants and EFBC parameters to fit the simulated nodal displacement to patient-specific DENSE MRI-derived targets. We hypothesize that the adventitial load distribution that replicates the in vivo translation and deformation of the aorta is representative of the active and passive periaortic interactions. We study 3 aortic locations: the infrarenal abdominal aorta, the descending thoracic aorta, and the distal arch with MRI scans from 9 individuals for each location. The optimal solutions showed good correspondence with DENSE-MRI data, producing averaged nodal displacement errors below 60% of the pixel-size resolution. Results include aortic wall properties, transmural net force distribution, and the share of deformation energy absorbed by the perivascular structures. The net transmural force peaks in regions corresponding to stiff or inwardly pushing boundaries, such as the interactions with the vertebra or with the moving heart. Soft tissues produce smaller force interactions and absorb a larger share of the pressure pulse energy. An adequate model of the periaortic interactions can bring a better understanding of the local differences of healthy and pathological growth and remodeling of the aortic wall. 1. Wilson, J. et al. J. Biomech. Eng. 141, 060901 (2019). 2. Bracamonte, J. et al. J. Biomech. Eng. 142, 121001 (2020).

16th U.S. National Congress on Computational Mechanics
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Title: Mesh Generation and NASA’s CFD Vision 2030

Author(s): *John Chawner, *Pointwise*;

Mesh generation has been described as the principle bottleneck and dominant cost in the application of computational fluid dynamics (CFD) within the aerospace industry. Complaints about mesh generation have been made since at least the 1980s but have reached a constructive zenith with publication of the NASA CFD Vision 2030 Study [1] which recommended several actions by which NASA’s CFD capability could achieve the desired level of performance by the year 2030. The Study’s recommendations regarding mesh generation cover the gamut of functionality from the relatively poor interoperability of geometry models to the inability to generate a mesh fit for a particular purpose on a complex geometry on the first attempt. This presentation will introduce the 2030 vision and provide a perspective on the vision’s current state as compiled in a 2020 progress report. REFERENCE [1] J. Slotnick, et al, “The NASA CFD Vision 2030 Study: A Path to Revolutionary Computational Aerosciences,” NASA NASA/CR-2014-218178, 2014.

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Title: Interactive Geometric Modification of Massively Parallel CFD Simulations

Author(s): *John Evans, *University of Colorado Boulder*; Corey Wetterer-Nelson, *Kitware Inc.*; Kenneth Jansen, *University of Colorado Boulder*;

In the context of high-performance finite element analysis, the cost of iteratively modifying a computational domain via re-meshing and restarting the analysis becomes time prohibitive as the size of simulations increases. In this talk, we present a new interactive simulation pipeline targeting high-performance fluid dynamics simulations where the computational domain is modified in situ, that is, while the simulation is ongoing. This pipeline is designed to be modular so that it may interface with any existing finite element simulation framework. A server-client architecture is employed to manage simulation mesh data existing on a high performance computing resource while user-prescribed geometric modifications take place on a separate workstation. In situ visualization techniques are leveraged to rapidly inform the user of simulation progression, enabling computational steering. By expressing the simulation domain in a reduced fashion on the client application, this pipeline manages highly refined finite element simulation domains on the server while maintaining good performance on the client application.

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Title: Using X-ray Angiography Images to Improve Accuracy of MR-Derived Patient-Specific Vascular Models

Author(s): *John Horn, *Texas Heart Institute*; Zbigniew Starosolski, *Texas Children's Hospital / Baylor College of Medicine*; Michael Johnson, *The University of Texas at Austin*; Avner Meoded, *Texas Children's Hospital*; Shaolie Hossain, *Texas Heart Institute / The University of Texas at Austin*;

Patient-specific computational modeling can be a valuable tool for analyzing local hemodynamics. We recently showed that by quantifying local wall shear rate (WSR), disease progression and stroke risk can be noninvasively assessed in pediatric patients with Moyamoya disease (MMD) – a steno-occlusive cerebrovascular disease that can lead to recurrent stroke. Because WSR is sensitive to vessel geometry, the predictive capability of these investigations is contingent on the ability to accurately reconstruct the patient's vascular anatomy. While computed tomography angiography (CTA) imaging is widely used for vascular model generation given its excellent resolution and signal to noise, CTA of pediatric MMD patients is uncommon due to radiation concerns. Magnetic resonance (MR) and x-ray angiography (XA) imaging are more commonly available for these patients. MR data can be used for CoW reconstruction, but often lacks sufficient spatial resolution, resulting in vessel diameter inaccuracies and failure to resolve features of interest (e.g., MMD-induced vessel narrowing). XA provides 2D projections that enable accurate measurement of vessel diameters and characterization of MMD-related narrowing. To improve accuracy of MR-derived vessel reconstructions, we have developed an approach for XA-based correction of modeled vessel geometries wherein virtual angiography, replicating the XA acquisition setup (i.e., spatial arrangement of x-ray source and detector), is performed on a MR-segmented model. Once aligned to the patient's position within the XA setup, the model is projected onto the detector plane. Automated algorithms employed in Rhino and Grasshopper CAD software are used to adjust vessel geometry until the model's 2D projections and the XA images are in good agreement. In blood flow simulations – using a Navier-Stokes solver within a NURBs-based isogeometric analysis framework – WSR distributions greatly vary among unadjusted and XA-adjusted models. In one XA-adjusted CoW model, high WSR (>45,000 s-1) in the left middle cerebral artery was observed suggesting elevated left-side stroke risk – a finding confirmed by the patient's clinical outcomes. In contrast, much lower WSRs (<20,000 s-1) were observed at multiple locations using the corresponding unadjusted model rendering the simulation inconclusive with respect to stroke risk. To verify the accuracy of our approach, we retrospectively identified a pediatric MMD patient with CTA, MR, and XA imaging data and compared the XA-adjusted MR-derived CoW model with the CTA-derived model. Agreement between the two models – with respect to vessel positions and diameters, especially in areas of vessel occlusion – suggests that our approach can accurately reconstruct patient-specific vascular geometries in the absence of CTA imaging data.

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Title: A Generalized Derivative Correction Methodology for Assuring Quadrature Consistency in Bubnov-Galerkin Polyhedral FEA

Author(s): *Joseph Bishop, *Sandia National Laboratories*;

Several types of shape functions are now available for use in defining H1-conforming polyhedral finite elements. These shape functions are more generally known as generalized barycentric coordinates (GBC) since they form a partition of unity and can reproduce linear functions. Even with the availability of shape functions for general polyhedra, one key challenge remaining for a viable polyhedral finite element formulation for nonlinear solid mechanics is developing an efficient and consistent quadrature scheme that results in a stable discretization. Quadrature for polyhedral elements with GBC shape functions is especially challenging given their non-polynomial nature. Development of an efficient quadrature scheme is especially crucial for applications in nonlinear solid mechanics where material constitutive models can be extremely expensive, e.g. for materials with a large number of internal state variables or for plasticity models with complex yield surfaces. In this work, a derivative correction scheme is proposed that ensures the necessary integration consistency in order to pass the patch test. The correction scheme involves projecting the true shape function derivatives to a finite-dimensional subspace. This projection results in the exact satisfaction of the patch test. The basis and dimension of the correction subspace determines the stability of the overall discretization. The derivative projection is facilitated through the use of the conjugate (dual) basis and covariant coordinates. There are several possibilities in choosing the correction subspace including using the given shape function basis directly. Several verification and nonlinear demonstration examples are presented along with observed rates of convergence.

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Title: Diffusion-Tensor Informed Finite Element Analysis of Shear Wave Propagation in Muscle Architecture

Author(s): *Joseph Crutison, *University of Illinois at Chicago*; Thomas Royston, *University of Illinois at Chicago*;

The combination of finite element models with medical imaging has been a valuable contribution to our understanding of tissue mechanics. In recent years, diffusion tensor imaging has aided in modeling axonal tracts in the brain to measure mechanical stresses related to traumatic brain injuries [Sahoo et al. Accid. Anal. Prev. 92, 53–70 (2016) doi: 10.1016/j.aap.2016.03.013]. However, other biological systems can benefit from this approach. Particularly, the development of diagnostic elastography for the musculoskeletal system could benefit from modeling shear wave propagation through better defined anisotropic models. The presented work demonstrates a pipeline from prior DTI to finite element models and preliminary results on the effects of prestress on shear wave propagation in these models. Dynamic elastography is a phase contrast imaging technique where contrast is based on the mechanical properties of the imaged tissue. Mechanical properties in this sense are characterized as estimations of tensile, shear or bulk moduli, obtained from solving an inverse system based on shear wave motion (inversion), typically under the assumption that the tissue is homogeneous, isotropic and without additional strains. Biological tissues, however, rarely have all three of these properties and the degree to which these assumptions are inaccurate can lead to poor estimates [Tweten et al. Magn. Reson. Med. 78(6), 2360–2372 (2017) doi: 10.1002/mrm.26600], [Chatelin et al. J. Biorheol. 27(1–2), 26–37 (2013) doi: 10.1007/s12573-012-0055-6]. Muscle typically violates all three major assumptions and requires more refined approaches for elastic moduli estimation. Using DTI to inform the generation of FE models addresses this problem by explicitly accommodating for variations in muscle architecture and allows us to compare and validate wave propagation in simulations to situational geometric changes induced by loading. Understanding wave propagation better could help derive anisotropic and prestressed relevant inversion algorithms improving the accuracy of muscle elastic moduli estimations. Initial results in the human soleus show that producing slow shear waves that are purely perpendicular to the axis of isotropy have no change in wave speed as prestress is increased, and fast and transverse shear waves vary with changing loads, in accordance to what we see analytically with transversely isotropic mediums. Differences arise based on the heterogeneity of the fiber directions, supporting the notion that the wave source and measurement location within a particular muscle needs to be considered when standardizing diagnostic protocol and comparing measurements.

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Title: Projection onto a Quadratic Manifold for Mitigating the Kolmogorov Barrier in Model Reduction

Author(s): *Joshua Barnett, *Stanford University*; Charbel Farhat, *Stanford University*;

In recent years, parametric, nonlinear, projection-based Model Order Reduction (PMOR) has significantly matured and demonstrated great success in many areas of computational mechanics, including structural dynamics, multiscale solid mechanics, and diffusion-dominated flows. For other applications such as convection-dominated flows, which are typically characterized by high Reynolds numbers, the efficiency if not feasibility of classical PMOR based on the concept of linear or affine subspace approximation is challenged by a slowly decaying Kolmogorov n-width -- defined as the worst-case error arising from a projection onto the best-possible linear subspace of dimension n -- which increases the dimension of the Reduced-Order Basis (ROB) needed to achieve the desired level of accuracy. While various approaches have been proposed to address this issue, only those based on piecewise linear subspace approximations and/or the concept of local ROBs have demonstrated so far successs for complex, convection-dominated flows such as turbulent viscous flows at high Reynolds numbers. While intellectually stimulating and interesting, alternative approaches based on deep convolutional autoencoders for constructing ROBs have been applied so far only to one-dimensional problems and the simplest of two-dimensional applications. However, the piecewise linear subspace approximation approach and associated concept of local ROBs only mitigate the Kolmogorov n-width challenge, in the sense that they only delay its manifestation -- for example, beyond a certain dimensionality of the parameter space or the ranges of its individual directions. For all these reasons, this lecture proposes a new approach for PMOR based on the approximation of the solution on a quadratic manifold. While the idea of PMOR based on a quadratic approximation has been recently attempted in the specific context of structural dynamic problems, the proposed approach is applicable to any dynamical system. More importantly, it features a versatile and cost-effective method for constructing the quadratic approximation of the solution manifold and is compatible with hyperreduction methods. The lecture also discusses the implementation of the proposed quadratic approximation approach in the Least-Square Petrov-Galerkin method for PMOR and highlights its superior accuracy and computational efficiency -- with respect to classical PMOR approaches based on linear or affine subspace approximations -- using several examples associated with convection-dominated flows of relevance to aerodynamics.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: TCB-Spline Based Isogeometric Method with High Quality Parameterization

Author(s): *Juan Cao, *Xiamen University*; Zhihao Wang, *Xiamen University*; Xiaodong Wei, *École polytechnique fédérale de Lausanne*; Yongjie Jessica Zhang, *Carnegie Mellon University*;

Isogeometric analysis (IGA) was introduced to integrate methods for analysis and computer-aided design (CAD) into a unified process. The computation of a high-quality parameterization of the physical domain plays a crucial role in IGA. However, it remains a challenge to obtain high-quality parameterization for complex geometries. Triangular configuration B-splines (TCB-splines) and their rational extensions are attractive alternatives of classical NURBS in the context of IGA, as they share many desired properties with NURBS and can be defined over general polygonal domains. In this work, we propose to use TCB-splines in IGA to overcome the limits posed by the tensor-product structure of NURBS. We present the methodology for IGA to use rational TCB-splines over general polygonal domains. Then we propose a method to generate the computational domain according to given physical domain boundaries. This allows us to easily obtain a high-quality parameterization without resorting to the optimization method. Several numerical examples with complex physical domains are provided to demonstrate the flexibility of our TCB-spline-based IGA method, the high quality of the parameterization, and the accuracy of the numerical solutions.

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Title: A New Regularization Approach for Topology Optimization with Discrete Objects

Author(s): *Julia Carroll, *Johns Hopkins University*; James Guest, *Johns Hopkins University*;

Density-based topology optimization discretizes a structure into a spatial mesh and the goal is to determine whether each element is solid or void. Due to the large design space, topology optimization typically relies on gradient-based optimization, requiring discrete outcomes (each element of the mesh is either solid or void) to be achieved using continuous variables (elements may be semi-solid, between solid and void). Interpolation approaches such as SIMP or RAMP can be combined with other techniques such as projection methods to achieve this goal at the finite element level. This talk will present a novel regularization technique that maps a field of continuous decision variables onto a discrete set of physical variables in order to enable the use of gradient-based algorithms in the topology optimization of components for fabrication by additive manufacturing. The technique was motivated by the capabilities of Electron Beam Freeform Fabrication, a wire-fed AM process. We introduce a manufacturing primitive tailored to this process and employ the proposed regularization technique to control the geometry of the primitive, as well as the interaction of the primitive with other primitives in the neighborhood. The proposed approach is demonstrated on the design of lightweight structural components, and geometric control is highlighted through various imposed manufacturing constraints. Extension of the new regularization approach to other topology optimization problems, and more general engineering optimization problems, is also discussed.

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Title: Application of Complex-Step Approximation to System Reliability-based Design Optimization

Author(s): *Junho Chun, *Syracuse University*;

This paper presents a method of complex-step approximation for sensitivity analysis and Hessian matrix computation, and its application to System Reliability-based Design Optimization (SRBDO). The system performance is a logical (Boolean) function of components having binary or multiple states based on associated performance criteria [1]. Efforts have been made to tackle the difficulties in the reliable estimation of the complex structural systems caused by various components and/or numerous failure modes and a high dimensionality. Sensitivity analysis of probabilistic constraints on system-level performance of structure is crucial for efficient gradient-based optimization. Additionally, local curvatures of probabilistic constraints are investigated through the Hessian matrix. The most derivative approximations for sensitivity analysis use a small step size to minimize subtractive cancellation and truncation errors. However, in the complex-step method [2], the step size utilizes an imaginary number. When compared to the finite difference method, the complex step approximation improves the first derivative accuracy by removing truncation error terms in Taylor's series expansion of a function. The proposed method utilizes the integration of complex-step method into a numerical integration scheme for sensitivity analysis of system probabilistic constraints, which involves the multi-fold integrals. For the Hessian matrix of the system probabilistic function, incorporation of Richardson extrapolation into the complex-step approximation is proposed to minimize truncation and subtraction errors. Results from Monte-Carlo simulations are compared with outcomes from the proposed method for numerical validation. Moreover, the computational efficiency of the proposed method for system reliability and sensitivity analysis involving high dimensionality is further improved by using a dimension reduction technique. Numerical examples of SRBDO are present to demonstrate the performance of the proposed method. References: [1] Der Kiureghian, A. 2006. "System reliability revisited." In: Integrating Structural Analysis, Risk & Reliability, Proc. the 3rd ASRANet International Colloquium. Glasgow. [2] Lyness, J. N. and Moler, C. B. 1967. "Numerical Differentiation of Analytic Functions," SIAM Journal on Numerical Analysis, 4(2):202–210

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Title: A Disconnection-Based Diffuse-Interface Approach to Model Grain Boundary Motion

Author(s): Himanshu Joshi, *University of Illinois at Urbana-Champaign*; *Junyan He, *University of Illinois at Urbana-Champaign*; Nikhil Admal, *University of Illinois at Urbana-Champaign*;

Disconnections, which are line defects that exist in grain boundaries (GBs), and defined by Burgers vectors and step heights, are instrumental in characterizing the coupling of GB motion and GB plasticity. The nucleation and subsequent migration of a disconnection in the presence of external driving forces gives rise to a shear-coupled GB motion, with a coupling factor equal to b/h, where b and h are the magnitude of the Burgers vector and step height of the disconnection, respectively. Depending on the nucleation barriers and the local stress states, multiple disconnection modes with different step heights can be activated, thereby allowing GBs to migrate with a multitude of shear-coupling factors. As a result, the disconnections framework for GBs recognizes that the mobility of a grain boundary is in fact a tensor that is not an intrinsic property of the GB, an important consequence for fundamental phenomena such as recrystallization and abnormal grain growth. In this talk, we present a continuum, large-deformation theory to model GB motion with disconnections being the primary carriers of GB plasticity. The model, based on a multi-phase field paradigm and crystal plasticity, is designed to converge to the small-deformation model of Wei et. al (2019) in the sharp-interface limit. Using stress and chemical potential as driving forces, and a diffuse-interface mobility tensor informed by atomistics, we demonstrate the consequence of coupled GB motion in polycrystals. Reference: Chaozhen Wei, Spencer L. Thomas, Jian Han, David J. Srolovitz, Yang Xiang, "A Continuum Multi-Disconnection-Mode model for grain boundary migration",Journal of the Mechanics and Physics of Solids,Volume 133,2019.

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Title: Multi-GPU MPM for Memory Intensive Engineering Projects

Author(s): *Justin Bonus, *University of Washington*; Pedro Arduino, *University of Washington*; Michael Motley, *University of Washington*; Marc Eberhard, *University of Washington*;

Graphics Processing Units (GPUs) accelerate Material Point Method (MPM) programs on the order of 100x, but limited memory and bandwidth restricts simulation size. Recent software advances in Computer Graphics now permit Multi-GPU MPM for engineering projects with many material points (10,000,000+) and grid-cells (1,000,000,000+). Hardware trends suggest rising GPU viability, with doubling of (i) video memory, (ii) bandwidth, (iii) computational cores, and (iv) increased accessibility in the next four years. We present our expansion of an optimized, open-source Multi-GPU MPM code (Claymore, https://github.com/penn-graphics-research/claymore) from computer graphics to engineering, where certain values (e.g. stress, strain, state-variables, forces) must be held to high standards. Building on open-source codes leverages prior development, requiring only basic I/O changes and vetting of physical accuracy (e.g. material models, shape-functions, transfer schemes). This code is used to model our real-world flume experiments, performed in 12m x 0.9m x 1.2m (UW Flume) and 104m x 4.6m x 3.7m (OSU Flume) facilities. Stochastic debris-field transportation, jammed debris formations, and precise loadings are captured and extrapolated for probabilistic structural design against tsunamis. In our presentation, the choice of Multi-GPU MPM over CPU codes is explained. Guidelines are detailed so others may discern short/long-term cost-benefits for their projects. GPU-rooted issues are confronted. Performance on three systems (Consumer Desktop, Mox Hyak, TACC Frontera) is shown.

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Title: Mapping the Spatial Variation of Mitral Valve Elastic Properties Using Air-Pulse Optical Coherence Elastography

Author(s): Dragoslava P. Vekilov, *Rice University*; Manmohan Singh, *University of Houston*; Salavat R. Aglyamov, *University of Houston / The University of Texas at Austin*; Kirill V. Larin, *University of Houston*; *K Jane Grande-Allen, *Rice University*;

The mitral valve is a highly heterogeneous tissue composed of two leaflets, anterior and posterior, whose unique composition and regional differences in material properties are essential to overall valve function. While mitral valve mechanics have been studied for many decades, traditional testing methods limit the spatial resolution of measurements and can be destructive. Optical coherence elastography (OCE) is an emerging method for measuring viscoelastic properties of tissues in a noninvasive, nondestructive manner. In this study, we employed air-pulse OCE to measure the spatial variation in mitral valve elastic properties with micro-scale resolution at 1 mm increments along the radial length of the leaflets. We analyzed differences between the leaflets, as well as between regions of the valve. We found that the anterior leaflet has a higher elastic wave velocity, which is reported as a surrogate for stiffness, than the posterior leaflet, most notably at the annular edge of the sample. In addition, we found a spatial elastic gradient in the anterior leaflet, where the annular edge was found to have a greater elastic wave velocity than the free edge. This gradient was less pronounced in the posterior leaflet. These patterns were confirmed using established uniaxial tensile testing methods. Overall, the anterior leaflet was stiffer and had greater heterogeneity in its mechanical properties than the posterior leaflet. This study measures differences between the two mitral leaflets with greater resolution than previously feasible and demonstrates a method that may be suitable for assessing valve mechanics following repair or during the engineering of synthetic valve replacements.

16th U.S. National Congress on Computational Mechanics
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Title: Latent Variable-Based Analysis with Machine Learning for Reduced-Order Modeling and Control of Fluid Flows

Author(s): *Kai Fukami, *University of California, Los Angeles*; Kazuto Hasegawa, *Keio University*; Taichi Nakamura, *Keio University*; Shoei Kanehira, *Keio University*; Koji Fukagata, *Keio University*;

Handling high-dimensional complex nonlinear systems in low-dimensional space while keeping its essential information is a well-known challenging task in a wide range of science and engineering. Effective modeling enables us to achieve not only controlling nonlinear systems in a practical manner but also understanding them in an explainable form. Although traditional linear-theory-based analyses have contributed to their developments, the recent advance of machine learning makes us possess the expectation for further progress of that on-going area. We here focus on the utilization of low-dimensional latent variables extracted from high-dimensional nonlinear dynamical systems with machine learning for reduced-order modeling and controls. As example problems governed by complex nonlinear nature, several canonical fluid flows are considered through the presentation. We first introduce the combination of convolutional neural network-based autoencoder (CNN-AE) and long short-term memory (LSTM) for reduced-order modeling[1,2]. The present framework founded on the CNN-AE and the LSTM enables us to drive spatiotemporal high- dimensional complex fluid flows on low-dimensional latent space extracted by the CNN-AE. Toward interpretable modeling, we also consider the use of sparse identification of nonlinear dynamics (SINDy) for deriving the time-evolving low-dimensional latent dynamics as a form of an ordinary differential equation[3]. Applicability of CNN-AE and LSTM/SINDy based modeling is demonstrated with both laminar and turbulent flow examples. At the end of our presentation, we will briefly exhibit a combination of machine-learning-based latent variables and a SINDy-based feedback control for the mitigation of unsteady vortex shedding. [1] K. Hasegawa, K. Fukami, T. Murata, and K. Fukagata, “Machine-learning-based reduced-order modeling for unsteady flows around bluff bodies of various shapes,” Theor. Comput. Fluid Dyn. 34, 367- 383 (2020). [2] T. Nakamura, K. Fukami, K. Hasegawa, Y. Nabae, and K. Fukagata, “Extension of CNN-LSTM based reduced order surrogate for minimal turbulent channel flow,” arXiv:2010.13351. [3] K. Fukami, T. Murata, and K. Fukagata, “Sparse identification of nonlinear dynamics with low-dimensionalized flow representations,” arXiv:2010.12177.

16th U.S. National Congress on Computational Mechanics
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Title: Interpretation of Convolutional Neural Networks for Predicting Volume Requirements in Studies of Microstructurally Small Cracks

Author(s): *Karen DeMille, *The University of Utah*; Ashley Spear, *The University of Utah*;

Understanding microstructurally small cracks (MSCs), or cracks whose lengths are on the order of the size of the predominant microstructural features, has remained an open problem in fracture mechanics. This is in part due to the strong dependence of MSC behavior on the local microstructural features. This dependence makes it necessary to measure and/or model microstructural features in MSC studies. However, the volume of microstructural features that should be included around an MSC in these studies is not clear. The question of how much volume should be included around an MSC was recently addressed through the determination of RVEMSC [1]. RVEMSC is defined as the minimum microstructural volume required around an MSC that ensures crack-front parameters are converged with respect to volume size. In the previous work, RVEMSC was determined via a finite element (FE)-based framework, in which J-integral values along a 3D crack front were tracked as the microstructural volume around an MSC was varied. Although successful in estimating RVEMSC, this FE-based framework proved to be computationally prohibitive for further studies [1]. To reduce the computational expense associated with determining RVEMSC, convolutional neural networks (CNNs) are deployed. Using data from the previous study [1], CNNs are trained to predict minimum microstructural volume requirements for the convergence of J-integral values with respect to volume size at individual crack-front points, or RVEMSC,ip. These CNNs make RVEMSC,ip predictions given 3D descriptions of the microstructure local to each crack-front point, as well as geometrical information about each crack. The CNNs make RVEMSC,ip predictions in a fraction of the time required by the FE-based framework. In addition to providing massive reductions in computational expense, CNNs also provide tools for investigating the complex relationship between microstructure and RVEMSC,ip. Although CNNs are commonly seen as “black box” models, methods for interpreting CNN models exist. Several of these methods are utilized to explore the role microstructure plays in RVEMSC,ip. These methods include input feature sensitivity analyses and saliency map [2] extractions. From these methods, the relative importance of microstructural and geometrical features to RVEMSC,ip are compared. Additionally, particular sets of microstructural features that most influence RVEMSC,ip are identified. [1] K. DeMille and A. Spear, Determination of representative volume elements for small cracks in heterogeneous, linear-elastic domains. Eng. Fract. Mech., Vol. 220, 106643, 2019. [2] K. Simonyan, A. Vedaldi, and A. Zisserman, Deep inside convolutional networks: visualising image classification models and saliency maps. In: ICLR, 2014. pp. 1-8.

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Title: Bayesian Genetic Programming Symbolic Regression with Preferential Search

Author(s): *Karl Garbrecht, *The University of Utah*; Nolan Strauss, *The University of Utah*; Geoffrey Bomarito, *NASA Langley Research Center*; Patrick Leser, *NASA Langley Research Center*; Jacob Hochhalter, *The University of Utah*;

Genetic Programming based Symbolic Regression (GPSR) is a non-discriminatory regression technique in which optimal model form and parameter values are sought via a Genetic Algorithm (GA). Contemporary GAs employ error-based fitness functions e.g. mean-squared error (MSE) to guide evolutionary processes and facilitate iterative convergence toward a solution(s). This project demonstrates the use of a Bayesian fitness metric, which incorporates model accuracy, complexity, and parameter distributions into a probabilistic selection process. The stochastic GPSR implementation is achieved through Sequential Monte Carlo (SMC) methods and is capable of simultaneous parameter calibration and model derivation. Model evolution within a GA is based on a trial and error process, which considers candidate model fitness to randomly generated new models (i.e. offspring) through recombination and mutation. Offspring are then calibrated and evaluated, thereby, allowing the algorithm to search the solution space and iteratively converge. This process has been proven to be reliable and an incredibly flexible strategy applicable to a wide variety of problems, albeit computationally expensive. A preferential search technique in which many offspring can be efficiently screened with a surrogate fitness prior to parameter optimization is also presented. Solution accuracy, generalizability, and computational efficiency of the contemporary and stochastic GPSR implementations, with and without the preferential search procedure, is evaluated on mechanical test data with a known governing model.

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Title: Adaptive Moving Mesh Methods through Optimal Transport Theory

Author(s): *Kelsey DiPietro, *Sandia National Laboratories*;

Adaptive moving mesh methods (r-adaptivity) have been critical to accurately solving partial differential equations with rapidly developing, fine scale solution features such as shock and singularities. Unlike other adaptive methods, r-adaptivity fixes the number of mesh points and polynomial approximation degrees. It shifts mesh points to improve accuracy in high interest areas while keeping data structures fixed. There are several ways to construct moving mesh methods, the two most common being variational approaches [2] and optimal transport approaches. This work builds upon the optimal transport approach from [1], which was restricted to finite difference methods and simply convex domains. In this work, we discretize the optimal transport problem, which can be represented as a PDE constrained optimization problem, with finite elements and solve the system using an SQP algorithm. The result is compared to the finite element solution to the Monge-Ampére equation, which is a convex solution to the optimal transport problem with quadratic costs. Once a solution to optimal transport problem is found, we pair it with a nonlinear partial differential equation posed on a convex domain and use it to generate an adaptive mesh that clusters mesh points where it requires additional resolution of the PDE. We present results of the method for a classical test bed of two-dimensional adaptivity problems including Burger's equation and semilinear blow up. [1] K. DiPietro, A. Lindsay. Adaptive solution to two-dimensional partial differential equations in curved domains using the Monge-Ampére equation. SIAM J. Sci. Comp. (2019). [2] W. Huang, Variational mesh adaptation: isotropy and equidistribution. J. Comp Phys (2001).

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Title: Upwind Summation By Parts Finite Difference Methods for Large Scale Elastic Wave Simulations In Complex Geometries

Author(s): *Kenneth Duru, *Australian National University*; Christopher Williams, *Australian National University*; Frederick Fung, *Australian National University*;

High-order accurate summation-by-parts (SBP) finite difference (FD) methods constitute efficient numerical methods for simulating large-scale hyperbolic wave propagation problems. Traditional SBP FD operators that approximate first-order spatial derivatives with central-difference stencils often have spurious unresolved wave-modes in their numerical solutions. On marginally resolved computational grids, these spurious wave-modes have the potential to destroy the accuracy of numerical solutions for a first-order hyperbolic partial differential equation, such as the elastic wave equation. To ensure the accuracy of numerical solutions of the three space dimensional (3D) elastic wave equation in complex geometries, we discretise the 3D elastic wave equation with a pair of non-central (upwind) finite-difference stencils, on boundary-conforming curvilinear meshes. Using the energy method we prove that the numerical method is stable, and energy conserving. Furthermore, computational results show the robustness of the scheme. We present numerical simulations of the 3D elastic wave equation in heterogeneous media with complex non-planar free surface topography, including numerical simulations of community developed seismological benchmark problems. Our results show that the upwind SBP operators are more robust and less prone to numerical dispersion errors on marginally resolved meshes when compared to traditional SBP operators, thereby increasing efficiency.

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Title: High-Order Finite Elements for Lumped-Mass Explicit Modeling in Nonlinear Solid Dynamics

Author(s): *Kent Danielson, *US Army Engineer Research and Development Center*; Robert Browning, *Synthetik Applied Technologies*;

This presentation discusses recent developments and current challenges with high-order finite elements for lumped-mass central difference type explicit time integration methods in nonlinear solid dynamics. Predictions are demonstrated for a wide range of applications, which includes linear wave propagation, but focuses particularly on complex highly nonlinear “hydro-code” problems involving large strains, inelasticity, and/or contact. Standard higher-order (p>1) finite element shape functions have negative interpolation regions that can produce non-positive lumped nodal masses and contact forces, which can preclude their use in common “hydro-code” lumped-mass explicit applications. Inclusion of bubble-like functions, such as those associated with internal and face nodes, can significantly reduce but may not eliminate negative regions. Newer elements based on NURBS (IGA), Bernstein/Bézier, and related functions may not have negative regions, but their associated non-physical points (knots/anchor/etc.) pose additional challenges for enforcing complex contact that may continue to evolve. The discontinuous nature of inelasticity and contact has led most hydro-code elements to be C0 continuous and non-hierarchical nodal interpolation functions are especially advantageous for discrete contact methods. Line, quadrilateral, and hexahedral elements using Lagrange polynomials with nodes placed at Legendre-Gauss-Lobatto (LGL) points have long been known to produce all positive lumped nodal masses with imprecise nodal quadrature [1]. In addition, the LGL nodal locations for the shape functions seem to minimize Runge phenomena [2]. More precise Gauss-Legendre quadrature rules with row-summation lumping is more accurate with distorted elements and also avoids the under-integration problems of spectral finite elements [3]. These Lagrange elements still have negative regions in their functions that can be problematic for some contact approaches, but they are shown to produce all positive nodal lumped masses that support workable explicit contact for high orders, e.g., up to at least p=9. For other elements with triangular faces, however, the choice and construction of appropriate interpolation functions for robust lumped-mass explicit analysis is not so straightforward nor unique, and viable such ones have not typically appeared past p=3. Elements with only vertex and mid-edge nodes are shown to provide mixed success using the Hinton-Rock-Zienkiewicz (HRZ) method to produce all positive nodal lumped masses. The discussion includes several classes of p=2 hexahedral, tetrahedral, wedge, and pyramid elements for Hex-Dominant modeling implemented into in-house meshing tools, a parallel FEA code (ParaAble), and visualization software, as well into popular production meshing (Cubit), parallel analysis (EPIC), and visualization (ParaView) software. ACKNOWLEDGMENTS Permission to publish was granted by Director, Geotechnical and Structures Laboratory

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Title: Geomiso ISA: A Cloud-Based Software for Static Isogeometric Analysis with Plate Elements

Author(s): Panagiotis Karakitsios, *Geomiso Company*; *Konstantinos Gogos, *Geomiso Company*; Konstantinos Mprellas, *Geomiso Company*;

In this paper, we present Geomiso ISA (www.geomiso.com), a new hybrid software for applications on isogeometric analysis and 3D design with splines. The isogeometric method, in combination with the plate theory, has attracted increasing attention in construction industry, as it achieves efficient design-through-analysis procedures and shows superior performance. Although NURBS are ubiquitous in CAD industry, the most promising spline technology is T-splines, which overcome limitations inherent to NURBS, ensure higher-order continuity across patches and permit local refinement. Geomiso ISA provides static isogeometric analysis with plate elements. This both stand-alone and cloud-based program satisfies the rising industrial need for seamless integration of computer-aided design and computer-aided analysis, while it appears to be more efficient to finite element software, as it facilitates the geometry modeling within analysis, eliminates geometric errors and achieves superior accuracy per degree-of-freedom with significantly reduced computational cost. It offers an innovative way to merge geometric design with mesh generation into a single procedure by designing, with its hybrid graphical user interface, models as tensor product grids in contrast to design programs. Applications to thin (Kirchhoff-Love) and thick (Mindlin-Reissner) plates are demonstrated with a comparison between Geomiso ISA and finite element programs. We compare the accuracy of the numerical results, such as displacement, strain and stress fields, and the matrix assembly and solver time for analysis of typical slab types widely used in construction. Parametric investigations were carried out on the effects of polynomial order and continuity of basis and shape functions, control point number and element number. This new hybrid software represents improvements over finite element software packages, as higher accuracy, robustness, and stability level is accomplished with drastically decreased computational time. This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T2EDK-00703). Keywords: Isogeometric analysis, Plate theory, Kirchhoff-Love, Mindlin-Reissner, Splines, Industrial applications, Buildings, Slabs, Software, Cloud References [1] P. Karakitsios, G. Karaiskos, A. Leontaris, P. Kolios, Geomiso TNL: A software for non-linear static T-spline-based isogeometric analysis of complex multi-patch structures, 14th World Congress in Computational Mechanics (WCCM), ECCOMAS Congress (2020). [2] A. Karatarakis, P. Karakitsios, M. Papadrakakis, GPU accelerated computation of the isogeometric analysis stiffness matrix, Comput. Methods Appl. Mech. Engrg., 269 (2014) 334-355. [3] T.J.R. Hughes, J.A. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry, and mesh refinement, Comput. Methods Appl. Mech. Engrg. 194 (2005) 4135-4195.

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Title: An Inverse Modelling Study on the Local Volume Changes During Early Morphoelastic Growth of the Fetal Human Brain

Author(s): Z. Wang, *University of Michigan*; B.T. Martin, *University of Michigan*; J. Weickenmeier, *Stevens Institute of Technology*; *Krishna Garikipati, *University of Michigan*;

We take a data-driven approach to deducing the local volume changes accompanying early development of the fetal human brain. Our approach uses fetal brain atlas MRI data for the geometric changes in representative cases. Using a nonlinear continuum mechanics model of morphoelastic growth, we invert the deformation obtained from MRI registration to arrive at a field for the growth deformation gradient tensor. Our field inversion uses a combination of direct and adjoint methods for computing gradients of the objective function while constraining the optimization by the physics of morphoelastic growth. We thus infer a growth deformation gradient field that obeys the laws of morphoelastic growth. The errors between the MRI data and the forward displacement solution driven by the inverted growth deformation gradient field are found to be smaller than the reference displacement by well over an order of magnitude, and can be driven even lower. The results thus reproduce the three-dimensional growth during the early development of the fetal brain with controllable error. Our findings confirm that early growth is dominated by in plane cortical expansion rather than thickness increase.

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Title: Calculation of Spin Hamiltonian Parameters Using Real-Space Density Functional Theory

Author(s): *Krishnendu Ghosh, *University of Michigan*; He Ma, *University of Chicago*; Mykyta Onizhuk, *University Of Chicago*; Vikram Gavini, *University of Michigan*; Giulia Galli, *University of Chicago / Argonne National Laboratory*;

Spin-defects have emerged as promising candidates for quantum information technologies like quantum computing and sensing. The efficacy of a spin-defect, also known as a quantum bit (qubit), depends largely on its ability to maintain quantum coherence. The primary physical phenomena responsible for causing decoherence are interactions of a spin qubit with its environment in the form of spin-spin interactions, spin-orbit interactions, and spin-lattice interactions. The interaction strengths are calculated using a model spin Hamiltonian (SH) whose parameters are obtained from the first principles. In this work we present an advance to the state-of-the art approach of calculating SH parameters. Pseudopotential based density functional theory (DFT) calculation of SH parameters relies on the artificial smoothness of electron densities inside the atomic core. But an accurate estimation of SH parameters requires capturing the cusps of the spin density even at the nuclei, thus necessitating either the use of corrective measures, like projected augmented wave (PAW), or carrying out an all-electron calculation with full details of the core electrons. While the former has been the state-of-the-art technique to compute SH parameters, we have recently proposed and benchmarked an all-electron SH parameter calculation methodology [1] based on real-space finite element based DFT [2]. This work shows systematic convergence of the SH parameters with respect to number of basis functions. Spin-spin interaction parameters are calculated in a 2x2x2 supercell (63 atoms) of nitrogen vacancy in diamond (NV-diamond) which is a well known qubit system. Although all-electron calculations provide a path for accurate estimation of SH parameters, the calculations become prohibitively expensive for large systems making it difficult for realistic defect densities. So we further propose a mixed approach [3] where only a few select atoms in a system are treated with all-electron description and the rest of the system is treated with pseudopotentials. We show that a judicious selection of the all-electron atoms in such a mixed approach can recover the same accuracy of a calculation with complete all-electron description. We demonstrate this method in NV-diamond as well as divacancies in 4H-SiC with system sizes going beyond 1000 atoms. [1] K. Ghosh et. al., Phys. Rev. Mat., 2019 [2] P. Motamarri et. al., Comp. Phys. Comm., 2020 [3] K. Ghosh et. al., under review, 2021

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Title: Continuous Artificial Viscosity Shock Capturing for Hybrid Discontinuous Galerkin Methods on Adapted Meshes

Author(s): *Krzysztof Fidkowski, *University of Michigan*;

One technique for capturing shocks with high-order methods is through artificial viscosity. Key considerations of this approach are (1) deciding the amount of artificial viscosity to add; (2) maintaining stability and efficiency of the nonlinear solver; and (3) ensuring the accuracy of the resulting solutions, particularly in the presence of strong shocks. To address (1), we present a method that employs a simple nonlinear switch based on intra-element solution variation. To address point (2), we forego a complete linearization of the artificial viscosity contribution to the residual, in order to keep the Jacobian stencil compact. To address (3), we introduce the viscosity in a piecewise-continuous fashion to avoid spurious entropy production. Furthermore, we use output-based error estimation and mesh optimization to minimize the output error. We test the method on aerodynamic flow applications ranging from transonic to supersonic, discretized using standard discontinuous Galerkin (DG) and hybridized/embedded DG. Out of these discretizations, the embedded DG method exhibits the best combination of high-order accuracy and efficiency in terms of fewer degrees of freedom and lower computational time.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A High-Order Spectral Difference Solver for 2D Ideal MHD Equations with Constrained Transport

Author(s): *Kuangxu Chen, *Clarkson University*; Chunlei Liang, *Clarkson University*;

When using the discontinuous Galerkin or spectral difference method to discretize magnetohydrodynamics (MHD) equations, it is challenging to satisfy the divergence-free constraint for the magnetic field. To tackle this challenge, an unstaggered constrained transport method is integrated with the spectral difference scheme. In addition to solving the two- dimensional ideal MHD equations, one more equation describing the transport of the magnetic potential is introduced. After each step of time marching, the magnetic field will be updated by computing the curl of the magnetic potential. This strategy could effectively control the magnitude of the divergence error. Meanwhile, the additional computational cost is also small, approximately 20% more than the spectral difference solver without constrained transport. Moreover, the inclusion of constrained transport does not obstruct the implementation of the artificial viscosity and resistivity and will not deteriorate the flexibility of the unstructured grids.

16th U.S. National Congress on Computational Mechanics
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Title: Multiphysics Modeling of Melt-Pool Dynamics in Metal Additive Manufacturing: Integration of Thermofluidics, Mechanics and Microstructure Evolution

Author(s): *Kunal Bhagat, *University of Wisconsin–Madison*; Kaila Bertsch, *University of Wisconsin–Madison*; Dan Thoma, *University of Wisconsin–Madison*; Shiva Rudraraju, *University of Wisconsin–Madison*;

In this work, we systematically build a numerical model that captures the spatio-temporal physics relevant to Metal Additive Manufacturing (MAM). The formation of the molten pool, the role of Marangoni and buoyancy forces on the convection currents, the coupling between temperature gradient and fluid velocity, and the melt-pool thermal variations are captured using a high fidelity thermo-fluidic model. The rapid solidification process and the role of the spatial temperature distribution in the building up of residual stresses are investigated by integrating a finite-strain mechanics model with the thermo-fluidic model. Cooling rates, thermal gradients, and laser scanning velocities are important process parameters that influence the microstructure and material properties of the final component. Hence, at the continuum scale, we present the comparison of cooling rates calculated using the thermo-fluidic model and the experimental results for the DED and SLM printed components. Further, we demonstrate the integration between a structural scale thermo-mechano-fluidic model of the melt-pool with the mesoscale phase-field model of dendritic solidification by comprehensively simulating test cases of microstructure evolution relevant to MAM. Time permitting, modeling insights into the role of nucleation, temperature gradients and dendrite tip velocities on the resulting microstructure evolution will be discussed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Spline Based Simulations of Structural Instabilities in Flexible Viscoelastic Composites

Author(s): *Kurtis Ford, *Sandia National Laboratories*; Aaron Bernreuether, *Kansas City National Security Campus*; Chris Whetten, *Coreform*;

Viscoelastic materials are commonly used as a bonding agent in thin composites. Buckling due to viscoelastic relaxation in thin flexible structures has been difficult to study however structural instabilities of a thin coating on an infinite viscoelastic substrate have been reported. Data has shown that densification of a viscoelastic substrate compresses a thin elastic film thereby increasing the chance of film buckling. Similarly, it has been shown mathematically that a time dependent loss in substrate stiffness reduces resistance to buckling in a thin coating under stress. Although the stress state of a thin flexible composite has additional complicating factors, both densification and loss of stiffness can lead to similar kinds of buckling. Despite the prevalence of viscoelastic bonding agents in thin flexible structures, studies are limited. Nonlinear viscoelastic material models that capture densification and fading memory of an epoxy require numerical methods that are not able to efficiently resolve the complex stress state of a thin flexible structure. In this work smooth spline shape functions are used to alleviate shear locking and capture stress fields due to global loading while also including viscoelastic effects that cause localized instabilities. To be presented at USNCCM16 - US National Congress on Computational Mechanics, July 25 - 29, 2021, Chicago, IL. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

16th U.S. National Congress on Computational Mechanics
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Title: The Origins of Plasticity During High-Rate Bending of Graphene

Author(s): *Landon Cordova, *Rutgers University*; Ryan Sills, *Rutgers University*;

While plasticity and fracture of graphene and other 2D materials under in-plane loading is relatively well-established, response to out-of-plane loading is less well understood. Recently, large electronic band gaps have been revealed in graphene processed via high-rate laser-shock forming, exhibiting plasticity in bending as a result of the out-of-plane loading from the laser shock [1]. In 3D solids, such plastic bending results from plastic strain gradients in the through-thickness dimension. However, since 2D materials lack a through-thickness dimension they cannot sustain such gradients, making the origins of this plastic bending unclear. Here we demonstrate through molecular dynamics simulations that plastic bending in graphene results from modulation of ripples at dislocations without motion of the dislocations. Starting with randomly arranged populations of dislocations in graphene sheets with zero average curvature, we determine the residual (plastic) curvature after high-rate forming with a nano-indenter. We demonstrate that the residual curvature increases with the dislocation density and the indenter velocity, indicating a microstructure-sensitive, rate-dependent plastic response. Analyzing the plastically deformed sheets, we demonstrate that plastic bending is sustained by changes in the rippled state of the sheet. The apparent rate-dependence of this process (sensitivity to indenter velocity) is due to the role of inertia in altering the rippled state. This work reveals a fundamentally new modality for plasticity in 2D materials, paving the way for innovations in processing and microstructure design. [1] Motlag et al., Asymmetric 3D Elastic-Plastic Strain-Modulated Electron Energy Structure in Monolayer Graphene by Laser Shocking, Advanced Materials, Vol. 31, 1900597, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A High-Order Fluid Structure Interaction Method: An Extended Approach

Author(s): *Lauritz Beck, *Technical University Darmstadt*; Florian Kummer, *Technical University Darmstadt*;

We present a high-order eXtended discontinuous Galerkin (XDG, also referred to as cut-cell DG or unfitted DG) method to simulate the interaction of multiple fluids with elastic solids. Originally, a XDG method is a discontinuous Galerkin method for multiple fluid phases with a sharp interface representation [1]. There, each interface is immersed in the numerical grid by defining it as the zero level set of a level set function, providing flexibility and high accuracy. In a novel approach, we employ the method's characteristic immersed interface representation to integrate an elastic solid. By utilizing the coupling approach proposed by Matthies and Steindorf [2], we detach our method from the detailed numerical representation of the elastic. It may be represented by a basic mass-spring system or an off-the-shelf structural solver. We will highlight the method's features by investigating a surprisingly complex test case: a water droplet sitting on an elastic solid surface. There, an elastic solid, a liquid and a gaseous phase meet at a three-phase contact line that poses substantial theoretical and practical obstacles. At the three-phase contact line, intricate tensions between the phases exert a singular force on the droplet, necessitating microscopic and macroscopic considerations. Depending on the material, this force deforms the solid, forming a bulge at the three-phase contact line. By focusing on the region of the three-phase contact line, we will detail the analytical foundation of the method. Since complex physical mechanisms are at work, all facets of the method are observable. Additionally, the intersection of multiple implicitly defined geometries in this region provides a substantial challenge for numerical integration, which constitutes the core of a XDG method. Finally, the deformation of the solid acts as a benchmark for the coupling. [1] Kummer, F., 2017. Extended discontinuous Galerkin Methods for two-phase flows: the spatial discretization. Int.J.Numer.Meth.Engng, 109: 259-289. [2] Matthies, H., Steindorf, J., 2003. Partitioned strong coupling algorithms for fluid-structure interaction, Computers & Structures, Volume 81, Issues 8-11, 805 - 812.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Compliant Mechanisms with Variable Loading and Supports Using Gaussian Function Parameterization

Author(s): *Lee Alacoque, *University of Illinois at Urbana-Champaign*; Kai James, *University of Illinois at Urbana-Champaign - https://publish.illinois.edu/designlab/*;

Key Words: Topology Optimization, Design Automation, Compliant Mechanisms, Variable Loading, Adjoint Sensitivity Analysis Topology optimization is typically used to generate optimal layouts of material within a design domain with boundary conditions predetermined by the user. For this work, we present a new method for efficiently designing loads and supports simultaneously with material distribution in density-based topology optimization. Taking inspiration from previous work on topology optimization of multi-body mechanisms [1], we use a super-Gaussian function to parameterize the locations of elastic supports and loads. With a continuous distance function as an input, the super-Gaussian function outputs a smooth, differentiable field of values with a plateau-shaped decay in the directions of increasing distance. Using different types of distance functions, we can model various types of boundary conditions with minimal numbers of additional design variables. As examples, we show that by using single points we can model concentrated loads and small fixed supports, and with one-dimensional lines we can simulate distributed loads and supports. The sensitivities of the objective function with respect to the loading and support locations can then be found by simply taking the derivatives of the Gaussian function and distance functions. These design sensitivities, as well as the ones with respect to element densities, are computed using the adjoint analytical method. Implementing this technique in a 2D topology optimization algorithm using the standard SIMP formulation with linear elasticity, we demonstrate the improvements that the Gaussian parameterization method makes to some common benchmark problems. By allowing the optimizer to move the loads and supports anywhere within the design domain, the method produces significant improvements to problems such as compliant mechanism design, where the location of the input load and fixtures in relation to the edges of the design domain can have a large effect on the magnitude of the output displacements. In the near future, we plan to apply the method to the design of structures with design-dependent concentrated loads and to multi-physics problems where manually choosing the optimal locations of boundary conditions is highly unintuitive. REFERENCES [1] K. Swartz and K.A. James, “Gaussian Layer Connectivity Parameterization: A New Approach to Topology Optimization of Multi-Body Mechanisms”, Computer-Aided Design. Vol. 115, pp. 42-51, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Transmural Distribution of Coronary Perfusion and Myocardial Work: an Insight from Computational Framework

Author(s): *Lei Fan, *Michigan State University*; Ravi Namani, *Michigan State University*; Jenny Choy, *California Medical Innovation Institute*; Ghassan Kassab, *California Medical Innovation Institute*; Lik Chuan Lee, *Michigan State University*;

There is a need for intimate balance between the transmural distribution of myocardial demand and supply to maintain normal cardiac function. A mismatch/imbalance of myocardial demand and supply is central to many heart diseases, e.g., ischemic heart failure [1]. How myocardial demand and supply are altered in heart diseases is difficult to answer from pure experimental or clinical studies. This is because in vivo measurements of myocardial blood flow in the deep layer of the heart wall is extremely challenging, and direct measurements of regional myofiber stress and work in the heart wall are currently not measurable. To resolve this issue, a computational framework coupling a left ventricular (LV) finite element (FE) model with coronary perfusion and systemic circulation is developed. In the model, a functional relationship between LV pressure and volume is obtained by minimizing a Lagrangian function consisting of a myocardial tissue strain energy function and terms associated with the enforcement of constraints on (1) myocardial tissue incompressibility, (2) zero-mean rigid body translation and rotation and (3) cavity volume. Mechanical behavior of the LV is modeled using an active stress formulation, in which the passive and active mechanical behaviors are described by a Fung-type strain energy function and a modified time-varying elastance model, respectively [2]. Four coronary flow networks each consisting of 400 vessels are located at four different transmural locations in the myocardium. Flow in each vessel is described by a nonlinear three-element Windkessel model [3], where the intramyocardial pressure (IMP) is prescribed using the local value of Lagrange multiplier associated with the incompressibility constraint. The model can predict circumferential and longitudinal strains, transmural distribution of IMP and coronary flow that match the experimental data measured in human and large animals under resting condition. The model is then applied to investigate how transmural demand (myocardial work)/supply (coronary perfusion) ratio changes in pathophysiological conditions. The key findings are: (1) Transmural distribution of IMP across the LV wall can explain the transmural distribution of passive coronary flow measured experimentally; (2) Myocardial demand/supply mismatch at the endocardium is exacerbated with an increase in contractility, preload, LV size and wall thickness, suggesting that the endocardium is vulnerable to ischemia in these conditions. References: [1] Algranati, D et al., Am. J. Physiol. - Hear. Circ. Physiol., 300: 1090-1100, 2011. [2] Guccione, J. M. et al., J. Biomech., 28, 1167–1177, 1995. [3] Fan, L. et al., Front. Physiol., 11: 915, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The DPG Method for Convection-Reaction Problems

Author(s): *Leszek Demkowicz, *The University of Texas at Austin*; Nathan Roberts, *Sandia National Laboratories*;

We present a progress report on the development of Discontinuous Petrov-Galerkin methods for the convection-reaction problem in context of time-stepping and space-time discretizations of Boltzmann equations [1]. The work includes a complete analysis for both conforming (DPGc) and non-nonconforming (DPGd) versions of the DPG method employing either globally continuous or discontinuous piece-wise polynomials to discretize the traces. The results include construction of a local Fortin operator for the case of constant convection and a global discrete stability analysis forboth DPGc and DPGd methods. The theoretical findings are illustrated with numerous numerical experiments in two space dimensions. [1] L. Demkowicz, N. Roberts, ``DPG Method for the Convection–Reaction Problem Revisited'', submitted.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Core Shells and Double Bubbles for a Three-Phase Nonlocal Model with Surface Tension

Author(s): Stan Alama, *McMaster University*; *Lia Bronsard, *McMaster University*; Xinyang Lu, *Lakehead University*; Chong Wang, *Trinity University*;

We consider a three-phase model for triblock copolymers in the plane, with unequal surface tension between the stable phases. We consider a blend with two dilute phases, in a “droplet phase” limit, which promotes condensation of the two minority phases into many small well-separated binary components in a sea of the third phase. The morphology of the droplets depends crucially on the weights imposed on the perimeters of the transitions between the phases, which must satisfy a triangle inequality. If this triangle inequality is strict, minimizing configurations prefer double-bubbles; in the degenerate case, centered core shells are energetically favorable.

16th U.S. National Congress on Computational Mechanics
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Title: Fast Characterization of Inducible Regions of Atrial Fibrillation Models with Multi-Fidelity Gaussian Process

Author(s): *Lia Gander, *Università della Svizzera italiana*; Simone Pezzuto, *Università della Svizzera italiana*; Paris Perdikaris, *University of Pennsylvania*; Rolf Krause, *Università della Svizzera italiana*; Francisco Sahli Costabal, *Pontificia Universidad Católica de Chile*;

Computational models of atrial fibrillation have successfully been used to predict optimal ablation sites. A critical step to assess the effect of an ablation pattern is to pace the model from different, potentially random, locations to determine whether arrhythmias can be induced in the atria. In this work, we propose to use multi-fidelity Gaussian process classification to efficiently determine the regions in the atria where arrhythmias are inducible. We will build a probabilistic classifier that operates directly in the atrial surface. To reduce the computational cost, we will use active learning to determine the optimal locations to pace the model and reduce the classification error. We will take advantage of lower resolution models to explore the atrial surface and combine seamlessly with high resolution models to identify region of inducibility. Finally, we will show some preliminary results in a sophisticated volumetric human atrial model with realistic fibrosis distribution and electrophysiology. We hope this new technique will allow faster and more precise clinical applications of computational models for atrial fibrillation.

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Title: Bayesian Calibration of Models for the Self-Assembly of Diblock Copolymers: Likelihood-Free Inference and Expected Information Gain via Measure Transport

Author(s): Richardo Baptista, *Massachusetts Institute of Technology*; *Lianghao Cao, *Oden Institute for Computational Engineering and Sciences*; Joshua Chen, *Oden Institute for Computational Engineering and Sciences*; Omar Ghattas, *Oden Institute for Computational Engineering and Sciences*; Fengyi Li, *Massachusetts Institute of Technology*; Youssef Marzouk, *Massachusetts Institute of Technology*; J. Tinsley Oden, *Oden Institute for Computational Engineering and Sciences*;

We consider the Bayesian calibration of models for the self-assembly of diblock copolymers (Di-BCPs) with observation data obtained via microscopy techniques. We identify two sources of uncertainties: the epistemic uncertainty due to noise in experimental measurements and the aleatory uncertainty that leads to the long-range disorder in equilibrium patterns of the self-assembly. Both uncertainties cause challenges in performing the Bayesian calibration, as they lead to intractable and non-analytical likelihood functions. We tackle these challenges with likelihood-free inference via a measure transport approach. Additionally, we show that the expected information gain based on various forms of noise and corruptions present in the imaging instruments can be computed with no significant additional cost via the proposed approach. Lastly, we present a particular numerical case study based on the Ohta-Kawaski (OK) model and top-down scanning electron microscope images of equilibrium patterns of the self-assembly of Di-BCPs. We demonstrate the power of the proposed approach for solving the OK model calibration problem and understanding the information retained by noisy instrumentation.

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Title: Data-Driven Analysis of Thermal Simulations, Microstructure and Mechanical Properties of Inconel 718 Thin Walls Deposited by Metal Additive Manufacturing

Author(s): *Lichao Fang, *Northwestern University*; Lin Cheng, *Northwestern University*; Jennifer Glerum, *Northwestern University*; Jennifer Bennett, *Northwestern University*; David Dunand, *Northwestern University*; Jian Cao, *Northwestern University*; Gregory Wagner, *Northwestern University*;

The rapid and repeated temperature variation during additive manufacturing of metal parts has a large effect on the resulting material microstructure and properties. The ability to accurately predict detailed temperature field, and quantitatively relate it to structure and properties, is a key step in predicting part performance and optimizing process design. In this work, a finite element model of the Directed Energy Deposition (DED) process is developed to predict the space and time dependent temperature field during the multi-layer build process for Inconel 718 walls. Three cases with different domain sizes and scan strategies are investigated. The thermal model is validated by the dynamic infrared (IR) images captured in-situ during the DED builds. Predicted thermal histories are shown to agree well with experimental measurements. Features of the temperature (cooling rate and solidification rate) at individual locations are then extracted and correlated with measurements of both the microstructure and mechanical properties at those same locations. Our results indicate that the reduced-order descriptions of the complicated thermal history curve can be related to the microstructure and to properties such as ultimate tensile strength (UTS), yield stress and failure stress. To improve the correlation between thermal history and properties even further, a 1D convolutional neural networks (CNN) data-driven framework is applied to automatically extract the dominant features from simulated temperature history. The relationship between the features, which are extracted by CNN, and the mechanical properties is studied. To interpret how CNN performs in intermediate layers, we visualize the extracted features produced on each convolutional layer by a trained CNN. Our results show that the results predicted by the CNN agree well with the experimental measurements. This study demonstrates that a machine learning-based analysis of the entire simulated thermal history of a part can be more effective than traditional simple-to-extract features, such as solidification cooling rate, in predicting mechanical properties of additively manufactured material. REFERENCES [1] DebRoy, Tarasankar, et al. "Additive manufacturing of metallic components–process, structure and properties." Progress in Materials Science 92 (2018): 112-224. [2] Heigel, J. C., P. Michaleris, and Edward William Reutzel. "Thermo-mechanical model development and validation of directed energy deposition additive manufacturing of Ti–6Al–4V." Additive manufacturing 5 (2015): 9-19. [3] Abdeljaber, Osama, et al. "Real-time vibration-based structural damage detection using one-dimensional convolutional neural networks." Journal of Sound and Vibration 388 (2017): 154-170.

16th U.S. National Congress on Computational Mechanics
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Title: A Fully Convolutional Neural Network Framework for Accelerating Representative Volume Element Analysis, Microscale Material Identification, And Defect Characterization

Author(s): *Lin Cheng, *Northwestern University*; Gregory Wagner, *Northwestern University*;

Representative volume element (RVE)-based analysis plays a central role in understanding the response of heterogeneous materials to properties and geometry of the constituents. However, the accuracy of RVE analysis on real-life materials requires extra efforts on the identification of material constituents, calibration of constituent properties, and characterization of imperfections (i.e., voids and cracks) introduced in the fabrication process. For these reasons, together with the multiscale and spatially varying nature of heterogeneities, analysis of heterogeneous materials can be prohibitively costly and time-consuming. In this work, a fully convolutional neural network (FCNN)-based framework called RVE-net is proposed to take advantages of the state-of-art use of FCNNs and feedforward neural networks in image segmentation to accelerate the discovery of effective macroscopic behavior, identify microscale material properties, and automatically characterize defects in materials. In contrast with standard numerical methods (e.g., the finite element method), which depend heavily on domain discretization and local interpolations, the RVE-net takes microstructure images, parameterized by a Heaviside representation coupled with a level-set field, and loading conditions as inputs. The aim is to directly learn the nonlinear interaction between the microstructures and their local responses in a hierarchical manner. This avoids the burdensome discretization and interpolations, makes it possible to transfer the learned structure-response from one microstructure to another microstructure, and thus significantly accelerates the modeling of heterogeneous materials. Several numerical examples are performed to examine the performance of the proposed RVE-net. It has been demonstrated that the RVE-net can leverage the power of graphics processing units in RVE analysis, inverse derivation of material constituents, and characterization of defects under both elastic and inelastic deformation.

16th U.S. National Congress on Computational Mechanics
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Title: Assessing Ideal Geometric Models of Woven Composites Using Image-Based Simulations

Author(s): *Lincoln Collins, *Sandia National Laboratories*; Collin Foster, *University of Illinois at Urbana-Champaign*; Scott Roberts, *Sandia National Laboratories*;

Mesoscale simulations of woven composites using ideal geometries offer a way to connect constituent material properties and arrangement to the effective behavior and performance of the composite. However, the reality of as-manufactured materials often differs from the ideal, both in term of the yarn geometry and manufacturing heterogeneity. As such, as-manufactured properties may different from ideal predictions and may show local variations within a material. We employ mesoscale finite element method simulations to compare ideal and as-manufactured woven composite materials and study the sensitivity of their properties to the mesoscale geometry. Three-dimensional unit cell geometries reconstructed from X-ray computed tomography are compared to ideal composite geometries and as-manufactured materials through calculated effective properties. Image segmentation is performed using deep learning methods and local fiber orientation is obtained using the structural tensor calculated from image scans. Suitable approximations to composite properties, using analytical unit cell calculations or effective media approximations are assessed. The result of this work is an assessment of how idealized geometries can be useful to predict the properties of as-manufactured composites. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: A Multi-Space-Time-Scale Generalized FEM with Transient Local Enrichment and Adaptivity Conditioning Control for Parabolic and Hyperbolic Problems

Author(s): *Lishen He, *University of Illinois at Urbana-Champaign*; Armando Duarte, *University of Illinois at Urbana-Champaign*; Albert Valocchi, *University of Illinois at Urbana-Champaign*;

Multiscale simulation of advection-diffusion problems has been the subject of many studies in recent years. Although methods like MsFEM and MsFVM have worked well for elliptic and some parabolic problems, there are challenges in extending them to general hyperbolic problems (Jenny, 2005). We equip the well-established Generalized FEM (GFEM) with transient local problems to address this challenge. The proposed method allows the discretization to be performed in multiple time and space scales. Each local problem can be solved efficiently in time by selecting its most appropriate time integration method and step size. One- and three-D numerical experiments of (mixed) parabolic and hyperbolic problems are performed to demonstrate that the proposed method 1) resolves multiple space and time scale; 2) is computationally efficient; 3) recovers fine scale fields on coarse global meshes. Certain mixed parabolic-hyperbolic problems pose a challenge to GFEM where enrichment functions may be nearly linear dependent among each other or can be nearly reproduced by the Partition of Unity. The resulting linear system is nearly singular thus impacting the numerical stability of the method. This is aggravated for time-dependent problems (Cui, 2020) where enrichment functions change over time, for example, when simulating the advection of a plume of contaminant. Prior research has only provided a solution to this issue for steady state problems with self-adjoint operators. In this presentation, we propose a general approach based on singular value decomposition. The proposed adaptive enrichment control can be performed efficiently as only diagonal blocks of the system of equations are used in the approach. The importance of proposed adaptive approach is that the well-known issue for near singularity in GFEM can be addressed for a broad class of enrichments, including those computed numerically. Bibliography Cui, C. a. (2020). Stable generalized finite element methods for elasticity crack problems. International Journal for Numerical Methods in Engineering, 3066-3082. Jenny, P. L. (2005). Adaptive multiscale finite-volume method for multiphase flow and transport in porous media. Multiscale Modeling & Simulation, 50-64.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Numerical Simulation of Cardiac Electromechanics: Multiscale Modeling and Coupling with Closed-Loop Blood Circulation

Author(s): *Luca Dede', *Politecnico di Milano*; Francesco Regazzoni, *Politecnico di Milano*; Matteo Salvador, *Politecnico di Milano*; Alfio Quarteroni, *Politecnico di Milano*;

We consider the numerical simulation of cardiac electromechanics with application to the left ventricle of the human heart [1]. We couple state–of–the art models for the electrophysiology of the tissue, mechanical activation at the cellular level, and the passive mechanical response of the muscle, thus yielding a coupled electromechanical problem within the active stress paradigm. Our multiscale model for cardiac electromechanics accounts for miscroscopic active force generation at the cellular level by exploiting model order reduction techniques based on Machine Learning algorithms [2]. In addition, our 3D electromechanical model for the left ventricle is coupled with a 0D, closed-loop model of the systemic and pulmonary blood circulations, other than of the remaining cardiac chambers [3]. We consider the spatial approximation of the Partial Differential Equations therein involved by means of the Finite Element method and the time discretization by using Backward Differentiation Formulas. We numerically solve the coupled electromechanics problem by exploiting intergrid transfer operators, as well as staggered approaches for realizing the numerical coupling. We present and discuss several numerical results of the cardiac electromechanics problem in the human left ventricle obtained in the high performance computing framework. This project has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme: grant agreement No 740132, iHEART –"An integrated Heart Model tor the Simulation of the Cardiac Function", 2017–2022. REFERENCES [1] Quarteroni A. Dede’ L., Manzoni A. and Vergara C. Mathematical Modelling of the Human Cardiovascular System. Cambridge University Press (2019). [2] Regazzoni F., Dede’ L. and Quarteroni A. Machine learning of multiscale active force generation models for the efficient simulation of cardiac electromechanics. Comput. Meth. Appl. Mech. Eng. (2020) 370:113268. [3] Regazzoni F., Salvador M., Africa P.C., Fedele M., Dede’ L. and Quarteroni A. A cardiac electromechanics model coupled with a lumped parameters model for closed-loop blood circulation. Part I: model derivation. arXiv (2020) 2011.15040.

16th U.S. National Congress on Computational Mechanics
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Title: A Fictitious Domain Formulation for FSI: Finite Element Approximation

Author(s): *Lucia Gastaldi, *University of Brescia*;

In this talk we present some results on the finite element approximation for a fictitious formulation of fluid-structure interaction. Our formulation originated from the Immersed Boundary Method and then moved toward Fictitious Domain approach. The finite element discretization of this formulation leads to an unfitted schemes. Our formulation for FSI offers an alternative to body-fitted approaches avoiding the difficulties related with mesh generation. Moreover, it allows the treatment of fluid and solid in their natural Eulerian and Lagrangian framework. We shall discuss the choice of the finite element spaces to be used in order to have a stable and convergent scheme.

16th U.S. National Congress on Computational Mechanics
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Title: Numerical Simulation of Incompressible Viscoelastic Flows and Elastic Deformations with Free Surfaces

Author(s): *Léo Diserens, *Ecole Polytechnique Fédérale de Lausanne / University of Applied Sciences Western Switzerland*; Alexandre Caboussat, *University of Applied Sciences Western Switzerland*; Marco Picasso, *Ecole Polytechnique Fédérale de Lausanne*;

We present a unified mathematical model and numerical framework for the modelling of both incompressible Oldroyd-B viscoelastic flows and Neo-Hookean elastic solid deformations in Eulerian coordinates with free surfaces. The model is based on a Volume Of Fluid (VOF) method and an extended form of the original Oldroyd-B constitutive extra-stress equation, in order to incorporate the description of an elastic solid constraint tensor. A time splitting strategy is applied in order to decouple the advection operators from the diffusive operators of the system of equations. The space discretization consists of a two-grid method mixing an unstructured finite element mesh, and a finer structured grid. A prediction step allows to solve the advection operators with a characteristics method on the structured grid, while the correction step allows to solve the diffusion operators using low order finite elements. Stability and convergence results of the numerical method are presented. We validate the model with several numerical experiments, including simulations of industrial processes, such as machining processes and traction experiments, in order to study stress-strain curves and failure experiments.

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Title: Recent Advances in Modeling Interfaces and Viscoelastic Flow Properties with Particles in Geodynamic Computations

Author(s): Elbridge Gerry Puckett, *University of California, Davis*; *Mack Gregory, *University of California, Davis*;

Combining finite element methods with particle-in-cell (PIC) methods is an important technique in computational geodynamics that has been widely used to model mantle convection, lithosphere dynamics, crustal-scale modeling, and other geodynamic processes. In these applications particles are used to advect properties of the medium such as the location of material boundaries, density, components of stress, chemical composition, and so on. Particle methods reduce the advection equation for each material property to an ordinary differential equation (ODE) for each particle, resulting in a problem that is simpler to solve than the original equation for which stabilization techniques are necessary to avoid oscillations. Since all of the material properties mentioned above may be advected on each individual particle simultaneously this reduces the solution of one advection equation per property to the solution of one system of ODEs for the particles. We have shown that this methodology has excellent weak and strong scaling over at least three orders of magnitude of model size on a uniform grid. For the adaptive grid case our methodology shows strong scaling that is nearly as good as for the uniform grid case, decreasing the total runtime essentially linearly from 96 to 3,072 cores. Thus, using particles to advect material properties is also very efficient. On the other hand, replacing field-based descriptions by quantities only defined at the locations of particles introduces numerical errors associated with the interpolation of the particle properties onto the finite element grid. These errors have previously been investigated, but a complete understanding from the practical point of view has been lacking. In particular, we are not aware of systematic guidance regarding how many particles one must choose per mesh cell to achieve a certain accuracy. We will describe several high-order accurate algorithms for interpolating the particle properties onto the mesh and, in some cases, back onto the particles. We demonstrate the accuracy of these methods with several benchmarks we have developed to assess the accuracy of our methodology. We also describe an algorithm for limiting the values of the properties in the interpolation step in order to eliminate overshoot and undershoot. Our presentation will include example computations of two or more materials with disparate properties evolving in a viscoelastic medium in which both the material interfaces and the viscoelastic rheology are modeled by properties carried on the particles and interpolated onto the underlying finite element grid at each time step.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Simulation of Microstructure Development in Additively Manufactured Nickel Superalloys through CA-FE Modelling Methods

Author(s): *Madie Allen, *NSIRC Ltd.*; Tyler London, *TWI Ltd.*; James Campbell, *Brunel University*;

James Campbell, Brunel University, james.campbell@brunel.ac.uk Additive manufacturing (AM) is becoming an increasingly popular method of production, due to the wide range of benefits it has to offer. However, its adoption in industry is limited by the reliability and repeatability of the process. This is largely due to the unique thermal profile experienced by additively manufactured material, which results in significantly different microstructures, and consequently material properties, when compared to traditionally manufactured parts. This work looks to address the reliability of metal AM by increasing understanding surrounding the relationship between process parameters and resultant microstructure, through the efficient use of numerical modelling. A weakly coupled cellular automata – finite element method has been employed to simulate crystal growth within the solidification of the melt pool. This is done by assigning a crystal growth envelope as presented by Gandin and Rappaz1. Within this presentation a number of case studies are presented showing the application of the modelling approach to nickel superalloys processed by both powder bed fusion (PBF) and direct energy deposition (DED) methods. The first case study focuses on the use of open source experimental data, made available as part of the NIST AM Benchmark 2018, to validate the microstructure model's capabilities. This is followed by a direct energy deposition case study, using extensively monitored thermal profiles to calibrate finite element thermal models as the input to the cellular automata models. Moreover, EBSD maps of the resultant microstructure of the samples have been obtained for comparison against simulated microstructures. The aim of this particular study is to investigate the capability of the microstructure model to simulate changes in microstructure as a result of a variation in process parameters in DED processes. Finally, the CA methods shown are utilised to demonstrate microstructural transitions as a result of an in-situ change of process parameters within a PBF build. References 1Gandin, Ch.-A. and Rappaz, M., 1997: 'A 3D Cellular Automaton Algorithm for the Prediction of Dendritic Grain Growth', Acta mater., Vol. 45, No.5, pp. 2187-2195

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Fast Multi-GPU Diffeomorphic Image Registration for Large-Scale Applications

Author(s): *Malte Brunn, *University of Stuttgart*; Naveen Himthani, *The University of Texas at Austin*; George Biros, *The University of Texas at Austin*; Miriam Mehl, *University of Stuttgart*; Andreas Mang, *University of Houston*;

3D image registration is a fundamental and computationally expensive operation in biomedical image analysis. We present an effective Gauss-Newton-Krylov solver for large deformation diffeomorphic registration of two images. Our work [1] extends the publicly available CLAIRE library [2, 3] to a multi-node multi-graphics processing units (GPUs) environment. We introduce several novel algorithmic modifications that significantly improve computational performance on the target architecture and allow us to tackle large-scale applications in biomedical imaging. Only few implementations of large deformation diffeomorphic registration packages are optimized for GPUs. Our contributions are the following: (i) efficient schemes for preconditioning the reduced-space Hessian system to further accelerate each Newton iteration using an approximate multi-level inverse Hessian; (ii) highly-optimized multi-node multi-GPU implementation exploiting direct device communication (i.e., CUDA-aware Message Passing Interface) for the main computational kernels - interpolation, high-order finite difference operators and Fast-Fourier-Transform; (iii) algorithmic options to adapt for available hardware resources to optimize utilization and runtime; and (iv) comparison with state-of-the-art CPU and GPU implementations an previous implementations of CLAIRE. We demonstrate the efficiency and scalability of our implementation on multiple NVIDIA Tesla V100 GPUs for a variety of test-cases, including high-resolution real-world biomedical imaging data for neuroimaging datasets of humans and CLARITY imaging datasets for murine neuroimaging. Most notably, we demonstrate that we can solve clinically relevant problem sizes (50M unknowns) in less than 5s on a single NVIDIA Tesla V100 and less than 3.5s on modern consumer grade hardware, with a peak performance speedup of 2x compared to the state-of-the-art [3]. We show scalability results for images with resolutions up to 2048^3 (25B unknowns; ~152x larger than the single GPU implementation) on 64 nodes with 256 GPUs on TACC's Longhorn system. [1] M. Brunn et al. "Multi-node multi-gpu diffeomorphic image registration for large-scale imaging problems", Conference on Supercomputing 2020. [2] A. Mang and G. Biros, "Constrained large deformation diffeomorphic image registration (CLAIRE)", 2019, https://andreasmang.github.io/claire [3] M. Brunn et al., "Fast GPU 3D diffeomorphic image registration", Journal of Parallel and Distributed Computing 149 (2021): 149-162.

16th U.S. National Congress on Computational Mechanics
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Title: Gaussian Process Regression Constrained by Boundary Value Problems

Author(s): *Mamikon Gulian, *Sandia National Laboratories*; Ari Frankel, *Sandia National Laboratories*; Laura Swiler, *Sandia National Laboratories*;

We develop a framework for Gaussian processes regression constrained by boundary value problems. The framework may be applied to infer the solution of a well-posed boundary value problem with a known second-order differential operator and boundary conditions, but for which only scattered observations of the source term are available. Scattered observations of the solution may also be used in the regression. The framework combines co-kriging with the linear transformation of a Gaussian process together with the use of kernels given by spectral expansions in eigenfunctions of the boundary value problem. Thus, it benefits from a reduced-rank property of covariance matrices. We demonstrate that the resulting framework yields more accurate and stable solution inference as compared to physics-informed Gaussian process regression without boundary condition constraints.

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Title: Solution of Ordinary Differential Equations Using Hypercomplex Numbers with Applications to Fracture Mechanics

Author(s): Mauricio Aristizabal, *Universidad EAFIT*; *Manuel Garcia, *Angelo State University*; Harry Millwater, *The University of Texas at San Antonio*;

The use of hypercomplex numbers have increased in the realm of computation of high-order derivatives since they provide highly-accurate arbitrary-order derivatives with low complexity of implementation. The method consists of perturbing the variables of interest in specific imaginary directions. Then, by using hypercomplex operations, the result contains the derivatives of the evaluated function with respect to the chosen variables, stored in the result's imaginary directions. Specific applications to fracture mechanics have been addressed recently. In this work, we present a novel method to solve first order Ordinary Differential Equations (ODEs) using hypercomplex algebras, i.e. solving y(t) given an equation of the form dy/dt = f(y(t),t). The method consists of using a hypercomplex algebra to compute the derivatives of the differential form (dy/dt) with respect to time at a given t and y. A Taylor series expansion of the value of dy/dt with respect to t is formed. Then, the same high order derivatives are used to calculate a feasible time step, such that a new evaluation time can be addressed. Two approaches are discussed, one consisting of computing partial derivatives of f(y,t) with respect to y and t and another one consisting of computing derivatives with respect to t, iteratively (both approaches use hypercomplex algebras). We apply this method to fracture mechanics problems. Some of the highlights of the method include: use of arbitrary order of derivatives on demand, highly accurate integration, no weights needed, lower computational cost than other methods such as Runge-Kutta pairs, and automatic step-size estimation.

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Title: Explicit VMDG: Synchronous and Concurrent Parallel Solution in Multi-Domain Problems

Author(s): *Marcelino Anguiano, *University of Illinois at Urbana-Champaign*; Paul Kuberry, *Sandia National Laboratories*; Pavel Bochev, *Sandia National Laboratories*; Arif Masud, *University of Illinois at Urbana-Champaign*;

One step towards faster design-to-analysis workflows is the ability to “tie” together subdomains with non-matching discretizations for analysis of the entire system. To this end, we consider the Variational Multiscale Discontinuous Galerkin (VMDG) method, which is a robust finite element approach for interface coupling where interface transmission conditions are consistently derived, and that accommodates non-matching discretizations of the subdomains at either side of an interface. In this talk, we present an explicit VMDG method for synchronous and concurrent parallel computations in transient multi-domain problems. In the context of linear elasto-dynamics, we show the derivation of the VMDG interface terms, in which the fine-scale modeling concept leads to variationally consistent coupling terms at the common interfaces. Then, the use of an explicit time integration algorithm decouples the solution of each subdomain, yielding a synchronous and concurrent parallel solution algorithm. We present numerical results showing optimal error convergence rates, energy conservation properties, and robustness under mismatches at the interface.

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Title: Flow of a Capsule Suspended in a Newtonian Liquid through a Constricted Capillary

Author(s): Jose Roca, *Pontificia Universidade Catolica do Rio de Janeiro*; Ivan Menezes, *Pontificia Universidade Catolica do Rio de Janeiro*; *Marcio Carvalho, *Pontificia Universidade Catolica do Rio de Janeiro*;

The flow of capsules suspended in a liquid phase through small channels and capillaries poses a complex problem presented in different applications, from red blood cells on hemodynamics to flow through porous media. In porous media applications, the understanding of micro-scale dynamics is fundamental to assess the macroscopic flow behavior of microcapsule suspension. Constricted channels and capillaries can be used to model a pore-throat connecting two adjacent pore-bodies. The flow of a suspended capsule through such models was analyzed to evaluate the flow characteristics, including the maximum pressure difference required to push a capsule through the constriction as a function of capsule radius, initial membrane tension, membrane material, channel and capillary geometries, as well as flow conditions. Inner and outer liquid phases were described by the Navier-Stokes equations and capsule membrane dynamics was modeled by a 1-D spring-like flexible structure. The fluid-structure interaction problem was solved using the finite element method coupled with the immersed boundary method. Results showed the mobility reduction of the continuous phase due to the presence of a capsule as it flows through the constriction. Such results can be used to design microcapsules to block preferential water flow paths in oil displacement process in porous media.

16th U.S. National Congress on Computational Mechanics
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Title: Static Solution of Crack Propagation Problems by Coupled Three-Dimensional Peridynamics and High-Order One-Dimensional Finite Elements

Author(s): Alfonso Pagani, *Politecnico di Torino*; *Marco Enea, *Politenico di Torino*; Erasmo Carrera, *Politecnico di Torino*;

A technique to couple —in a global/local sense– three-dimensional peridynamics with one-dimensional high-order finite elements based on classical elasticity is proposed in this work. The refined finite elements employed are based on the well-established Carrera Unified Formulation, which the previous literature has shown to provide structural formulations with unprecedented accuracy and optimized computational efficiency [1]. The coupling is realized by using Lagrange multipliers that guarantee versatility and physical consistency [2]. The proposed methodology is, hence, utilized for the static solution of crack propagation problems by sequentially linear analyses and is demonstrated to be an efficient way to find both the failure load of a structure and the shape of the crack pattern. References: [1] Carrera, E., Cinefra, M., Petrolo, M. & Zappino, E., Finite Element Analysis of Structures through Unified Formulation. John Wiley & Sons Ltd (2014). ISBN 978-1-119-94121-7. [2] Pagani, A. & Carrera, E., Coupling three-dimensional peridynamics and high-order one-dimensional finite elements based on local elasticity for the linear static analysis of solid beams and thin-walled reinforced structures. Int. J. Numer. Methods Eng. 5066–5081 (2020). doi:10.1002/nme.6510.

16th U.S. National Congress on Computational Mechanics
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Title: Comparative Study of Constitutive Models for EPS Foam Under Combined Compression and Shear Loading

Author(s): *Marcus Arnesen, *KTH Royal Institute of Technology / Mips AB*; Artem Kulachenko, *KTH Royal Institute of Technology*; Peter Halldin, *KTH Royal Institute of Technology / Mips AB*; Jonathan Bergström, *Mips AB*;

Finite Element Analysis (FEA) is widely used to explore/understand the behavior of Expanded Polystyrene (EPS) in energy absorbing applications such as packaging, sandwich cores, and protective gear. However, simulation accuracy is highly dependent on a reliable estimation of the material properties and appropriate constitutive relations. The non-linear mechanical behavior of EPS under pure compression has been well characterized and modelled as crushable foam in commercial FEA software. Recently, this modelling approach was experimentally shown to be inaccurate for representing EPS behavior under combined compression and shear – a loading mode which typically occurs in helmets during collisions. The aim of this study is to investigate to what extent the constitutive models available in commercial FEA software can adequately capture EPS behavior in combined compression and shear loading states. FEA simulations are compared against experimental data available in the literature and complementary in-house experiments. Results show that the existing models in LS-DYNA can capture the compression part, strain rate dependency and unloading compared to the experimental tests, but the description of shear deformations can potentially be improved through new material model designs.

16th U.S. National Congress on Computational Mechanics
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Title: Novel Space-Time Finite Element Simulation Methods in Material Processes

Author(s): *Marek Behr, *RWTH Aachen University*;

Moving-boundary flow simulations are an important design and analysis tool in many areas, including civil and biomedical engineering, as well as production engineering. Interface-capturing offers flexibility for complex free-surface motion, while interface-tracking is very attractive due to its mass conservation properties at low resolution. We focus on these alternatives in the context of flow simulations based on stabilized finite element discretizations of Navier-Stokes equations, including space-time formulations that allow extra flexibility concerning grid design at the interface. Space-time approaches offer some not-yet-fully-exploited advantages; among them, the potential to allow some degree of unstructured space-time meshing. A method for generating simplex space-time meshes has been developed, allowing arbitrary temporal refinement in selected portions of space-time slabs. The method increases the flexibility of space-time discretizations, even in the absence of dedicated space-time mesh generation tools. The resulting tetrahedral and pentatope meshes are being used in the context of cavity filling flow simulations, such as those necessary to design injection molding processes.

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Title: System Inference for the Spatio-Temporal Evolution of Infectious Diseases: COVID-19 in Michigan and in Mexico

Author(s): *Mariana Carrasco-Teja, *University of Michigan*; Zhenlin Wang, *University of Michigan*; Gregory Teichert, *University of Michigan*; Krishna Garikipati, *University of Michigan*;

We extend the classical SIR model of infectious disease spread to account for time dependence in the parameters, which also include diffusivities. The temporal dependence accounts for the changing characteristics of testing, quarantine and treatment protocols, while diffusivity incorporates a mobile population. This model has been applied to data on the evolution of the COVID-19 pandemic in Mexico, and in the US state of Michigan. For system inference, we use recent advances; specifically our framework for Variational System Identification (Wang et al.,Comp. Meth. App. Mech. Eng., 356, 44-74, 2019; arXiv:2001.04816 [cs.CE]) as well as Bayesian machine learning methods.

16th U.S. National Congress on Computational Mechanics
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Title: A Data-Enhanced, Multifidelity, Feasible, Robust, and Versatile Modeling Method

Author(s): *Marie-Jo Azzi, *Stanford University*; Charbel Farhat, *Stanford University*;

The recently proposed Nonparametric Probabilistic Method (NPM) is a multi-faceted, data-enhanced, computational modeling method. Originally developed for modeling and quantifying model-form uncertainties, it is equally suitable for updating a computational model so that it matches target values obtained from data. This data can be experimental and/or higher-fidelity numerical. Hence, NPM is also a multi-fidelity modeling approach. It is grounded in projection-based model order reduction, which makes it also data-driven and computationally tractable. Essentially, NPM is a physics-based, machine learning method for extracting from data fundamental information and/or knowledge that are not captured by a deterministic computational model and infusing them into a counterpart stochastic model. Starting from a conventional, deterministic, high-dimensional model, NPM constructs in three steps a counterpart stochastic, projection-based, reduced-order model (SPROM). First, it builds a deterministic PROM and hyperreduces it using the Energy-Conserving mesh Sampling and Weighting method. Next, it substitutes the deterministic Reduced-Order Basis (ROB) underlying the PROM with a stochastic counterpart (SROB) that it constructs on a subset of a compact Stiefel manifold using a small number of hyperparameters. Finally, it identifies these hyperparameters by: formulating a statistical inverse problem grounded in the construction of an SROB such that the mean value and statistical fluctuations of some quantities of interest predicted using the resulting SPROM match target values obtained from data; and solving the corresponding optimization problem. While the potential of NPM for quantifying model-form uncertainties has been successfully demonstrated for a number of realistic applications including the vibration analysis of a real, small-scale replica of an X-56 type aircraft for which experimental data is available, it remains a computationally intensive method for two reasons: the optimization problem underlying the identification of its hyperparameters is both non-convex and stochastic; and so far, this optimization problem has been solved using gradient-based optimization methods where the sensitivities of the objective function with respect to the hyperparameters are computed by finite differencing. In this talk however, an analytical approach is presented for exactly computing these aforementioned semi-discrete sensitivities. This approach tracks the complex web of operations underlying the construction of the stochastic objective function, including those associated with stochastic model reduction and hyperreduction. Most importantly, it is shown that this analytical approach dramatically improves the robustness and wall-clock performance of NPM and enables its application to realistic problems in structural dynamics pertaining to uncertainty quantification, model updating, and the design of digital twins.

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Title: Adjoint Computations of Relaxation Runge-Kutta Methods

Author(s): *Mario Bencomo, *Rice University*; Jesse Chan, *Rice University*;

Relaxation Runge-Kutta (RK) methods reproduce a fully discrete dissipation/conservation of entropy for entropy stable semi-discretizations for nonlinear conservation laws. In this talk, we derive the discrete adjoint for relaxation RK schemes, which are applicable to discretize-then-optimize approaches to optimal control problems. Furthermore, we prove that the derived relaxation RK adjoint preserves time-symmetry when applied to linear skew-symmetric systems of ODEs. Numerical experiments verify these theoretical results while demonstrating the importance of appropriately treating the relaxation parameter when computing the discrete adjoint.

16th U.S. National Congress on Computational Mechanics
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Title: Bayesian Optimal Sensor Placement for Damage Detection under Steady-State Dynamics

Author(s): *Mark Chen, *Duke University*; Kavinayan Sivakumar, *Duke University*; Gregory Banyay, *Westinghouse Electric*; Timothy Walsh, *Sandia National Laboratories*; Michael Zavlanos, *Duke University*; Wilkins Aquino, *Duke University*;

Identification and monitoring of structural damage have growing importance in the maintenance of aging structures. We propose a robust active sensing framework through the integration of model-based inference and optimal sensing. Our approach is to address the monitoring problem from a holistic view in which inference from data and data acquisition are tightly integrated. We will present preliminary damage identification capabilities coupled with optimal sensor placement. We adopt a partial differential equation (PDE)-constrained formulation for damage detection, thus allowing for a large-scale implementation. The optimal sensor placement problem is then cast within a decision-centric, utility maximization framework. We use mutual information (or relative entropy) as our utility criteria, and thus find sensors that maximize information about damage parameters. We demonstrate the performance of our implementations through three numerical examples of increasing complexity. Our damage detection capability is shown to identify damage parameters with error commensurate with the level of measurement noise. Additionally, we quantify the performance of sensor placements using a mean-squared error (MSE) metric, and we show that optimally-selected sensors outperform randomly selected sensors, in general. We also provide a potential heuristic in selecting a sensor budget through the consideration of utility. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

16th U.S. National Congress on Computational Mechanics
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Title: Mechanics of Architected 2D Materials

Author(s): *Markus Buehler, *Massachusetts Institute of Technology*;

We review progress in using a combination of atomistic modeling and machine learning to predict the mechanics of 2D materials, assembled into hierarchical structures. We review elastic and fracture behavior, and the elucidation of bio-inspired mechanism for materials design. Complementing the numerical work, we validate the predicted material behaviors by 3D printing, and elucidate fundamental design principles. Specific questions explored include the mechanics of grain boundaries, and the assessment of 3D gyroid-like graphene structures optimized for mechanical and thermal performance.

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Learning of Nonlocal Models: From High-Fidelity Simulations to Constitutive Laws

Author(s): *Marta D'Elia, *Sandia National Laboratories*; Huaiqian You, *Lehigh University*; Yue Yu, *Lehigh University*; Stewart Silling, *Sandia National Laboratories*;

In this talk we show that machine learning can improve the accuracy of simulations of stress waves in one-dimensional composite materials. We propose a data-driven technique to learn nonlocal constitutive laws for stress wave propagation models. The method is an optimization-based technique in which the nonlocal kernel function is approximated via Bernstein polynomials. The kernel, including both its functional form and parameters, is derived so that when used in a nonlocal solver, it generates solutions that closely match high-fidelity data. We apply this technique to wave propagation within a heterogeneous bar with a periodic microstructure. Several one-dimensional numerical tests illustrate the accuracy of our algorithm. The optimal kernel is demonstrated to reproduce high-fidelity data for a composite material in applications that are substantially different from the problems used as training data.

16th U.S. National Congress on Computational Mechanics
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Title: Time Integration Advances and Challenges in the Material Point Method.

Author(s): *Martin Berzins, *University of Utah*;

The material point method has been tremendously successful in solving a great many challenging problems in science and engineering. One of the challenges with the method is achieving high accuracy in time integration. Experiments with different methods with both low and high accuracy are presented and are complemented by theoretical results. The results show that the individual errors that arise for instance when moving from particles to mesh nodes and back again have a noticeable impact on the global time accuracy that is attained. Different strategies to address this problem are presented including using very high order methods in space and different time integration methods as well as experiments with a novel MPM variant that is substantially different from present methods. The experimental results shown are explained in the light of current theoretical results relating to both energy conserving integration methods and Runge-Kutta Methods in general.

16th U.S. National Congress on Computational Mechanics
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Title: Computational Modeling of Fluid-Porohyperelastic Structure Interaction

Author(s): *Martina Bukac, *University of Notre Dame*; Anyastassia Seboldt, *University of Notre Dame*;

We consider a moving domain, fluid-porohyperelastic structure interaction problem in a dual-mixed formulation. The fluid is described using the Navier Stokes equations and the porohyperelastic structure is described using the Biot equations. To solve this problem numerically, we propose two novel, partitioned, loosely-coupled methods based on the generalized Robin boundary conditions. In the first partitioned method, the Navier-Stokes problem is solved separately from the Biot problem. In the second proposed method, the problem is further split by separating the Biot problem into a mechanics sub-problem and a Darcy sub-problem. The performance of both methods, as well as the applications to problems in hemodynamics, is investigated in numerical examples.

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Title: Phase Field Models of the Growth of Tumors Embedded in an Evolving Vascular Network: Dynamic 1D-3D Models of Angiogenesis

Author(s): Prashant K. Jha, *The University of Texas at Austin*; *Marvin Fritz, *Technical University of Munich*; Tobias Koppl, *Technical University of Munich*; J. Tinsley Oden, *The University of Texas at Austin*; Andreas Wagner, *Technical University of Munich*; Barbara Wohlmuth, *Technical University of Munich*;

In this talk, we present a coupled 3D-1D model of tumor growth within a dynamically changing vascular network to facilitate realistic simulations of angiogenesis. Additionally, the model includes ECM erosion, interstitial flow, and coupled flow in vessels and tissue. We employ continuum mixture theory with stochastic Cahn–Hilliard type phase-field models of tumor growth. The interstitial flow is governed by a mesoscale version of Darcy's law. The flow in the blood vessels is controlled by Poiseuille flow, and Starling's law is applied to model the mass transfer in and out of blood vessels. The evolution of the network of blood vessels is orchestrated by the concentration of the tumor angiogenesis factor (TAF) by growing towards increasing TAF concentration. The process is not deterministic, allowing random growth of blood vessels and, therefore, due to the coupling of nutrients in tissue and vessels, stochastic tumor growth. We demonstrate the performance of the model by applying it to a variety of scenarios. Numerical experiments illustrate the flexibility of the model and its ability to generate satellite tumors. Simulations of the effects of angiogenesis on tumor growth are presented as well as sample-independent features of cancer. This is joint work with Dr. J. T. Oden at the University of Texas at Austin, M. Fritz, Dr. T. Köppl, A. Wagner, and Dr. B. Wohlmuth at the Technical University of Munich. The work of PKJ and JTO was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Mathematical Multifaceted Integrated Capability Centers (MMICCS), under Award Number DE-SC0019303.

16th U.S. National Congress on Computational Mechanics
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Title: An Immersed Isogeometrics-Peridynamics Approach for Fluid-Structure Interaction Modeling

Author(s): *Masoud Behzadinasab, *Brown University*; Georgios Moutsanidis, *Stony Brook University*; Nathaniel Trask, *Sandia National Laboratories*; Yuri Bazilevs, *Brown University*;

Analysis of Fluid-Structure Interaction (FSI) is an inseparable part of many engineering systems. FSI problems are complicated as they involve interaction of a deformable structure with an internal or surrounding fluid flow. Air-Blast-Structure Interaction (ABSI) problems are extreme events involving additional complexity as the structure undergoes severe damage and fragmentation due to explosion. Immersed methods have been used in FSI analysis, where the fluid is represented on an Eulerian domain and the structure is modeled using a Lagrangian frame. The monolithic approach is attractive in the simulation of FSI problems for capturing the interaction between fluid and solid without the need to explicitly track the fluid-solid interface. Isogeometric analysis (IGA) is a computational technique that combines exact representation of complex geometry and smooth approximation of the solutions. Peridynamics (PD) is a continuum mechanics theory well suited for modeling material failure and fragmentation, and without the need for explicitly tracking crack interfaces. We present a novel framework for FSI analysis based on an immersed, monolithic approach coupling of IGA and PD. Numerical examples are provided to showcase the model applicability to ABSI problems. A discussion on numerical challenges for performing the noted simulations is given.

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Title: An Efficient Preconditioner for a Monolithic High-Order Fluid-Structure Interaction Solver

Author(s): *Matteo Franciolini, *NASA Ames Research Center*; Anirban Garai, *NASA Ames Research Center*; Scott Murman, *NASA Ames Research Center*;

As there are many engineering problems involving the coupling of multiple physics, there is a growing interest in developing solution strategies that account for multiphysics effects, leveraging the variety of methods and tools available to accurately solve single physics discretizations. To this end, monolithic approaches are consistent, stable, and high-order accurate, at the expense of a higher software development effort. Previous research efforts at NASA focused on the development of a high-order monolithic implicit multiphysics solver [1] which supports the use of discontinuous-, continuous-, and C1-discontinuous-Galerkin numerical methods in a space-time manner, along with adjoint and tangent solver capability, and can be applied to the parachute-capsule fluid structure interaction problem. However, challenges arise when solving these nonlinear problems in massively parallel platforms, as the memory requirements and time-to-solution are typically too high with the use of standard preconditioning methods. The objective of the current work is to introduce a preconditioning suite that allows for the efficient solution of linear systems arising from the space-time monolithic implicit discretization of multiphysics problems up to 16th-order of accuracy both in space and time. The solver relies on a matrix-free implementation of the linearization operator to avoid the computation and storage of the Jacobian matrix. Since standard preconditioning strategies still require the use of parts of the iteration matrix, it is mandatory to develop memory lean operators to maintain the limited memory footprint of the matrix-free implementation. At the same time, those operators need to be effective to precondition the system and lead to satisfactory convergence rates for the solver. The talk will report on recent advances related to preconditioning each physics module. First, we will report on results of a matrix-free tensor-product multigrid algorithm [2] for the discontinuous-Galerkin solution of the Navier--Stokes equation. Second, we will describe an efficient entity-by-entity factorization algorithm to precondition the structural solver used for the continuous-Galerkin discretization of the elasticity equations. Third, we discuss the extension of this algorithm to the C1-discontinuous-Galerkin discretization of the linear shell equations used for the parachute-fabric simulation, and its use within a multigrid cycle. The talk will finally assess the performance of those strategies for the simulation of the fully coupled fluid structure interaction of the parachute-capsule system. [1] Carton de Wiart et al. "Design of a modular monolithic implicit solver for multi-physics applications". AIAA Paper 2018-1400. [2] Franciolini et al. "Multigrid preconditioning for a space-time spectral-element discontinuous-Galerkin solver". AIAA Paper 2020-1314

16th U.S. National Congress on Computational Mechanics
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Title: On Coupling Hydrologic and Surge Processes in Coatal Watersheds

Author(s): *Matthew Bilskie, *University of Georgia*; Haihong Zhao, *Arcadis International*; Don Resio, *University of North Florida*; John Atkinson, *Arcadis International*; Zachary Cobell, *The Water Institute of the Gulf*; Scott Hagen, *Louisiana State University*;

Traditional coastal flood hazard and risk studies only consider coastally-driven flooding mechanisms and do not consider rainfall-runoff. Recent hurricane events (e.g., Florence & Harvey) have highlighted the need to consider rainfall and direct runoff when computing total water levels within coastal watersheds (i.e., compound flooding). To begin to address this (modeling) challenge, we developed a rain-on-mesh module within the ADCIRC model framework to route spatially and temporally variable rainfall excess across wet and dry regions. A series of simulations were conducted that include plausible realizations of antecedent (pre-hurricane) rainfall followed by a hurricane passage. These modeling methods were applied to two distinct coastal watersheds in southeast Louisiana and lead to the delineation of various flood hazard zones (rainfall-runoff, coastal, or coastal transition). We demonstrate how antecedent conditions alter total water levels and how the inclusion of hurricane-induced rainfall amplifies coastal flooding. Our findings emphasize the need to develop and refine coastal flood inundation models to include various flooding mechanisms and related physics. Such improvements can enhance our preparedness and resilience strategies across low-lying coastal landscapes.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Reduced Order Models Using a Non-Local Calculus on Finite Weighted Graphs

Author(s): *Matthew Duschenes, *University of Michigan*; Krishna Garikipati, *University of Michigan*;

Partial differential equation-based numerical solution frameworks for initial and boundary value problems have attained a high degree of sophistication. Solutions can contain upwards of billions of degrees of freedom and this computational expense and complexity do not lend themselves to typical engineering design. Reduced-order models with controlled approximations must therefore be relied on for efficient, intuitive decision-making. Here we present an approach to reduced-order modelling that builds off of recent graph theoretic work for representation, exploration and analysis on computed states of physical systems (Banerjee et al., Comp. Meth. App. Mech. Eng., 351, 501-530, 2019). This graph theoretic framework consists of representing a physical system with a discrete manifold, where high fidelity and high dimensional states are mapped to vertices on a graph, with a lower dimensional state vector associated with each vertex. Weighted edges between vertices can then be assigned, or found through graph theoretic principles, indicating relationships or transitions between states, and the magnitude of such correlations. Reversible linear systems lead to undirected graphs that are fully connected, whereas dissipative dynamical systems are represented by directed trees. Path-dependence can be thought of as being associated with an absence of cycles. Many other associations between dynamics and specific graph structures follow, some due to definitions in graph theory, others as corollaries or theorems. Notions of centrality reveal insights to the relations between states, and path traversal properties are induced on graphs by equilibrium or dynamical transitions on the physical system. On this manifold we seek to define functional representations and differential equations for the evolution of certain components of the state vector. To construct a basis of operations to form these representations, we show how it is possible to extend a non-local calculus on finite weighted graphs (Gilboa et al., Multiscale Model. Simul., 7, 1005-1028, 2008), by exploiting first order dynamics, polynomial expansions, and Taylor series. Some aspects of the non-local calculus related to convergence of the models, and consistency with classical definitions from differential calculus are explored, and implementation details are discussed. Finally, we will show the intuitive and general nature of this approach through applications to a variety of physical systems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Additive Manufacturing Process-Informed Topology Optimization

Author(s): *Matthew Ireland, *University of Maine*; Masoud Rais-Rohani, *University of Maine*; Brett Ellis, *University of Maine*;

Topology optimization (TO) often results in complex part geometries that are much better suited to additive manufacturing (AM) than traditional manufacturing processes. However, large thermal-gradient AM processes, such as powder bed fusion (PBF), exhibit process-dependent microstructures and properties that are ignored in process-agnostic TO solutions, thus, excluding valuable process-structure-property relationships from the purview of optimum design search [1] and raising doubts about the validity of the TO results. This work seeks to address this shortcoming by implementing a process-informed topology optimization (PITO) algorithm for PBF AM of IN718. The iterative PITO algorithm augments a density-based TO search technique with a process simulation model to calculate as-solidified porosity. The design density field is polarized to form a discrete geometry in a manner that reflects the common industry practice of isodensity surface extraction, and the discrete geometry is then translated into a set of manufacturing instructions as inputs to the process simulation model. Spatially-dependent porosities in manufactured regions of the PBF build volume are calculated as a function of scan strategy, beam diameter, beam power, and thermomechanical properties of powdered IN718. The position- and process-dependent porosity data are utilized to calculate isotropic elastic moduli via a Mori-Tanaka homogenization scheme. Direct update of design variables, where porosity data is used to initialize the next position in the design domain, and indirect update of design variables, where element-wise mechanical properties are updated but position in the design domain is preserved between iterations, are implemented and their effects contrasted. A set of design envelopes, boundary conditions, manufacturing and response constraints, objective functions, and manufacturing orientations are chosen and presented to convey the impact of including processing outcomes into the TO algorithm. Where process-agnostic TO results exhibit symmetry, PITO design solutions are parameter-dependent and exhibit asymmetry in the build direction. Importantly, a numerical comparison of post-design TO and PITO solutions shows improved discrepancy between as-designed and anticipated performance. This work contains two significant contributions. First, this work demonstrates PITO solutions more accurately predict performance than traditional TO solutions. Second, this work demonstrates an approach to incorporate the manufacturing processes into part design, providing a framework for integrated process-product optimization toward improved performance. [1] Yoder, S., Morgan, S., Kinzy, C., Barnes, E., Kirka, M., Paquit, V., Nandwana, P., Plotkowski, A., Dehoff, R. R., & Babu, S. S. (2018). Characterization of topology optimized Ti-6Al-4V components using electron beam powder bed fusion. Additive Manufacturing, 19, 184–196. https://doi.org/10.1016/j.addma.2017.12.001

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Learning Optimal Priors

Author(s): *Matthias Chung, *Virginia Polytechnic Institute and State University*;

Emerging fields such as data analytics, machine learning, and uncertainty quantification heavily rely on efficient computational methods for solving inverse problems. With growing model complexities and ever increasing data volumes, state of the art inference method exceeded their limits of applicability and novel methods are urgently needed. In recent year new approaches for optimal experimental design for inverse problem have been investigated. Optimal experimental design for inverse problems require well suited prior to obtain meaningful solutions. In this talk, we will discuss and utilize new optimal experimental design frameworks for obtaining optimal priors. Hence priors are design specific to its experiments. We also discuss alternative neural network learning techniques. In various numerical experiment, such as medical tomography, we illustrate advantages and limitations of our methods.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Buckling Analysis of Functionally Graded Curvilinearly Stiffened Plates using Ritz Method with Jacobi Polynomials

Author(s): *Mayank Agarwal, *Virginia Polytechnic and State University*; Wei Zhao, *Virginia Polytechnic and State University*; Rakesh Kapania, *Virginia Polytechnic and State University*;

With the recent advancement in the manufacturing technology, functionally graded materials (FGMs) are now becoming one of the most widely used materials in the aerospace industry because of their adaptability to different situations by changing the material constituents as per the requirement. In addition, curvilinear stiffeners have been found to increase the buckling load significantly by modifying its buckling mode wavelength only with slight weight penalty [1, 2]. This study presents an efficient way for buckling analysis of FGM panels stiffened with curvilinear stiffeners using the Ritz Method. The present approach enables rapid analysis towards obtaining static and buckling responses, which helps to conduct a fast design analysis of FGM stiffened panels. Both the plate as well as the stiffener are being modelled using the first-order shear deformation theory. The material properties vary continuously in the thickness direction of the FGM panel and the variation is governed by the Power law. Compared to using FEM for studying such stiffened plates, the implementation of Ritz method makes it much simpler to apply the compatibility condition between the panel and the stiffener displacements as the stiffeners can be placed arbitrarily and do not have to share nodes with the plate. Orthogonal Jacobi Polynomials as trial functions are used to approximate the displacement field, which makes the present method more robust even for predicting higher mode shapes [3]. The accuracy of the method is then demonstrated by validating the obtained numerical results against reference solutions available in the literature for unstiffened FGM plates and straight as well as curvilinearly stiffened isotropic plates. Parametric studies show that the buckling load of FGM plates increases with decrease in the Power Law index. The present method will be used to analyze the system under thermal loads as ceramic-based FGMs can both, withstand higher temperatures and avoid buckling under in-plane compressive loads. References: [1] R. K. Kapania and A. Y. Tamijani, "Buckling and static analysis of curvilinearly stiffened plates using mesh-free method," AIAA Journal, vol. 48, no. 12, pp. 2739-2751, 2010. [2] W. Zhao and R. K. Kapania, "Buckling analysis of unitized curvilinearly stiffened composite panels," Composite Structures, vol. 135, pp. 365-382, 2016. [3] B. Alanbay and R. K. Kapania, "On the use of classical Jacobi orthogonal polynomials in the Ritz method," in AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, 2018.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analytical and Machine Learning Based Uncertainty Quantification for Metallic Microstructures

Author(s): *Md Mahmudul Hasan, *Virginia Polytechnic Institute and State University*; Pinar Acar, *Virginia Polytechnic Institute and State University*;

Microstructure uncertainty is unavoidable as it arises from different thermo-mechanical effects during the processing and manufacturing of materials. This uncertainty can propagate over multiple length-scales and alter the material properties and performance. Neglecting the effects of the microstructure uncertainty may lead to unexpected material failure. In this study, we aim to optimize the volume-averaged material properties of metallic microstructures by considering the effects of the microstructure uncertainty in design. The microstructure is represented in terms of the Orientation Distribution Function (ODF). A linear programming (LP) based analytical method is introduced to quantify the effects of the microstructure uncertainty on the desired volume-averaged material properties that are linearly dependent on the ODF. The solutions of the LP problems provide us with the mean values and covariance of the ODFs which maximize a volume-averaged linear material property. However, the LP-based analytical procedure is not applicable to the maximization of non-linear material properties under microstructural uncertainties. Therefore, an artificial neural network (ANN) based sampling method is developed to estimate the mean values and covariance of the ODFs that satisfy the design constraints and maximize the volume-averaged non-linear material properties. Applications are demonstrated for the Titanium-7wt%Aluminum (Ti-7Al) alloy, which is a candidate material for different aerospace components. A couple of other design problems are also illustrated to clarify the applications of the proposed models for both linear and non-linear properties.

16th U.S. National Congress on Computational Mechanics
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Title: Meshing Algorithm to Increase the Accuracy of Li-ion Batteries 3D Models

Author(s): *Mehdi Chouchane, *Laboratoire de Réactivité et Chimie des Solides*; Alejandro A. Franco, *Laboratoire de Réactivité et Chimie des Solides*;

With the increasing electricity demand, energy storage devices such as batteries need to be improved to accommodate the expected growth of renewable energies. A standard Li-ion battery is composed of two electrodes in which there are three phases, the Active Material (AM), the inactive phase (Carbon-Binder Domains, i.e. CBD), and a liquid phase, namely the electrolyte. Until recently in the energy storage literature, reported 3D-resolved battery models relied on oversimplifications, such as an implicit representation of the inactive phase using effective parameters for porosity and tortuosity factor or merging CBD with the AM as a single solid phase with the same physical properties. This work's novelty relies on the explicit representation of CBD, leading to a new level of accuracy in terms of electrochemical modeling. This achievement is made possible thanks to an in-house MATLAB algorithm, INdefinite Number Of phases meshing through Voxelization (INNOV)1. The explicit consideration of the inactive phase is of the utmost importance because the electrochemical reaction responsible for the flow of electrons in the cell occurs at the interface between the active material and the electrolyte. Having the CBD meshed as an individual phase allows to capture a decrease of the surface of reaction (when the CBD is in contact with the active material) and to create hotspots for the reaction to take place thanks to higher electronic conductivity. These conclusions have been highlighted in one of our published works where we investigate the impact of the mesostructure of the electrode (mainly CBD location) thanks to finite element method simulations.2 INNOV is now integrated into the overall multiscale computational workflow for the simulation of electrodes manufacturing process within our ARTISTIC project.3 In conclusion, INNOV offers a time-efficient tool to perform meshing without requiring substantial computational resources. Simulations can later be performed to characterize these meshes with the CBD explicitly considered. It can lead to new approaches to characterize battery microstructures and the impact of each component. 1. Chouchane, M., Rucci, A. & Franco, A. A. A Versatile and Efficient Voxelization-Based Meshing Algorithm of Multiple Phases. ACS Omega 4, 11141–11144 (2019). 2. Chouchane, M., Rucci, A., Lombardo, T., Ngandjong, A. C. & Franco, A. A. Lithium ion battery electrodes predicted from manufacturing simulations: Assessing the impact of the carbon-binder spatial location on the electrochemical performance. Journal of Power Sources 444, 227285 (2019). 3. Alejandro A. Franco. ARTISTIC Homepage. https://www.u-picardie.fr/erc-artistic/.

16th U.S. National Congress on Computational Mechanics
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Title: Bounding Discretization Errors of Physics-Informed Neural Network Solutions in Elasticity

Author(s): *Mengwu Guo, *University of Twente*; Ehsan Haghighat, *Massachusetts Institute of Technology*;

In this talk, an energy-based a posteriori error bound is presented for the physics-informed neural network solutions of elasticity problems. The proposed error bound is formulated as the constitutive relation error defined by a solution pair, consisting of a kinematically admissible displacement solution and a statically admissible stress solution. In this work, such an admissible displacement-stress pair is obtained from a mixed form of physics-informed neural networks. The proposed error estimator can provide an upper bound of the global error of neural network discretization. From the perspective of neural network training, the generalization errors of physics-informed neural networks can be quantified through the proposed energy-based error bounds in elasticity problems. The asymptotic behavior of the physics-informed neural network solutions are discussed with the constitutive relation error bounds as well. [1] E. Haghighat, M. Raissi, A. Moure, H. Gomez, and R. Juanes. A deep learning framework for solution and discovery in solid mechanics. arXiv: 2003.02751, 2020. [2] M. Guo, and E. Haghighat. An energy-based error bound of physics-informed neural network solutions in elasticity. arXiv: 2010.09088, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: An Updated Lagrangian Framework for Isogeometric Kirchhoff–Love Thin–Shell Analysis

Author(s): *Mert Alaydin, *Brown University*; Yuri Bazilevs, *Brown University*;

In this talk, we present a new comprehensive isogeometric Kirchhoff-Love shell analysis framework that is capable of undergoing large elasto-plastic deformations. Primarily targeting industry-level problems, the proposed framework can support existing 3-D constitutive laws and operate on multi-patch scenarios in the isogeometric analysis (IGA) context. Central to this development, we reformulate the governing thin-shell equations in terms of the mid-surface velocity degrees of freedom, therefore accommodating the 3-D material response in the time-rate form while ensuring objectivity. To handle complex multipatch geometries, we propose a penalty coupling technique consistent with the underlying Updated Lagrangian format for enforcing the continuity conditions at the patch interfaces. This penalty technique is further extended to weakly enforce rotational and mid-surface velocity symmetry boundary conditions. A recently proposed non-local penalty contact algorithm [1] is adopted as part of the formulation to treat dynamic problems with self-contact. Numerical examples, ranging from static elasto-plastic shell obstacle course to highly dynamic crushing scenarios, validate the accuracy, efficiency, and robustness of the proposed framework. References: [1] D. Kamensky, F. Xu, C.-H. Lee, J. Yan, Y. Bazilevs, and M.C. Hsu, “A contact formulation based on a volumetric potential: Application to isogeometric simulations of atrioventricular valves”, Computer methods in applied mechanics and engineering, 330 (2018) 522–546.

16th U.S. National Congress on Computational Mechanics
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Title: Enhancing Multifidelity UQ with Model Tuning

Author(s): *Michael Eldred, *Sandia National Laboratories*; Gianluca Geraci, *Sandia National Laboratories*; Alex Gorodetsky, *University of Michigan*; John Jakeman, *Sandia National Laboratories*;

Multifidelity Uncertainty Quantification (MF UQ) is an efficient tool for enabling predictive analyses of high-fidelity systems. MF UQ strategies can be divided in sampling based approaches, e.g. multilevel and multifidelity Monte Carlo (MLMC, MFMC) and Approximate Control Variate (ACV) [1], and surrogate based approaches, e.g. multilevel polynomial chaos/hierarchical stochastic collocation/functional tensor train (ML PCE/HSC/FTT) and MFNets [2]. Both families of MF UQ methods are based on a common idea: a prescribed accuracy of the statistics of interest can be reached more efficiently, i.e. with a lower computational cost, by fusing information obtained from several sources of varying accuracy and cost. In this work, we plan to build on some numerical observations, e.g. [3], that corroborate the idea that some of the numerical hyper-parameters of the lower fidelity models, for instance configuration parameters that control discretization and convergence details and which manage physical assumptions/closure models that are not shared among models, can be optimized to select the values that maximize the MF UQ estimator efficiency. Moreover, these controls generally encompass a mixture of continuous and discrete hyper-parameters, leading to mixed-integer nonlinear programming approaches for the optimization of predictive utility. We will formulate the optimization problem in the context of specific MF UQ estimators, e.g. MLMC, MFMC, and ACV, and solve it to demonstrate the viability of the approach and its robustness and performance compared to the corresponding MF UQ benchmark without hyper-parameter optimization. We plan to discuss several verification test problems and progress towards more complex numerical applications in the areas of wind energy and fusion energy. [1] Gorodetsky, A.A., Geraci, G., Eldred, M.S., and Jakeman, J.D., “A Generalized Approximate Control Variate Framework for Multifidelity Uncertainty Quantification”, J. Comput. Phys., 408:109257, 2020. [2] Gorodetsky, A. A., Jakeman, J.D., Geraci, G., Eldred, M.S., "MFNETS: multifidelity datadriven networks for Bayesian learning and prediction." International Journal of Uncertainty Quantification 10:6, pp. 595-622, 2020. [3] Geraci, G., Crussell J., Swiler, L., Debusschere, B., Exploration of multifidelity UQ sampling strategies for computer network applications, Accepted for publication, International Journal of Uncertainty Quantification, 2021. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
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Title: Variationally Consistent Naturally Stabilized Thermo-Mechanical Meshfree Formulation

Author(s): Kuan-Chung Lin, *National Cheng Kung University*; *Michael Hillman, *The Pennsylvania State University*;

Coupled thermo-mechanical problems are present in several applications such as the popular three-dimensional printing technique of fused deposition modeling (FDM), which is the focus of the present work. For FDM, this problem includes phase change, thermoelasticity, finite strain thermomechanical analysis, and thermoviscous fluid flow. For thermoelasticity, and the classical constitutive laws of Fourier and Duhamel Neumann for heat flux and stress, respectively, provide an infinite wave propagation speed for the temperature, which is arguably unacceptable. In this work, we consider both the parabolic type of classical thermo-elasticity and thermo-mechanics, and hyperbolic type generalized theories with finite propagation speed of temperature, for example, Lord and Shulman [1]. These latter alternative theories are also more amenable to explicit dynamic calculations as they ease the critical time step restriction significantly. A meshfree approach for solving the associated fully coupled governing equations is developed in this work. In order to obtain an effective meshfree solution, accurate, low order node-based quadrature is desired, such as a stabilized and corrected nodal integration. To this end, a naturally stabilized nodal integration [2] is proposed for the thermo-mechanical problem to provide a stable nodal integration technique. A Taylor series expansion is performed for both the strains and the gradient of the temperature field, resulting in a stabilized bilinear form. The variational consistency conditions are then derived for the coupled two-field problem, where it is shown that the conditions differ in several ways from pure elasticity. A variationally consistent integration method [3] to correct the error in nodal integration is then introduced by modifying the test function gradients. Several benchmark problems solved to demonstrate the effectiveness of the proposed method for fully coupled classical and generalized thermoelasticicity, finite-strain thermoplasticity, and thermoviscous fluid flow. FDM simulations are also presented. References [1] Harold Wesley Lord and Y Shulman. A generalized dynamical theory ofthermoelasticity. Journal of the Mechanics and Physics of Solids, 15(5):299–309, 1967. [2] Michael Hillman and Jiun-Shyan Chen. An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics. International Journal for Numerical Methods in Engineering, 107:603–630, 2016. [3] Jiun-Shyan Chen, Michael Hillman, and Marcus Ru?ter. An arbitrary order variationally consistent integration for Galerkin meshfree methods. International Journal for Numerical Methods in Engineering, 95(5):387–418, 2013.

16th U.S. National Congress on Computational Mechanics
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Title: Polyhedral Nonconforming Discretization Methods for Multiple-Network Poroelasticity

Author(s): *Michele Botti, *Politecnico di Milano*; Paola F. Antonietti, *Politecnico di Milano*; Lorenzo Botti, *University of Bergamo*; Daniele A. Di Pietro, *Université de Montpellier*;

The numerical modeling of poroelastic media is relevant in several geoscience applications, including subsidence due to fluid withdrawal, waste disposal, injection-production cycles in geothermal fields, and CO2 storage in saline aquifers. Reservoir and aquifer systems are often formed by fractured rocks containing fissured networks. The simultaneous presence of pores and interconnected fractures requires a modification of the classical Biot poroelasticity model in which the flow processes in the different networks are coupled by a exchange terms. In this work, we develop and analyze nonconforming discretization methods for multiple-network geomechanical problems describing seepage through deformable fissured media. The proposed methods are designed to support general polygonal and polyhedral elements. This is a fundamental feature in geological modeling, where the need for general elements arises, e.g., due to the presence of fracture and faults, to the onset of degenerate elements to account for compaction or erosion, or when nonconforming mesh adaptation is performed. We focus on fully coupled methods based on discontinuous Galerkin and Hybrid High-Order methods, which have several appealing features: they supports general meshes and arbitrary approximation order; they can be applied to any number of pore networks; they are well-behaved for quasi-incompressible porous matrices; and they deliver error estimates that are robust in the entire range of geophysical parameters. The stability and convergence results rely on a novel abstract framework for the analysis of nonconforming monolithic discretizations that rest on mild regularity assumptions. The theoretical results are demonstrated on a complete panel of numerical tests.

16th U.S. National Congress on Computational Mechanics
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Title: Traces on General Sets without Differentiability

Author(s): *Mikil Foss, *University of Nebraska-Lincoln*;

A common class of nonlocal operators has a convolution like structure. If the kernel is integrable with an integrable then the operator is generally insensitive to the values of a function on sets of zero measure. Thus, for associated nonlocal problems, the analogue of a Dirichlet-type boundary condition is a volume-constraint, where the value of a solution is prescribed on a region of positive measure. I will present some conditions under which a trace for a function can be identified on a set with strictly positive codimension. The conditions are compatible with nonlocal problems where operators with integrable kernels are employed. The functions are required to satisfy an oscillation constraint that does not require any differentiability away from the boundary. The assumptions also allow domains with very rough boundaries that possess cusp-like features.

16th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in Immersogeometric Analysis

Author(s): *Ming-Chen Hsu, *Iowa State University*;

Immersogeometric analysis, which was heavily inspired by Isogeometric Analysis, was first introduced as a geometrically flexible technique for solving computational fluid dynamics (CFD) and fluid-structure interaction (FSI) problems involving large, complex structural deformation. This novel method makes direct use of the CAD boundary representation (B-rep) of a complex design structure by immersing it into a non-body-fitted discretization of the surrounding fluid domain, thereby eliminating the challenges associated with time-consuming and labor-intensive geometry cleanup and mesh generation/manipulation. The key ingredients to achieving high simulation accuracy include imposing the kinematic constraints weakly using augmented Lagrangian or Nitsche's methods and faithfully capturing the geometry in intersected elements. In this talk, I will discuss the fundamentals and some recent advances of the method and demonstrate its effectiveness through several industrial applications.

16th U.S. National Congress on Computational Mechanics
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Title: An Efficient Numerical Algorithm for Modeling of Seismic Cycles: Effect of Low Velocity Zones

Author(s): *Mohamed Abdelmeguid, *University of Illinois at Urbana-Champaign*; Xiao Ma, *University of Illinois at Urbana-Champaign*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*;

Modeling earthquake ruptures is a complex challenge due to the eclectic sources of nonlinearities and heterogeneities, in addition to the multi-scale nature of the problem, both spatially and temporally. In this study, we utilize FEBI and efficient numerical scheme that couples finite element (FE) and spectral boundary integral (SBI) method to study the long-term behavior of a rate and state fault subjected to slow tectonic loading over a long duration intermittent by episodes of dynamic fracture in the presence of a near fault low velocity zone. The proposed scheme combines the numerical superiority of SBIM with the flexibility of FEM to handle nonlinear problems with varying length scales at a substantially reduced computational cost. We handle the different time scales during the periods of loading and dynamic rupture by alternating between a quasi-dynamic and a dynamic solver. The periods with long inter-seismic tectonic loading are simulated using the quasi-dynamic approximation that allows for larger time steps, while during the periods of dynamic rupture we utilize an explicit time stepping algorithm to capture the wave propagation properties within the simulated domain. The impact of the LVZ in altering the overall pattern and behavior of the earthquake cycle is highlighted. Specifically, the introduction of the LVZ contributes to the emergence of sub-surface events that fails to propagate to the free surface and produces residual stresses which impact subsequent ruptures resulting in larger slip rates. In addition, the material mismatch result wave reflections that contributes toward the generation of pulse like ruptures that are absent from the homogeneous case. Finally, we comment on the overall changes to the earthquake patterns in the presence of LVZ such as inter event times, event patterns and magnitude scaling.

16th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in the VoroCrust Algorithm for Automatic Generation of Conforming Voronoi Meshes

Author(s): *Mohamed Ebeida, *Sandia National Laboratories*; Tara LaForce, *Sandia National Laboratories*; Joseph Bishop, *Sandia National Laboratories*; William Mclendon, *Sandia National Laboratories*;

Over the past decade, polyhedral meshing has been gaining popularity as a better alternative to tetrahedral meshing in certain applications. Within the class of polyhedral elements, Voronoi cells are particularly attractive thanks to their special geometric structure. In 2020, We introduced VoroCrust, the first automated algorithm to generate Voronoi meshes for non-convex and non-manifold domains. In this talk we will discuss the recent advances we achieved to increase the speed of the code by two orders of magnitude. VoroCrust can now generate a 3d mesh with one million random cells in less than 10 minutes using a modern laptop and few OpenMP threads. The generated mesh is provably good in terms of aspect ratio and dihedral angles. We will also demonstrate the impact of VoroCrust meshes via Earth science Simulations where fluid flow have been run on models of the subsurface generated by geological modelling software and meshed using VoroCrust. Furthermore, simulations of benchmark problems have shown that fluid flow simulations on automated Vorocrust meshes have similar accuracy to ideal (hard-to generate) structured meshes. Vorocrust generated polyhedral elements are also being studied for applications in solid mechanics with comparisons to traditional hexahedral and tetrahedral discretizations. Ref: 1. Ahmed Abdelkader, Chandrajit L. Bajaj, Mohamed S. Ebeida, Ahmed H. Mahmoud, Scott A. Mitchell, John D. Owens, and Ahmad A. Rushdi. 2020. VoroCrust: Voronoi Meshing Without Clipping. ACM Trans. Graph. 39, 3, Article 23 2020. 2. LaForce, T., Chang, K.W., Perry, F.V., Lowry, T.S., Basurto, E., Jayne, R., Brooks, D., Jordan, S., Stein, E.R., Leone, R., Nole, M. GDSA Repository Systems Analysis Investigations in FY 2020. SAND2020-12028 R, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Neural Gaussian Processes for Robust Systems Identification Under Uncertainty

Author(s): *Mohamed Aziz Bhouri, *University of Pennsylvania*;

We present a machine learning framework for Bayesian systems identification from partial, noisy, sparse and irregular observations of nonlinear dynamical systems. The proposed method takes advantage of recent developments in differentiable programming to propagate gradient information through ordinary differential equation solvers and perform Bayesian inference with respect to unknown model parameters using Markov Chain Monte Carlo sampling and Gaussian Processes. This allows us to efficiently infer posterior distributions over plausible models with quantified uncertainty, while the use of sparsity-promoting priors such as the Finnish Horseshoe distribution enables the discovery of interpretable and parsimonious representations for the underlying latent dynamics. A series of numerical studies is presented to demonstrate the effectiveness of the proposed methods including predator-prey systems, systems biology, and a 50-dimensional human motion dynamical system. Taken all together, our findings put forth a novel, flexible and robust workflow for data-driven model discovery under uncertainty.

16th U.S. National Congress on Computational Mechanics
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Title: Mechanical Behavior of Additively Manufactured Metallic Cellular Scaffold Structures for Bone Tissue Engineering

Author(s): *Mohammad Al-Barqawi, *University of Wisconsin–Milwaukee*; Adeeb Rahman, *University of Wisconsin–Milwaukee*; Dan Thoma, *University of Wisconsin–Madison*;

Critical-sized bone defects represent a significant challenge in the orthopedic field. Limitations on autograft and allograft as treatment techniques led researchers to explore the implantation of artificial bone tissue scaffolds. Bone scaffolds are three-dimensional cellular structures that provide mechanical support and behave like a template for bone tissue formation. Stress shielding in bones is defined as the bone weakening and reduction in bone density as a result of stiffness mismatch between the bone and the scaffold. The main hypothesis in this research is that the stress shielding phenomenon is the main cause of bone resorption (loss) that leads to eventual failures of bone implants. The availability of additive manufacturing facilitated the fabrication of bone scaffolds with precise architectural and structural configurations. This study aimed to reduce the stress shielding effect by designing and manufacturing a numerically optimized stainless steel bone scaffold with an elastic modulus that matches the structural modulus of the human cortical bone. Diagonal and cubic cell scaffold designs were explored. Strut and cell sizes were numerically optimized with a predetermined pore size to achieve the target structural modulus. The optimized scaffold designs were manufactured using the direct metal laser sintering (DMLS) technique and experimentally tested in compression to validate the finite element analysis (FEA) model and explore the failure mechanisms of both scaffold designs. Scanning electron microscopy (SEM) was used to characterize the structural configuration of the manufactured scaffolds. Minimal porosity was found in struts and minor variations in strut sizes were observed between the manufactured scaffolds and CAD models. Rough surfaces were noticed due to the metal powder sintering process. FEA results were found to agree with the experimental findings validating the FEA model. Stretch-dominated failure was noticed in the cubic scaffold, while bending-dominated failure was observed in the diagonal scaffold. The bending and torsional stiffnesses of both scaffold designs have been numerically evaluated. Higher bending and torsional moduli were observed in the diagonal scaffold compared with the cubic scaffold. In conclusion, this research presented the ability to optimize, design, and manufacture bone scaffolds using additive manufacturing with mechanical properties that relate to the cortical bone as part of bone tissue engineering. Also, it highlighted the need to investigate the biomechanical loading behavior and osteointegration properties of the designed scaffolds.

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Title: Accelerating Random Heterogeneous Material Design via Supervised ML: A Physically-Aware Approach

Author(s): *Mohammad Hashemi, *Iowa State University*; Azadeh Sheidaei, *Iowa State University*;

Random heterogeneous material systems include a large class of materials such as ceramics, amorphous metals, and polymeric composites. Their specific microstructures necessitate using complex and expensive computational models, such as the Young-Torquate method of reconstruction, to realize and characterize their microstructure. Furthermore, their inverse design, i.e., finding the optimum representative material microstructures or RVEs to achieve a target set of material properties, is a challenging task considering that their results should be physically feasible and manufacturable. Recent advancements in manufacturing techniques have enabled us to make heterogeneous materials with a variety of phase materials at length scales that were not achievable a decade ago. In this work, we introduce a supervised ML-assisted computational framework of inverse material design for a specific type of heterogeneous materials with applications in Fuel cells. An efficiently-designed database of material microstructures has been generated with their properties or labels found through our recently-developed FFT method. An ML model was trained on our generated dataset to serve as a surrogate model of the forward structure-property relationships in conjunction with a back-propagation optimization method for solving the inverse design problem. To link the results of this framework to the process part, we used different statistical functions such as Two-point Correlation and Clusteredness ones augmenting the microstructure features for the microstructure characterization and realization.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An LBM/MD/IBM Method for the Simulation of Composite Foam Processing

Author(s): *Mohammadmehdi Ataei, *University of Toronto*; Erfan Pirmorad, *University of Toronto*; Franco Costa, *Autodesk, Inc*; Sejin Han, *Autodesk, Inc*; Chul Park, *University of Toronto*; Markus Bussmann, *University of Toronto*;

Polymer foams are manufactured by injecting supercritical gas at high pressure into a molten polymer, dissolving the gas in the polymer melt, and then reducing the pressure suddenly to nucleate gas bubbles. The nucleated bubbles grow and form a low-density cellular structure that has many applications. Polymer foam composites improve on the properties of such foams by addition of fibers (such as glass fibers, carbon fibers, carbon nanotubes, and nanowires) that serve to stabilize and strengthen the foam, and may also enhance properties such as thermal and electrical conductivity. The alignment and distribution of these fibers (resulted from the interaction with growing bubbles and the bulk shearing flow of the polymer during the foaming process) and the fiber content significantly influences the foam properties and manufacturing costs. Lower fiber content is favorable, as it reduces manufacturing costs and processing time, provided that the properties of the composite foam are maintained. A number of earlier studies developed analytical and semi-analytical solutions to analyze the motion of fibers in a foam, all based on simplifying geometrical and physical assumptions. In this work, we present a comprehensive fluid-solid foaming simulation solver for both the foaming process and the movement and interaction of fibers with growing bubbles. The Lattice-Boltzmann Method (LBM) is used to resolve the foaming process (fluid flow and gas diffusion / bubble growth), and a Molecular Dynamics (MD) model accounts for bubble-fiber interaction, considering the fiber structural constraints. These two solvers are coupled by a direct forcing Immersed Boundary Method (IBM). The hybrid LBM/MD/IBM solver has been implemented in an efficient and scalable parallel way that enables large-scale simulations involving many bubbles and fibers. For the first time, this solver relaxes most of the simplifying assumptions in polymer foam composites modeling, and will pave the way for further research on the control and manipulation of such foaming processes, to enhance the mechanical, electrical, and electromagnetic properties of foams.

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Title: Stable Midpoint Integration Method for Galerkin Meshfree Method

Author(s): *Mohammed Mujtaba Atif, *University of Illinois at Chicago*; Sheng-Wei Chi, *University of Illinois at Chicago*;

Despite extensive research, the domain integration in the Galerkin meshfree method remains a challenge for high strain rate simulations. Although higher-order quadrature rules can achieve stability and accuracy, they become computationally expensive in extreme deformation problems. Several nodal integration methods were developed to resolve the efficiency issue; nonetheless, some suffer from instability or suboptimal convergence [1]. Recent-developed nodal integration methods such as Natural Stabilized Nodal Integration (NSNI) with Variationally Consistent Integration (VCI) alleviate the above issues [2] through enforcing the integration constraint. However, the required contour integral to impose the variationally consistent condition is not straightforward in the meshfree approximation, especially for contact and material separation problems. In this work, a stable nodal integration called Midpoint Integration Method (MPIM) is developed based on the extension of modified Simpson's rule [3]. The method is derived in such a way that the evaluation point relies on the nodal point without the need of conforming subdomains. To enhance computational efficiency, an implicit gradient reproducing kernel is applied to the MPIM. The resultant method is free from the conforming subdomains and does not require VCI correction. Two variants of the MPIM are developed to reduce the overall computational cost of the integration method. Several numerical analyses are carried out to verify the stability and convergence. The effectiveness of the proposed method in the large deformation problems is tested in penetration simulations. Overall MPIM shows better performance when compared with other nodal integration schemes. Keywords: NSNI, semi-Lagrangian, VCI, Modified Simpson's rule, Meshfree method. [1] M. Hillman, J.S. Chen, S.W. Chi (2014). Stabilized and variationally consistent nodal integration for meshfree modeling of impact problems. Computational Particle Mechanics 1 (3), 245-256. [2] M. Hillman, and J. S. Chen, (2016). An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics. Int. J. Numer. Methods Eng. 107 (7): 603–630. [3] P. Cerone and S. S. Dragomir, (2000). Midpoint-type Rules from an Inequalities Point of View. Handbook of Analytic-Computational Methods in Applied Mathematics, CRC Press, 135–200.

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Title: Applied Machine Learning Method to Predict Crack Propagation Path in Polycrystalline Graphene Sheet

Author(s): *Mohan Surya Raja Elapolu, *University of North Carolina at Charlotte*; Alireza Tabarraei, *University of North Carolina at Charlotte*; MD Imrul Reza Shishir, *University of North Carolina at Charlotte*;

We are employing machine learning techniques to predict crack growth path during brittle fracture in polycrystalline graphene sheet. Computational modeling of crack propagation involves atomic bond breaking which often requires atomistic level modeling techniques. These techniques are computationally expensive and hinders rapid prediction of material behavior. On the other hand, due to their ability to learn complex nature of data and make predictions, machine learning techniques has found applications in a wide range of industries. Recently, researchers are employing them to predict material and fracture properties. We employ machine learning models for rapid prediction of the fracture process in polycrystalline graphene sheet. The polycrystalline graphene sheet considered is of dimensions 20 X 40 nm with an edge crack of 0.7 X 4 nm. We conducted simulations on 700 sheets where each sheet has randomly oriented grains. The grain sizes considered are in the range of 3 – 9 nm. We simulate tensile loading using LAMMPS molecular dynamics package [1]. Our simulation results show that polycrystalline graphene sheet fails through brittle crack propagation. Careful observation of crack propagation path shows that the crack path is dependent on the orientation of the grain, and the grain boundary. We are employing machine learning architecture which is a combination of convolutional neural network (CNN) and recurrent neural network (RNN) to predict crack propagation path. One of the challenging tasks is to build the training set to train the machine learning model. Our training set is composed of images of dimension 128 X 256 pixels. Input image is the initial configuration of polycrystalline graphene sheet with edge crack. Each grain in the image is colored based on its orientation. The corresponding output image is the one which shows the fully grown crack in the graphene sheet. Our machine learning model can predict the crack propagation path in the polycrystalline graphene sheet. [1] Plimpton, Steve. "Fast parallel algorithms for short-range molecular dynamics." Journal of computational physics 117, no. 1 (1995): 1-19.

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Title: Deep Learning-Based Reduced Order Modeling with Application to Prediction of Riverine Flow Velocity

Author(s): *Mojtaba Forghani, *Stanford University*; Yizhou Qian, *Stanford University*; Jonghyun Lee, *University of Hawaii at Manoa*; Matthew Farthing, *US Army Engineer Research and Development Center*; Tyler Hesser, *US Army Engineer Research and Development Center*; Peter Kitanidis, *Stanford University*; Eric Darve, *Stanford University*;

The prediction of riverine flow velocity for varying boundary conditions (BCs) plays a crucial role in many applications, such as the successful operation of shipping and navigation, the study of river morphodynamics, the study of flood routing and risk assessment, and sediment transport. The shallow water equations (SWEs) are commonly used for predicting the riverine flow velocity, given the BCs and the riverbed profile (bathymetry). However, accurate and fast prediction with standard SWE solvers is challenging. Traditional numerical techniques are computationally expensive and require high-resolution bathymetry measurements for accurate velocity prediction. Consequently, they are a poor fit in situations where they need to be evaluated repetitively, for example, when exploring the effect of different BCs or different bathymetry profiles. In this work, we propose a two-stage process to tackle these issues. First, using the principal component geostatistical approach (PCGA), a scalable Hierachical Bayesian inverse modeling approach, we estimate the bathymetry from flow velocity measurements. Then we use multiple machine learning algorithms to obtain a fast solver of the SWEs, given the posterior bathymetry distribution generated by PCGA and the prescribed range of potential BCs. The first step of the proposed approach allows us to predict flow velocities without any direct measurement of the bathymetry. Furthermore, during the second stage, our approach allows incorporating additional measurements into the flow velocity prediction for improved accuracy and generalization, even if the bathymetry changes over time due, for example, to erosion or sediment deposition by assimilating new data and updating bathymetry using the constructed reduced order models. We benchmarked three different fast forward solvers, referred to as the principal component analysis-deep neural network (PCA-DNN), the supervised encoder (SE), and the supervised variational encoder (SVE). We validated them on a reach of the Savannah River near Augusta, GA, USA. Our results show that these fast solvers can predict flow velocities with variable bathymetry and BCs with reasonable accuracy at a computational cost that is significantly lower than the cost of solving the full boundary value problem with traditional numerical approaches.

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Title: The Spatial and Temporal Heterogeneity of Lung Specimens

Author(s): Crystal Mariano, *University of California, Riverside*; Samaneh Sattari, *University of California, Riverside*; Mohammad Maghsoudi-Ganjeh, *University of California, Riverside*; *Mona Eskandari, *University of California, Riverside*;

Respiratory biomechanics research has been cast to the forefront due to the world-gripping COVID-19 pandemic. Even before the virus, lung disease constituted the leading cause of morbidity and mortality. Pulmonary macromechanics, the pressure-volume behavior of inflated ex-vivo lung specimens, are standard means of characterizing the behavior of the tissue and yield insights regarding the bulk, comprehensive response of the organ. Understanding the local tissue behavior in response to global-level breathing is central to determining fundamental physiological behaviors [1], and examining potential load amplifications in diseased states [2]. To address this need, we introduce a validated, custom-designed apparatus capable of imitating breathing in large porcine specimens collected from an abattoir (no IACUC required). The system is retrofitted with a digital image correlation interface, resulting in associative measures between local tissue strains and global pressure-volume loads [3]. While isolated parenchymal tissue is known to be isotropic, its combination with the anisotropic interwoven airways and encapsulating stiff visceral pleura layer produces spatially heterogenous strain contours with lobal regions evolving differently over time. The magnitude, range, and distribution of strains, and relative degree of spatial anisotropy and heterogeneity is non-uniformly dependent on the variable volumes and breathing rates imposed on the specimens. This data is used to establish these local-to-global relationships in an inverse finite element model and enable in-silico means of potentially optimizing ventilation protocols in the clinic to improve patient outcomes. [1] Arora, Hari, et al. “Correlating Local Volumetric Tissue Strains with Global Lung Mechanics Measurements.” Materials 14.2 (2021): 439. [2] Sarabia-Vallejos, Mauricio A., Matias Zuñiga, and Daniel E. Hurtado. “The role of three-dimensionality and alveolar pressure in the distribution and amplification of alveolar stresses.” Scientific reports 9.1 (2019): 1-11. [3] Mariano, Crystal A., et al. “Novel Mechanical Strain Characterization of Ventilated ex vivo Porcine and Murine Lung using Digital Image Correlation.” Frontiers in Physiology 11 (2020): 1536.

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Title: Recent Developments and Numerical Experiments Regarding Recovery Strategies, a Posteriori Error Estimation and Adaptivity for the GFEM.

Author(s): *Murilo Bento, *University of Sao Paulo*; Caio Ramos, *University of Sao Paulo*; Sergio Proença, *University of Sao Paulo*;

The Generalized Finite Element Method (GFEM) is widely used nowadays to efficiently and accurately solve classes of problems that present challenging behaviors and demand high computational costs when treated with conventional methodologies. For instance, problems within the Linear Elastic Fracture Mechanics (LEFM) context, depending on the crack shape, can become difficult to be analyzed using standard procedures. Despite being an efficient methodology for the generation of displacement approximations, studies on its stability, reliability, and applicability are still under investigation [1]. In this contribution, we address a recent formulation for a stress-based recovery procedure [2] that is compatible with the Partition of Unity (PU) framework. This new formulation can significantly expand the applicability of the recovery strategy and the a posteriori error estimator derived from it. Some advantages are related, for example, to the use of reduced number of recovery degrees of freedom and to the implication of well-conditioned projection matrices. Moreover, it is worth highlighting its ability to deal with problems for which no previous information about the stresses is available. Herein, we assess the accuracy of this procedure when applied to standard low- and high-order FEM, as well as to the GFEM combining different enrichment strategies with non-conventional PUs to attain optimal convergent approximations. A straightforward tool extracted from the recovery procedure is an a posteriori ZZ error estimator, which can be efficiently used to estimate the discretization error when no exact analytical solution is known. These resources can therefore be applied to adaptively solve the problem and return a solution that meets an user's pre-specified tolerance, starting with any initial discretization. This type of analysis is attractive in practical situations, when the user wants to avoid multiple simulations and unwanted computational costs. We illustrate our findings by a set of numerical experiments, therefore demonstrating their advantages and potentialities. [1] A.G. Sanchez-Rivadeneira and C.A. Duarte. A stable generalized/eXtended FEM with discontinuous interpolants for fracture mechanics. Computer Methods in Applied Mechanics and Engineering, 345: 876-918, 2019. [2] R. Lins, S.P Proença and C.A. Duarte. Efficient and accurate stress recovery procedure and a posteriori error estimator for the stable generalized/extended finite element method. International Journal for Numerical Methods in Engineering, 119: 1279-1306, 2019.

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Title: Isogeometric Optimal Design of Auxetic Lattice Structures Considering Frictionless Beam-to-Beam Contact of Hyperelastic Cosserat Rods with Extensible Directors

Author(s): *Myung-Jin Choi, *RWTH Aachen University*; Roger A. Sauer, *RWTH Aachen University / Gdansk University of Technology*; Sven Klinkel, *RWTH Aachen University*;

In this research, we develop an optimal design method for three-dimensional lattice structures considering beam-to-beam contact interactions of constituent ligaments, where a gradient-based optimization method is combined with a stochastic algorithm to explore multiple local minima. Our design objective is to achieve an extremal and constant negative Poisson's ratio during large deformations. The previous work of [1], which presents an optimal design of auxetic beam lattice structures, has the several limitations. For example, it uses a linear elastic constitutive model that assumes small strains and rigid cross-section. Moreover, the contact interaction between ligaments in large compressive deformation was not considered, so that the amount of compressive load was limited to avoid unphysical overlap. In this work, we employ an isogeometric finite element formulation of Cosserat rods with extensible directors in [2,3], where three-dimensional hyperelastic constitutive laws can be straightforwardly employed without zero stress conditions, and in-plane cross-sectional deformation is described by two director vectors. To alleviate Poisson locking, we enrich the transverse normal and in-plane shear strain of the cross-section by using the enhanced assumed strain (EAS) method. Using isogeometric analysis (IGA), the convected coordinates of the lateral boundary surface can be straightforwardly expressed by the coordinate along the beam central axis and the initial director vectors. This enables us to derive the differential quantities on the boundary surface in terms of the beam kinematic variables, from which we consistently derive the surface-to-surface frictionless contact formulation. (*) Acknowledgements: M-J. Choi gratefully acknowledges the financial support by a Humboldt post-doctoral research fellowship from the Alexander von Humboldt foundation. (*) References: [1] Myung-Jin Choi, Se-Hyeon Kang, Myung-Hoon Oh, and Seonho Cho. Controllable optimal design of auxetic structures for extremal Poisson's ratio of -2. Composite Structures, 226:111215, 2019. [2] Myung-Jin Choi, Roger A. Sauer, and Sven Klinkel. An isogeometric finite element formulation for geometrically exact timoshenko beams with extensible directors. arXiv: 2010.14454, 2020. [3] Damien Durville. Contact-friction modeling within elastic beam assemblies: an application to knot tightening. Computational Mechanics, 49(6):687–707, 2012.

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Title: The Shifted Boundary Method for Embedded Solid Mechanics

Author(s): *Nabil Atallah, *Duke University*; Claudio Canuto, *Politecnico di Torino*; Guglielmo Scovazzi, *Duke University*;

We propose a new embedded/immersed framework for computational solid mechanics, aimed at vastly speeding up the cycle of design and analysis in complex geometry. In many problems of interest, our approach bypasses the complexities associated with the generation of CAD representations and subsequent body-fitted meshing, since it only requires relatively simple representations of the surface geometries to be simulated, such as collections of disconnected triangles in three dimensions, widely used in computer graphics. Our approach avoids the complex treatment of cut elements, by resorting to an approximate boundary representation and a special (shifted) treatment of the boundary conditions to maintain optimal accuracy. Natural applications of the proposed approach are problems in biomechanics and geomechanics, in which the geometry to be simulated is obtained from imaging techniques. Similarly, our computational framework can easily treat geometries that are the result of topology optimization methods and are realized with additive manufacturing technologies. We present a full analysis of stability and convergence of the method, and we complement it with an extensive set of computational experiments in two and three dimensions, for progressively more complex geometries.

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Title: Multilevel Ensemble Kalman-Bucy Filters

Author(s): *Neil Chada, *King Abdullah University of Science and Technology*; Ajay Jasra, *King Abdullah University of Science and Technology*; Fangyuan Yu, *King Abdullah University of Science and Technology*;

In this talk we consider the linear filtering problem in continuous-time. We develop and apply multilevel Monte Carlo (MLMC) strategies for ensemble Kalman--Bucy filters (EnKBFs). These filters can be viewed as approximations of conditional McKean--Vlasov-type diffusion processes. They are also interpreted as the continuous-time analogue of the \textit{ensemble Kalman filter}, which has proven to be successful due to its applicability and computational cost. We prove that our multilevel EnKBF can achieve a mean square error (MSE) of $\mathcal{O}(\epsilon^2), \ \epsilon>0$ with a cost of order $\mathcal{O}(\epsilon^{-2}\log(\epsilon)^2)$. This implies a reduction in cost compared to the (single level) EnKBF which requires a cost of $\mathcal{O}(\epsilon^{-3})$ to achieve an MSE of $\mathcal{O}(\epsilon^2)$. In order to prove this result we provide a Monte Carlo convergence and approximation bounds associated to time-discretized EnKBFs. To the best of our knowledge, these are the first set of Monte-Carlo type results associated with the discretized EnKBF. We test our theory on a linear problem, which we motivate through a relatively high-dimensional example of order $\sim 10^3$

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Title: Carotid Plaque Segmentation, Classification, 3D Reconstruction and Risk Stratification Using Ultrasound Images

Author(s): *Nenad Filipovic, *University of Kragujevac*; Branko Arsic, *University of Kragujevac*; Tijana Djukic, *BioIRC*; Smiljana Djorovic, *BioIRC*;

The carotid arteries are major blood vessels in the neck that supply blood to the head. Disease started when fatty deposits (plaques) clog the blood vessels. Ultrasound (US) images are used most often for screening patients for blockage or narrowing of the carotid arteries. Complete insight into the characterization and 3D visualization of carotid morphological structures are very important for understanding the etiology of carotid atherosclerosis. In this study we are presented: segmentation of carotid lumen and wall using deep learning model, computer-based automated 3D carotid reconstruction using previously segmented US images, carotid plaque segmentation and classification of three different plaque types using deep learning model, computer-based automated 3D reconstruction of carotid plaque including different plaque types. This is important step further into development of computational tools for atherosclerotic risk assessment and computational analysis of carotid atherosclerosis, using conventional 2D ultrasound images as the input. However, manual segmentation requires highly intensive labor and the results are operator depending. The overcoming of US technical limitations that had been discussed in many papers in the literature and it leaves space for further improvement and refinement of computational tools in the US processing. The presented approach and methodology which combine the data mining and computer-based 3D reconstruction of carotid artery enable efficient segmentation, extraction of the morphological parameters (plaque characterization, geometrical features) and creation of 3D meshed volume models, ready for the further computational examinations. The integration and implementation of additional US datasets from other clinical images is very important for clinical decision making. Enlarged input datasets will improve the robustness and validation of developed tools. Also, the used US images from the baseline timepoint are compared with the follow-ups of the clinical study. Presented computational models will be incorporated in the future prospective clinical study (baseline and follow-up visits) in order to make better clinical decision and change the current medical paradigm which will provide predictive medicine and risk stratification for carotid artery disease.

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Title: Accounting for Model Errors in Probabilistic Linear Identification of Nonlinear PDE Systems

Author(s): *Nicholas Galioto, *University of Michigan*; Alex Gorodetsky, *University of Michigan*;

System identification of dynamical systems is important in many applications for discovering dynamical properties and behavior of a given system from data. Recent work has focused on advancements in modeling complex systems through the model parameterization by increasingly sophisticated neural networks and through introducing model structure that enforces certain dynamical properties of the desired model, e.g., stability or energy conservation. Across all of these different contributions, however, nearly every method suffers from at least one of two common drawbacks: the method requires a large amount of data to train and/or the method's performance drops dramatically when the training data are sparse/noisy and the models are mismatched with the truth. We propose to mitigate these issues through the use of an objective function that accounts for the uncertainty in the model that other methods struggle to manage. Our objective is derived from first principles utilizing a probabilistic model of the system dynamics such that the three primary sources of uncertainty present in every system identification problem are addressed: model, measurement, and parameter uncertainty. In contrast, the methods mentioned earlier most commonly rely on a least squares-based approach, which effectively bundles these three sources of uncertainty into one, often ignoring how they may interact. In fact, it can be provably shown that some of the most common objective functions do not account for at least one source of uncertainty, resulting in the method's performance suffering greatly. The most notable difference in our modeling from least squares-based algorithms is the inclusion of process noise regardless of whether we are interested in learning a deterministic or stochastic system. We empirically show that directly accounting for these three sources of uncertainty significantly increases the robustness of our algorithm compared to approaches that exclude these uncertainties. In this work specifically, we present an objective function for learning linear subspace models. We demonstrate that this algorithm can effectively capture nonlinear dynamics through the approximation of the Koopman operator, can learn low-dimensional representations of high-dimensional PDE systems, and can even learn chaotic systems due to our robust management of uncertainty. Furthermore, we show that our method consistently outperforms existing least squares-based algorithms and is able to closely approximate a given dynamical system when the data are noisy and/or sparse beyond what most existing algorithms can handle.

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Title: Continuous Modal Bases for Parameter-Varying Dynamical Systems

Author(s): *Nicholas Hamilton, *National Renewable Energy Laboratory*;

By construction, reduced order models (ROMs) defined through modal decomposition methods are able to approximate the dynamics of a full state-system around a single operating point. Sufficiently far from the point of their definition, no ROM can be expected to accurately represent the target system dynamics. In the case of energy systems, normal operation may include a wide range of environmental and operational conditions. An alternative to driving reduce order models toward a single set point is to have defined dynamics for a range of parameter spaces representing external forcing and operational settings. Attempts to support the natural response of the target system dynamics to changes in exogenous forcing states have been proposed, most notably the dynamic mode decomposition (DMD) with control or input-out DMD. However, the addition of a control vector or process block to the definition of the modeled dynamical system does not help the ROM response; the structures identified through DMDc or ioDMD cannot contain target system dynamics in conditions outside of their definition. Representation of system dynamics over a parameterized operational space is requires that those dynamics be available to the ROM definition in order to include them in the modal basis retained for modeling, either significantly increasing the computational costs associated with modal decompositions or building a library of individual model bases that represent the target system response to different operating conditions. Because the modes or coherent structures in a ROM are derived from dynamics embedded in input data, changes to the operational state of a target system that are represented in the data can be seen in the resultant modal basis. A smooth transition of modes reflect changes in the operating environment of a target system indicates a continuity between Krylov subspaces. This work explores the smooth transition of DMD modes representing turbulent structures in an offshore wind turbine wake due to changes imposed on the wind turbine operation. The state-adaptive continuity of modal structures are considered as a continuous manifold of Krylov subspaces that can be characterized by a smooth surface in the parameter space. Subspace manifolds reflect the inherent variability of a reduced order model under the influence of operational parameters, including regions of attenuated dynamics and unstable operation. In the present case, the manifold highlights the emergence of turbulent structures in the wake and the increase of their relative importance as the turbine yaws with respect to the incident wind.

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Title: Sensor Selection for Configuration-Dependent Linear Bayesian Inverse Problems

Author(s): *Nicole Aretz, *RWTH Aachen University*; Peng Chen, *The University of Texas at Austin*; Denise Degen, *RWTH Aachen University*; Karen Veroy, *Eindhoven University of Technology*;

In numerical simulations, mathematical models are widely used to predict the behavior of a physical system. The uncertainty in the prediction caused by unknown parameters can be decreased by incorporating measurement data: by means of Bayesian inversion a posterior probability distribution can be obtained that updates prior information on the uncertain parameters. As experimental measurement data can be expensive, sensor positions need to be chosen carefully to obtain informative data despite a limited budget. In this talk we consider a group forward models that are characterized through different configurations of the physical system. The configuration is a non-linear influence on the solution, and can, for instance, be the geometry or material of any individual work piece in a production chain. Our goal is to choose one set of sensors for the estimation of an uncertain linear influence hat yields informative data for all possible configurations. We identify an observability coefficient that links the experimental design to the covariance of the posterior. We then present a sequential sensor selection algorithm that, supported by model order reduction for computational feasibility, improves the observability coefficient uniformly for all configurations.

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Title: Continuity with Respect to Data and Stability due to Changes in Parameters of Nonlocal Models

Author(s): *Nicole Buczkowski, *University of Nebraska-Lincoln*; Mikil Foss, *University of Nebraska-Lincoln*; Michael Parks, *Sandia National Laboratories*; Petronela Radu, *University of Nebraska-Lincoln*;

Background and Motivation: Nonlocal operators are advantageous choices in modeling due to their flexibility in handling discontinuities, incorporating nonlocal effects, and modeling a range of interactions through different choices for kernels. Using these operators in models has several applications, notably peridynamics. Continuous dependence implies that changes in data and parameters yield comparable changes in solutions. Since measured data is never exact, for a mathematical model to be physically relevant, small changes in data or parameters will yield appropriate changes in the solution. These continuity properties are also imperative for useful results in numerical analysis, where small variations that are beyond computer precision should not be reflected in the numerical solutions produced. For the nonlocal boundary value problem we prove that changes in the forcing, collar, or kernel bound the changes in the solution in some appropriate norm. Main Results for Continuous Dependence of Nonlocal Operators: A first result regarding the dependence of solutions on the forcing term uses a mean-value type property and convolution properties, however, it requires a condition on the size of the collar. A second theorem that does not require such a condition is based on an energy argument and utilizes nonlocal versions of classical results. We can further adapt this theorem to the nonlinear setting, given some added conditions on the forcing term. We are also able to quantify the dependence of solutions on boundary (collar) data using this adapted energy method. Finally, we are able to quantify variations of the solution with kernel changes, thus recording the system's sensitivity to the type of nonlocal interactions.

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Title: Mesoscale Modeling of Facet Formation in Graphene-Metal Interfaces

Author(s): *Nikhil Chandra Admal, *University of Illinois at Urbana-Champaign*; Tusher Ahmed, *University of Illinois at Urbana-Champaign*; Mitisha Surana, *University of Illinois at Urbana-Champaign*;

The chemical vapor deposition (CVD) of graphene on metal serves as a robust method to synthesize high quality graphene flakes. Therefore, understanding the thermodynamics and kinetics of graphene-metal interface is an important step towards synthesizing high quality graphene during CVD. The focus of this talk is on the modeling of the formation of facets in graphene-metal interfaces during CVD. The size of the facets on a graphene-metal interface are about 100 nm in width and 10 nm in height. Materials characterization clearly shows variations in the nature of facets across grain boundaries of the metal clearly highlighting the role of crystallography of the substrate. Recent molecular dynamics and experimental studies of Yi et al. [2018] suggest bunching of atomic-sized steps on vicinal surfaces of metal driven by the bending rigidity of graphene as a possible mechanism for the formation of facets. In this talk, we will present an atomistically informed mesoscale continuum model that is based on the work of Gurtin and Jabbour [2002] to model the evolution of graphene-metal interfaces. Equipped with orientation-dependent surface energy and a bending rigidity obtained from molecular dynamics, the evolution of a graphene-metal interface is enabled by surface diffusion of metal atoms. The direction and scale of facets predicted by the model, simulated using the finite element method, is compared with those observed in experiments. This work lays the groundwork to explore the relationship between the atomic scale interactions at graphene-metal interfaces and the facets observed at a mesoscale. References: Morton E Gurtin and Michel E Jabbour. Interface evolution in three dimensions with curvature-dependent energy and surface diffusion: Interface-controlled evolution, phase transitions, epitaxial growth of elastic films. Archive for rational mechanics and analysis, 163(3):171–208, 2002. Ding Yi, Da Luo, Zhu-Jun Wang, Jichen Dong, Xu Zhang, Marc-Georg Willinger, Rodney S Ruoff, and Feng Ding. What drives metal-surface step bunching in graphene chemical vapor deposition? Physical review letters, 120(24):246101, 2018.

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Title: Modeling Photo-Sensitive Polymeric Gels

Author(s): *Nikola Bosnjak, *Cornell University*; Shawn Chester, *New Jersey Institute of Technology*;

Exposing a dry polymeric network to a suitable solvent, causes the network to imbibe the solvent molecules and undergo a volumetric deformation known as swelling. A polymeric network in this mixed and swollen state is known as a polymeric gel. It is well known that the stress and solvent content are coupled and together affect the overall behavior of the polymeric gel. In addition, many polymeric gels are known to respond or activate when exposed to a light stimulus. This light-driven alteration of the behavior is known to be caused by the photochemical reactions occurring inside the polymeric network. Thus, the overall response of photo-sensitive polymeric gels is affected by the (i) mechanical stress, (ii) solvent content, and (iii) the extent of photochemical reaction caused by light irradiation. Photo-sensitive polymeric gels find a vast range of applications due to their mechanical properties and environmental responsiveness. The responsiveness of polymeric gels to irradiation has been widely utilized in soft robotics, and has also showcased a promising potential in microfluidics and drug delivery. While influence of the photochemical reactions on swelling has been well documented, recent experimental studies suggest the influence of the photochemical reactions goes beyond the degree of swelling. More specifically, the studies report the viscoelastic response of gels, alongside the polymer-solvent interaction, is affected by the photochemical reactions. The objective of this work is to develop a continuum-level constitutive model and numerical implementation, which takes into account experimentally observed change in behavior of gels due to photochemical reactions. The proposed model takes into account the limited extensibility of the polymer chains through a non-Gaussian statistical mechanics model. Further, the mixing between the polymeric network and solvent molecules is implemented using a Flory-Huggins model. Lastly, the influence of light is taken into account through a photochemical reaction, which affects the degree of volumetric swelling and visoelasticity. The photo-chemo-mechanical continuum framework involves the three balance laws, represented by the coupled partial differential equations, i.e., (i) the balance of forces and moments, (ii) the balance of solvent content and (iii) the radiative transfer. For solving this coupled set of equations, we employ the finite element method and numerically implement the framework in the finite element software Abaqus/Standard as a user element (UEL) subroutine. Along with the framework, we implement the developed constitutive model, thus providing robust simulation capabilities for the photo-chemo-mechanically coupled behavior of photo-sensitive polymeric gels in general boundary value problems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Model for 3D Deformation and Reconstruction of Contractile Microtissues

Author(s): Jaemin Kim, *Cornell University*; Erik Mailland, *École polytechnique fédérale de Lausanne*; Selman Sakar, *École polytechnique fédérale de Lausanne*; *Nikolaos Bouklas, *Cornell University*;

Engineered fibrous tissues consisting of cells encapsulated within collagen gels are widely used three-dimensional in vitro models of morphogenesis and wound healing. While biological characteristics have been extensively studied, the importance of their mechanical behavior has been recently recognized. Microtissue modeling has mainly been restricted to 2D models. This work is concerned with studying complex 3D deformation patterns that arise in microtissues prior and post-damage. The complex mechanics of contractile fibrous microtissues, are captured from a novel continuum model which considers a distinct contractile response on the surface and in the bulk, necessary to capture wound healing. The main goal of this contribution consists in the development of constitutive modeling developments and the numerical implementation and the 3D experimental characterization of the shape of the microtissues. We used microelectromechanical systems technology to generate arrays of fibrous microtissues and robot-assisted microsurgery to perform local incisions. The model simulations, which reproduced the experimentally observed shape changes after surgical operations, indicate that fitting of only bulk and surface contractile moduli is enough for the prediction of the equilibrium shape of the microtissues and indicate a lower Poisson’s ratio is necessary to model the evolution of the deformation from the initial uncontracted state in the micro-wells. The computational and experimental methods we have developed provide a general framework to study and predict the morphogenic states of contractile fibrous tissues under external loading at multiple length scales

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Title: Stability and Length Scales of Dislocation Walls: Analysis via Monte Carlo-Discrete Dislocation Dynamics

Author(s): *Nipal Deka, *Rutgers University*; Ryan Sills, *Rutgers University*;

One of the long-standing questions in dislocation theory is: what gives rise to the broad array of dislocation patterns that are observed in deformed metals? These patterns are believed to significantly influence work hardening and strain localization, among many other phenomena. Often these patterns are comprised of dense wall structures (e.g., cell walls) interspersed with regions of low density (e.g., cells). In order for such patterns to form, these confined wall structures must be stable and their width must be much less than the cell diameter. To date, there have been few studies of confined wall structures which provides insight into their stability and intrinsic length scales. To enable such a study, we have developed a new, Monte Carlo (MC) based solver for discrete dislocation dynamics (DDD) whereby dislocation lines are added to the system one-by-one, subject to a user-defined acceptance criterion. Using this solver, dislocation structure evolution can be studied in a controlled way that is not possible using conventional DDD methods. Using the MC-DDD method, we have evaluated the evolution of planar dislocation structures as new lines are introduced. Interestingly, we find that after reaching a critical dislocation density, the dislocation walls adopt a characteristic width which does not change as additional dislocation lines are added. This characteristic width is sensitive to the acceptance criterion used during MC steps. We have further evaluated the dislocation storage rate within the walls and variation in boundary misorientation with dislocation addition. Our results demonstrate for the first time that dislocation structures can adopt characteristic length scales that naturally arise from elastic interactions within the network. We believe that the new MC-DDD method will enable systematic studies of dislocation patterns, providing unprecedented insight into the underlying mechanics.

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Title: Edge-Promoting Adaptive Bayesian Experimental Design for X-Ray Imaging

Author(s): Tapio Helin, *LUT University*; *Nuutti Hyvönen, *Aalto University*; Juha-Pekka Puska, *Aalto University*;

This work considers edge-promoting sequential Bayesian experimental design in (discretized) X-ray imaging. The process of computing a total variation type reconstruction of the internal absorption of the imaged body via the lagged diffusivity iteration [1] is interpreted in the Bayesian framework. Assuming a Gaussian additive noise model, this leads to a Gaussian posterior with a covariance structure that contains information on the location of the edges in the reconstruction that is formed based on the currently available projection images. The next projection geometry is then chosen through A-optimal design (cf. [2]); as is well known, in the considered linear and finite-dimensional setting with Gaussian prior and noise models, this corresponds to minimizing the trace of the posterior covariance matrix after the new projection. Two and three-dimensional numerical examples demonstrate the functionality of the introduced approach. [1] Vogel, C. R., and Oman, M. E. Iterative methods for total variation denoising. SIAM J. Sci. Comput. 17 (1996), 227–238. [2] Burger, M., Hauptmann, A., Helin, T., Hyvönen, N., and Puska, J.-P. Sequentially optimized projections in x-ray imaging. arXiv preprint arXiv:2006.12579 (2020).

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Title: Nanoscale Investigation of Shock Wave Propagation Through Amorphous Polymers and Their Interfaces with Hard Materials

Author(s): *Nuwan Dewapriya, *Carleton University*; Ronald Miller, *Carleton University*;

Recent advances in microprojectile impact tests have enabled experimentalists to explore the mechanics of nanomaterials under extreme conditions. However, the existing experimental techniques are unable to elucidate some of the complex atomistic mechanisms associated with the ballistic impacts, which can only be realized through atomistic simulations. For example, in contrast to the macroscopic experimental observations, our molecular dynamics (MD) simulations revealed that placing a nanoscopic polymer layer on the strike face is more effective than placing it on the back face of a nanoscopic metallic target [1]. Moreover, MD simulations have also demonstrated that the ballistic limit velocity and the specific penetration energy of the nanoscale multilayers are significantly higher than the experimentally measured values for other nanomaterials [2]. In this work, we conducted a comprehensive MD study of shock wave propagation through amorphous polyurea and polyurethane as well as polymer/aluminum and polymer/silicon-carbide interfaces. We first computed the shock Hugoniot of polymers, using an MD simulation method called multiscale shock technique [3], and compared them with the existing experimental data to evaluate the fidelity of a classical non-reactive force field in modeling polymers under extreme conditions. This investigation helped us to establish the upper limits of the particle velocity that can be accurately modeled using the classical MD force field. Subsequently, density functional theory calculations were performed to obtain accurate MD force field parameters to model the adhesive interactions of selected material interfaces. Thereafter, we explicitly model the dynamic shock wave propagation and spallation of polymers as well as polymer/ceramic and polymer/metal multilayers. Our MD simulations provide significant insight into the nanoscale mechanisms associated with the dynamic behavior of materials under extreme conditions. References [1] M.A.N. Dewapriya, R.E. Miller, Comput. Mater. Sci. 184, 109951 (2020). [2] M.A.N. Dewapriya, R.E. Miller, J. Appl. Mech. 87, 121009 (2020). [3] E. J. Reed, L.E. Fried, and J.D. Joannopoulos, Phys. Rev. Lett. 90, 235503 (2003).

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Title: The Modified Error in Constitutive Equation Formulation for the Shear Wave Elastography Inverse Problem

Author(s): *Olalekan Babaniyi, *Rochester Institute of Technology*; Wilkins Aquino, *Duke University*;

Shear wave elastography (SWE) is a technique used to estimate the mechanical proper- ties of soft tissue from measurements of its deformation field. These mechanical properties can be used to noninvasively diagnose and help with the treatment of various diseases. Es- timating the mechanical properties requires solving an inverse problem that is challenging because of noisy and sometimes missing measurements, and ill posedness of the governing equations (due to unknown boundary conditions, resonances etc). We present a modified error in constitutive equations (MECE) formulation to recon- struct the mechanical properties from noisy shear wave deformation data, without knowl- edge of the boundary conditions in the forward model [2]. The formulation leads to stable solutions of the inverse problem without the need for regularization, and has been shown to have a well posed forward model [1]. The formulation achieves this by treating the measurements, constitutive equations, and unknown boundary data as unreliable. We successfully use the formulation to reconstruct the mechanical properties from sim- ulated data, and measurements collected from a tissue mimicking phantom manufactured to have the same acoustic and mecnaincal properties as soft tissue. We also show the ef- fect of using quasi-newton optimization strategy, and a alternating directions minimization strategy to solve the nonlinear inverse problem. Finally, we show the effect of adding total variation regularization to the MECE formulation. References [1] Wilkins Aquino and Marc Bonnet. Analysis of the error in constitutive equation ap- proach for time-harmonic elasticity imaging. SIAM Journal on Applied Mathematics, 79(3):822–849, 2019. [2] Manuel I Diaz, Wilkins Aquino, and Marc Bonnet. A modified error in constitutive equation approach for frequency-domain viscoelasticity imaging using interior data. Computer methods in applied mechanics and engineering, 296:129–149, 2015.

16th U.S. National Congress on Computational Mechanics
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Title: Nonlocal Phase-Field Models for Describing Sharp Interface Dynamics

Author(s): *Olena Burkovska, *Oak Ridge National Laboratory*;

Phase-field models are a popular choice in computational physics to describe complex dynamics of substances with multiple phases and are widely applied in various applications including solidification or fracture mechanics. Usually, diffuse interface models that are governed by local differential operators are employed, such as Cahn-Hilliard or Allen-Cahn. In contrast, we analyze models where the interface evolution is represented by a coupled system of local-nonlocal dynamics. While the classical local phase-field models always lead to a diffuse interface, we demonstrate that under certain conditions and with a careful choice of the nonlocal operator we can obtain a model that allows for a sharp interface in the solution. We study different models of Cahn-Hilliard and Allen-Cahn type involving a nonsmooth obstacle double-well potential. Here, the lack of smoothness of the potential is essential to guarantee the aforementioned sharp-interface property. Mathematically, this introduces additional inequality constraints that, in a weak form, lead to a coupled system of variational inequalities. We prove the well-posedness and regularity properties of the solutions and present efficient space-time discretizations that can handle these sharp interfaces. Finally, we discuss extensions to more complex models arising in the context of solidification, where the nonlocal phase-field model is additionally coupled to local diffusion equations. We develop appropriate numerical methods that can be realized efficiently, investigate energy stability properties, and support our findings with several numerical experiments.

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Title: A Unified Approach for Topology Optimization with Local Stress Constraints Considering Various Failure Criteria: von Mises, Drucker-Prager, Tresca, Mohr-Coulomb, Bresler-Pister, and William-Warnke

Author(s): *Oliver Giraldo-Londoño, *University of Missouri*; Glaucio H. Paulino, *Georgia Institute of Technology*;

An interesting, yet challenging problem in topology optimization consists of finding the lightest structure that can withstand a given set of applied loads without experiencing local material failure. Most studies consider material failure via the von Mises criterion, which limits the designs to structures made of ductile metals. To extend the range of applications to structures made of a variety of different materials, we introduce a unified failure function that can represent several failure criteria including von Mises, Drucker-Prager, Tresca, Mohr-Coulomb, Bresler-Pister, and William-Warnke, and use it to solve topology optimization problems with local stress constraints. The unified failure function not only represents all these failure criteria but also provides a smooth representation of the Tresca and the Mohr-Coulomb criteria—an attribute that is desired when using gradient-based optimization techniques. In this presentation, we provide details of the unified formulation and present numerical examples to illustrate how the unified failure function can be used to obtain different designs, depending on the type of material used to fabricate the topology-optimized parts.

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Title: Uncertainty Quantification in the Vibration Analysis of a Spent Nuclear Fuel Container with High Modal Density

Author(s): *Olivier Ezvan, *Université Gustave Eiffel*; Xiaoshu Zeng, *University of Southern California*; Roger Ghanem, *University of Southern California*; Bora Gencturk, *University of Southern California*;

The context of this work is the vibration analysis of a fully-loaded canister used for transportation and storage of spent nuclear fuel assemblies (FA). The vibration analysis is restricted to the external surface of the cylindrical canister and is aimed at probing the structural integrity of the canister internals (i.e., the FA). Each FA is comprised of a bundle of numerous slender rods (the fuel rods) and the canister exhibits separate structural levels. The fine description of the structural levels leads to a finite element model with more than 100 million degrees of freedom. In addition, the modal analysis entails around half a million modes that arise from the isolated vibrations of the small components (mainly, the fuel rods). As the numerous components and several structural levels are connected together through narrow interfaces, Craig-Bampton (CB) substructuring is efficiently implemented with Schur complement factorization and Shift-Invert Lanczos algorithm for solving the CB eigenvalue problem. There are parameter uncertainties and modeling errors, which need to be taken into account for a robust prediction of the structural response. In particular, to distinguish the variations in the structural response pertaining to inherent uncertainty from variations due to internal damage to FA or fuel rods, a stochastic model of uncertainties is necessary. The nonparametric approach of uncertainties in structural dynamics, based on random matrix theory, has been introduced by C. Soize in the early 2000s. In this approach, instead of considering the physical parameters (such as the Young modulus), it is the mathematical operators (in their matrix form) that are randomized. In this work, the nonparametric approach is used and adapted to the unusual case of a high modal density. The matrices to be randomized are very large and their entries are associated with different types of modes. For the nonparametric approach to be computationally tractable, a removal of the least dominant modes is carried out, leading to a reduction of a factor ten, without significant loss of accuracy. Due to the diverse nature of the numerous modes, the equal treatment of uncertainty between modes leads to spurious behavior of the classic nonparametric model. A sensitivity analysis is carried out and it is found that removing the random matrix coupling terms, equating the statistical dispersion levels for mass and stiffness, and randomizing only a subset of dominant modes, leads to an improved behavior.

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Title: Unfitted Hybrid High-Order Methods for the Wave Equation

Author(s): Erik Burman, *University College of London*; *Omar Duran, *Ecole des Ponts ParisTech*; Alexandre Ern, *Ecole des Ponts ParisTech*;

We design an unfitted hybrid high-order (HHO) method for the wave equation. The wave propagates in a domain where a curved interface separates subdomains with different material properties. The key feature of the discretization method is that the interface can cut more or less arbitrarily through the mesh cells. We address both the second-order formulation in time of the wave equation and its reformulation as a first-order system. We prove H1-error estimates for a space semi-discretization in space of the second-order formulation, leading to optimal convergence rates for smooth solutions. Numerical experiments illustrate the theoretical findings and show that the proposed numerical schemes can be used to simulate accurately the propagation of acoustic waves in heterogeneous media, with meshes that are not fitted to the geometry. For the second-order formulation, the implicit, second-order accurate Newmark scheme is used for the time discretization, whereas (diagonally-implicit or explicit) Runge-Kutta schemes up to fourth-order accuracy are used for the first-order formulation. In the explicit case, we study the CFL condition on the time step and observe that the unfitted approach combined with local cell agglomeration leads to a comparable condition as when using fitted meshes [1]. [1] E. Burman, O. Duran, and A. Ern. Unfitted hybrid high-order methods for the wave equation. Available at https://hal.archives-ouvertes.fr/hal-03086432, 2020.

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Title: Artificial Generation of Representative Single Li-Ion Electrode Particle Architectures From Microscopy Data

Author(s): *Orkun Furat, *Ulm University*; Donal Finegan, *National Renewable Energy Laboratory*; Kandler Smith, *National Renewable Energy Laboratory*; Volker Schmidt, *Ulm University*;

Accurately capturing the shape and intergranular architecture of lithium-ion electrode particles in 3D is essential for quantifying their influence on material properties, like, for example, sub-particle lithium transport, rate limitations, and degradation mechanisms. Microscopy techniques like X-ray nano-computed tomography (CT) and focused ion beam (FIB) - electron backscatter diffraction (EBSD) can provide representative 3D images of the particles' shape (outer shells) and their grain architecture, respectively. However, it can be quite time-consuming and costly to rely solely on imaging techniques for generating a sufficient amount of data for the analysis of structure-property relationships. In this talk, we present an alternative approach using stochastic geometry models. More precisely, using machine learning supported image processing followed by parametric stochastic geometry modeling, we leverage data from X-ray nano-CT and FIB-EBSD to generate artificial but representative single particle architectures completed with grain morphological details. Therefore, the FIB-EBSD data depicting the 3D architecture of a single lithium-ion electrode particle is segmented into individual grains. To do so, grain boundaries depicted in the image data were enhanced by deploying a convolutional neural network, followed by the application of a marker-controlled watershed algorithm [1]. Then, a random Laguerre tessellation model is fitted to the segmented FIB-EBSD data from which we can generate virtual, but statistically representative grain architectures [2]. Analogously, we utilize nano-CT data depicting the outer shells of numerous particles to derive a random outer shell model, using parametric random field models on the sphere [2]. By combining both models, we can generate a large number of virtual particles with statistically representative shapes and grain morphologies, which can be used as input for numerical simulations, i.e., for virtual materials testing to study the influence of a material's geometry on its physical properties. Moreover, by systematic variation of model parameters, a wide range of virtual particles with statistically distinct morphologies can be generated to increase the database for the investigation of structure-property relationships in the search for ideal particle architectures for high energy- or power-density cells.
References [1] O. Furat, D. P. Finegan, D. Diercks, F. Usseglio-Viretta, K. Smith and V. Schmidt, Mapping the architecture of single electrode particles in 3D, using electron backscatter diffraction and machine learning segmentation. Journal of Power Sources 483 (2021), 229148. [2] O. Furat, L. Petrich, D. P. Finegan, D. Diercks, F. Usseglio-Viretta, K. Smith and V. Schmidt, Artificial generation of representative single Li-ion electrode particle architectures from microscopy data. Preprint (submitted)

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Title: A Quadrature Free Approach for Isogeometric and Immersed Method in Trimmed Domains

Author(s): *Pablo Antolin, *École Polytechnique Fédérale de Lausanne*;

The computation of the integrals involved in the numerical solution of PDEs defined in immersed and trimmed isogeometric volumetric domains is a very challenging task. In this work we present an approach for computing them based on the exploitation of the polynomial representation of the volume's boundary. The integrals of polynomials can be computed by means of the divergence theorem, transforming volume integrals into face integrals. Due to the polynomial nature of both, the initial integrand and the boundary's geometrical representation, the integrands of the new face integrals are also polynomials themselves. By applying again the divergence theorem, face integrals are transformed into line integrals, along polynomials curves, whose integrands are also polynomials. Finally, the line integrals of polynomials can be computed explicitly without the use of numerical quadratures. This approach in based on two main hypotheses: 1) the domain's boundary is represented by means of (non-rational) polynomials; and 2) the integrand of the initial volumetric integral is also a polynomial itself. In the case in which the geometry is not described through non-rational polynomials (e.g., NURBS or primitive geometries), it is still possible to apply the described approach by first creating a polynomial approximation of the geometry. According to [1], in the case of elliptic problems it is possible to preserve the method's optimality by approximating the geometry with the same polynomial degree used for solution discretization. Regarding the second hypothesis, it is very common to encounter non-polynomial terms in the involved integrals. E.g., in the case of second (or higher) order problems in which the basis functions are mapped with non-affine transformations, or when non-polynomial coefficients appear. In such cases it is still possible to replace those terms with polynomial approximations that preserve the method's optimal approximation properties (as proved in [2]). These polynomial approximations require the calculation of local projections computed by means of standard quadrature rules. References: [1] Antolin, P., Buffa, A. and Martinelli, M. Isogeometric Analysis on V-reps: First results. Comput. Meth. Appl. Mech. (2019) 335:976–1002. [2] Mantzaflaris A. and Jüttler, B. Integration by interpolation and look-up for Galerkin-based isogeometric analysis. Comput. Meth. Appl. Mech. (2015) 284:373–400.

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Title: Surrogate Modeling For 3-D Patient-Specific Hemodynamics Using Statistical Shape Modeling and Deep Learning

Author(s): *Pan Du, *University of Notre Dame*; Xiaozhi Zhu, *University of Notre Dame*; Jian-Xun Wang, *University of Notre Dame*;

Due to the rising demand for acquiring comprehensive hemodynamic flow information for the diagnosis of cardiovascular diseases, image-based Computational Fluid Dynamics (CFD) has been widely employed to enable the derivation of functional information that is not accessible by medical images alone (e.g., pressure distribution, shear stress contour, velocity vector field), facilitating quantitative analysis and risk assessment in clinical therapy. However, such modeling requires numerically solving mesh-based discretization of partial differential equations, which is computationally expensive, particularly for complex flow or when considering fluid-structure interaction. This has largely limited the translation of image-based CFD to clinical treatments that require timely feedback for further therapeutic assessment and treatment planning. Moreover, it has posed a significant challenge to many-query applications, including uncertainty quantification, parameter estimation, and optimization problems arising in cardiovascular modeling. To enable efficient cardiovascular hemodynamic simulations, reduced-order or surrogate models have received increased attention and been developed as an alternative to predict functional information with a significantly less computational cost. For example, Lumped Parameter or 1-D reduced-order models are widely used to rapidly predict volumetric flow rate and have been an area of intense investigation. However, those approaches only focus on global information and are incapable of providing local flow information such as spatiotemporal fields of velocity or wall shear stresses, which is more crucial to advancing cardiovascular research/healthcare. Deep neural network (DNN) is renowned for its capability of approximating complex nonlinear functions and fast online inference speed. As a result, trained DNN shows a great potential of serving as a surrogate model for high-dimensional CFD simulations. In this work, we propose a novel deep learning surrogate modeling framework for image-based computational fluid simulations, enabling fast predictions of hemodynamics given complex 3-D patient-specific geometries.

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Title: An Overlapping Approach for Modelling the Filtration of Fluids in Porous Media

Author(s): *Paola Gervasio, *University of Brescia*;

The Navier-Stokes/Darcy problem modeling the filtration of incompressible fluids through porous media is the topic of this talk. To make this coupling, I consider the Interface Control Domain Decomposition (ICDD) method proposed in [1, 2]. The global computational domain, occupied by both the free fluid and the porous medium, is split into two overlapping subdomains in which I solve Navier-Stokes and Darcy equations, respectively. The overlap region is in fact the transition region between the two regimes. ICDD introduces virtual control variables on the subdomain internal boundaries (named “interfaces” even if they do not represent the classical interfaces typical of substructuring domain decomposition methods) that play the role of the unknown trace of the Stokes velocity and the unknown trace of the Darcy pressure. Such virtual controls are determined by minimizing a suitable cost functional that measures the jump between the Stokes velocity and the Darcy velocity as well as the jump between the Stokes pressure and the Darcy pressure at the interfaces of the decomposition. We solve an optimal control problem in which both controls and observation are defined on the interfaces and whose constraints are the PDEs on the overlapping subdomains ([3]). In this talk, we discuss both theoretical and computational aspects of the ICDD method applied to Stokes-Darcy coupling, and we show some numerical results. Then we compare our approach with classical coupling techniques based on non-overlapping decompositions and the well-known Beavers-Joseph-Saffman interface conditions. REFERENCES [1] M. Discacciati, P. Gervasio, and A. Quarteroni 2013 The interface control domain decomposition (ICDD) method for elliptic problems. SIAM J. Control Optim., vol. 51 (5), pp 3434-3458. [2] M. Discacciati, P. Gervasio, and A. Quarteroni 2014 Interface control domain decomposition methods for heterogeneous problems. Int. J. Numer. Meth. Fluids. Vol. 76 (8), pp 471-496. [3] M. Discacciati, P. Gervasio, A. Giacomini, and A. Quarteroni 2016 The interface control domain decomposition method for Stokes-Darcy coupling. SIAM J. Numer. Anal. vol. 54 (2), pp 1039-1068.

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Title: A Numerical Study of Extensional Flow-Induced Crystallization in Filament Stretching Rheometry

Author(s): *Patrick Anderson, *Eindhoven University of Technology*; Frank van Berlo, *Eindhoven University of Technology*; Gerrit Peters, *Eindhoven University of Technology*; Ruth Cardinaels, *Eindhoven University of Technology*;

A finite element model is presented to describe the flow, resulting stresses and crystallization in a filament stretching extensional rheometer (FiSER). This model incorporates nonlinear viscoelasticity, nonisothermal processes due to heat release originating from crystallization and viscous dissipation as well as the effect of crystallization on the rheological behavior. To apply a uniaxial extension with constant extension rate, the FiSER plate speed is continuously adjusted via a radius-based controller. The onset of crystallization during filament stretching is investigated in detail. Even before crystallization starts, the rheology of the material can change due to the effects of flow-induced nucleation on the relaxation times. Both nucleation and structure formation are found to be strongly dependent on temperature, strain rate and sample aspect ratio. The latter dependence is caused by a clear distribution of crystallinity over the radius of the filament, which is a result of the nonhomogeneous flow history in the FiSER. Therefore, this numerical model opens the possibility to a priori determine sample geometries resulting in a homogeneous crystallinity or to account for the nonhomogeneity.

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Title: Least-Squares Petrov--Galerkin Reduced-Order Models for Steady Hypersonic Aerodynamics

Author(s): *Patrick Blonigan, *Sandia National Laboratories*; David Ching, *Sandia National Laboratories*; Marco Arienti, *Sandia National Laboratories*; Francesco Rizzi, *NexGen Analytics*; Jeffrey Fike, *Sandia National Laboratories*;

High-fidelity simulations are becoming indispensable across a range of scientific and engineering disciplines. These simulations often employ extreme-scale nonlinear dynamical system models that require substantial computational resources. Such computational costs impose a barrier to using high-fidelity simulations for many-query and real-time applications such as uncertainty propagation, design optimization, model calibration, and control. While a range of surrogate models (e.g., data fits, lower-fidelity models) could be used to mitigate this computational burden, projection-based reduced-order models (ROMs) provide a particularly promising mechanism for doing so. This is due to the fact that ROMs remain strongly ‘tied’ to the high-fidelity physics, as they achieve computational savings by executing a projection process directly on the equations governing the high-fidelity model. While a wide range of ROM techniques has been developed for myriad applications, we focus on the least-squares Petrov—Galerkin (LSPG) projection [1], due to its observed accuracy and stability on large-scale problems, and its flexible optimization-based formulation that readily admits integration of structure-preserving constraints. LSPG has been demonstrated extensively on small-scale problems, but there have only been a few successful demonstrations of LSPG on large-scale steady-state applications [2,3]. This talk presents the application of LSPG to steady hypersonic computational fluid dynamics (CFD) simulations using Pressio, a novel “minimally-intrusive” ROM library developed at Sandia National Laboratories. The results presented are an extension of previous work [3], with wider input parameter ranges and different state approximation schemes than had been previously investigated. Additionally, the accuracy of the LSPG ROM is compared with other surrogate models. Finally, we discuss implications for model reduction of hypersonic CFD and other high-fidelity simulations. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2021-1303 A References [1] K. Carlberg, C. Bou-Mosleh, and C. Farhat. “Efficient non-linear model reduction via a least-squares Petrov–Galerkin projection and compressive tensor approximations,” International Journal for Numerical Methods in Engineering, Vol. 86, No. 2, p. 155–181 (2011). [2] K. M. Washabaugh, "Fast Fidelity for Better Design: A Scalable Model Order Reduction Framework for Steady Aerodynamic Design Applications", PhD Thesis, Department of Aeronautics and Astronautics, Stanford University, August 2016. [3] P. Blonigan, F. Rizzi, M. Howard, J. Fike and K. Carlberg, “Model reduction for steady hypersonic aerodynamics via conservative manifold least-squares Petrov–Galerkin projection” Accepted for publication by AIAA Journal, in press.

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Title: Quasistatic Fracture Using Nonliner-Nonlocal Elastostatics withan Analytic Tangent Stiffness Matrix

Author(s): *Patrick Diehl, *Louisiana State University*;

We apply a nonlinear-nonlocal field theory for numerical calculation of quasistatic fracture. The model is given by a regularized nonlinear pairwise (RNP) potential in a peridynamic formulation. The potential function is analytic and smooth. This fact allows us to write the entries of the tangent stiffness matrix analytically thereby saving computational costs during the assembly of the tangent stiffness matrix. We validate our approach against classical continuum mechanics for the linear elastic material behavior. In addition, we compare our approach to a state-based peridynamic model that uses standard numerical derivations to assemble the tangent stiffness matrix. The numerical experiments show that for elastic material behavior our approach agrees with both classical continuum mechanics and the state-basedmodel. The fracture model is applied to produce a fracture simulation for a ASTME8 like tension test. We conclude with an example of crack growth in a pre-cracked square plate. Our approach is novel in that only bond softening is used as opposed to bond breaking. For the fracture simulation we have shown that our approach works with and without initial damage for two common test problems

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Title: Surface Fluctuating Hydrodynamics Methods for the Drift-Diffusion Dynamics of Proteins and Microstructures within Curved Lipid Bilayer Membranes

Author(s): *Paul Atzberger, *University of California, Santa Barbara*;

We introduce surface fluctuating hydrodynamics approaches for investigating transport and fluid-structure interactions arising in cell mechanics within curved lipid bilayer membranes. We focus particularly on drift-diffusion dynamics of interacting proteins and microstructures. We show how a mesoscale stochastic description of the mechanics can be formulated (SPDEs) accounting for geometric contributions, hydrodynamic coupling, and thermal fluctuations. The underlying stochastic equations (SPDEs) pose practical challenges for use in simulations, including, (i) a need for accurate and stable discretizations of geometric terms and differential operators on curved geometries, (ii) techniques for hydrodynamics handling surface incompressibility constraints, and (iii) stiffness from rapid time-scales introduced by the thermal fluctuations. We show how practical spectral methods and meshfree computational approaches can be developed for simulations over long spatial-temporal scales. We then present results for protein and microstructure interactions within membranes and the roles played by hydrodynamic coupling and geometry.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Data-Driven Computational Approach Applied to a FE2 Multiscale Method for History-Dependent Materials

Author(s): *Paul-William Gerbaud, *ENS Paris-Saclay*; Pierre Ladevèze, *ENS Paris-Saclay*; David Néron, *ENS Paris-Saclay*;

As data-driven methods are making their way into the world of computational mechanics, we present our vision applied to multiscale calculation. Here, a classical FE2 calculation on a heterogeneous history-dependent material becomes a simple FE calculation. From an RVE combining two history-dependent materials, we build a homogenized Experimental Constitutive Manifold (ECM) which replaces the homogenized behaviour, using the method presented in [1,2] and applied in [3] to single materials. This ECM can then be used directly in a classical FE solver. Through this method, a calculation that would usually require a FE resolution at the RVE level for each element at the macroscopic level becomes a simple FE problem where the material model equations are replaced by the ECM. Therefore, we present our ECM building method applied to a multiscale calculation. An illustration is performed considering an RVE with two different viscoplastic materials and periodic boundary conditions.

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Title: Data-Driven Modeling of Subgrid-Scale Processes Using Deep Neural Nets and Transfer Learning

Author(s): *Pedram Hassanzadeh, *Rice University*; Ashesh Chattopadhyay, *Rice University*; Yifei Guan, *Rice University*; Adam Subel, *Rice University*;

Resolving all the relevant length and time scales in many CFD simulations, particularly of turbulent flows, is computationally challenging. In practice, low-resolution CFD solvers resolve the large-scale processes while the effects of the small-scale processes are often parameterized in terms of the large-scale variables. In the past few years, non-parametric data-driven parameterization (DD-P) using deep learning has shown promising results, but numerical stability (in online or a posteriori simulations) and generalization (i.e., extrapolation) have remained as challenging and important issues to address. In this talk, using 1D forced Burgers and 2D turbulent flows as testbeds, we 1) Show the promises of DD-P in representing subgrid-scale effects, in particular by capturing energy backscattering, while remaining numerically stable, and 2) Demonstrate how transfer learning enables DD-P to generalize to flows with higher Reynolds numbers.

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Title: Construction and Inverse Identification of Stochastic Models for Soft Biological Tissues Based on Experiments

Author(s): *Peiyi Chen, *Duke University*; Johann Guilleminot, *Duke University*;

This work focuses on the construction of stochastic models and inverse identification strategies for soft biological tissues. We specifically consider the modeling of anisotropic strain energy functions in nonlinear elasticity and investigate the definition of information-theoretic and deep-learning-based models ensuring well-posedness for the associated stochastic boundary value problem. We then discuss model calibration and validation using experimental data sets on artery walls.

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Title: Bayesian Learning of Heterogeneous Epidemic Models: Application to COVID-19 Spread Accounting for Long-Term Care Facilities

Author(s): *Peng Chen, *The University of Texas at Austin*; Keyi Wu, *The University of Texas at Austin*; Omar Ghattas, *The University of Texas at Austin*;

We propose a high dimensional Bayesian inference framework for learning heterogeneous dynamics of a COVID-19 model, with a specific application to the dynamics and severity of COVID-19 inside and outside long-term care (LTC) facilities. We develop a heterogeneous compartmental model that accounts for the heterogeneity of the time-varying spread and severity of COVID-19 inside and outside LTC facilities, which is characterized by time-dependent stochastic processes and time-independent parameters in 1500 dimensions after discretization. To infer these parameters, we use reported data on the number of confirmed, hospitalized, and deceased cases with suitable post-processing in both a deterministic inversion approach with appropriate regularization as a first step, followed by Bayesian inversion with proper prior distributions. To address the curse of dimensionality and the ill-posedness of the high-dimensional inference problem, we propose use of a dimension-independent projected Stein variational gradient descent method, and demonstrate the intrinsic low-dimensionality of the inverse problem. We present inference results with quantified uncertainties for both New Jersey and Texas, which experienced different epidemic phases and patterns. Moreover, we also present forecasting and validation results based on the empirical posterior samples of our inference for the future trajectory of COVID-19.

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Title: Residual stress modeling of a 17-4PH cantilever beam under additive manufacturing conditions

Author(s): *Phil DePond, *Stanford University*; Adrian Lew, *Stanford University*; Yi Shu, *Stanford University*; Wei Cai, *Stanford University*; Brandon McWilliams, *ARL*;

Though promising progress has fueled an intensely active research and design ecosystem in additive manufacturing (AM) of metals, there are still many challenges ahead for L-PBF technologies. For example, mechanical properties of AM metallic parts are known to be strongly affected by the strong thermal histories induced by the processing laser and residual stresses arise due to these large temperature gradients. These residual stresses and often unacceptable levels of distortion compromise the geometrical accuracy of printed parts. In addition, the variability from part-to-part and from machine to machine can challenge the certification of structural components for industries with strict material requirements. In the hope of informing the printing process, avoiding defects and controlling the quality of printed parts, it is desirable to ensure that models produce accurate enough predictions. Validation experiments are therefore necessarily conducted. We have designed deflection experiments of metallic substrates monitored by a high-speed camera, which would benefit calibrating thermo-mechanical models for residual stresses because of the substrate's simple thermal and mechanical history. In this thermo-mechanical model, a rate dependent thermo-elastic-viscoplastic constitutive behavior with isotropic hardening, dynamic recovery, static recovery/annealing and yield surface softening occurs below the melting point, with viscoelastic behavior at and above the melting point. The material constants for this internal variable model are guided by fitting to uniaxial stress strain data. By reproducing the deflection experiments with the model based on heat conduction and elasto-viscoplasticity, we conclude that the solid state phase transformation plays an indispensable role in the evolution of residual stresses of 17-4PH SS. We also highlight the necessity of monitoring time evolution instead of the end state when evaluating models for residual stress of alloys with volume change during phase transformation.

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Title: A Variational Multiscale Method for Heterogeneous Structures

Author(s): *Philipp Diercks, *Bundesanstalt für Materialforschung und -prüfung (BAM)*; Karen Veroy, *Eindhoven University of Technology*; Annika Robens-Radermacher, *Bundesanstalt für Materialforschung und -prüfung (BAM)*; Jörg F. Unger, *Bundesanstalt für Materialforschung und -prüfung (BAM)*;

In analyzing large scale structures, it is necessary to take into account the material heterogeneity for accurate failure prediction. However, this greatly increases the degrees of freedom in the numerical method, thus making it infeasible. Moreover, in applications where scale separation as the basis of classical homogenization schemes does not hold, the influence of the fine scale on the coarse scale has to be modelled directly. This work aims to develop an efficient methodology to model heterogeneous structures combining the variational multiscale method [1] and model order reduction techniques. Superposition-based methods assume a split of the solution field into coarse and fine scale contributions. In deriving practical methods, some form of localization is necessary to eliminate the fine-scale part from the coarse-scale equation. Hund and Ramm [2] discussed different locality constraints and resulting solution procedures in the context of solid mechanics. Particularly, zero jump conditions ensuring continuity of the fine scale solution which are enforced by a Lagrange-type method lead to a coupled solution procedure. In this contribution, a combination of the variational multiscale method and model order reduction techniques is applied to model the influence of the fine scale on the coarse scale directly. First, possible coarse and fine scale solutions are exploited for a representative volume element (RVE), specific to the material of interest, to construct local approximation spaces. The local spaces are designed such that local contributions of RVEs can be coupled in a conforming way. Therefore, the resulting global system takes into account, the effect of the fine scale on the coarse scale, is sparse, and has much lower dimensions compared to the full system in the direct numerical simulation. The authors gratefully acknowledge financial support by the German Research Foundation (DFG), project number 394350870. This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 818473). References [1] Hughes, T.J.R. and Feijoo, G.R. and Mazzei, L. and Quincy, J.-B. The variational multiscale method - a paradigm for computational mechanics. Comput. Methods Appl. Mech. Engrg. (1998) 166:3--24. [2] Hund, A. and Ramm, E. Locality constraints within multiscale model for nonlinear material behaviour. Int. J. Num. Meth. Engng. (2007) 70:1613--1632.

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Title: Multiscale Analysis and Design of Heterogeneous Materials Using an GFEM-Based Reduced-Order Modeling Approach

Author(s): David Brandyberry, *University of Illinois at Urbana-Champaign*; Xiang Zhang, *University of Wyoming*; *Philippe Geubelle, *University of Illinois at Urbana-Champaign*;

This work is motivated by advances made over the past few decades in (i) the mathematical formulations and numerical methods used for the multiscale analysis of complex materials, and (ii) additive manufacturing techniques, which allow the creation of heterogeneous materials with increasing complexity and precision. Motivated by advances in these two complementary fields, we have developed a multiscale modeling framework focused on the multiscale analysis and design of nonlinear heterogeneous materials, with as ultimate goal the optimization of the material microstructure to achieve a desired macroscopic constitutive response. The framework relies on three components: - The Interface-enriched Generalized Finite Element Method (IGFEM) that allows for the accurate and efficient analysis of the nonlinear response of heterogeneous materials using finite element discretizations that do not conform to the material microstructure. - A multiscale sensitivity analysis to quantify the sensitivity of the macroscopic response on the material and shape parameters that define the microstructure. The sensitivities are then combined with an optimization scheme to design the material microstructure that minimizes the gap between computed and desired macroscopic responses. - Reduced-order models (ROM) for the efficient multiscale analysis of the nonlinear constitutive and failure response of heterogeneous materials described by a combination of volumetric damage and cohesive interfacial failure models. The presentation will focus on the ROM-based multiscale analysis and design of 3D particulate composites. We will show how the GFEM/ROM-based approach allows for substantial (multiple orders of magnitude) savings in computational effort compared to traditional finite-element-based methods in the multiscale analysis of heterogeneous materials with small loss in precision. This computational efficiency is then taken advantage of to perform the top-down design of the composite microstructure to achieve a desired nonlinear homogenized constitutive response. Brandyberry, D., Zhang, X., and Geubelle, P. H. (2021) “A GFEM-based reduced-order homogenization model for heterogeneous materials under volumetric and interfacial damage”. To appear in Computer Methods in Applied Mechanics and Engineering.

16th U.S. National Congress on Computational Mechanics
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Title: Model-Free Data-Driven Fracture Mechanics

Author(s): *Pietro Carrara, *ETH Zurich*; Laura De Lorenzis, *ETH Zurich*; Laurent Stainier, *EC Nantes*; Michael Ortiz, *California Institute of Technology*;

We present a new paradigm for variational brittle fracture mechanics where the fracture-related material modeling assumptions are removed from the formulation, while retaining the epistemic laws of fracture that stem from variational principles [1]. In this approach, the fracture constitutive behavior is encoded exclusively in a discrete material data set, leading thus to a data-driven model-free approach [2]. We consider approaches based on both local and global stability principles, fulfilling in the former case the Kuhn–Tucker conditions for the energy release rate and, in the latter, the minimization of the total free energy. The data-driven solution of the fracture mechanics problem relies on the definition of a discrete quantity, generally termed distance, which attains its minimum in correspondence of the data point that best fulfills the conditions imposed by the global and local minimization principles, leading to the data-driven counterparts of both variational principles. Furthermore, the solution is constrained so as to fulfill the crack irreversibility condition. In this non-conservative framework, the crack extension plays the role of a history variable and the proposed approach belongs to the class of differential materials [3]. The data-driven solution relying on the global minimization approach is based on the minimization of a generalized distance coinciding with the total free energy computed in correspondence of each material point. For local minimization, two alternative data-driven distances are proposed, one based on the closest-point projection of the material data set onto the (analytically known) energy-release rate function and another based on the Kuhn–Tucker conditions. Both approaches are tested on double-cantilever-beam examples with different geometries, using artificially generated material data sets, with or without random noise, which reproduce or randomize Griffith and R-curve type fracture models. A convergence study with respect to the number of points and the noise amplitude of the data set is also performed. [1] Carrara, P., De Lorenzis, L., Stainier, L., Ortiz, M. (2020). Data-driven fracture mechanics. Computer Methods in Applied Mechanics and Engineering, 372, 113390. [2] Kirchdoerfer, T., Ortiz, M. (2016). Data-driven computational mechanics. Computer Methods in Applied Mechanics and Engineering, 304, 81–101. [3] Eggersmann, R., Kirchdoerfer, T., Reese, S., Stainier, L., Ortiz, M. (2019). Model-Free Data-Driven inelasticity. Computer Methods in Applied Mechanics and Engineering, 350, 81–99.

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Title: Hyperelastic Material Properties of Brain Myelinated Axons

Author(s): *Poorya Chavoshnejad, *Binghamton University*; Mir Jalil Razavi, *Binghamton University*;

The characterization of the mechanical properties of the human brain in microscopic or macroscopic scales is an important task to understand the normal or pathological development of human brain as well as the studying of brain trauma and developing therapeutic treatments. To date, most of the experimental studies by classical tension/compression/shear tests or magnetic resonance elastography (MRE) have reported the mechanical properties of brain averaged over the gray and white matters or over the specific macroscopic regions of interest. As the result, there is a missing correlation between the mechanical properties of the microscopic constituent elements and the bulk material properties of the brain. Specifically, white matter shows a higher anisotropic behavior than gray matter owing to including the high density of axonal fibers embedded in the extracellular matrix (ECM). In this study, we develop a representative volume element (RVE) model with the embedded element technique to exclusively find the hyperelastic material properties of the myelinated axons and their surrounding ECM. We implement a multi-objective optimization technique to caliber our model to find the material properties of axons according to the reported seven experimental tests for the bulk white matter tissue. These tests include three different modes in simple shear and two different modes in compression (axial and transversal) and tension (axial and transversal) of corpus callosum section that has highly aligned axonal fibers. Result of the study shows that the discrepancy between the reported values for the elastic behavior of white matter in literature stems from the anisotropic behavior of the tissue in the microscopic scale. Shear modulus of the myelinated axons is much larger than the ECM, and the shear modulus of the bulk tissue is significantly correlated with the fiber volume fraction (FVF). Moreover, the distribution of the axonal caliber has a small effect on the shear modulus of the white matter in tension, while this effect is considerable in compression and shear. The findings of this study provide the accurate hyperelastic material properties of the axonal fibers that can be used directly in the computational modeling of traumatic brain injury (TBI) and brain folding.

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Title: Multi-Scale Mechanical Model Coupled with an Energy-Based Criterion for Predicting Fracture Initiation in Strain-Crystallizing Rubbers

Author(s): *Prajwal Kammardi Arunachala, *Stanford University*; Reza Rastak, *Stanford University*; Christian Linder, *Stanford University*;

Strain Induced Crystallization (SIC) is a key phenomenon in enhancing the fracture toughness of polymers like Natural Rubber. This ensues in unique properties like high stretchability, which in turn finds myriad applications in fields like stretchable electronics and implantable sensors. Thus, models capable of explaining material behavior for different deformation states and eventually predicting fracture initiation in these polymers become vital in quantifying their stretchability. Although there are copious models describing SIC phenomenon, most of them restrict attention to uniaxial tensile loading cases. Additionally, there is a scarcity of models quantifying the effect of crystallization on fracture initiation in strain-crystallizing rubbers. Thus, we propose a multi-scale mechanical model capable of predicting material behavior when subjected to both uniaxial and biaxial deformation states, in conjunction with an energy-based criterion to predict crack initiation in rubber-like materials. Non-Gaussian statistical mechanics is utilized to describe the behavior of microscale polymer chains and crystallization is also considered in them at higher stretches. The rate-dependent evolution law of crystallization considered ensures the satisfaction of the second law of thermodynamics. Unlike the classical theories, the molecular bond deformation is considered by modeling the chain segments as elastic. A failure criterion based on the internal energy due to these bond stretches is used for predicting fracture initiation. The deformation at the macroscale is connected to the chain dynamics at the microscale with the help of a non-affine network homogenization model called Maximal Advance Path Constraint [1]. Its potential to account for anisotropy in the stretched network compels the model to be preferable due to its physical significance, for the purpose of fracture modeling. Continuous crystallization distributions [2] along the principal stretch directions are used at the macroscopic level to connect with crystallinity in the chains at microscopic level. The model is validated by comparison with existing experimental results for both crystallizing and non-crystallizing rubbers. In addition to its potential to predict the material behavior when subjected to uniaxial and biaxial loading, the capability of the model to quantitatively estimate the effect of crystallization on fracture initiation of strain-crystallizing rubbers is also verified. 1. M. Tkachuk, C. Linder, The maximal advance path constraint for the homogenization of materials with random network microstructure, Philosophical Magazine 92 (2012) 2779–2808. 2. R. Rastak, C. Linder, A non-affine micro-macro approach to strain-crystallizing rubber-like materials, JMPS 111 (2018) 67–99.

16th U.S. National Congress on Computational Mechanics
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Title: A Symphony of Data-Based, Physics-Based, and Agent-Based Models to Create a COVID-19-Safe Corridor for International Travel

Author(s): *Prathamesh Desai, *Rice University*; Nihar Sawant, *Courant Institute of Mathematical Sciences / New York University*; Achal Khilnani, *Mumbai University*;

Keywords: Artificial Intelligence, COVID-19 forecast, Multiphysics modeling, pollutant transport, cellular automata, automated transit systems The on-going existential threat of coronavirus pandemic has exposed the world to the flaws of over-optimized and low liquidity systems such as transportation, manufacturing, logistics, and supply chain. This crisis will result in a leapfrog towards a speedy adoption of autonomous systems controlled by artificial intelligence (AI) and their associated digital avatars or twins. Such systems would include autonomous driving cars, robotic personal rapid transit systems (PRT), and simulation guided engineering design. The general public would rely more on personal vehicles for inter-city, intra-state, and inter-state travel. Such transport means can provide a controlled and COVID-19-safe environment compared to rental cars or public transit. However, the public would continue to use commercial aircraft for international travel. Thus, there is a need to establish an individual-specific COVID-19 mitigation strategy for international travel. This series of works focuses on developing three computational models that can aid in creating such a COVID-19-safe corridor. The first one is a new data-based AI model [1], viz., Sentiment Informed Timeseries Analyzing AI (SITALA), to predict county-specific COVID-19 test positivity as a function of historical test positivity data and news sentiment obtained using IBM Watson Discovery News. SITALA is inspired by the Google-Wavenet architecture and makes use of TensorFlow. The second model is a physics-based one [2] to predict the distribution of the orally or nasally released pollutant inside the cabins of international aircrafts. The model is a full CFD RANS k-epsilon model with species transport. The model was executed on the Pittsburgh Supercomputer. The third and final model is an agent-based one to simulate a last-mile connectivity system in the form of a PRT loop at an international airport. PRT comprises automated pods on tracks and offers easy sanitation means compared to public transit systems such as monorails, trains, and buses. This cellular automata model simulates the traffic of PRT pods and predicts the percent capacity utilization of the system. [1] Desai, P.S., 2020. Sentiment Informed Timeseries Analyzing AI (SITALA) to curb the spread of COVID-19 in Houston. Expert Systems with Applications (under revision); Preprint medRxiv:2020.07.22.20159863. [2] Desai, P.S., Sawant, N. and Keene, A., 2020. On COVID-19-safety ranking of seats in intercontinental commercial aircrafts: A preliminary multiphysics computational perspective. Building Simulation (accepted); Preprint medRxiv:2020.08.17.20176909.

16th U.S. National Congress on Computational Mechanics
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Title: One Dimensional Nonlinear Elastic Wave Propagation in a Reid's Rate-Independent Pinched Hysteretic Material

Author(s): *Pravinkumar Ghodake, *Indian Institute of Technology Bombay*;

Single frequency (f) elastic wave propagating in a damaged material generate higher harmonics (2f, 3f, 4f,…), known as the acoustic nonlinear effect. The nonlinear effect in rocks observed experimentally due to the interaction of the wave with damages like micro-cracks and pores. In metals, elastic waves produce micro-plastic deformations due to movement and breakaway of dislocations, micro-cracks, and internal frictions. In theoretical and computational studies damaged materials are modeled as quadratic, cubic, and hysteretic nonlinearities. Acoustic nonlinearity is correlated to plasticity and micro-cracks that include hysteresis. Hysteretic models like Preisach-Mayergoyz, Hodgdon, Power Law, etc. were implemented for nonlinear elastic wave propagation studies to capture various shapes of hysteretic loops. Experimentally, pinched and non-pinched curves are observed in metals and rocks mainly due to micro-cracks dynamics. Nazarov (1888) and Gusev (1997) used two different constitutive models for hysteretic materials in their theoretical studies. Here in this study, a numerical study is carried out to understand the interaction of single and two frequency sinusoidal and Gaussian input pulses with a pinched hysteretic material model. A spatial domain is discretized as a long-chain of spring-mass elements along with a hysteretic spring element added in parallel. The hysteretic element is modeled as Reid’s pinched model (1956). Reid’s model is computationally less intensive as it surpasses the problem of singularities due to pinching. Interaction of single-frequency wave with Reid’s rate-independent pinched hysteretic material generates only odd harmonics and very nice pinched triangular hysteretic loops are observed both in the case of sinusoidal and Gaussian pulse inputs. The hysteretic loops obtained due to Gaussian pulse are evolving dynamically. For two-frequency input pulse, sum and difference frequency combinations along with the corresponding odd frequencies of the input frequencies are observed. Sharp vertical minor loops are captured effectively in two-wave mixing studies. In one-way two-wave mixing, two collinear longitudinal waves of different input frequencies are sent from the left end of the spatial domain. One-way mixing generates resonant waves with sum and difference frequency combinations. In two-way two-wave mixing, two longitudinal waves with different input frequencies are sent from the left and right end of a spatial domain independently and mixed at the center of the domain. Sum and difference frequency combinations are observed only in the mixing zone and the resonant wave is not generated. In the non-mixing domain both the waves propagate independently along with the generated odd harmonics corresponding to the input frequencies.

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Title: A Diffused Interface Based Non-local Crystal Plasticity Model to Capture the Effect of Slip Transmission Across Grain Boundaries on Elasto-Plastic Response of Polycrystals

Author(s): *Pritam Chakraborty, *Indian Institute of Technology Kanpur*; Devesh Tiwari, *Indian Institute of Technology Kanpur*; Jothi Mani Thondiraj, *Indian Institute of Technology Kanpur*; Pierre-Antony Deschenes, *Hydro Quebec*; Daniel Paquet, *Hydro Quebec*;

Transmissibility of dislocations across grain boundaries strongly influences the mechanical behavior of polycrystalline metals and alloys. Thus, incorporation of this mechanism in polycrystalline scale models of plasticity, creep, fracture and fatigue can significantly improve their accuracy. However, such grain boundary physics based polycrystal models are scarce owing to the difficulties in deducing appropriate physical laws of slip transmission and their subsequent numerical treatment. The present work addresses these shortcomings through the development of a diffused interface based grain boundary model of slip transmission. In the diffused interface representation, a grain boundary has been modeled as a region of coexisting grains where the slip rates have been penalized depending on misorientation [1]. Furthermore, the possibility of obstruction in motion of dislocations across a grain boundary has been included in the model from the direction of slip in the grains with respect to the local normal of the grain boundary. These considerations lead to misorientation dependent strain gradients at the grain boundary region, which has been physically related to geometrically necessary dislocations and the slip resistances thereof, by a non-local crystal plasticity model [2]. The non-local grain boundary dependent crystal plasticity model has been numerically integrated using Finite Element Method (FEM). A structured mesh could be used in the FEM simulations owing to the diffused representation of the grain boundaries. However, due to the use of small mesh size required to resolve the grain boundary regions, the number of degrees of freedom becomes extremely large. This limitation has been overcome by using a hanging node based biased mesh with refinement at and near the grain boundaries and coarser elements in the interior of grains. The model has been applied to understand the influence of grain size and misorientation on the macroscopic stress-strain response of polycrystalline face centered cubic grains. The analysis reveals that the Hall-Petch factor increases with the increase of average misorientation in the fundamental zone. [1] A.Ma, F.Roters, D.Raabe, "Studying the effect of grain boundaries in dislocation density based crystal-plasticity finite element simulations", International Journal of Solids and Structures, Volume 43, Issue 24, November 2006, Pages 7287-7303. [2] M. Anahid, M. K. Samal, S. Ghosh, "Dwell fatigue crack nucleation model based on crystal plasticity finite element simulations of polycrystalline titanium alloys", Journal of the Mechanics and Physics of Solids, Volume 59, Issue 10, October 2011, Pages 2157-2176.

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Title: A Data-Driven, Real-Time Thermal Process Simulation Model for Laser Powder Bed Fusion via Convolutional Neural Network and Long Short-Term Memory (CNN-LSTM)

Author(s): *Qian Chen, *University of Pittsburgh*; Albert To, *University of Pittsburgh*; Florian Dugast, *University of Pittsburgh*;

Laser powder bed fusion (L-PBF) has become one of the most widely used additive manufacturing technologies in academia and industry. The complex thermal conditions during the fabrication process highly depend on the geometry and have a significant impact on the part quality such as microstructure, grain texture, density and residual deformation. However, predictions for detailed thermal history with rapid heating and cooling are usually computationally expensive and time-consuming for part scale model because of the incompatible spatial scale between the laser beam (μm) and part (cm). In this work, a sequential machine learning model including convolutional neural network (CNN) and recurrent neural network (RNN), long short-term memory unit, is proposed for real-time thermal prediction. In this model, each sliced layer of the input geometry is processed by the CNN to extract feature vector. The feature vector is then taken as input by the RNN unit to predict the detailed thermal histories. This model is trained by nodal temperatures collected from ten geometries and shows the capability of accurate prediction on the test dataset. A 100x prediction speed improvement is achieved compared to the finite element analysis which makes the prediction faster than real fabrication process and real-time temperature profile available.

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Title: Robust Finite Element Method on Poor Grids via Discontinuous Galerkin Stabilized Meshfree Approximation: Fast Implementation and Theory

Author(s): *Quang-Thinh Ha, *Boston University*; Paul Kuberry, *Sandia National Laboratories*; Paul Barbone, *Boston University*; Nathaniel Trask, *Sandia National Laboratories*;

A finite element mesh serves two purposes: (1) defining the geometry of the model, and (2) representing the interpolating function. Task (1) is relatively easily accomplished. Task (2), on the other hand, is limited by mesh quality and is one of the key factors that determines the performance of the finite element method. Poor quality meshes may result from automated mesh generators, or by deformation of an initially high quality mesh. REBAR is a novel finite element framework recently introduced that divorces these two tasks. The geometry of the simulation domain is represented in the traditional way. REBAR uses compactly supported discontinuous shape functions which are generated from a meshfree method called Generalized Moving Least Squares. These discontinuous polynomials are then applied within a Discontinuous Galerkin (DG) with Interior Penalty (IP) variational framework. Since the basis functions definition is separated from the shape of the underlying elements, the dependence on mesh quality is removed. This presentation describes an a priori error analysis of this formulation. Our scalable implementation in COMPADRE, a COMpatible PArticle Discretization and REmap Toolkit, demonstrated the expected convergence behaviour, even on poor quality meshes.

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Title: Physics-Defined Deep Learning Frameworks on Mechanics of Moving Interfaces: Application to Fluid-Structure Interaction

Author(s): *Rachit Gupta, *University of British Columbia*; Rajeev Jaiman, *University of British Columbia*;

We introduce hybrid deep learning (DL) architecture focused on the physics of moving interface and predicting unsteady flow involving fluid-solid interaction (FSI). The full-order flow snapshots and point-cloud displacements are created using the discretized Navier-Stokes (NS) in the Arbitrary Lagrangian-Eulerian (ALE) reference frame as target physical data for combined dynamical learning and inference. The combined operation of the physics-related models with the reduced-order modeling based on DL makes our framework hybrid. Our proposed multi-level architecture consists of two data-driven physics-DL drivers that forecast unsteady flow and track moving point cloud displacements respectively while sharing force information at the physical interface. As a semi-supervised framework, the first driver relies on the proper orthogonal decomposition-based recurrent network (POD-RNN) to infer the ALE description of the moving point cloud. This model cardinally relies on physics-based POD basis modes to reduce dimensionality and evolve these modes as such. As a self-supervised DL tool, the second driver uses the convolution-based recurrent autoencoder network (CRAN) to predict the nonlinear flow dynamics on static Eulerian probes. We add these probes as spatially organized query nodes in the moving point cloud to address the Lagrangian to Eulerian field conflict and train the CRAN driver conveniently. We detail a novel snapshot-field transfer and load recovery (FTLR) algorithm to optimally select these Eulerian probes. They are selected in a way that the two drivers are constrained at the interface to recover bulk force quantities. Ultimately, these hybrid physics-DL drivers depend on recurring neural networks (RNNs) to transform the low-dimensional state. To assess the efficacy of this framework, the benchmark problem of flow past a free oscillating cylinder is chosen. This two-level system is capable of reliably recording the exact definition of the interface and forecasting extremely non-linear wake dynamics with minimal feedback demonstration. These findings inspire us to further explore the application of this hybrid framework to the idea of digital twinning of engineering structures, especially those with moving boundaries.

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Title: Data Assimilation and Mixed-Variable Metamodeling with Latent Map Gaussian Processes

Author(s): Nicholas Oune, *University of California, Irvine*; *Ramin Bostanabad, *University of California, Irvine*;

Gaussian processes (GPs) are ubiquitously used in sciences and engineering for metamodeling, uncertainty quantification, or Bayesian analyses. Standard GPs, however, can only handle numerical or quantitative variables. In this talk, I will introduce latent map Gaussian processes (LMGPs) that inherit the attractive properties of GPs but are also applicable to mixed data that have both quantitative and qualitative inputs. I will elaborate on the core idea of LMGPs which consists of learning a low-dimensional manifold where all qualitative inputs are represented by some latent quantitative features. Through a wide range of analytical and real-world examples, I will demonstrate the advantages of LMGPs over state-of-the-art methods in terms of accuracy and versatility. In particular, I will show that LMGPs (1) can handle variable-length inputs, (2) have a nice neural network interpretation, and (3) can assimilate multi-fidelity data without imposing any hard constraints on how low and high fidelity data sources are related.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Accurate Multi-Phase Flow Simulation in Faulted Reservoirs Using Mimetic Finite Difference Methods on Polyhedral Cells

Author(s): *Rencheng Dong, *The University of Texas at Austin*; Faruk O. Alpak, *Shell International E&P Inc.*; Mary F. Wheeler, *The University of Texas at Austin*;

Faulted reservoirs are commonly modeled by corner-point grids. Since the two-point flux approximation (TPFA) method is not consistent on non-orthogonal grids, multi-phase flow simulation using TPFA on corner-point grids may have significant discretization errors if grids are not K-orthogonal. To improve the simulation accuracy, we propose a novel method where the faults are modeled by polyhedral cells, and mimetic finite difference (MFD) methods are used to solve flow equations. We use a cut-cell approach to build the mesh for faulted reservoirs. A regular orthogonal grid is first constructed, and then fault planes are added by dividing cells at fault planes. Most cells remain orthogonal while irregular non-orthogonal polyhedral cells can be formed with multiple cell divisions. We use a standard IMPES algorithm for two-phase flow and MFD methods to solve the pressure equation over general polyhedral cells. First, we compared flux accuracy in faulted reservoirs between TPFA and MFD methods by solving a single-phase flow problem. The reference solution is obtained on a rectangular grid while the same problem is solved by TPFA and MFD methods on a grid with distorted cells near a fault. The fault did not have additional seal-factors applied on it such that the test problem fully focuses on grid non-orthogonality across the fault. As the grid becomes more distorted, fluxes computed using TPFA exhibit larger errors while fluxes computed using MFD methods are still as accurate as the reference solution. MFD methods reduce flux errors substantially on distorted non-orthogonal cells in faulted reservoir models. We also compared saturation accuracy of multi-phase flow in faulted reservoirs between TPFA and MFD methods. A two-phase (oil and water) flow problem is solved in a faulted reservoir with distorted cells using both TPFA and MFD methods while a reference solution is obtained on rectangular cells. Compared with the reference solution, saturation from TPFA exhibits non-physical errors near the fault while the saturation error from MFD is smaller than TPFA thanks to more accurate fluxes from MFD. Grid distortion is more local in the cut-cell paradigm than corner-point grids. Grid distortion errors can be significantly reduced over the reservoir model since most cells retain orthogonality. We quantitatively demonstrate that MFD methods are robust and yield highly accurate fluxes on non-orthogonal polyhedral cells near faults. This novel modeling method can substantially improve the accuracy of multi-phase flow simulations in faulted reservoirs while incurring a relatively small computational overhead over TPFA.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analysis of Higher Order Scattering Modes in Parameter Retrieval Method for the Characterization of Dispersive Media

Author(s): *Reza Abedi, *University of Tennessee*; Alireza Amirkhizi, *University of Massachusetts Lowell*;

The parameter retrieval method based on scattering data is used to derive dynamic constitutive parameters of 2D solids with periodic structure. The details of the parameter retrieval method and the causal spacetime discontinuous Galerkin (cSDG) method used for time domain simulations can be found in [1,2]. In the parameter retrieval method, an incident wave enters a slab of n unit cells from an ambient material on one side of the slab and exits from the other side. An equivalent homogeneous material is sought such that its transmission and reflection coefficients match those of the composite material. The characterized overall properties are valid from static to low frequency ranges. In its common form, only the averages of the stress and velocity fields are used for parameter retrieval. Herein, we perform a Fourier series expansion on the reflected and transmitted waves for both normal and shear waves. The first term of the expansion corresponds to the conventional parameter retrieval method. We demonstrate that the higher order modes have nonzero energy transmission and reflection that are missed by the conventional method. Specifically, we demonstrate that beyond a certain frequency, the higher order modes have a nonzero net energy input to the slab. If these modes are not considered, for a lossless unit cell design, some loss will be introduced into the overall properties beyond this frequency. We will relate this frequency limit to the diffraction phenomena. Finally, we discuss how the number of unit cells and the properties of the ambient material affect this frequency limit. This analysis is also helpful to determine the frequency range in which the characterized overall properties accurately represent the energy response of the composite. References: [1] A.V. Amirkhizi, "Homogenization of layered media based on scattering response and field integration." Mechanics of Materials 114: 76-87. 2017. [2] R. Abedi, A.V. Amirkhizi, “Use of loss limit approach to zero in scattering-based parameter retrieval of elastic micro-structured media”, International Journal of Solids and Structures, 200: 34-63. 2020

16th U.S. National Congress on Computational Mechanics
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Title: Low-Dimensional Structure in Bayesian Inference Problems with Mixture Models

Author(s): *Ricardo Baptista, *Massachusetts Institute of Technology*; Jayanth Jagalur Mohan, *Massachusetts Institute of Technology*; Youssef Marzouk, *Massachusetts Institute of Technology*;

Efficient solutions to many Bayesian inference problems exploit the low-dimensional structure in the prior-to-posterior update. Such structure typically arises when the data are informative only on a subspace of the parameters. Identifying the subspace, often labeled as the likelihood-informed subspace (LIS) is particularly challenging when using non-gaussian priors, and/or non-linear maps between parameters and data. When the likelihood and/or the prior are prescribed using Gaussian mixture models, the LIS for each component of the posterior mixture is easily identified, and cumulatively they describe the data informed directions for the full problem. We rigorously analyze the ability of these component LIS in approximating the posterior distribution, and demonstrate the utility of the underlying ideas in a high-dimensional atmospheric retrieval problem.

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Title: A 19-Node ‘Lagrangian’ Second-Order Pyramid Element for Explicit Dynamic Nonlinear Solid Mechanics

Author(s): *Robert Browning, *Synthetik Applied Technologies*; Kent Danielson, *US Army Engineer Research and Development Center*; David Littlefield, *The University of Alabama at Birmingham*;

Recent advances in second-order elements have made hex-dominant meshing an attractive option for explicit dynamic nonlinear solid mechanics. Such methods rely on robust element formulations capable of mass-lumping with all-positive masses at the nodes. One of the recent developments is a 19-node second-order pyramid element (Browning 2020) capable of serving as a transition element for hex-dominant meshing. The pyramid is referred to here as a “Lagrangian” pyramid, indicating that it has the same nodes as would be achieved by collapsing the classic 27-node Lagrangian hexahedral to a uniform pyramid with one quadrilateral face and four triangular faces. The 19-node pyramid (PYR19), however, uses rational shape functions, rather than polynomials, which permits it to mass-lump positively while also being compatible with 27-node hexahedral (Danielson and O’Daniel 2011) and 15-node tetrahedral (Danielson 2014) elements. These elements are supported in the meshing software Cubit and in the analysis codes EPIC and ParaAble, while Visualization is supported in ParaView. This presentation will focus on the numerical integration (i.e., quadrature) rules and extrapolation rules that are necessary for successful solution and post-processing, respectively. Examples of the pyramid’s utility in hex-dominant meshing will also be discussed. 1. Browning, R. S. (2020). “A second-order 19-node pyramid finite element suitable for lumped mass explicit dynamic methods in nonlinear solid mechanics.” Ph.D. dissertation, University of Alabama at Birmingham, Birmingham, AL. https://doi.org/10.13140/RG.2.2.26801.20322. 2. Danielson, K. T., and O’Daniel, J. L. (2011). “Reliable second-order hexahedral elements for explicit methods in nonlinear solid dynamics.” International Journal for Numerical Methods in Engineering, 85(9), 1073–1102. https://doi.org/10.1002/nme.3003. 3. Danielson, K. T. (2014). “Fifteen node tetrahedral elements for explicit methods in nonlinear solid dynamics.” Computer Methods in Applied Mechanics and Engineering, 272, 160–180. https://doi.org/10.1016/j.cma.2014.01.012.

16th U.S. National Congress on Computational Mechanics
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Title: Stabilized Coupled-Space-and-Time Framework to Model Periodic Flows

Author(s): *Robert Dyja, *Czestochowa University of Technology*; Biswajit Khara, *Iowa State University*; Saurabh Kumar, *Iowa State University*; Anupam Sharma, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

Flow past bluff and streamlined bodies exhibit multiscale periodic characteristics. Simulating these characteristics is important to quantify and design cruising performance -- for instance for ground vehicles, airplanes and marine vehicles. However, most of the computational effort in simulating these phenomena is in removing the transients, with over 90% of computing time usually taken for removing transients before data can be collected for analysis. Here we build on our prior work to formulate a variationally stabilized coupled-in-space-and-time framework that solves for large slabs of space-time. We show that by applying periodic conditions across the time dimension, we can directly extract periodic behavior. We detail how careful stabilization is critical for this approach to succeed. We illustrate this approach on canonical problems of flow past a cylinder and oscillatory bluff bodies.

16th U.S. National Congress on Computational Mechanics
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Title: Multi-Institution R&D for Computational Mechanics Solutions

Author(s): *Robert Ferencz, *Lawrence Livermore National Laboratory*;

In this talk we discuss computational mechanics research and development in the context of a multi-mission national security laboratory. Two LLNL examples are used to illustrate multiple phases of R&D that can engage different collaborations to support capability delivery to internal and/or external customers. The first case study is the Blast Protection for Platforms and Personnel Institute led by the US Army Research Laboratory through support by the Department of Defense HPC Modernization Program. This six-year project for simulation of blast-structure interaction sustained full production-capable implementations (and testing!) of embedded mesh algorithms [1] that were first researched through an academic collaboration [2]. The second case study pertains to thermomechanical modeling of laser powder bed fusion (PBF) to gain insights into residual stresses and distortions arising during this metal additive manufacturing process. This example illustrates an inverted staging, where first internal research efforts created an initial capability for modeling part-scale response [3]. Publications of these successful efforts then created interest from academic and industrial researchers leading to collaborations that have extended and enriched our modeling capabilities [4]. We will also touch more generally on other funding opportunities in the Department of Energy national laboratory ecosystem. References [1] M.A. Puso, E. Kokko, R. Settgast, J.D. Sanders, B. Simpkins, B. Liu, “An embedded mesh method using piecewise constant multipliers with stabilization: mathematical and numerical aspects,” IJNME 104 (7) 697-720 (2015). [2] J.D. Sanders, T.A. Laursen and M.A. Puso, “A Nitsche embedded mesh method”, Computational Mechanics, 49 (2) 243-257 (2012). [3] N.E. Hodge, R.M. Ferencz, J.M, Solberg, “Implementation of a thermomechanical model for the simulation of selective laser melting”, Computational Mechanics 54 (1), 33-51 (2014). [4] J. Nitzler, C.A. Meier, K.W. Müller, W.A. Wall, N.E. Hodge, “A Novel Physics-Based and Data-Supported Microstructure Model for Part-Scale Simulation of Ti-6Al-4V Selective Laser Melting”, preprint arXiv:2101.05787v1 (2021).

_____ This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

16th U.S. National Congress on Computational Mechanics
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Title: A Scalable Distributed Architecture for a Spacetime Parallel–Adaptive Hyperbolic Solver

Author(s): *Robert Haber, *University of Illinois at Urbana-Champaign*; Amit Madhukar, *University of Illinois at Urbana-Champaign*; Christian Howard, *University of Illinois at Urbana-Champaign*; Volodymyr Kindratenko, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Space Institute*;

The causal Spacetime Discontinuous Galerkin (cSDG) method is a powerful scheme for solving hyperbolic systems [1],[2]. In lieu of synchronous time marching, it constructs unstructured spacetime meshes according to a causality constraint that localizes the solution to small clusters of spacetime elements called patches. The solution on each patch depends only on adjacent, previously-solved elements and prescribed initial and boundary data. This structure supports patch-by-patch solution procedures with an intrinsic, fine-grained parallel structure. The causal spacetime meshes are constructed incrementally as part of the patch-wise solution procedure by advancing a space-like front mesh through the spacetime analysis domain. Each local advancement of the front creates a new patch that is solved immediately. In adaptive solvers, each new patch solution is tested with various error indicators. If the solution error is too large, the patch is discarded and the front mesh is refined to produce local refinement in both the spatial and temporal diameters of the spacetime mesh. The result is an extremely dynamic form of adaptive meshing capable of tracking fast-moving solution features such as dynamic fractures. The adaptive meshing evolves so rapidly that conventional load-balancing schemes cannot keep up. We describe a new scalable framework for parallel–adaptive cSDG schemes intended for large-scale distributed-memory systems. The front mesh is the only global data structure, and we freely distribute its data across the distributed memory system. This flexibility enables new probabilistic data and load-balancing techniques that can keep pace with embarrassingly parallel cSDG adaptive meshing and solution procedures. Dedicated MPI processes perform gather/scatter operations to construct front-mesh fragments in local memory, while dedicated solver processes, each running on its own dedicated cpu, perform embarrassingly-parallel patch-generation, patch-solution, and local adaptive meshing operations. We describe latency hiding methods for the MPI processes and techniques for isolating the solver processes from the rest of the system that are key to scalability. We present scaling results for the new architecture on an IBM POWER9 cluster. [1] R. Abedi, R. B. Haber and B. Petracovici. A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum. Comp Methods Appl Mechs Engrg 195 (2006), pp 3247–3273. [2] R. Abedi, R. B. Haber and P. L. Clark. Effect of random defects on dynamic fracture in quasi-brittle materials, Int J Fract 208 (2017), pp 241–268.

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Title: DG Methods for Layered Ocean Modeling: Thin Layers and Variable Bottom Topography

Author(s): *Robert Higdon, *Oregon State University*;

In a numerical model of ocean circulation, one possible choice of vertical coordinate is a density-based (isopycnic) coordinate. Such a coordinate can be discretized by approximating the fluid as a stack of layers, each having constant density but variable thickness. In this context, one issue to be addressed is the representation of the lateral pressure forcing. In the case of a discontinuous Galerkin (DG) numerical method, one approach is to consider the volume of fluid lying on a given grid cell in a given layer, multiply the horizontal pressure gradient by a test function, integrate on that volume, and then integrate by parts. In the case of the shallow water equations for a single-layer hydrostatic fluid, this approach yields a numerical representation of the pressure forcing that is automatically well-balanced in the presence of variable topography along the bottom of the fluid region. Similar results apply for the case of a multi-layer fluid, provided that suitable care is taken at locations where layer interfaces intersect the bottom topography, and thus where certain layers reduce to negligible thickness. The measures taken include suitable limiting related to those layers and locations. This analysis is supported by numerical computations, with one horizontal spatial dimension, in which layer interfaces move upward and downward along sloping bottom topography.

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Title: Simulation of Unsteady Compressible Navier Stokes Equations Using a Data-Enriched Finite Element Method

Author(s): *Rohit Deshmukh, *The Ohio State University*; Vilas Shinde, *The Ohio State University*; Troy Shilt, *The Ohio State University*; Jack McNamara, *The Ohio State University*;

Exorbitant costs of carrying out high-fidelity analyses of large, parametric, nonlinear fluid flow systems pose significant challenges for the analysis and design of multi-physics systems. Specifically, highly refined grids are necessary for accurate resolution of a large spectrum of spatial scales present in turbulent flows. Researchers have long sought efficient, data-driven parametric models; however, the state-of-the-art techniques suffer from several shortcomings: 1) the data-driven functions don't generalize well to varying parameters, requiring large numbers of training points; 2) feature learning algorithms require large amounts of training data to extract converged functions; and 3) intrusive methods require access and modifications to the high-fidelity solvers, thereby limiting the applications of the developed tool. In a recent study, the authors developed a novel 'data-enriched finite elements' framework in which the enrichment functions are learned from a small amount of training data using a feature learning technique. The learned features are then embedded in the low-order finite element space to enrich it. The developed approach is demonstrated on large scale three-dimensional turbulent flows at different operating conditions. The generated enrichment learning process has several advantages: 1) the training is carried out using a single observation of the unsteady flow instead of a long time-series; 2) the extracted enrichment functions are valid over a large parameter space, and 3) the training is carried out in a non-intrusive, 'offline' manner – the source of training data is not limited to a particular computer software, and the process also allows learning from experimental data. However, the predictive capabilities of the data-enriched finite elements for turbulent flows are yet to be assessed. The authors have successfully developed predictive models for canonical systems, such as steady Stokes flow, unsteady linear advection-diffusion equations, and nonlinear Burgers' equation. For the current study, the authors are developing an unsteady compressible Navier Stokes solver using the nonintrusive data-driven enrichment functions. Flows inside a two-dimensional lid-driven cavity at various Reynolds numbers will be considered for this study. The high-fidelity training and evaluation datasets are generated using a high-order finite difference solver. The performance of the developed models will be compared to the standard finite elements and higher-order finite difference-based models.

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Title: Localized Non-Intrusive Reduced-Order Modeling in the Operator Inference Framework

Author(s): *Rudy Geelen, *The University of Texas at Austin*; Karen Willcox, *The University of Texas at Austin*;

In this talk we introduce a new approach for the non-intrusive derivation of projection-based reduced-order models based on concepts of Operator Inference (OpInf) [1] and localization [2]. Projection-based model reduction constructs the operators of a reduced model by projecting the equations of the original full model onto a reduced space. Instead of approximating the solution of interest in a fixed low-dimensional subspace of global basis vectors, the proposed method approximates this solution in a subspace generated by most appropriate local basis vectors. To achieve this, the solution space is partitioned into subregions after which a local reduced-order basis is constructed and assigned to each subregion offline. During the solution procedure of the online reduced problem, a local basis is chosen according to the subregion of the solution space where the current high-dimensional solution lies. The OpInf framework is employed to find the local reduced matrix operators that yield the reduced model that best matches the projected snapshot data in a minimum-residual sense. The proposed approach is non-intrusive in nature and can be applied to a host of nonlinear systems by exposing its inherent polynomial structure. It is particularly suited for problems characterized by different physical regimes and parameter variations. We demonstrate the localized OpInf approach for different nonlinear systems and investigate its potential for maintaining high levels of accuracy when the number of degrees of freedom associated the data-driven regression problem is low. [1] Peherstorfer, B. and Willcox, K., 2016. Data-driven operator inference for nonintrusive projection-based model reduction. Computer Methods in Applied Mechanics and Engineering, 306, pp.196-215. [2] Amsallem, D., Zahr, M.J. and Farhat, C., 2012. Nonlinear model order reduction based on local reduced?order bases. International Journal for Numerical Methods in Engineering, 92(10), pp.891-916.

16th U.S. National Congress on Computational Mechanics
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Title: Peeling and Sliding of Graphene Nanoribbons with Coupled Adhesive and Frictional Interactions

Author(s): Zhiming Xue, *Harbin Institute of Technology*; *Rui Huang, *The University of Texas at Austin*;

The peeling and sliding behaviors of monolayer graphene nanoribbons (GNRs) atop a rigid crystalline substrate are studied by a continuum mechanics model and finite element simulations. The coupled interactions in both the normal and tangential directions of the interface are simulated by using a periodic interlayer potential function, which is formulated based on atomistic calculations and implemented numerically as a user-defined subroutine (UINTER) within ABAQUS for the finite element simulations. It is found that the 90-degree peeling behavior of a GNR is determined primarily by the adhesive interactions in the normal direction with negligible tangential interactions at the interface. In contrast, the sliding behavior is generally more complicated, with coupled normal and tangential interactions as well as lateral sliding. The stick-slip sliding is related to formation and gliding of strain solitons in the GNRs, depending on the chiral orientation as well as the ribbon width. Finally, a coupled peeling and sliding process is considered, based on which both the adhesive and frictional properties of GNRs can be deduced from measurements of the reaction forces in both the normal and tangential directions.

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Title: On the Computational Modelling of Plasticity in the Martensite Phase of TRIP Alloys

Author(s): *Rui Pedro Cardoso Coelho, *University of Porto*; Miguel Vieira de Carvalho, *University of Porto*; Francisco Manuel Andrade Pires, *University of Porto*;

Over the last years, increasing attention has been given to the development of high-strength multiphase alloys with enhanced mechanical properties. TRIP (transformation induced plasticity) and dual-phase steels are examples of such materials, exhibiting both high strength and elongation at failure. Their constitutive response results from the complex interactions of multiple deformation mechanisms at the micro-scale, for instance, plastic slip and martensitic transformation. Multi-scale models promote a natural framework for the representation of the complex response inherent to the several microscopic phenomena occurring in these alloys. Directly modelling the multiple constituent phases (crystalline ferrite, martensite and austenite) as well as phase transformations within Representative Volume Elements (RVEs) allows inferring the overall macroscopic behaviour by RVE homogenisation. In contrast, phenomenological models often require several parameters calibrated experimentally whereas the homogenisation based approach leads to a direct connection between the microstructure and the material response. A fully implicit algorithm for slip plasticity and martensitic transformation [1] with a volume-preserving exponential map is used, as well as a rate-dependent regularisation to circumvent the non-smooth yield functions and the non-unique solutions for linearly dependent systems. Further sub-stepping strategies at the stress level and iterative refinements to the rate-sensitivity parameters are performed to sidestep equation stiffness in the rate-independent limit of viscoplastic formulations. The generalisation of Patel and Cohen’s [2] energy-based criterion is employed to introduce the effect of mechanically-induced martensitic transformation. The described model does not predict yielding in the martensitic phase after transformation. In this work, slip plasticity is introduced to this phase [3]. Relevant aspects of the new formulation and its respective computational treatment are addressed and discussed. The resulting model is evaluated in a large-strain fully implicit multi-scale finite element program by RVE homogenisation. [1] de Bortoli, D. and Adziman, F. and de Souza Neto, E.A. and Andrade Pires, F.M. "Constitutive modelling of mechanically induced martensitic transformations: Prediction of transformation surfaces", Engineering Computations, 35, 772–799 (2018). [2] Patel, J. R. and Cohen, M. "Criterion for the Action of Applied Stress in the Martensitic Transformation". Acta Metallurgica 1.5 (1953). [3] Kouznetsova, V.G. and Geers, M.G.D. "A multi-scale model of martensitic transformation plasticity", Mechanics of Materials, 40 (8), 641-657 (2008)

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Title: Topology Optimization of Binary Structures for Soil-Structure Interaction Problems Using IBEM-FEM Coupled Analysis

Author(s): *Rômulo Cortez, *University of Sao Paulo*; Raghavendra Sivapuram, *University of California, San Diego*; Persio Barros, *University of Campinas*; Josue Labaki, *University of Campinas*; Renato PIcelli, *University of Sao Paulo*;

Topology optimization has brought up new scenarios to structural engineering design through optimized layouts. One of its current challenges is the optimization of structures subject to complex loads, which requires the development of new computational methodologies. This article proposes and investigates the topology optimization method applied to problems of soil-structure interaction. In this case, the structure is built on an elastic soil instead of having rigid supports. The objective is to investigate how the flexibility of soil affects the topology optimization of the structure in a static soil-structure interaction problem. This problem is important when topology optimization is used in the design of structures that are sensitive to the behavior of the soil, such as in particle accelerators, nuclear power plants, and offshore platforms on the seabed. In this work, the soil is modeled with the Indirect Boundary Element Method (IBEM), and the structure with the Finite Element Method (FEM). Coupling between soil and structure is obtained by imposing kinematic compatibility and stress balance conditions at their shared interface. The problem of minimizing structural compliance subject to a volume restriction is solved using the Topology Optimization of Binary Structures (TOBS) method. TOBS is a topology optimization method that accommodates binary design variables {0,1} and employs integer linear programming. Numerical results with different values of soil and structure stiffness show that the flexibility of the soil must be taken under consideration in the design of a structure via topology optimization.

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Title: Simple H-R-H Adaptation for Immersed Geometries for CFD Applications

Author(s): *Sacha El Aouad, *Mines ParisTech - CFL - CEMEF*; Aurélien Larcher, *Mines ParisTech - CFL - CEMEF*; Elie Hachem, *Mines ParisTech - CFL - CEMEF*;

A new simple geometric adaptation is introduced to build a body fitted mesh for immersed geometries. Since the success of the finite element method lies in its flexibility to represent the geometry, the Immersed Volume Method [1] is extended towards a sharp adaptation to accurately define the geometry at the interface without the need of a narrow band region. The adaptive anisotropic local grid refinement based on the geometric implicit distance representation (Level-set function) offers a great tool to capture the sharp discontinuities of the fluid-solid interface. After the use of anisotropic adaptation, the interpolation free Moving Mesh Model [2] is first applied on specific nodes of the isolated cut elements relocating them to the interface. Then a simple topology change of the mesh (swapping) is applied. With the algorithm proposed, fluid-solid interactions and CFD problems with complex geometries can be addressed and solved more accurately without the need of enrichment functions or penalty terms that alter the numerical scheme [3]. [1] Elie Hachem, Stephanie Feghali, Ramon Codina, and Thierry Coupez. Anisotropic adaptive meshing and monolithic variational multiscale method for ?uid– structure interaction. Computers & Structures, 122:88– 100, 2013. [2] Tao Tang. Moving mesh methods for computational fluid dynamics. Contemporary mathematics, 383(8): 141–173, 2005. [3] Alex Main and Guglielmo Scovazzi. The shifted boundary method for embedded domain computations. part ii: Linear advection–diffusion and incompressible Navier–Stokes equations. Journal of Computational Physics, 372:996–1026, 2018.

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Title: Reduced-Order Modeling of Parameteric Simulations with Bayesian Matrix Completion

Author(s): *Saibal De, *University of Michigan*; Hadi Salehi, *Michigan State University*; Alex Gorodetsky, *University of Michigan*;

Matrix completion, where we attempt to infer the full matrix from a few known matrix entries, is a classical problem in data science with many applications, such as recommender system design, drug-protein interaction prediction, and image completion. In the context of data-driven modeling, we can also pose the exploration of discretized two-dimensional parameter space as a matrix completion problem. In fact, low-rank Bayesian matrix completion can serve as a reduced-order model for a parametric simulation with robust uncertainty estimates. A standard Bayesian inference approach is to assign zero-mean Gaussian priors on the columns or rows of factor matrices to create a conjugate system. This choice of prior leads to simple implementations; however, it also causes symmetries in the posterior distribution that can severely reduce the efficiency of Markov-chain Monte-Carlo (MCMC) sampling approaches. In this talk, we propose a simple modification to the prior choice that provably breaks these symmetries and maintains/improves accuracy. Specifically, we provide conditions that the Gaussian prior mean and covariance must satisfy so that the posterior does not exhibit invariances that yield sampling difficulties. For example, we show that using non-zero linearly independent prior means significantly lowers the autocorrelation of MCMC samples, and can also lead to lower reconstruction errors.

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Title: An Arc-Length Stabilized Adaptive Wavelet-Enriched Hierarchical Finite Element Method for Crack Propagation Using Phase Field Models

Author(s): *Saikat Dan, *Johns Hopkins University*; Thirupathi Maloth, *Johns Hopkins University*; Preetam Tarafder, *Johns Hopkins University*; Somnath Ghosh, *Johns Hopkins University*;

This work presents a novel adaptive wavelet-enriched hierarchical finite element method for solving coupled displacement-phase field problems to simulate crack propagation in brittle multi-phase microstructures. The advantage of the multi-resolution nature of wavelets accounts for the selection of an optimal set of basis-functions that is capable of adaptively enriching the solution space around a crack with a prescribed level of accuracy [1]. A second-generation family of wavelets with a lifting scheme is employed to generate hierarchical interpolation functions. The adaptive enrichment can resolve the high gradients in the solution of the phase field order parameter with the evolution of the crack. Moreover, phase field models are known to experience numerical convergence issues with regular Newton-Raphson type solvers which might cause simulations to terminate as soon as the material starts to degrade. To address this issue, a dissipation-based arc-length stabilization scheme is adopted in this work. A constraint equation for the load step is solved in conjunction with the coupled displacement-phase field problem [2]. Crack propagation under finite deformation kinematic assumptions is driven by stored elastic energy that accounts for material anisotropy and tension-compression asymmetry. The phase field model is augmented with an auxiliary phase field order parameter to regularize the displacement jump across an interface. Traction-separation laws are utilized at cohesive interfaces to prescribe bond strength and predict crack nucleation sites [3]. The resulting finite element model is used to simulate complex failure mechanisms including crack nucleation, propagation, branching and their subsequent interactions in fiber-matrix and particle embedded multi-phase microstructures. [1] Y. Azdoud and S. Ghosh (2017), “Adaptive wavelet-enriched hierarchical finite element model for polycrystalline microstructures”, Comput. Methods Appl. Mech. Engrg., Vol. 321, pp. 337-360 [2] N. Singh, C. V. Verhoosel, R. De Borst, E. H. Van Brummelen (2016), “A fracture-controlled path-following technique for phase-field modeling of brittle fracture”, Finite Elems. in Analysis and Design, Vol. 113, pp. 14-29 [3] P. Tarafder, S. Dan and S. Ghosh (2020), “Finite Deformation Cohesive Zone Phase Field Model for Crack Propagation in Multi-Phase Microstructures”, Comput. Mech., Vol. 66, pp. 723-743

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Title: DFT-FE --- a Massively Parallel Real-Space Density Functional Theory Code Using Adaptive Finite-Element Discretization, and its Application to Study Dislocation Core Energetics in Magnesium

Author(s): *Sambit Das, *University of Michigan*; Phani Motamarri, *Indian Institute of Science*; Vikram Gavini, *University of Michigan*;

Kohn-Sham density functional theory (DFT) calculations have been instrumental in providing many crucial insights into materials behavior. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons. In the first part of this work, we present a massively parallel real-space DFT framework (DFT-FE) [1, 2], which is based on a local real-space variational formulation of the Kohn-Sham DFT energy functional discretized with higher-order adaptive spectral finite-element, and handles pseudopotential and all-electron calculations in the same framework. We will present the efficient and scalable numerical algorithms in conjunction with mixed precision strategies for the solution of Kohn-Sham equations, that has enabled computationally efficient, fast and accurate DFT calculations on generic material systems reaching ~100,000 electrons, and demonstrate an order of magnitude performance advantage over widely used plane-wave codes both in CPU-times and wall-times. Finally, in the second part of this work, we study the core energy difference between the <c+a> screw dislocations on pyramidal I and II planes in pure magnesium (EpyrI-II), which forms a crucial and sensitive input to a quantitative model predicting the ductility of magnesium alloys. Accurate estimation of EpyrI-II using explicit DFT calculations has so far been out of reach using plane-wave codes as large system sizes containing thousands of atoms are required to accurately resolve the relevant physics in the dislocation core. Using DFT-FE, we conducted a systematic cell size study to obtain EPyrI-II up to an estimated cell-size error of ~10 meV/nm at a cell-size of ~2,000 atoms (20,000 electrons) per periodic layer along the dislocation line, with further simulations at larger cell sizes ongoing to improve the accuracy to better than 5 meV/nm. Obtaining EPyrI-II accurately has significant implications for achieving high ductility in light-weight magnesium alloys. [1] Motamarri, P., Das, S., Rudraraju, S., Ghosh, K., Davydov, D., Gavini, V., 2020, DFT-FE --- A massively parallel adaptive finite-element code for large-scale density functional theory calculations, Comput. Phys. Commun. 246, 106853. [2] Das, S., Motamarri, P., Gavini, V., Turcksin, B., Li, Y.-W., Leback, B., 2019, Fast, scalable and accurate finite-element based ab initio calculations using mixed precision computing: 46 PFLOPS simulation of a metallic dislocation system, Proceedings of SC19, The International Conference for High Performance Computing, Networking, Storage, and Analysis.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Symmetry-Breaking and Selection in Colloidal Assemblies on Curved Elastic Substrates

Author(s): *Sanjay Dharmavaram, *Bucknell University*; Luigi Perotti, *University of Central Florida*;

In recent decades, colloidal assemblies have been extensively used as model systems to explore fundamental questions concerning the crystal structure of materials on curved substrates. Experimental and theoretical studies have provided significant insights into the role of substrate topology and its curvature on various aspects of colloidal packing, including the ability to self-assemble and the structure of their defects. While most studies have so far focused on fixed substrate geometries, there is growing interest in understanding assemblies on elastic substrates, with potential applications to designing functional materials, e.g., energy harvesting, self-healing, shape programmable, and structural color, to name a few. In this work, we will present a hybrid-continuum model for such systems, where colloids are modeled as interacting point-particles and the substrate as an elastic shell. We use a Lagrangian finite element scheme to explore the interplay between particle assembly and substrate elasticity. We show that for a small to a moderate number of particles the system exhibits a variety of highly symmetric equilibrium configurations with symmetries that are sensitive to the elastic material parameters of the substrate. Some of these states have symmetries equivalent to those of the classical Thompson problem, but many others have no corresponding analogs. We will discuss the use of group-theoretic techniques to efficiently explore phase transitions between different symmetry states. Such group-theoretic techniques significantly increase computational efficiency as, due to symmetry, only a subset of the degrees of freedom needs to be determined. This approach allows the analysis of energetically close (and potentially easily tunable) symmetry transitions that would otherwise be very difficult to detect and leverage.

16th U.S. National Congress on Computational Mechanics
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Title: Toward Improved Heat Transfer Models for Strongly-Coupled, Gas-Solid Flows

Author(s): *Sarah Beetham, *University of Michigan*; Aaron Lattanzi, *University of Michigan*; Jesse Capecelatro, *University of Michigan*;

At sufficient mass loading, gas-solid flows exhibit the development of large-scale, coherent structures (clusters) due to coupling between the phases. This behavior is particularly prevalent in the context of circulating fluidized bed reactors, commonly used in the upgrading of feedstock into fuel. Due to the momentum coupling between phases, the development of these structures effectively `de-mixes' the underlying flow, which degrades gas-solid contact. This significantly impedes heat transfer and subsequent devolatilization, which has important implications for reactor design and efficiency. Here, we use a volume-filtered Euler-Lagrange (EL) method to quantify the role of clustering on heat transfer. This is done using a two-step approach, in which statistically steady clustering is first established with cold-flow conditions and then fed into a secondary simulation with a defined particle-fluid thermal gradient. This results in the thermal development toward equilibrium to occur in 1D (e.g., over the length of the riser). In this talk, the effect of clustering on heat transfer between the phases will be quantified and models for relevant terms will be proposed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Experimental and Computational Mechanical Characterization of Heterogeneous Fibrin Gels

Author(s): *Sarah Calve, *University of Colorado Boulder*; Julian Jimenez, *Purdue University*; Yifan Guo, *Purdue University*; Adrian Buganza - Tepole, *Purdue University*;

Biological tissues are made up of heterogeneous mixtures of cells and extracellular matrix (ECM). This leads to variable material properties, particularly at interfacial boundaries where composition, organization, and density differ drastically; for example, a wound surrounded by healthy tissue. Characterizing the non-uniform mechanics of tissues is critical to understanding how variations in material properties influence cellular behavior; however, this is challenging to analyze within the complex in vivo environment. Our long-term goal is to generate in vitro models that capture the heterogeneity of biological tissues in a controlled environment. As a first step, we mechanically characterized fibrin-based constructs that contained two discrete regions with varying material properties. Fibrin is naturally occurring and polymerized from fibrinogen and thrombin following injury, providing a temporary structure for remodeling during wound healing [1]. The construct base was 2mg/mL fibrin containing a circular inclusion of 4 mg/mL fibrin. To visualize the different materials, and provide a means to optically measure strain, 2 and 4 mg/mL gels were fluorescently labeled with AF488 and AF546, respectively. A confocal microscope was used to photobleach fiducial lines, visualize geometry and obtain cross-sectional areas. A custom tensile tester was used to collect force data (0.01s-1) and sample deformation videos as previously described [2]. Strain was calculated from videos using MATLAB and Python algorithms. An FE model was created in Abaqus to simulate the heterogeneous fibrin gel. The geometry was extracted from confocal images, and the material was simulated using the model from [3], with parameters from the material response of homogenous 2 or 4 mg/mL gels. During tensile testing, the interface between the 2 and 4mg/mL gels remained cohesive. An FE model based on the mechanical properties of homogenous fibrin allowed us to determine the stress-strain response within different regions of the heterogeneous gels. Regions within the stiffer 4mg/mL fibrin experienced a lower strain than the surrounding less stiff 2mg/mL fibrin. The overall stress-strain response of the heterogeneous gel fell in between the response for the homogeneous 2 and 4mg/mL gels. We anticipate this approach will enable us to design and characterize novel biomaterial combinations that seek to recapitulate in vivo mechanics and elucidate the mechanisms of tissue repair.
Acknowledgement: NSF1911346-CMMI to Tepole and Calve. [1] Janmey, P et al., J R Soc Interface, 6: 1-10, 2009. [2] Enríquez, A et al., Adv Funct Mater, 31:2005021, 2021. [3] Gasser, TC et al., J R Soc Interface, 3: 15-35, 2006.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling the Interplay Between Deep Subsurface Pressure Perturbation, Fault Stability, Surface Deformation and Earthquake Cycles

Author(s): *Saumik Dana, *University of Southern California*; Birendra Jha, *University of Southern California*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*;

A 2012 study by National Research Council on Induced Seismicity in Energy Technologies [carbon capture/storage, enhanced geothermal systems, post fracking waste water disposal] identified the following goals from the modeling standpoint (1) Linking geomechanical and earthquake simulation models to identify critical geological characteristics controlling induced seismicity (2) Developing simulation capabilities integrating reservoir and earthquake simulation modeling for hazard and risk assessment and (3) Scaling these models to field scale simulations. We present the numerics of an integrated framework in which we study the interplay between deep subsurface pressure and stress perturbations pre- and post- fault slippage and the deformation of the earth's surface. The integration is a combined outcome of the numerics presented in (1) Dana et al. [2], which allows for the effects of pressure perturbations to be upscaled to model uplift or subsidence, (2) Jha et al. [1], which couples the effects of pressure perturbations to fault stability and earthquake triggering and (3) Elbanna et al. [3], which determines the fault slip rate and post-slip stress perturbations in the domain. [1] Birendra Jha and Ruben Juanes. “Coupled multiphase flow and poromechanics: A computational model ofpore pressure effects on fault slip and earthquake triggering”. In:Water Resources Research50 (5 2014),pp. 3776–3808 [2] Saumik Dana, Benjamin Ganis, and Mary F. Wheeler. “A multiscale fixed stress split iterative scheme forcoupled flow and poromechanics in deep subsurface reservoirs”. In:Journal of Computational Physics352(2018), pp. 1–22 [3] Mohamed Abdelmeguid, Xiao Ma, and Ahmed Elbanna. “A Novel Hybrid Finite Element-SpectralBoundary Integral Scheme for Modeling Earthquake Cycles: Application to Rate and State Faults withLow-Velocity Zones”. In:Journal of Geophysical Research: Solid Earth(2019), 2019JB018036

16th U.S. National Congress on Computational Mechanics
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Title: Patient Specific CFD Models Investigated in a Novel 0D-3D Numerical Framework, Based on 4D-MRI and CT Imaging

Author(s): *Scott Black, *University of Strathclyde*; Konstantinos Ritos, *University of Strathclyde*; Craig Maclean, *Terumo Aortic*; Robbie Brodie, *Terumo Aortic*; Pauline Hall-Barrientos, *NHG Greater Glasgow & Clyde*; Asimina Kazakidi, *University of Strathclyde*;

Regions of the thoracic aorta affected by an aneurysm or dissection may require surgical intervention using vascular stent-grafts. Such grafts must generate physiological branch perfusion distribution and in-stent haemodynamics. Therefore, enhanced understanding of pre- and post-operative perfusion in patient-specific cases is critical to improving clinical practice and patient outcomes. The aim of this study was to create patient-specific computational fluid dynamics (CFD) models from 4D-MRI and computed tomography (CT) via a multi-modality, multi-dimensional approach, and extract clinically relevant haemodynamic parameters. Arterial blood flow in healthy and diseased cases was investigated from 4D-MRI data. Thereafter, a novel methodology was employed to reconstruct a healthy, three-dimensional (3D) geometry from retrospective 4D-MRI images. Additionally, diseased geometries incorporating a dissection were reconstructed from CT images. To generate patient-specific boundary conditions (BCs), the arterial geometry was reduced to a one-dimensional (1D) model. Thereafter, the terminal branches were coupled to zero-dimensional (0D) 3-Element Windkessel models (3EWM), which are representative of downstream vasculature. In this 0D-1D numerical framework, the 3EWM parameters were changed iteratively to generate branch flow waveforms, minimising the error between computed and in-vivo 4D-MRI data. These BCs were coupled to the terminal branches of the 3D models, and the MRI-obtained velocity profile at the ascending aorta was prescribed at the inlet of the CFD domain. Thus, blood flow was investigated in a fully patient-specific 0D-3D numerical framework. The results of this study highlight the importance of generating patient-specific 3EWM BCs, which can be generated without requiring invasive measurements to capture in-vivo pulse waveforms. From the CFD simulations, clinically relevant haemodynamic parameters including time averaged wall shear stress and oscillatory shear index were extracted, elevated values of which are associated with post-surgical dissection formation and graft limb occlusion. Additionally, qualitative analysis of 4D-MRI data can highlight regions of stagnation and recirculation. Consequently, this study showed the combination of 4D-MRI, CT, and CFD grants unparalleled visualisation and quantification of arterial blood flow. In future work, multiple stent-graft configurations will be included within the CFD model to estimate post-surgical haemodynamics. The presentation will outline arterial pathology and the need for surgical intervention. Subsequently, a description of 4D-MRI blood flow analysis and a novel methodology for arterial reconstruction will follow. The CFD set-up and boundary condition optimisation will then be described, highlighting the use of 4D-MRI and CT. Finally, results from the haemodynamic analysis of healthy and diseased cases will be presented, with conclusions and future work.

16th U.S. National Congress on Computational Mechanics
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Title: Simulations of an Active Surface Immersed in Viscous Fluids

Author(s): *Sebastian Aland, *Dresden University of Applied Sciences / Technical University Freiberg*;
Lucas Wittwer, *Dresden University of Applied Sciences*;

The surface of biological cells is connected to the cell cortex - a thin layer of active material. This layer exerts an active contractile tension which regulates cellular shape by deforming the surface. The strength of the active tension is controlled by the concentration of force-generating molecules. Advective transport of these molecules leads to a complex interplay of surface deformation, hydrodynamics and molecule concentration which gives rise to pattern formation and self-organized shape dynamics. In this talk, we present a numerical model to simulate such an active viscous surface immersed in viscous fluids. We show the resulting patterning and cell shape dynamics for different parameter configurations as well as the flow profiles in the two bulk phases and discuss implications to the functioning of biological cells.

16th U.S. National Congress on Computational Mechanics
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Title: A Surface Correction Technique for Bond Based Peridynamics

Author(s): *Semsi Coskun, *Western Michigan University*; Jinseok Kim, *Western Michigan University*;

The peridynamic parameters such as micro-modulus constant, and critical bond stretch are calculated for bulk material points which has complete neighborhood. These parameters are used throughout the problem domain, yielding the "surface effects" at the nodes having incomplete neighborhood. This causes softer material response at the boundary nodes compared to bulk material nodes [1]. Therefore, a surface correction algorithm is needed to improve the accuracy of the prediction of material behavior. When problems involve fractures, the correction algorithm must be adoptively applied to newly formed boundaries in addition to pre-de fined problem boundaries. There are various correction methods suggested in the literature to minimize surface effects. Le and Bobaru [2] has implemented surface correction methods available in the literature and demonstrated their performance in reducing surface effects. This study shows that surface correction algorithms improve results significantly compared to uncorrected cases. On the other hand, the performance of these methods strongly depend on the deformation types, i.e. homogeneous or inhomogeneous, and the geometry of the problem domain. The goal of this study is to clarify the accuracy and convergence of a prototype micro-elastic brittle (PMB) material model enriched with a surface correction algorithm which is more suitable in numerical applications. The surface effects are aimed to be eliminated by using discrete form of PD parameters [3]. In this study, 2D formulations of the discrete form of micro-modulus constant, and critical bond stretch are derived for general loading cases, and the comparisons with other corrections factors are presented. With the proposed algorithm, it is shown that the PD parameters can be computed numerically in the simulation progress, and hence not only the problem boundaries but also any emerging free-surfaces, such as cracks, can be treated accordingly. References [1] E. Madenci and E. Oterkus, Peridynamic theory and its applications, vol. 17. New York: Springer, 2014. [2] Q. V. Le and F. Bobaru, Surface corrections for peridynamic models in elasticity and fracture, Computational Mechanics, vol. 61, no. 4, pp. 499-518, 2018. [3] G. C. Ganzenm■uller, S. Hiermaier, and M. May, Improvements to the prototype micro-brittle model of peridynamics, in Meshfree methods for partial differential equations VII, pp. 163-183, Springer, 2015.

16th U.S. National Congress on Computational Mechanics
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Title: Interface Learning: Towards Seamless Integration of Multi-Scale, Multi-Physics and Multi-Fidelity (M3) Models

Author(s): *Shady Ahmed, *Oklahoma State University*; Suraj Pawar, *Oklahoma State University*; Omer San, *Oklahoma State University*; Adil Rasheed, *Norwegian University of Science and Technology*;

A multitude of natural and engineered systems comprise multiple characteristic scales, multiple spatiotemporal domains, multiple physical closure laws, and even multiple disciplines. In a naïve implementation of numerical simulation, the stiffest part dictates the spatial mesh resolution and time stepping requirements, making the solution of such systems computationally daunting. Instead, an ensemble of solvers and modeling approaches with varying levels of complexity can be selected for efficient simulation of multi-scale, multi-physics and multi-fidelity (M3) models. This includes domain decomposition techniques, multi-fidelity solvers, and multi-geometrical abstractions. However, effective communications and information sharing among heterogeneous computational entities have to be accomplished to guarantee solution convergence and reduce idle times. To this end, we propose a series of interface learning (IL) paradigms [1-3] to pave the way for seamless integration of M3 models using hybrid analysis and modeling (HAM) techniques. We exploit a robust HAM approach combining a physics-based full order model (FOM) and a data-driven reduced order model (ROM) to form the building blocks of an integrated approach among mixed fidelity descriptions toward predictive digital twin technologies. We focus on a multi-fidelity formulation targeting domain decomposition type problems that consist of multiple zones with different characteristics as well as multi-physics systems where different levels of solvers are devoted to coupled physical phenomena. A key aspect of the zonal multi-fidelity approach is its ability to handle intrinsic heterogeneous physical properties, varying geometries, and underlying governing dynamics. At the interface, we introduce a long short-term memory network to bridge these high and low-fidelity models in various forms of interfacial error correction and prolongation. The proposed IL approaches are tested as a new way to address ROM-FOM coupling problems solving nonlinear advection-diffusion flow situations with a bifidelity setup that captures the essence of a broad class of transport processes. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research under Award Number DE-SC0019290. [1] Ahmed, S. E., San, O., Kara, K., Younis, R., \& Rasheed, A. (2020). Interface learning of multiphysics and multiscale systems. Physical Review E 102, 053304. [2] Ahmed, S. E., San, O., Kara, K., Younis, R., \& Rasheed, A. (2021). Multifidelity computing for coupling full and reduced order models. PLOS ONE (to appear). [3] Pawar, S., Ahmed, S. E., \& San, O. (2020). Interface learning in fluid dynamics: Statistical inference of closures within micro–macro-coupling models. Physics of Fluids 32, 091704.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling Failure Mechanisms of Topologically Interlocked Structures

Author(s): *Shai Feldfogel, *ETH Zurich*; David Kammer, *ETH Zurich*;

Topological Interlocking (TI) structures are block assemblies that rely on a typical spatial arrangement and on inter-block force transfer for structural integrity. The blocks in TI structures are shaped and assembled so that they are fully kinematically constrained, meaning no block can move without disturbing its neighbors. This defining property eliminates the need for inter-block connectors, and it provides TI structures with unique properties, including excellent crack resistance, high tolerance to missing blocks, recyclability, and great shape and material versatility. With modern manufacturing technologies, complex shapes of TI blocks and structures across a wide range of size scales have become a reality, making topological interlocking a powerful design concept for architectured materials. The discrete nature of TI assemblies means that local friction failure at blocks' interfaces is the main driver of global collapse mechanisms, which are a foremost consideration for design. These failure mechanisms tend to become unstable and dynamic, as numerous experimental studies have revealed. The current understanding of these failure mechanisms, as well as the available computational tools for their analysis, is insufficient. Thus, the ability to predict the failure of TI structures is lagging the practical knowledge of exploiting their unique structural properties. The challenges holding back the development of effective computational tools are due to the unstable and dynamic nature of the local interfacial slips where they nucleate; the multi-body contact and friction interactions between blocks; the geometrical irregularity, and often nonconvexity, of the blocks; and the large displacements and rotations that typify TI structures. The lack of effective computational tools for TI structures sets back their fuller exploitation and widespread application. Here, we propose a new computational methodology to address the failure mechanisms of TI assemblies. This methodology is based on the adaptation of the Level Set Discrete Element Method (LSDEM), typically used to analyze the flow-like mechanics of granular media, to structural analysis. LSDEM's ability to handle the multiple interfacial interactions in a dynamic framework, and principally, its unique ability to represent arbitrarily shaped blocks sets it apart from commonly used methodologies and make it a uniquely suitable to address the behavior of TI structures. Comparisons of the performance of the LSDEM-based tool against experimental results reported in the literature show the former's ability to well capture and shed new light on the failure mechanisms of the topologically interlocked structural form.

16th U.S. National Congress on Computational Mechanics
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Title: Stochastic Modeling and Identification of Material Properties on 3D-Printed Structures, with Application to Orthopedic Implants

Author(s): *Shanshan Chu, *Duke University*; Johann Guilleminot, *Duke University*;

In this talk, an uncertainty quantification framework enabling the modeling of non-Gaussian random fields of material properties on complex geometries is proposed. The approach involves stochastic partial differential equations, which are specifically defined to capture the features of the underlying geometry, and information-theoretic prior models. We also discuss the identification and validation of the stochastic model, using physical experiments on 3D printed titanium structures.

16th U.S. National Congress on Computational Mechanics
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Title: In Silico Modeling and Data-Driven Analysis of a Novel Transcatheter Valve with Embedded Pressure Sensors

Author(s): *Shantanu Bailoor, *Johns Hopkins University*; Jung Hee Seo, *Johns Hopkins University*; Lakshmi Prasad Dasi, *Georgia Institute of Technology*; Stefano Schena, *Johns Hopkins University*; Rajat Mittal, *Johns Hopkins University*;

Transcatheter heart valves (THV) suffer from asymptomatic complications like subclinical leaflet thrombosis (SLT) which may result in fatal outcomes for the patient. Such malfunction may develop either early or late post implantation and may progress to clinical valve thrombosis, remain stable or even regress over time. SLT is detected incidentally during post-implant follow-up, and common imaging techniques are either invasive or expose the patient to radiation, prohibiting their regular use. Moreover, SLT progression mechanism is not clearly understood, in that SLT has been observed progress to clinical valve thrombosis, remain stable and even resolve over time. This makes it difficult to prescribe the same anticoagulant therapy regimen across a cohort of patients. These issues inform a critical need for a non-invasive and non-toxic, continuous monitoring modality of THVs which can alert to the onset of potential adverse outcomes at an early stage. We present a data-driven, in-silico proof-of-concept assessment for a novel, microsensor-based technology for THVs which can provide persistent and longitudinal monitoring of prosthesis function. We generate a dataset of high-fidelity simulations of transvalvular flow in a canonical aorta with healthy and mildly stenotic aortic valves. Reduced leaflet motion associated with unequal leaflet thickening results in aortic jet tilting and consequently, asymmetric pressure loading on the aorta wall. Particularly, we identify a region in the valve vicinity where pressure fluctuations show greatest sensitivity to changes in leaflet mobility. We hypothesize that extracting pressure measurements from this region can be analyzed to predict individual leaflet mobility. The strong coupling between leaflet mobility and downstream hemodynamics facilitates correlating pressure measurements at strategic locations in the vicinity of the THV with leaflet mobility. Linear discriminant analysis is used to relate pressure measurements from strategic locations on the stent to the presence of abnormal leaflet motion and logistic regression is used to quantify its severity. Testing various candidate locations, we determine the optimal sensor placement for detection of anomalous leaflet motion. Preliminary results demonstrate pressure measurements at as few as two discrete locations per valve leaflet can accurately detect the presence of anomalous leaflet motion.

16th U.S. National Congress on Computational Mechanics
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Title: Image-Based Patient-Specific Flow Simulations are Consistent with Stroke in Pediatric Cerebrovascular Disease

Author(s): *Shaolie Hossain, *The University of Texas at Austin*; Zbigniew Starosolski, *Texas Children's Hospital*; Travis Sanders, *The University of Texas at Austin*; Michael Johnson, *The University of Texas at Austin*; Michael Wu, *Brown University*; Ming-Chen Hsu, *Iowa State University*; Dianna Milewicz, *University of Texas Health Science Center at Houston*; Ananth Annapragada, *Texas Children's Hospital*;

Objective: Moyamoya disease (MMD) is characterized by narrowing of the distal internal carotid artery and the circle of Willis (CoW) and leads to recurring ischemic and hemorrhagic stroke. Neurosurgical interventions are used to augment blood flow to the affected region and avert future stroke events. A retrospective review of 50 pediatric MMD patients revealed that, among the 24 who suffered a unilateral stroke and were surgically treated, 11 (45.8%) went on to have a subsequent contralateral stroke. There is no reliable way to predict these events. After conducting a pilot study in Acta-/- mice that have features of MMD, we hypothesized that local hemodynamics are predictive of contralateral strokes and sought to develop a patient-specific analysis framework to non-invasively assess this stroke risk. Methods: Computational models of the complex CoW were reconstructed from patient imaging data. Realistic blood flow simulations were performed over several cardiac cycles using an unsteady Navier-Stokes solver within an isogeometric analysis framework. Vascular regions with critical WSR values above the coagulation limit (> 5000 s-1) were identified as having a higher probability of clot formation leading to stroke. Results: A pediatric MMD patient with an occlusion in the right middle cerebral artery and right-sided stroke, who was surgically treated and then suffered a contralateral stroke, was selected for patient-specific analysis and the results were compared with an age/gender matched control subject. WSR > 60, 000 s-1 (12X higher than the coagulation threshold of 5000 s-1 and 9X higher than control) occurred in the terminal left supraclinoid artery and coincided with the location of the subsequent post-surgical left stroke event. The results suggest that an occlusion in the CoW could result in excessive contralateral WSRs leading to stroke and WSR could be a reliable parameter in predicting the occurrence and location of future stroke. Conclusion: The computational toolset presented in this paper could be useful in non-invasively identifying vascular regions that could evolve into severe stenosis or occlusion causing stroke, which could help ensure that unilateral MMD patients likely to progress to bilateral disease are properly followed and treated before contralateral strokes occur.

16th U.S. National Congress on Computational Mechanics
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Title: Thermo-Mechanical Behavior of Dielectric Viscoelastomers

Author(s): Keven Alkhoury, *New Jersey Institute of Technology*; *Shawn Chester, *New Jersey Institute of Technology*;

Soft dielectrics are electrically-insulating elastomeric materials, which are capable of large deformation and electrical polarization, and are used as smart transducers for converting between mechanical and electrical energy. While much theoretical and computational modeling effort has gone into describing the ideal, time-independent behavior of these materials, they are known to be viscous and temperature sensitive. Viscoelasticity and the associated thermo-mechanically coupled behavior is a crucial component of the observed mechanical response and hence have a significant effect on the observed electro-mechanical behavior. e have a calibrated constitutive model for the soft dielectric VHB4910 that is able to describe electromechanical coupling, large-deformations, chain-locking, and the thermo-mechanically coupled time-dependent mechanical response.

16th U.S. National Congress on Computational Mechanics
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Title: Material Characterization from Non-Equilibrium Data using the Jarzynski Equality

Author(s): *Shenglin Huang, *University of Pennsylvania*; Chuanpeng Sun, *University of Pennsylvania*; Prashant Purohit, *University of Pennsylvania*; Celia Reina, *University of Pennsylvania*;

The Jarzynski equality is a remarkable relation that links the free energy difference between two states and the non-linear ensemble average of the work done along a non-equilibrium process between these states. Here, by leveraging the Jarzynski equality and a local equilibrium assumption, we provide a strategy to extract both equilibrium and non-equilibrium information, i.e., the free energy and the dissipation potential of the system, to recover the continuum model. This strategy is demonstrated for pulling experiments on a mass-spring model, which is a prototype for biological macromolecules, polymers or nanorods. The inferred continuum model is then validated over different mechanical excitations, therefore demonstrating the usefulness of the proposed strategy for fully characterizing the material from non-equilibrium data.

16th U.S. National Congress on Computational Mechanics
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Title: Reduced-Order Multiscale Modeling of Elasto-Plastic Porous Metal Alloys

Author(s): *Shiguang Deng, *University of California, Irvine*; Carl Soderhjelm, *University of California, Irvine*; Ramin Bostanabad, *University of California, Irvine*;

Cast aluminum alloys are increasingly utilized as light-weight materials in automobile industry due to their superior capability in withstanding high mechanical loads. A major challenge in casting is the presence of manufacturing-induced localized pores of various topologies and spatial distributions. To understand the effect of porosity on the mechanical properties of casting components, multiscale simulations are required as these components possess a hierarchical structure that spans multiple length-scales. In this talk, we will introduce a computationally efficient, data-driven, reduced-order multiscale framework to simulate the behavior of porous metal alloys under irreversible deformations. The major components of our approach are: (1) data compression which decomposes the domain into topologically connected clusters; and (2) deflation algorithm which projects homogenized solution variables on a lower dimensional space. We will compare our approach against state-of-the-art methods to demonstrate its performance and versatility.

16th U.S. National Congress on Computational Mechanics
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Title: BeltramiNet: A Deep Forward Neural Network for Predicting the Solution of Thermally Coupled Steady State Incompressible Navier Stokes Equations

Author(s): *Shoaib Goraya, *University of Illinois at Urbana-Champaign*; Nahil Sobh, *University of Illinois at Urbana-Champaign*; Arif Masud, *University of Illinois at Urbana-Champaign*;

Recently, Deep Learning methods have been an active area of research for developing approximate solutions to high dimensional nonlinear partial differential equations (PDEs). These methods strive to generate approximate solutions to PDEs by minimizing a loss functions over their domain, boundary values and possibly initial conditions. Although physics constraint deep learning models are witnessing a tremendous growth in publications, a thorough investigation of error and uncertainty quantification of the method has been lacking. To address this issue, we have designed a deep feedforward neural network, BeltramiNet, that approximates the solution of the incompressible Navier Stokes equations that are thermally coupled with an energy conservation equation via the Boussinesq assumptions. BeltramiNet approximates three PDEs: (i) Thermally coupled momentum balance PDE (ii) Incompressibility constraint PDE, and (iii) Thermal advection-diffusion PDE. We present the architecture of BeltramiNet and provide an interpretation of the hidden layers including the spectral representation of the approximating functions in the context of collocation method. We performed a systematic convergence study to investigate the role of the dataset size, batch size, and other hyperparameters as to their impact on the quality of the approximate solution. Preliminary results show that domain dataset size exhibits a correlation with the size of the boundary dataset that leads an optimal partition ratio resulting in best performance. We also observed that the incompressibility constraint is hard to satisfy during the training where the error in the pressure field is relatively high compared to the rest of the field variables (velocities and temperature). However, adding the Poisson pressure equation as “augmented” constraint significantly reduces this error. Finally, we propose a practical, accurate, and scalable boundary representation. References: [1] Shin, Yeonjong, Jerome Darbon, and George Em Karniadakis. "On the convergence and generalization of physics informed neural networks." arXiv preprint arXiv:2004.01806 (2020). [2] Zhang, D., Lu, L., Guo, L., & Karniadakis, G. E. (2019). Quantifying total uncertainty in physics-informed neural networks for solving forward and inverse stochastic problems. Journal of Computational Physics, 397, 108850.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Utilizing the Orthogonality Relation of the Thickness-Averaged Structural Intensity to Extract the Mode Scattering Coefficients in Multi-Mode and Multi-Directional Wave Field

Author(s): *Shuai Cao, *Agency for Science, Technology and Research (A*STAR)*; Yue Hu, *Agency for Science, Technology and Research (A*STAR)*; Jing Xiao, *Agency for Science, Technology and Research (A*STAR)*; Fangsen Cui, *Agency for Science, Technology and Research (A*STAR)*;

The scattering of the ultrasonic guided wave becomes complex when the wave traveling in plate structures with defects. The far-field scattered wave can be regarded as the resultant wave of both Lamb wave and shear horizontal wave. Apart from different modes of the wave in the scattered field, the propagating direction of each mode might be different, which increases the difficulties to interpret the scattered wave. In this paper, a more complex wave field (multi-mode and multi-directional wave field) is explored by extracting the wave scattering coefficients, which is based on the existing studies of separating the modes of the scattering wave field. The orthogonality relations of the thickness-averaged structural intensity (SI) of different modes are verified by the semi-analytical finite element method (SAFE). Besides the unidirectional wave modes, the wave modes propagating in different directions are also considered. It is shown that the orthogonality of different modes is still well-founded, namely, the thickness-averaged SI is zero, while the value of the coupling thickness-averaged SI is not zero when the modes of different directional waves are the same. Next, on the basis of the established orthogonality relations, an algorithm is proposed to obtain the coefficients of each mode in the complex wave field. These coefficients include the information of the complex amplitude and directions of the mode. Furthermore, to validate the proposed method, the case of a plate with a rivet hole is analyzed. The scattering coefficients of the wave can be used as the damage indicator of the structures

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Title: A Spatially Varying Robin Interface Condition for Fluid-Structure Coupled Simulations

Author(s): *Shunxiang Cao, *California Institute of Technology*; Guangyao Wang, *Tianjin University*; Alex Main, *Ansys Inc.*; Kevin Wang, *Virginia Polytechnic Institute and State University*;

We present a spatially varying Robin interface condition for solving fluid-structure interaction problems involving incompressible fluid flows and non-uniform flexible structures. Recent studies have shown that for uniform structures with constant material and geometric properties, a one-parameter Robin interface condition can improve the stability and accuracy of partitioned numerical solution procedures. In this work, we generalize the constant parameter to a spatially varying function that depends on the structure's local material and geometric properties, without varying the exact solution of the coupled fluid-structure system. We present an algorithm to implement the Robin interface condition in an embedded boundary method for coupling a projection-based incompressible viscous flow solver with a nonlinear finite element structural solver. We demonstrate the numerical effects of the spatially varying Robin interface condition using two example problems: a simplified model problem featuring a non-uniform Euler-Bernoulli beam interacting with an inviscid flow, and a generalized Turek-Hron problem featuring a non-uniform, highly flexible beam interacting with a viscous laminar flow. Both cases show that a spatially varying Robin interface condition can clearly improve numerical accuracy (by up to 2 orders of magnitude in one instance) for the same computational cost. Using the second example problem, we also demonstrate and compare two models for determining the local value of the combination function in the Robin interface condition.

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Title: Optimal Time Filtering Methods as General Linear Methods

Author(s): *Sigal Gottlieb, *University of Massachusetts Dartmouth*; Zachary Grant, *Oak Ridge National Laboratory*; Victor DeCaria, *Oak Ridge National Laboratory*; William Layton, *University of Pittsburgh*;

In this talk I will describe our work on time filtering methods for the Navier Stokes equations as well as other applications. Time filtering has been used to enhance the order of accuracy of given methods. This is particularly useful in the context of legacy codes, in which the time-stepping module is given and difficult to change. However, modifying the inputs and outputs is simple and allows for higher order. In this talk, we show how time filtering approaches can be seen as equivalent to generating a general linear methods. We use this GLM approach to develop an optimization routine that enabled us to find new time-filtering methods with high order and efficient linear stability properties. We will present our new methods and show their performance when tested on sample problems.

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Title: A Hybrid Black-Box Optimization for Efficient Calibration of Heat Conduction Model in Additive Manufacturing

Author(s): *Sirui Bi, *Oak Ridge National Laboratory*; Benjamin Stump, *Oak Ridge National Laboratory*; Jiaxin Zhang, *Oak Ridge National Laboratory*; Yousub Lee, *Oak Ridge National Laboratory*; Matt Bement, *Oak Ridge National Laboratory*; Guannan Zhang, *Oak Ridge National Laboratory*;

Solidification dynamics play an important role in determining microstructure properties in additively manufactured products. A high-fidelity simulation model offers an opportunity to predict heat conduction effects at length and time scales. However, it is often computationally intensive, specifically for complex multi-physics numerical models. To address this challenge, a recent study proposes a low-fidelity heat conduction model using a semi-analytical approach with an adaptive integration scheme. The mismatch between the low-fidelity model and the high-fidelity model (e.g., Truchas) can be penalized by calibrating the model parameters via optimization. In this work, we develop a novel hybrid black-box optimization method and apply it for efficient calibration of the heat conduction model. This hybrid method leverages recent advances in evolutionary strategies with directional Gaussian smoothing and Bayesian optimization. We show that the proposed method has superior performance on optimal solution search, computational efficiency and stability, and demonstrate it on several analytical benchmarks and the real-world heat conduction problem in additive manufacturing

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Title: Reduced-Order Modeling for Hydrodynamics Simulation of the Rayleigh–Taylor Instability

Author(s): *Siu Wun Cheung, *Lawrence Livermore National Laboratory*; Youngsoo Choi, *Lawrence Livermore National Laboratory*; Dylan Copeland, *Lawrence Livermore National Laboratory*; Kevin Huynh, *Lawrence Livermore National Laboratory*;

In this talk, we present some novel model reduction techniques for computational methods which simulate the Rayleigh-Taylor instability phenomenon which occurs at interfaces between two fluids of different densities, where the lighter fluid is pushing the heavier fluid due to external forces. Real-world applications include the formation of mushroom clouds from volcanic eruptions and atmospheric nuclear explosions, and supernova explosions in which expanding core gas is accelerated into denser shell gas. Classical model reduction schemes are built on linear subspaces for solution representation and limited to the assumption that the intrinsic solution space falls into a subspace with a small dimension, i.e., the solution space has a small Kolmogorov n-width. However, the Rayleigh-Taylor instability phenomenon is advection-dominated in nature, which hinders these model reduction schemes from being practical. We investigate to improve the performance of model reduction schemes by enhancing the solution representability of the linear subspace by introducing some special treatments and adaptive schemes or replacing the linear subspace solution representation with the nonlinear manifold.

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Title: Immersed Finite Elements Based on Local Cauchy Problems: Convergence and Stability

Author(s): *Slimane Adjerid, *Virginia Polytechnic Institute and State University*; Tao Lin, *Virginia Polytechnic Institute and State University*; Ruchi Guo, *University of California, Irvine*;

We present a high-order immersed finite element (IFE) method for elliptic interface problems with nonhomogeneous interface jump conditions. We allow elements in a given mesh to be cut by the interface leading to two types of elements: (i) elements that are not cut by the interface, referred to as non-interface elements and (ii) elements that are cut by the interface referred to as interface elements. The finite element spaces consists of standard polynomial spaces on non-interface elements and piecewise polynomial IFE functions obtained by solving a local Cauchy problem on each interface element. The proposed IFE method consists of a discontinuous Galerkin formulation on interface elements and a continuous Galerkin formulation on non-interface elements. We show that this method converges optimally under mesh refinement and we present new stability results for the proposed IFE method by establishing upper bounds for the condition numbers of associated stiffness matrices.

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Title: Continuum-Kinematics-Inspired Peridynamics

Author(s): *Soheil Firooz, *University of Erlangen-Nuremberg*; Paul Steinmann, *University of Erlangen-Nuremberg*; Ali Javili, *Bilkent University*;

Peridynamics (PD) is a non-local continuum formulation and has been extensively used in different fields of study to date [1]. The original version of PD was restricted to bond-based interactions. Bond-based PD is geometrically exact. However, bond-based PD fails to capture the Poisson effect correctly. This shortcoming was later addressed via introducing state-based PD where the kinematics of the problem was not accurately preserved. Continuum-kinematics-inspired peridynamics (CPD) developed by Javili et al. [2] provided a geometrically exact framework whose underlying kinematics coincide with that of CCM and is capable of capturing the Poisson effect correctly. In CPD, one distinguishes between one-, two- and three-neighbour interactions. One-neighbour interactions are equivalent to the bond-based interactions of the original PD formalism. However, two- and three-neighbour interactions are fundamentally different from state-based interactions. This presentation briefly introduces CPD and elaborates on its computational aspects, and provides detailed derivations that are essential for its implementation [3]. The proposed strategy is robust and the quadratic rate of convergence associated with the Newton--Raphson scheme is observed. Key features of the resulting computational CPD are elucidated via a series of numerical examples. Both two- and three-dimensional problems examples are provided at both small and large deformations. As promised, CPD eliminates the zero-energy mode instabilities associated with non-ordinary state-based peridynamics and thus, it proves to be a compelling alternative. 1- A. Javili, R. Morasata, E. Oterkus, S. Oterkus, Peridynamics Review, Mathematics and Mechanics of Solids. Vol. 24, pp. 3714--3739, (2019). 2- A. Javili, A. T. McBride, P. Steinmann, Continuum-kinematics-inspired peridynamics. Mechanical problems, Journal of the Mechanics and Physics of Solids. Vol. 131, pp. 125--146, (2019). 3- A. Javili, S. Firooz, A.T. McBride, P. Steinmann, The computational framework for continuum-kinematics-inspired peridynamics, Computational Mechanics. Vol. 66, pp. 795--824, (2020).

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Title: A VMS Method for Advection-Diffusion Anisotropic Problems with Spectral Approximation of Sub-grid Scales

Author(s): *Soledad Fernández-García, *Universidad de Sevilla*; Tomás Chacón Rebollo, *Universidad de Sevilla*; Macarena Gómez-Mármol, *Universidad de Sevilla*;

In this talk, we consider the extension of the Variational Multi-scale method with spectral approximation of the sub-scales to two-dimensional advection-diffusion problems. The spectral VMS method is cast for low-order elements as a standard VMS method with specific stabilized coefficients. These coefficients are anisotropic in the sense that they depend on two grid Péclet numbers, each one associated to a different component of the advection velocity. The stabilized coefficients are computed for grids of isosceles right triangles and right quadrilaterals, based upon the explicit computation of the eigen-pairs of the advection-diffusion operator with Dirichlet boundary conditions. In order to reduce the computing time, they are pre-computed at the nodes of a grid in an off-line step, and then interpolated by a fast procedure in the on-line computation. Finally, we present several numerical tests, with the aim to compare our results with those provided by other stabilization coefficients, both isotropic and anisotropic ones. We consider tests for advection-diffusion equations with constant and anisotropic velocities, as well as tests in structured and unstructured meshes. The method is also tested for the solution of Navier-Stokes equations. We observe a relevant accuracy gain for moderately large grid Péclet numbers for variable advection velocity.

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Title: Adaptive and Efficient Rare Event Analysis Using a Gaussian Process Modeling Fidelity Recommender System

Author(s): *Som Dhulipala, *Idaho National Laboratory*; Michael Shields, *Johns Hopkins University*; Benjamin Spencer, *Idaho National Laboratory*; Chandrakanth Bolisetti, *Idaho National Laboratory*; Andrew Slaughter, *Idaho National Laboratory*; Vincent Laboure, *Idaho National Laboratory*; Promit Chakroborty, *Johns Hopkins University*;

Accurately characterizing rare events is vital in many engineering fields. However, due to the low failure probabilities and the high computational costs of models, characterizing rare events is very time consuming. To this end, we propose a modeling fidelity recommender system using Gaussian Processes and combine it with the variance reduction method Subset Simulation for an adaptive and efficient rare event analysis. For each input parameters sample in the Subset Simulation, a fast-running, but less accurate, low-fidelity model (may also be a surrogate mod-el) is first evaluated. Then, Gaussian Process decides whether a computationally expensive, but accurate, high-fidelity model evaluation is necessary, or a low-fidelity model evaluation is sufficient, given the input parameters sample. The aim is to call the high-fidelity model as few times as possible while accurately estimating the failure probability. Our proposal has three ad-vantages over other methods that use Gaussian Processes for rare event analysis: (1) Quicker Gaussian Process since only a small fraction of the input samples (i.e., those samples using which the high-fidelity model is evaluated) are used for its training and evaluation; (2) Flexibility to choose the low-fidelity model, which can be a reduced degrees of freedom or reduced physics finite element model or even a Deep Neural Network surrogate; (3) Potentially more accurate Gaussian Process for a given training set since it has to only learn the differences be-tween the low- and high-fidelity model outcomes, and not the outcomes of the high-fidelity mod-el. We demonstrate our modeling fidelity recommender system using diverse test cases where the failure probabilities are small, including the steady state Navier-Stokes equations and maximum Von Mises stress in a transversely isotropic material. In general, we find that our proposed methodology gives accurate predictions of the failure probability while calling the high-fidelity model very few numbers of times in comparison to the total number of calls to the low-fidelity model. We will conclude the presentation with a brief overview of the implementation of the proposed algorithm and other Uncertainty Quantification methods in the Multiphysics Object Oriented Simulation Environment (MOOSE) developed at Idaho National Lab, and its usage in Nuclear Energy simulations.

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Title: WATMUS: Wavelet Transformation Induced Multi-Time Scaling for Accelerating Fatigue and Multi-Physics Simulations

Author(s): *Somnath Ghosh, *Johns Hopkins University*;

Multiple time scales are commonly encountered in the multifunctional response of many structure-material systems that are governed by multi-physics relations. These systems exhibit disparate frequencies in their time-dependent behavior, transcending time-scales that span several orders of magnitude. Time-scales in structural response can range from those of defect nucleation and propagation at the atomic scale to deformation and crack propagation in the material microstructure, and the overall material deformation and damage evolution at the macroscopic scale of the component. Important classes of problems that are often challenged by the need to address multiple time-scales in their behavior include the prediction of fatigue failure in structural components under cyclic loading conditions and analysis of the transient response of multi-functional electro-magnetic and piezo-electric systems. Computational methods are generally used for simulating the time-dependent response of evolving variables in these systems. A majority of these methods employ semi-discrete models, where the spatial domain is discretized into finite element meshes and the temporal domain is discretized into time steps and integrated using conventional single-scale time integration methods. A major shortcoming of these single-scale time integration methods is the lack of efficiency for providing adequate temporal resolution to variables and phenomena at their respective time-scales. This paper describes a novel wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerating computational simulations of the two classes of problems mentioned above [1,2]. Furthermore, temporal multiscaling will be presented in the context of spatial multiscaling to address the evolution of fatigue crack evolution, both at the material and component scales. The wavelet decomposition naturally retains the high-frequency response through the wavelet basis functions and transforms the low-frequency material response into a ``cycle scale'' problem undergoing monotonic evolution. No assumption of scale separation or any homogenization is needed with the WATMUS method and hence is significantly advantageous over other multi-time scale methods. [1] P. Chakraborty and S. Ghosh, “Accelerating cyclic plasticity simulations using an adaptive wavelet transformation based multi-time scaling method'', Int. J. Num. Meth. Engng., Vol. 93, pp. 1425-1454, 2013. [2] R. Yaghmaie and S. Ghosh, “Multi-time scale-based modeling of piezoelectric materials coupling transient electrical and dynamic fields with finite deformation damage”, Int. J. Sol. Struct., Vol. 202, pp. 338-355, 2020.

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Title: Spatially Local Reduced-Order Bases for Accelerating Nonlinear Projection-Based Reduced-Order Models

Author(s): *Spenser Anderson, *Stanford University*; Charbel Farhat, *Stanford University*;

Classical projection-based Model Order Reduction (PMOR) approaches rely on the pre-computation of a linear subspace approximation defined by a Reduced-Order Basis (ROB) that, despite having a dimension much smaller than that of the High-Dimensional Model (HDM) constructed for the solution of a problem of interest, exhibits the ability to capture the dominant features of the HDM-based solution of this problem. It is common to construct such a ROB by collecting many HDM-based solution snapshots into a snapshot matrix and compressing this matrix using the Singular Value Decomposition (SVD) method. However, for highly nonlinear problems such as convection-dominated flow problems and applications characterized by multiple distinct scales or physical regimes -- or more generally, for any problem with a high Kolmogorov n-width -- a single, global ROB often needs to be prohibitively large to deliver sufficient accuracy. One approach for addressing this issue is to substitute the linear subspace approximation with a piecewise linear counterpart, or more generally, an approximation on some appropriate nonlinear manifold. In particular, one such approach is the method of local ROBs based on the aforementioned piecewise linear or affine subspace approximation. It partitions the state space into regions by clustering the solution snapshots, then constructs local ROBs that are accurate in their assigned subregions of the state space. Because each local ROB needs to be accurate only in a subregion of the state space, it can have a relatively small dimension, which achieves computational efficiency. In this talk, a complementary approach is presented to boost even further computational efficiency. This approach accelerates the performance of a Projection-Based Reduced-Order Model (PROM) by also partitioning the computational domain underlying the HDM into subdomains and building for each one of them a separate, locally-supported ROB. In this case, the full state vector over the entire spatial domain can be approximated in the span of the union of the aforementioned spatially-local bases. Effectively, this leads to constructing a sparse global ROB and therefore to accelerating the computation of the PROM-based solution by exploiting this sparsity. Algorithms for clustering the spatial domain and constructing spatially local ROBs are presented, and techniques for exploiting the resulting sparsity in PROM-based simulations are discussed. The overall performance of the proposed local ROB approach for PMOR is demonstrated for several CFD applications using the Least-Squares-Petrov-Galerkin PMOR method.

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Title: Convergence of the TFDW Energy to the Liquid Drop Model

Author(s): Lorena Aguirre Salazar, *McMaster University*; *Stan Alama, *McMaster University*; Lia Bronsard, *McMaster University*;

We consider two nonlocal variational models arising in physical contexts. The first is the Thomas-Fermi-Dirac-von Weizsacker (TFDW) model, introduced in the study of ionization of atoms and molecules, and the second is the liquid drop model with external potential, proposed by Gamow in the context of nuclear structure. It has been observed that the two models exhibit many of the same properties, especially in regard to the existence and nonexistence of minimizers. We show that, under a "sharp interface" scaling of the coefficients, the TFDW energy with constrained mass Gamma-converges to the liquid drop model, for a general class of external potentials. Finally, we present some consequences for global minimization of each model.

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Title: Parallel Simulations of High-Power Optical Fiber Amplifiers

Author(s): *Stefan Henneking, *The University of Texas at Austin*; Jacob Grosek, *Air Force Research Laboratory*; Leszek Demkowicz, *The University of Texas at Austin*;

Fiber laser amplifiers are of interest in communication technology, medical applications, and military defense capabilities. Silica fiber amplifiers can achieve high-power operation with great efficiency. At high optical intensities, multi-mode amplifiers suffer from undesired thermal coupling effects such as the transverse mode instability (TMI). The TMI is a major obstacle in power-scaling of large mode area, active gain, fiber amplifiers. A better understanding of these nonlinear coupling effects is beneficial in the design of new fibers. We present details on the implementation and numerical results for a high-fidelity fiber amplifier model. This model is based on the 3D vectorial time-harmonic Maxwell equations for two weakly coupled electromagnetic fields. The high-frequency nature of the wave propagation problem requires the use of high-order discretizations to effectively counter numerical pollution. The discontinuous Petrov-Galerkin (DPG) finite element method provides a stable discretization with a built-in error indicator. For simulating a significant fiber length of more than one thousand wavelengths, a scalable parallel implementation is critical. For this, we have developed an MPI/OpenMP finite element software that supports high-order discretizations for complex multiphysics problems. In particular, we have implemented a parallel nested dissection solver suited for the DPG linear system. We show scalability results for modern manycore compute architectures.

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Title: Active-Set Solution of Mortar Contact Between Higher-Order Elements in Explicit Dynamics

Author(s): *Stephen Beissel, *Southwest Research Institute*;

In simulations of wave motion in solids, higher-order finite elements demonstrate much greater accuracy than the industry-standard first-order elements over the entire range of asymptotic convergence. Exploiting this accuracy in problems of practical interest requires commensurate accuracy of the algorithms enforcing boundary conditions on bodies in contact. This presentation details a mortar formulation of the contact boundary conditions applied to higher-order elements and subjected to explicit time integration, and the solution of the resulting equations by an active-set method. The formulation is tailored to higher-order elements by accounting for both the curvature of the higher-order surfaces in the contact constraints, and the order of the shape functions in computing the contact forces. The performance of the proposed contact algorithm is then compared to the performance of a widely used legacy contact algorithm for explicit dynamics. The transmission of a planar wave through a contact interface demonstrates correct enforcement of the contact boundary conditions along the interface by the proposed contact algorithm, regardless of element order or alignment of opposing elements. In contrast, the legacy contact algorithm only enforces the boundary conditions correctly when opposing elements are the same order and aligned with one another. The oblique impact of a rounded projectile on a plate, resulting in large plastic strains in the plate and subsequent ricochet of the projectile, is simulated at several levels of mesh refinement to study convergence. A posteriori error estimates of the velocities in the projectile from the legacy contact algorithm are several times larger than those from the proposed contact algorithm. The proposed contact algorithm thereby appears to better extend the superior accuracy of higher-order elements to problems involving contact.

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Title: Machine Learning for Fluid Mechanics

Author(s): *Steven Brunton, *University of Washington*;

Many tasks in fluid mechanics, such as design optimization and control, are challenging because fluids are nonlinear and exhibit a large range of scales in both space and time. This range of scales necessitates exceedingly high-dimensional measurements and computational discretization to resolve all relevant features, resulting in vast data sets and time-intensive computations. Indeed, fluid dynamics is one of the original big data fields, and many high-performance computing architectures, experimental measurement techniques, and advanced data processing and visualization algorithms were driven by decades of research in fluid mechanics. Machine learning constitutes a growing set of powerful techniques to extract patterns and build models from this data, complementing the existing theoretical, numerical, and experimental efforts in fluid mechanics. In this talk, we will explore current goals and opportunities for machine learning in fluid mechanics, and we will highlight a number of recent technical advances. Because fluid dynamics is central to transportation, health, and defense systems, we will emphasize the importance of machine learning solutions that are interpretable, explainable, generalizable, and that respect known physics.

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Title: Progress Toward Global to Coastal Modelling Capabilities within E3SM

Author(s): *Steven Brus, *Argonne National Laboratory*; Luke Van Roekel, *Los Alamos National Laboratory*; Mark Petersen, *Los Alamos National Laboratory*; Qing Li, *Los Alamos National Laboratory*; Nairita Pal, *Los Alamos National Laboratory*; Giacomo Capodaglio, *Los Alamos National Laboratory*; Kristin Barton, *University of Michigan*; Brian Arbic, *University of Michigan*; Andrew Roberts, *Los Alamos National Laboratory*;

The U.S. Department of Energy's (DOE) Energy Exascale Earth System Model (E3SM) is a fully coupled Earth system model which includes atmosphere, ocean, sea ice, land ice, land, and runoff model components. E3SM is unique in that each of these components supports the use of variable resolution meshes. Our goal is to use this regional refinement capability to represent coastal scale processes and water cycle extremes within the global coupled climate system. This talk gives an overview of several efforts to incorporate the features and processes necessary to bridge the global and coastal scales to address DOE mission questions. This includes regional refined mesh design, vertical mixing parameterizations, wetting and drying, coupled wave modeling, tidal forcing, and variable time stepping. The combination of these advancements will allow for a better understanding of the impact of flooding and biogeochemistry in dynamic coastal zones under multi-decadal climate change scenarios.

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Title: An Adaptive-Sparse Spline Dimensional Decomposition Method for High-Dimensional Uncertainty Quantification

Author(s): *Steven Dixler, *The University of Iowa*; Ramin Jahanbin, *The University of Iowa*; Sharif Rahman, *The University of Iowa*;

This work introduces a novel adaptive-sparse spline dimensional decomposition (SDD) method for solving high-dimensional uncertainty quantification (UQ) problems, which arise in numerous fields of science and engineering. The proposed method enhances the efficiency of the standard SDD expansion by employing global sensitivity analysis to guide the selection of SDD component functions to be retained according to their degree of contribution to the approximation. While selectively adjusting the number of subintervals in the spline knot sequence associated with each input variable, the tensor product structure of the SDD approximation is trimmed by eliminating the component functions corresponding to weak variable interactions. Therefore, in contrast to the standard SDD method in which truncation of the expansion is controlled on a global level by parameters that are specified a priori and arbitrarily, the adaptive-sparse SDD method accounts for differences in the degree of influence of individual input variables and their interactions. As such, the resulting approximation further alleviates the curse of dimensionality and is therefore better equipped to solve practical engineering problems that involve many input variables. The utility of the proposed method is demonstrated with three numerical examples, one involving two mathematical functions, another involving a random field input, and the last one solving a practical high-dimensional engineering problem. The results obtained indicate that the adaptive-sparse SDD method requires significantly fewer coefficients to reach a desired level of accuracy when compared with the standard SDD method.

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Title: Use of Stochastic Gradient Descent for Topology Optimization under Reliability Constraints

Author(s): *Subhayan De, *University of Colorado Boulder*; Kurt Maute, *University of Colorado Boulder*; Alireza Doostan, *University of Colorado Boulder*;

In many design applications, practitioners are interested in designs that ensure the structure's probability of failure does not exceed a certain limit. This presentation focuses on topology optimization under reliability constraints. We propose a novel approach for evaluating failure probabilities in the optimization process. For most applications, the acceptable probability of failure is very small. As a result, a random sampling-based approach is prohibitively expensive when the structural response needs to be predicted by finite element analysis. These computational costs increase significantly in the context of design optimization which requires repeated prediction of the failure probability. Thus, instead of sampling-based approaches, traditional reliability-based topology optimization (RBTO) methods adopt some form of approximate reliability analysis, using a Taylor-series approximation of the limit-state function. This approach, however, may introduce errors in the failure probability and its gradient estimation. In this talk, we present a stochastic gradient-based approach to reduce the cost of RBTO. In this approach, we estimate the failure probability and its gradients using efficient sampling strategies that use surrogate models for the limit-state function. To show its efficacy, we illustrate the proposed approach with a benchmark problem that has an analytical solution and a topology optimization problem.

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Title: Combined Modeling and Experimental Study to Explain Air Trap During Droplet Impact onto Dielectric Surface

Author(s): *Subhayan Halder, *University of Illinois at Chicago*; Vitaliy Yurkiv, *University of Illinois at Chicago*; Rafael Granda Neto, *University of Illinois at Chicago*; Abhilash Sankaran, *University of Illinois at Chicago*; Jingwei Wu, *University of Illinois at Chicago*; Alexander Yarin, *University of Illinois at Chicago*; Farzad Mashayek, *University of Illinois at Chicago*;

Controlled droplet deposition onto a dry surface is important for various technologies such as spray cooling and spray painting, pesticide deposition, inkjet printing and coating. An uncontrolled air entrapment during droplet deposition may significantly alter the quality of aforementioned processes. In this contribution, we present the results of a combined phase-field modeling (PFM) and experimental study of air entrapment during water droplet impact onto a dry hydrophobic dielectric surface. The PFM is formulated using the Cahn-Hilliard and Navier-Stokes (NS) equations, where the local and global characteristics of the droplet impact are taken into account. The model includes the description of the droplet and air bulk phases, as well as of the smooth interface between the phases. The PFM is validated by predicting the experimentally measured equilibrium contact angle between the droplet and hydrophobic surface as well as by simulating the water droplet impact without the air entrapment. Then, several cases with varying the Weber and Froude numbers are considered to study air entrapment. The modeling results of water droplet impact allow for direct comparison with our experimental measurements in terms of maximum spreading and rebound height. The PFM results reveal that air may be entrapped under water droplet during the initial deposition as well as retraction after maximum spreading. The volume of the entrapped air bubble varies during both processes significantly influencing droplet spreading and rebound height. Furthermore, the simulation results reveal a huge pressure build up in the entrapped air (up to an order of magnitude higher than in the surrounding water phase), which has a detrimental influence on the process of droplet impact and spreading. Based upon our predictions and experimental results a contour map (the Weber vs. the Froude numbers) of the air entrapment is created. Thus, the present combined modeling and experimental study allows for a physical interpretation of the reasons behind the change of wettability of dry hydrophobic surfaces, which is an important phenomenon for controlled droplet deposition in various technological applications.

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Title: Viscoelastic Finite Element Study of Metal-Ceramics and Porcelain-Veneered Lithium Disilicate Material Systems used in Dental Crowns

Author(s): *Sukirti Dhital, *University of Connecticut*; Camila Rodrigues, *Federal University of Santa Maria, Brazil*; Yu Zhang, *University of Pennsylvania*; Jeongho Kim, *University of Connecticut*;

Metal-ceramics (MC) are one of the oldest dental restorative systems in use, owing to their long-term survival rate. However, MC restorations show clinical complications due to veneer chipping in addition to biological mishaps. The main cause of veneer chipping is the residual stress stored in crowns during the cooling phase of veneer firing cycle [1]. The grayish metallic color also makes these crowns visually unappealing and has led to the rise of all-ceramic combinations, such as porcelain-veneered lithium disilicate (PVLD) restorations. Incidences of veneer chipping in PVLD is lower than that for MC crowns and they perform biologically better [2]. However, there is a lack of information on stresses developed in PVLD restorative systems as they have been in use recently. Hence, a comparative study of PVLD with MC crowns against various parameters such as veneer to core thickness ratios (2:1, 1:1, 1:2) and cooling rates (fast or slow), can give us a better understanding of properties that govern structural stability of these restorations. For this, Viscoelastic Finite Element modeling (VFEM) of axisymmetric bilayer crowns was performed in ABAQUS, capturing the viscoelastic behavior of porcelain veneer layer [1]. Experimentally validated user subroutines (UEXPAN and UTRS) and temperature-dependent properties were applied to determine transient and residual stresses induced in the veneer layer during the cooling phase. VFEM showed higher residual stresses in the veneer layer of MC (~7MPa more), located in the inner cusp area, as compared to the PVLD system where maximum stress was at the central fossa. Both the material systems had lower residual as well as transient stresses for slow cooling (1.74E-5W/mm2?) relative to fast cooling (1.74E-4W/mm2?). PVLD system had an increase of 52-66% in residual stresses during fast cooling relative to slow cooling and the MC system had an increase of 35%-43%. The effect of thickness ratio was more prominent in MC than in PVLD. Thus, PVLD crowns produce lower (or, at least comparable), stresses relative to their traditional MC counterparts and can be a suitable replacement for MC systems. Acknowledgment: This research was funded by NIH/NIDCR (Grant Nos: R01DE026772/R01DE026279). [1] Kim J, Dhital S, Zhivago P, Kaizer MR, Zhang Y. Viscoelastic finite element analysis of residual stresses in porcelain-veneered zirconia dental crowns. J Mech Behav Biomed. 2018. [2] Sailer, I., Makarov, N.A., Thoma, D.S., Zwahlen, M., Pjetursson, B.E. All-ceramic or metal-ceramic tooth-supported fixed dental prostheses? A systematic review of the survival and complication rates.Dent. Mater. 2015.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: CMLMC algorithms for the estimation of risk measures for optimal design

Author(s): Quentin Ayoul-Guilmard, *École polytechnique fédérale de Lausanne*; *Sundar Ganesh, *École polytechnique fédérale de Lausanne*; Fabio Nobile, *École polytechnique fédérale de Lausanne*;

Risk-averse wind engineering design requires the accurate and efficient estimation of risk measures, as well as their sensitivities with respect to system design parameters. These sensitivities are important for the implementation of gradient-based algorithms for solving the optimal design problem. Since the input uncertainties are typically high-dimensional, Monte Carlo methods are often used to carry out the statistical estimation of these risk measures and their sensitivities. Multi-Level Monte Carlo (MLMC) methods have shown promise in improving the performance of Monte Carlo simulations by exploiting a sequence of approximations of the underlying problem. We propose novel Continuation MLMC (C-MLMC) algorithms to compute risk measures such as the Conditional Value at Risk, as well as their sensitivities. The C-MLMC algorithms rely on error estimators and adaptivity to achieve a prescribed tolerance with minimal computational cost. They are implemented with parallelization in the publicly available Python library XMC. We will also show how C-MLMC can be used within an optimization algorithm for risk-averse optimization and demonstrate it on a simple example of optimal design, as well as on an example of practical relevance to the wind-engineering community.

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Title: Development of a Computational Model for Prediction of Long-Term Behavior in Timber Structures

Author(s): *Susan-Alexis Brown, *Northwestern University*; Danyang Tong, *Northwestern University*; David Corr, *Northwestern University*; Gianluca Cusatis, *Northwestern University*;

Rising global emissions have led to a renewed popularity of timber as a structural material, including timber-concrete tall buildings up to 18 stories [1]. In spite of this surge in wood construction, there remains a gap in understanding of long-term structural behavior, particularly wood creep. Unlike concrete, code prescriptions for wood design lack in robust estimates for structural shortening. Computational prediction models for wood creep have therefore become increasingly necessary due to the potential for unforeseen shortening, especially with respect to differential shortening in concrete-timber hybrid structures. These effects can have serious impacts as timber building heights continue to grow. In addition to viscoelastic creep, wood also experiences moisture effects in two ways. First, the material shrinks and swells in response to decreases or increases in moisture content, respectively. Second, the viscous effect is magnified by changes in response to absolute change in moisture content, regardless of direction [2]. These effects must also be considered in any computational model for timber structures. This study lays the groundwork for wood compliance prediction models for use in timber design. A thorough review of wood creep studies was conducted, and viable experimental results were compiled into a database. Studies were chosen such that experimental conditions matched realistic building environments. An unbiased parameter identification method, originally applied to concrete prediction models, was used to fit multiple compliance functions to each data curve. Based on individual curve fittings, statistical analysis was performed to determine the best fit function and average parameter values for the collective database. A power law trend in wood creep, with lognormal parameter distribution, was confirmed by the results. A material subroutine was developed via strain superposition, where the viscoelastic strain was implemented numerically via a non-aging Kelvin chain. A stress-dependent mechanosorbtive linear strain was added, as well as a stress-independent linear shrinkage term, both dependent on change in humidity. The compliance model was verified against experimental data. Then the long-term behavior of laminated timber was predicted based on the orthotropic implementation of the developed subroutine. The results show promising use for such a model in structural design applications. [1] C. Hill and K. Zimmer, "The Environmental Impacts of Wood Compared to Other Building Materials," Norsk Institutt for Bioøkonomi, 2018. [2] Ross, R.J. (2010). “Wood Handbook: Wood as an Engineering Material.” Forest Prod. J.

16th U.S. National Congress on Computational Mechanics
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Title: A Backward Compatible Physics Informed Neural Networks for Solving Nonlinear and Higher Order Partial Differential Equations

Author(s): Revanth Mattey, *Michigan Technological University*; *Susanta Ghosh, *Michigan Technological University*;

We propose a backward compatible physics informed neural networks (xPINN) scheme that can be applied to systems described by non-linear and higher order partial differential equations as the current state of the art PINN suffers in approximating the solution. A continuous time inference model has been adopted where the neural network approximates the function between the output and the spatio-temporal input. The backward compatible physics informed neural network uses a novel training approach through domain decomposition which makes the method computationally efficient. An adaptive training scheme has been developed which can solve partial differential equations of high order and high nonlinearity effectively. Additionally, we have also shown that using techniques like logarithmic loss function and phase space could further improve the accuracy. To illustrate these ideas, we have used the classical Cahn Hilliard and Allen Cahn equations which are widely used to describe phase separation and reaction diffusion systems.

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Title: Space-Time Discontinuous Galerkin Methods for Fluid-Rigid Body Interaction Problems

Author(s): *Tamas Horvath, *Oakland University*;

Fluid-rigid body interactions are often encountered in real-world applications, such as airflow around turbines, bridges, or tall antennas. We present a higher-order accurate Space-Time Hybridizable-Embedded Discontinuous Galerkin method to solve fluid-rigid body interaction problems. The rotation and/or the translation of the rigid body is described by ordinary differential equations coupled to the fluid equation through the lifting and the pitching force. We use a sliding mesh approach that allows us to use precomputed meshes to incorporate arbitrary rotation.

16th U.S. National Congress on Computational Mechanics
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Title: Solving Bayesian Inverse Problems via Variational Autoencoders

Author(s): Hwan Goh, *Oden Institute of Computational Sciences and Engineering*; Sheroze Sherriffdeen, *Oden Institute of Computational Sciences and Engineering*; Jonathan Wittmer, *Oden Institute of Computational Sciences and Engineering*; *Tan Bui-Thanh, *Oden Institute of Computational Sciences and Engineering*;

In recent years, the field of machine learning has made phenomenal progress in the pursuit of simulating real-world data generation processes. One notable example of such success is the variational autoencoder (VAE). In this work, with a small shift in perspective, we leverage and adapt VAEs for a different purpose: uncertainty quantification in scientific inverse problems. We introduce UQ-VAE: a flexible, adaptive, hybrid data/model-informed framework for training neural networks capable of rapid modelling of the posterior distribution representing the unknown parameter of interest. Specifically, from divergence-based variational inference, our framework is derived such that most of the information usually present in scientific inverse problems is fully utilized in the training procedure. Additionally, this framework includes an adjustable hyperparameter that allows selection of the notion of distance between the posterior model and the target distribution. This introduces more flexibility in controlling how optimization directs the learning of the posterior model. Further, this framework possesses an inherent adaptive optimization property that emerges through the learning of the posterior uncertainty.

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Title: Modeling and Analysis of Air Flow in Parallel and Tilt Opening Windows

Author(s): Yihe (Grace) Huang, *Schuco-USA LLLP*; Chenzhang Wang, *Schuco-USA LLLP*; *Tejav DeGanyar, *Schuco-USA LLLP*;

The recent interest in natural ventilation for high-rise residential buildings has resulted in the need for innovative window solutions that allow natural ventilation. Simultaneously, the safety requirements, mechanical and structural constraints, acoustic efficiency, and aesthetic demands pose an exciting optimization problem. Mainly one that requires maintaining the smallest opening size while allowing the maximum airflow to meet the governing standards. Natural ventilation is the passive process of exchanging air between indoor and outdoor environments without using mechanical systems. It refers to external airflow to an indoor space due to pressure differences arising from natural forces. In practice, natural ventilation characteristics are hard to predict. Natural ventilation is categorized by wind-driven ventilation and buoyancy-driven ventilation. Wind-driven ventilation arises from the different pressures created by wind around a building or structure, which is generally unstable. Buoyancy-driven ventilation occurs due to the directional buoyancy force that results from the controllable temperature differences between the interior and exterior. Design considerations are further constrained because acoustic efficacy is the antithesis of airflow, so unique features using metamaterial concepts are also needed to mitigate sound energy. All these elements create a unique challenge that crosses the boundaries of conventional computational mechanics techniques and requires a multi-physics approach to the problem. In fact, this seemingly trivial problem requires a somewhat complicated and intricate solution approach that ranges from sophisticated CFD analysis, acoustic and structural simulations to parametric studies that result in simplified empirical relations that design engineers can readily utilize to design the window system. This study presents the journey through this process. It describes the various stages of the product development process, from concept design and laboratory testings to developing tools for the design and configuration windows. It showcases how complex and time-consuming coupled computational methods are transformed into straightforward methodologies which are adopted in the routine design procedures and production of highly efficient façade elements.

16th U.S. National Congress on Computational Mechanics
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Title: Learning Constitutive Models with a Non-Intrusive Reduced Basis Method

Author(s): *Theron Guo, *Eindhoven University of Technology*; Karen Veroy, *Eindhoven University of Technology*;

Recently, there has been a growing demand in designing microstructures with optimally tailored macroscopic properties. To avoid the high costs of empirical testing, two-scale simulation models based on computational homogenization have been used, where the microstructure is explicitly defined on so-called representative volume elements, thus essentially replacing the macroscopic constitutive model. Unfortunately, such simulations are computationally expensive and infeasible in multi-query contexts such as design, optimization, and control. To make such analyses possible, several authors have suggested data-driven approaches to replace the microscopic simulation with a computationally inexpensive surrogate model. Although these methods work quite well, they require large training datasets and, more importantly, the connection to the microstructure is lost. In this work, an approach based on reduced basis methods [1] is proposed. We construct the surrogate model in two steps: first, a proper orthogonal decomposition is applied on the microscopic stress field to discover an optimal low-dimensional basis that can accurately represent the stress. Subsequently, a deep neural network [2, 3] is employed to construct a mapping between the input parameters and the basis coefficients, yielding a non-intrusive model. For a new set of input parameters, the microscopic stress field is swiftly obtained by inferring the basis coefficients, from which the effective stress and stiffness can then be derived. Moreover, the derivatives of the effective stress with respect to material parameters are also at hand and could be used for inverse or optimization problems. The framework is tested on a two-scale problem involving a fiber-reinforced composite microstructure with varying material parameters. The simulation results obtained with the surrogate model are compared to the full two-scale results and illustrate the accuracy of the surrogate on both macro- and microscale despite using a relatively small training dataset. The speedup obtained is of several orders of magnitude. Acknowledgement: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (Grant agreement No. 818473). [1] Quarteroni, A., Manzoni, A. and Negri, F., 2015. Reduced basis methods for partial differential equations: an introduction (Vol. 92). Springer. [2] Hesthaven, J.S. and Ubbiali, S., 2018. Non-intrusive reduced order modeling of nonlinear problems using neural networks. Journal of Computational Physics, 363, pp.55-78. [3] Mohan, A.T. and Gaitonde, D.V., 2018. A deep learning based approach to reduced order modeling for turbulent flow control using LSTM neural networks. arXiv preprint arXiv:1804.09269.

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Title: Global-in-Time Domain Decomposition Methods for the Coupled Stokes and Darcy Flows

Author(s): *Thi Thao Phuong Hoang, *Auburn University*; Hyesuk Lee, *Clemson University*; Hemanta Kunwar, *Clemson University*;

We study decoupling iterative algorithms based on domain decomposition for the time-dependent Stokes-Darcy model, in which different time step sizes can be used in the flow region and in the porous medium. The coupled system is formulated as a space-time interface problem based on either physical interface conditions or equivalent Robin-Robin interface conditions. Such an interface problem is solved iteratively by a Krylov subspace method (e.g. GMRES) which involves at each iteration parallel solution of time-dependent Stokes and Darcy problems. Consequently, local discretizations in both space and time can be used to efficiently handle multiphysics systems with discontinuous parameters. Numerical results with nonconforming time grids are presented to illustrate the performance of the proposed methods.

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Title: Stable High-Order Discretizations of Spectrally Convergent Radiation Boundary Conditions

Author(s): *Thomas Hagstrom, *Southern Methodist University*;

As the radiation of energy to the far field is a central feature of wave physics, convergent near-field domain truncation techniques are an essential component of any comprehensive software for simulating waves. Many methods have been proposed to address this issue. Focusing on time-domain formulations, examples include retarded potential integral equations, fast low-memory methods for applying space-time integral operators arising in exact formulations, damping layers such as the perfectly matched layer or simpler combinations of grid stretching and artificial viscosity, as well as sequences of local radiation boundary conditions. Here we advocate the latter technique. First, in comparison with methods based on integral operators, local methods are more easily parallelized and are more memory-efficient. Second, in comparison with damping layers, there is a straightforward way to choose optimized parameters associated with sharp error estimates. These are the complete radiation boundary conditions (CRBC) constructed in (Hagstrom and Warburton, SINUM 47 2009). The implementation of local radiation boundary condition sequences is built on the introduction of a collection of auxiliary functions which formally obey simple recursions. For first order hyperbolic systems, these auxiliary functions may be restricted to the faces of the radiation boundary as in (Hagstrom and Warburton Wave Motion, 39 2004). For second order systems they can be evolved in a thin, one-element, double absorbing boundary layer (Hagstrom, Givoli, Rabinovich and Bielak, JCP 259 2014). In both cases edge and corner closures can be imposed to support polygonal artificial boundaries. Although the evolution equations for the auxiliary equations are provably hyperbolic, they do not seem to admit simple energy estimates. Therefore, standard techniques for proving the stability of Galerkin discretizations do not directly apply. We present theoretical and experimental studies of stable, high-order discretizations of the auxiliary equations as well as a discussion of their coupling with popular volume discretizations. These are the necessary ingredients for our development of a generally usable CRBC library.

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Title: The Cut FEM for Structural Membranes and Shells

Author(s): *Thomas-Peter Fries, *Graz University of Technology*;

The Cut FEM is a fictitious domain method (FDM), herein applied to partial differential equations on manifolds such as they appear, e.g., in the modelling of structural membranes and shells [1,2]. The governing equations are formulated based on the Tangential Differential Calculus (TDC) [3]. The geometries of the structures are implied by the level-set method, prescribed at the nodes of some higher-order background mesh and interpolated in-between. As for any other FDM, the Cut FEM has to address the following three issues: (1) The numerical integration of the weak form in the (three-dimensional) background elements which are cut by the membrane or shell. Therefore, the zero-level sets of the level-set functions have to be identified and integration points defined. (2) The application of boundary conditions within the background elements which is done based on Nitsche's method here. (3) The stabilization with respect to shape functions with extremely small supports on the structure. In the context of the Cut FEM for PDEs on manifolds, a stabilization is also required to tackle linear dependencies of the three-dimensional shape functions of the background mesh when applied to the analysis of the (curved) two-dimensional structures. Numerical results show the success of the proposed formulation. References [1] T.P. Fries, D. Schöllhammer: A unified finite strain theory for membranes and ropes, Comp. Methods in Appl. Mech. Engrg., 365, 2020 (doi.org/10.1016/j.cma.2020.113031). [2] D. Schöllhammer, T.P. Fries: A Higher-order Trace Finite Element Method for Shells, Internat. J. Numer. Methods Engrg., early view, (doi.org/10.1002/nme.6558). [3] M.C. Delfour, J.P. Zolésio: Shapes and geometries - Metrics, Analysis, Differential Calculus, and Optimization. SIAM, Philadelphia, PA, 2011.

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Title: A Variational Phase-Field Model For Ductile Fracture with Coalescence Dissipation

Author(s): *Tianchen (Gary) Hu, *Duke University*; John Dolbow, *Duke University*; Brandon Talamini, *Sandia National Laboratories*; Andrew Stershic, *Sandia National Laboratories*; Michael Tupek, *Sandia National Laboratories*;

A novel phase-field for ductile fracture model is presented. The model is developed within a consistent variational framework in the context of finite-deformation kinematics. A novel coalescence dissipation introduces a new coupling mechanism between plasticity and fracture by degrading the fracture toughness as the equivalent plastic strain increases. The proposed model is compared with a recent alternative where plasticity and fracture are strongly coupled. Several representative numerical examples motivate specific modeling choices. In particular, a linear local fracture dissipation function provides an “unperturbed” ductile response prior to crack initiation, and Lorentz-type degradation functions ensure that the critical strength remains independent of the phase-field regularization length. In addition, the response of the model is demonstrated to converge with a vanishing phase-field regularization length. The model is then applied to calibrate and simulate a three-point bending experiment of an aluminum specimen with a complex geometry. The effect of the proposed coalescence dissipation coupling on simulations of the experiment is first investigated in a two-dimensional plane strain setting. The calibrated model is then applied to a three-dimensional calculation, where the calculated load-deflection curves and the crack trajectory show excellent agreement with experimental observations. Finally, the model is applied to simulate crack nucleation and growth in a specimen from a recent Sandia Fracture Challenge.

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Title: High-Order Implicit Shock Tracking: Robust Solvers and Applications

Author(s): *Tianci Huang, *University of Notre Dame*; Matthew Zahr, *University of Notre Dame*;

Shock tracking, as an alternative method to shock capturing, aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods have been shown to enable high- order approximation of high-speed flows and do not require extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the solution basis approximates the remaining smooth features. In previous work [1], we introduced an implicit shock tracking framework that re-casts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conservation, stability, and high-order approximation (both solution and geometry). By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh. In this talk, we present a number of extensions to the implicit shock tracking method aimed at improving robustness for complex problems, including: (1) introduction of shock-preserving, arbitrary-order element collapses in arbitrary dimensions to preserve solution features; (2) in- corporation of pseudo-transient continuation to improve solver robustness with respect to the initial guess; and (3) the use of vanishing-viscosity as part of the optimization solver to prevent severe mesh motion and distortion. We use the proposed framework to solve a number of relevant inviscid, steady and unsteady, transonic and supersonic, inert and reacting flows in two and three dimensions, and demonstrate the potential of the method to provide accurate approximations to these difficult problems with local features on coarse, high-order meshes. REFERENCES [1] Matthew J. Zahr, Andrew Shi, and Per-Olof Persson. Implicit shock tracking using an optimization-based high-order discontinuous Galerkin method. Journal of Computational Physics, 410:109385, 2020.

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Title: Direct Serendipity and Mixed Finite Elements on Convex Polygons

Author(s): *Todd Arbogast, *The University of Texas at Austin*; Zhen Tao, *The University of Texas at Austin*; Chuning Wang, *The University of Texas at Austin*;

The classical serendipity and mixed finite element spaces suffer from poor approximation on nondegenerate, convex quadrilaterals. We develop direct serendipity and direct mixed finite element spaces on convex polygons, which achieve optimal approximation properties and have minimal local dimension. The set of local shape functions for either the serendipity or mixed elements contains the full set of scalar or vector polynomials of degree r, respectively, defined directly on each element (i.e., not mapped from a reference element). Because there are not enough degrees of freedom for global H^1 or H(div) conformity, additional supplemental shape functions must be added to each element. The specific choice of supplemental functions gives rise to different families of direct elements. These new spaces are related through a de Rham complex. The new families of serendipity spaces are the precursors under the curl operator of our direct mixed finite element spaces, which can be constructed to have reduced or full H(div) approximation properties. One choice of direct serendipity supplements on quadrilaterals gives the precursor of the recently introduced Arbogast-Correa spaces [1]. Other fully direct serendipity supplements can be defined without the use of mappings from reference elements, and these give rise in turn to fully direct mixed spaces. Our development is constructive, so we are able to give global bases for our spaces. Numerical results are presented to illustrate their properties. [1] T. Arbogast and M. R. Correa, Two families of H(div) mixed finite elements on quadrilaterals of minimal dimension, SIAM J. Numer. Anal., 54:6 (2016), pp. 3332-3356, DOI 10.1137/15M1013705.

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Title: Large Eddy Simulation Reduced Order Models

Author(s): *Traian Iliescu, *Virginia Polytechnic Institute and State University*; Changhong Mou, *Virginia Polytechnic Institute and State University*; Birgul Koc, *Virginia Polytechnic Institute and State University*;

We present reduced order models (ROMs) that are constructed by using ideas from large eddy simulation (LES) and variational multiscale (VMS) methods. These LES-ROMs are built by using ROM spatial filters, e.g., the ROM projection and the ROM differential filter. The LES-ROMs capture the large scale ROM features and model the interaction between these large scales and the small scale ROM features. We present results for LES-ROMs in the numerical simulation of under-resolved engineering flows (e.g., flow past a cylinder and turbulent channel flow) and the quasi-geostrophic equations (which model the large scale ocean circulation).

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Title: Towards Structural Health Monitoring of a Miter Gate through a Computationally Efficient Digital Twin

Author(s): *Travis Fillmore, *Coastal and Hydraulics Laboratory, ERDC, USACE*; Zihan Wu, *University of California, San Diego*; Manuel Vega, *University of California, San Diego*; Zhen Hu, *University of Michigan-Dearborn*; Michael Todd, *University of California, San Diego*;

Keywords: Structural health monitoring, digital twin, miter gates, real-time diagnosis, multi-scale ABSTRACT Lock gates are a critical element of the United States inland waterway system, supporting a barge industry whose value adds $33.8 billion to the United States gross domestic product. While the United States Army Corps of Engineers (USACE) spends hundreds of millions of dollars each year maintaining these navigational structures, not enough money is available to fix every need identified in this deteriorating infrastructure. If the USACE had better knowledge about the current state of their gates and establish a risk profile, they could optimize their maintenance decisions over the life cycle. Structural health monitoring (SHM) offers critical insights into the health of gate structures, and therefore can be a major asset to the USACE. Supervised SHM algorithms are effective in many applications for which the data can be tagged based on the degree of damage or by a binary category (e.g. damaged or undamaged). However, lock gates are so large and many are so old that such tagging is nearly impossible. Consequently, continous damage monitoring of lock gates through the digital-twin paradigm has been pursued. A computational lock gate can be interrogated to tell us whether the gate is damaged or undamaged given certain SHM data. Our academic partnership with UCSD has produced a number of fruitful inquiries into lock gate digital twins. One challenge is that the USACE SHM system commonly gathers data at the rate of one reading a second. Since miter gates are large fifty foot structures, cracks are inches long, and both scales individually are computionally demanding, serious advances need to be made in the speed of any digital twin employed. We show that for a miter gate, a machine learning based global-local method brings the computational speed much closer to the SHM-required speed necessary for real-time structural health diagnosis.

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Title: A Locking-Free Variational Multiscale Meshfree Method for Reissner-Mindlin Plate Formulation

Author(s): *Tsung-Hui (Alex) Huang, *National Tsing Hua University*;

The Reissner-Mindlin plate formulation in the thin-plate limit will encounter the well-known shear-locking phenomenon that must be overcome. The meshfree nodal integration can easily handle the locking issue, but it may suffer from zero and low energy instability. Although the conventional domain-subdivision-based or nodal gradient-based stabilization can avoid the low energy instability, they may cause the violation of the bending exactness (BE) in the Galerkin framework. In this research, a variational multiscale approach [1] is employed for the proposed meshfree Reissner-Mindlin plate formulation, where the solution is decoupled into coarse-scale and fine-scale under the variational equation. The coarse-scale solution utilizes the mesh-free reproducing kernel particle method (RKPM), with the stabilized conforming nodal integration (SCNI). The RK approximation in second-order monomial basis stratifies the Kirchhoff mode reproducing condition (KMRC), and SCNI guarantees the bending exactness in the Galerkin meshfree equation [2] without triggering zero-energy instability. The fine-scale solutions represent the residual of the coarse-scale equation, and the embedment of the fine-scale solutions in the coarse-scale system results in a residual-based Galerkin Least-Square (GLS) stabilization, which eliminates the spurious oscillatory modes. In order to ensure the fine-scale solution is also locking-free, a smoothed stress divergence (SSD) is employed in the stabilization term such that the bending exactness is satisfied. RKPM naturally avoids computational challenges associated with low-quality meshes, allows efficient adaptive refinement, and provides flexible control of continuity and locality in numerical approximations [3]. The proposed framework, termed VMS-RKPM, is verified by different numerical examples, and it exhibits a better convergence rate than the conventional approach with comparable efficiency. Reference [1] Hughes, T. J., Feijóo, G. R., Mazzei, L., & Quincy, J. B. (1998). The variational multiscale method—a paradigm for computational mechanics. Computer methods in applied mechanics and engineering, 166(1-2), 3-24. [2] Wang, D., & Chen, J. S. (2004). Locking-free stabilized conforming nodal integration for meshfree Mindlin–Reissner plate formulation. Computer Methods in Applied Mechanics and Engineering, 193(12-14), 1065-1083. [3] Chen, J. S., Hillman, M., & Chi, S. W. (2017). Meshfree methods: progress made after 20 years. Journal of Engineering Mechanics, 143(4), 04017001.

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Title: How to Reduce the Surface Effect and to Apply the Boundary Conditions in 1D Peridynamic Models

Author(s): *Ugo Galvanetto, *University of Padova*; Francesco Scabbia, *University of Padova*; Mirco Zaccariotto, *University of Padova*;

Peridynamics is a recently proposed continuum theory which has been specially devised to describe fracture phenomena in solid bodies [1, 2, 3]. The non-local nature of the theory causes an undesired stiffness fluctuation near the boundaries (known as surface effect [4]) as well as some difficulties in the application of the boundary conditions [2, 3]. The authors propose an innovative method to mitigate the surface effect and to rationally impose boundary conditions. The basic idea [5] is to introduce a fictitious boundary layer and to define the displacements of its nodes by means of a Taylor expansion based at the closest real node. Therefore, the fictitious nodes are bound to move according to the displacements of the nodes of the real body close to the boundary. In this way the neighbourhoods of all real boundary points are completed in a rational way. The proposed method is presented with the use of a 1D bond-based example and then applied to a 1D ordinary state-based body under various constraints and loads for which the same solution of classical mechanics is expected. The numerical results recover the classical solution exactly in the whole domain, even near the boundaries. U. Galvanetto and M. Zaccariotto would like to acknowledge the support they received from MIUR under the research project PRIN2017-DEVISU and from the University of Padua under the research project BIRD2018 NR.183703/18. References [1] S.A. Silling, M. Epton, O. Weckner, J. Xu, E. Askari. Peridynamic states and constitutive modeling. Journal of Elasticity, 88(2), 2007. [2] E. Madenci, E. Oterkus. Peridynamic Theory and its Applications. Springer-Verlag, 2014. [3] F. Bobaru, J.T. Foster, P.H. Geubelle, S.A. Silling. Handbook of Peridynamic Modeling. CRC press, Boca Raton (FL), 2016. [4] Q.V. Le, F. Bobaru. Surface corrections for peridynamic models in elasticity and fracture. Computational Mechanics, 61(4), 2018. [5] Scabbia F., Zaccariotto M., Galvanetto U., ‘A novel and effective way to impose boundary conditions and to mitigate the surface effect in 1D state-based Peridynamics’, submitted.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Data-Driven Nonlinear Aeroelastic Models of Morphing Wings for Control

Author(s): *Urban Fasel, *University of Washington*; Nicola Fonzi, *Politecnico di Milano*; Steven L. Brunton, *University of Washington*;

Accurate and efficient aeroelastic models are critically important for enabling the optimization and control of highly flexible aerospace structures, which are expected to become pervasive in future transportation and energy systems. Advanced materials and morphing wing technologies are resulting in next generation aeroelastic systems that are characterized by highly coupled and nonlinear interactions between the aerodynamic and structural dynamics. In this work, we leverage emerging data-driven modelling techniques to develop highly accurate and tractable reduced-order aeroelastic models that are valid over a wide range of operating conditions and are suitable for control. In particular, we develop two extensions to the recent dynamic mode decomposition with control (DMDc) algorithm to make it suitable for aeroelastic systems: 1) we introduce a formulation to handle algebraic equations, and 2) we develop an interpolation scheme to smoothly connect several linear DMDc models developed in different operating regimes. Thus, the innovation lies in accurately modelling the nonlinearities of the coupled aerostructural dynamics over multiple operating regimes, not restricting the validity of the model to a narrow region around a linearization point. We demonstrate this approach on a high-fidelity, three-dimensional numerical model of an airborne wind energy system, although the methods are generally applicable to any highly coupled aeroelastic system or dynamical system operating over multiple operating regimes. Our proposed modelling framework results in real-time prediction of nonlinear unsteady aeroelastic responses of flexible aerospace structures, and we demonstrate the enhanced model performance for model predictive control. Thus, the proposed architecture may help enable the widespread adoption of next generation morphing wing technologies.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Oblique Scattering and Wave Propagation in Layered Media: Band Structure, Scattering, and Homogenization

Author(s): *Vahidreza Alizadeh, *University of Massachusetts Lowell*; Alireza Amirkhizi, *University of Massachusetts Lowell*;

The band structure of infinitely periodic layered media and scattering off of finite slabs of such materials can be analyzed using the transfer matrix method. In this work, the analysis of low frequency resonant micro-structured media with viscoelastic constituent layers will be presented. The scattering response may be used to produce a homogenized description in the sense of Willis-type constitutive formulation. It is shown that the constitutive model is inherently spatially dispersive or it cannot reproduce all possible scattering responses. Moreover, such representation is not unique. Utilizing a consistent field integration technique, Onsager’s principle and elastodynamic reciprocity, a reduced set of constitutive tensors will be introduced. Finally, a detailed study on the behavior of the eigenvalues and eigenvectors near the mode collapse will be discussed. Multiple configurations for the layered media are presented to assess the homogenization method's robustness and influence of mode collapse on the scattering response of these systems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Peridynamic Micromechanics of Composites Materials (CM) of Random Structures

Author(s): *Valeriy Buryachenko, *Micromechanics & Composites LLC*;

Summary: There are four correspondences between the properties of constituents of CM and the effective properties of CM: 1) local +homogenization=local (see Chapters 8-10 in [1]), 2) local + homogenization =nonlocal (see Chapter 12 in [1]), 3) nonlocal + homogenization=local [2], 4) nonlocal + homogenization=nonlocal [3]. We will consider the problem classes 3) and 4). It is established formal similarity of the operator forms of general integral equation (GIEs) proposed by the author for both locally elastic CMs and nonlocal ones (in the senses of either Eringen or Silling) that opens the opportunities to straightforward generalization of their solutions for locally elastic CMs [1] to their nonlocal counterparts. Background, variational principles, and basic methods of locally elastic CMs [1] are generalized to peridynamic micromechanics for 3) (see [2] and references therein). Effective moduli in 3) are expressed through the introduced new notions of both the micropolarization tensor and the average local interface polarization tensor (although the local interface polarization tensor is not defined). The averages are accomplished over the surface of the extended inclusion phase rather than inside entire composite. Any spatial derivatives of local displacement fields are not required (al hough the effective constitutive equation contains a macro strain). For 4), we estimate the effective deformations of statistically homogeneous peridynamic CMs for the prescribed self-equilibrated body-forces. A subsequent simplification is described by the dilute approximation method assuming coincidence of the effective field with the applied field when interaction of inclusions is negligible. The method is based on estimation of a perturbator introduced by one inclusion that is, in fact, the solutions of the basic problem for one inclusion inside the infinite peristatic matrix subjected to the body-force. The effective nonlocal operator (which is not necessarily peridynamic one with a priory unknown structure, such as, e.g., some type of kernel) is obtained by averaging of both the displacements and stresses estimated by summation of these perturbators for all possible locations of inclusions. [1] Buryachenko V. A. (2007) Micromechanics of Heterogeneous Materials. Springer, NY. [2] Buryachenko V. (2020) Generalized effective field method in peridynamic micromechanics of random structure composites. J. Solids Structures 202:765-786 [3] Buryachenko V. (2020) Effective deformation of peridynamic random structure bar subjected to inhomogeneous body-force. J. Multiscale Comput. Enging 18:1–17

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Numerical Analysis of the Mixed and the Primal Hybrid Finite Element Methods to Solve the Poisson's Equation: Accuracy, Simulation Time and A-Posteriori Error Estimation

Author(s): *Victor Bringhenti Oliari, *Unicamp*; Denise de Siqueira, *Universidade Tecnológica Federal do Paraná*; Philippe Remy Bernard Devloo, *Unicamp*;

The diffusion of monophasic fluids through porous media is described by the Poisson's equation. In particular, two finite element formulations used to model the Poisson's problem are the mixed [1] and the primal hybrid [2], each of which locally preserve the mass. The mixed method seeks the pressure and the flux (Darcy's velocity) satisfying the source term and the boundary conditions, whereas the primal hybrid, seeks the pressure and the normal-component of the flux. When these formulations are approximated by polynomial spaces of similar orders, the flux space requires a greater number of degrees of freedom (DOF) to be described than the space describing the normal-component of the flux. On the other hand, the primal hybrid formulation is not numerically stable when approximated using low-order polynomial spaces. Considering that in practice the simulations are usually carried out using low-order approximation spaces, it is not clear which method is numerically more efficient. Moreover, the authors have not found studies which evaluate a a-posteriori error estimator for the primal hybrid method. The objective of this work is to clarify these issues by carrying out a numerical analyses that: compare the approximation errors and the simulation times of both methods, and evaluate an error estimator formulation for the primal hybrid method. [1] FORTIN, M.; BREZZI, F.Mixed and hybrid finite element methods. [S.l.]: New York:Springer-Verlag, 1991. [2] RAVIART, P.-A.; THOMAS, J.-M. A mixed finite element method for 2-nd order elliptic problems. In:Mathematical aspects of finite element methods. [S.l.]: Springer,1977. p. 292–315.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Learning Coarse-Grained Dynamics from High Fidelity Models

Author(s): *Victor Churchill, *The Ohio State University*; Kailiang Wu, *The Ohio State University*; Dongbin Xiu, *The Ohio State University*;

Molecular dynamics simulations can be used to replicate a wide variety of physical phenomena. However, long simulations are computationally expensive. Coarse-grained variables are able to capture complex behavior from large-scale simulations without needing to keep track of individual atoms, but explicit equations for these variables are not always available. Therefore, in this talk, the long-term dynamics of coarse-grained variables are learned using deep residual neural networks with memory trained on short bursts of coarse-grained trajectories.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Phase Field Modeling of Crack Propagation, Deflection and Delamination in Engineered Interfaces

Author(s): *Vinamra Agrawal, *Auburn University*; Brandon Runnels, *University of Colorado Colorado Springs*;

Nanolayered composites with engineered interfaces offer excellent potential for damage resistance and improved fracture toughness. For instance, Cu/Nb metallic nanolayered composite has been shown to exhibit different crack propagation paths and distances. By varying the geometry of the interface, the stiffness, strength, toughness, and failure mechanisms of the composite can be tuned. In this work, we use phase field model to study the crack propagation in nanolayered composites with engineered interfaces. We study the case of a notch crack propagating under mode-I loading. The domain comprised of two isotropic materials with different elastic properties and fracture energies, with an interface of a different fracture energy. As the crack propagates and approaches the interface, depending on the moduli, fracture energy ratios and geometry of the interface, the crack can either deflect towards or away from the interface leading to either delamination or material fracture. We implement the phase field model using Alamo, a finite difference multilevel multigrid and multicomponent solver, on a block structured adaptively refined grid. Using a hybrid isotropic-anisotropic model for fracture, we solve for elastic equilibrium and crack propagation with a staggered solution approach. We solve elastic equilibrium equations in their strong form implicitly using finite difference scheme, followed by a Ginzberg-Landau type evolution dynamics for evolving crack field. The block structured mesh is adaptively refined using a reflux-free scheme near the crack tip and the interface. We first validate our code by a) obtaining stress fields around a Mode I crack and comparing with analytical values and b) applying standard Mode-I test with varying meshes to study crack propagation. We conduct a systematic analysis of crack interaction with interface by varying moduli, fracture energies and interface geometries. Finally, we compare interface designs in their ability to arrest crack growth.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Finite Element Modeling of Contact Formation in an External Gear Pump

Author(s): *Vincent de Bie, *VMI Holland B.V. / Eindhoven University of Technology*; Martien Hulsen, *Eindhoven University of Technology*; Patrick Anderson, *Eindhoven University of Technology*;

External gear pumps are very efficient for the transport of fluids. In these pumps, the rotation of one gear is imposed. This gear drives the other gear by means of contact. In previous work of the authors [1], two-dimensional fi nite element simulations of an external gear pump are performed with the rotation of both gears imposed. The reasoning behind this is that modeling a moving contact point is quite complex using the finite element method. It is assumed that the effect of driving both gears is small when the minimum distance between the gears is set small enough. In this work, we want to verify if contact formation is always the case, or if there are exceptions. This is done by studying the effect of material and processing parameters on the formation of contact. The mesh re finement routines ensure that a set number of elements is present between the boundaries of the geometry. This enables us to follow the contact formation in the simulations up to micrometer scale. The aim of the study is to understand what conditions could drive the formation of a lubrication layer between the gears. The prevention of contact would result in less wear on the gears of the external gear pump. Numerically, the persistence of a lubrication layer enables fi nite element simulations of multiple rotations. [1] V. G. de Bie, M. A. Hulsen, and P. D. Anderson. Finite element modeling of a viscous fluid flowing through an external gear pump. Macromolecular Theory and Simulations, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Peridynamic Analysis of Crushing Behavior in Ceramic Open Cell Foams

Author(s): *Vinzenz Guski, *University of Stuttgart*; Kim Lars Haeussler, *CeramTec*; Anne Uhlenbrock, *CeramTec*; Siegfried Schmauder, *University of Stuttgart*;

Since decades open cell foams show their potential for lightweight components in automobile, aerospace or medical industry as crash relevant parts or implants. Usually, for these applications a high demand on safety and reliability of the components is required. Thus, the development of new products is time- and cost extensive. Especially, products for medical applications such as implants have to prove their reliability and bio-compatibility in long-term investigations. In this regard, simulation methods can help to drastically reduce the experimental efforts to develop new products. The focus in the present investigation is directed towards the crushing behaviour of ceramic foam structures, which are employed as bone substitutes for implants. Computed tomography (CT) has emerged as a useful technique to quantify the foam characteristics and to reconstruct such 3D foam structures. For the simulation in this study, a new continuum mechanics approach called peridynamics is employed to investigate the crushing behaviour of the reconstructed 3D foam structures. Based on bond-based peridynamics theory the dynamic process of compression and crushing in the brittle material is simulated. Finally, in combination with the determined foam characteristics a structure-property-relationship is obtained.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Microstructure-guided Deep Material Network for Nonlinear Material Modeling

Author(s): Tianyu Huang, *Northwestern University*; Zeliang Liu, *Livermore Software Technology, an ANSYS company*; *Wei Chen, *Northwestern University*;

For nonlinear and heterogeneous materials, simultaneously simulating many alternative microstructures under arbitrary loads is crucial in high-fidelity multiscale analyses but remains computationally inefficient. We propose an efficient deep-learning-based material modeling approach for composites to predict their nonlinear behavior considering constituent plasticity for (1) any loading paths and (2) microstructure phase configurations described by descriptors (e.g., volume fraction and orientation). Our work is built upon the deep material network (DMN) [1], a specially architected deep learning model that is trained from the linear finite element analysis data of a given microstructure and predicts its nonlinear response when an arbitrary loading path is provided. The proposed method, named microstructure-guided deep materials network (MGDMN), generalizes DMN's capability from considering only loading as inputs to any microstructure configurations while keeping the cost of collecting training data manageable. To accomplish this goal, we introduce a way of generating a DMN model's parameters for a new microstructure by directly interpolating those from a few carefully selected trained DMNs, the minimum number of which is only Np + 2 where Np is the number of phases in the material. Unlike existing data-driven material modeling work, the creation of new microstructures' models via MGDMN does not require additional data and optimization-based model training. This approach provides significant computational cost savings, and the efficiency becomes more prominent when a large number of different microstructures (e.g., several orders of magnitude) are to be simulated. Our framework enables new studies of nonlinear structural and material behavior with complex microstructures. Examples include high-fidelity multiscale simulations with heterogeneous microstructures and uncertainty quantification (UQ) of nonlinear material behaviors for random microstructures. We demonstrate our approach and show its accuracy and efficiency via short carbon fiber reinforced polymer (CFRP) composites modeling and its UQ considering heterogeneous microstructures. [1] Z. Liu and C. T. Wu, "Exploring the 3D architectures of deep material network in data-driven multiscale mechanics," Journal of the Mechanics and Physics of Solids, vol. 127, pp. 20–46, 6 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Atomistic Mechanism of Stress Modulated Phase Transition of 2D TMDC Materials

Author(s): *Wei Gao, *The University of Texas at San Antonio*;

Monolayer transition metal dichalcogenides TMDC materials have two most stable phases: semiconducting 2H phase and metallic 1T' phase. The dynamic control of transitions between these two phases on a single atomically thin sheet holds promise for variety of revolutionary applications. Particularity, it is quite promising that stress field can be utilized to dynamically modulate such phase transitions. The mechanism of stress dependent phase transition is that stress field can be applied to change transition energy barriers and pathways. The barriers determine phase transition rates. Transition pathways reveal the atomistic process of phase transition such as new phase nucleation and propagation. So far, the role of stress on these phase transition behaviors of 2D TMDC is not clear. The central objective of this study is to determine transition barriers and pathways of 2D TMDC as a function of applied stress field, in order to build a mechanics foundation for phase engineering of 2D TMDC at the atomic level.

16th U.S. National Congress on Computational Mechanics
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Title: A New Procedure for Implementing the Modified Inherent Strain Method with Improved Accuracy in Predicting Both Residual Stress and Deformation for Laser Powder Bed Fusion

Author(s): *Wen Dong, *University of Pittsburgh*; Xuan Liang, *University of Pittsburgh*; Qian Chen, *University of Pittsburgh*; Shawn Hinnebusch, *University of Pittsburgh*; Zekai Zhou, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

During the metal additive manufacturing process like laser powder bed fusion (L-PBF), the fast, intense, and repetitive laser scanning usually causes residual stress and deformation in the as-built parts, thereby compromising their quality and performance. The modified inherent strain (MIS) method has been proved to be able to predict the residual deformation of the as-built part accurately. However, the present work finds that the residual stress predicted by the existing MIS method is inaccurate. Therefore, a new procedure for implementing the MIS method is proposed, which can provide predictions in both residual stress and deformation with good accuracy. Compared with the existing method, the new procedure only modifies how to apply inherent strains to the part-scale finite element model. The extraction of inherent strains from the detailed process model is not changed. In the simulation using the part-scale model, the new procedure introduces material properties not only at ambient temperature but also at an elevated temperature corresponding to the intermediate state that is defined during the extraction of inherent strains. Both numerical and experimental examples show that after adopting the new procedure, the MIS method can effectively predict residual stress, and its ability to predict residual deformation will not be impaired.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Over-Coming Fluid-Structure Instabilities for Incompressible Flows and Light Bodies

Author(s): *William Henshaw, *Rensselaer Polytechnic Institute*;

The added-mass instability has, for decades, plagued partitioned fluid-structure interaction (FSI) simulations of incompressible flows coupled to light solids and structures. Many current approaches require tens or hundreds of expensive sub-iterations per time-step. In this talk some new stable partitioned algorithms are described for coupling incompressible flows with (1) elastic bulk solids, (2) thin structural beams and (3) rigid bodies. These added-mass partitioned (AMP) schemes require no sub-iterations, can be made fully second- or higher-order accurate, and remain stable even in the presence of strong added-mass effects. These schemes are implemented on moving and deforming overlapping grids using the Overture framework.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multiscale FEM for Statics and Eigenvibration Analysis

Author(s): *Witold Cecot, *Cracow University of Technology*; Marta Oleksy, *Cracow University of Technology*;

We present an improvement of the Multiscale Finite Element Method (MsFEM) [1] for problems with highly oscillating material coefficients. The concept of MsFEM is based on a two-mesh analysis. The coarse, macro-scale mesh discretizes the whole domain with a relatively small number of degrees of freedom and the auxiliary fine mesh, generated independently for each coarse element, captures the micro-scale details of the material. The MsFEM essential component is an online computation of special trial shape functions by the solution of local boundary value problems in each coarse element. Our enhancement uses either the static [2] or dynamic condensation that transmits the construction of the oscillatory basis functions exclusively to the coarse mesh skeleton (element interfaces). This way, both the approximation error and computational cost are reduced. Moreover, one may use arbitrary polytopal coarse elements. Higher-order shape functions increase the efficiency of calculations, and the DPG methodology [3] provides the discrete stability for the mixed formulations. Good accuracy and convergence of the improved method will be illustrated by solutions of selected plane strain (statics or eigen-vibration) problems. REFERENCES: 1. T. Hou and X. Wu, "A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media", Journal of Computational Physics, 1997, 134:169-189 2. W. Cecot and M. Oleksy, "The Discontinuous Petrov-Galerkin Methodology for the Mixed Multiscale Finite Element Method", Computers and Mathematics with Applications, 2020, In Press. 3. L. Demkowicz and J. Gopalakrishnan, "A class of discontinuous Petrov-Galerkin methods. Part II. Optimal test functions", Numerical Methods for Partial Differential Equations, 2011, 27:70-105.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multiphysics Design on Si/C Composite Nanostructures for High-Energy-Density and Robust Lithium-Ion Battery Anode

Author(s): *Xiang Gao, *University of North Carolina at Charlotte*; Jun Xu, *University of North Carolina at Charlotte*;

Generally, most of the current material fabrication guidelines for novel designs of Si/C composite nanostructure materials focus on electrochemical behavior and redox reactions at the nano/micro level. However, such guidance cannot provide detailed information for predicting the mechanical behaviors of the composite particles, especially when the mechanical field coupled with electrochemical and thermal fields. In this study, we establish an electro-chemo-mechanical model and implement it to quantitatively analyze the multiphysics behavior of five representative Si/C composite nanostructures, that are the core-shell structure, yolk-shell structure, dual-shell structure, hollow core-shell structure, and multicore-shell structure. We mainly consider two types of mechanical failure here, i.e. shell fracture and core-shell debonding. Modeling and computational results discover that yolk-shell and dual-shell structures are more robust in terms of particle fractures. For electrochemical performance, we propose a factor to evaluate the structure considering the charging/discharging capacity and diffusion capability. When considering electrochemical performance, the yolk-shell structure is the best among the compared five Si/C composites. Finally, we map design guidance to further illustrate quantitative structure-property relationships. This study provides novel insights on Si/C composite nanostructure anode material design and additional powerful design tools for next-generation high-energy-density lithium-ion batteries.

16th U.S. National Congress on Computational Mechanics
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Title: Deep Autoencoders for Physics-Constrained Data-Driven Nonlinear Materials Modeling

Author(s): *Xiaolong He, *University of California, San Diego*; Qizhi He, *Pacific Northwest National Laboratory*; J. S. Chen, *University of California, San Diego*;

Physics-constrained data-driven computing that performs physical simulation directly from material data has attracted considerable attention, but it remains challenging to deal with high-dimensional applications and extrapolation generalization. This study introduces autoencoder based deep manifold learning to the data-driven framework for nonlinear materials modeling to address these fundamental issues. An autoencoder is a special architecture of deep neural networks that extracts a low-dimensional representation (embedding) of data and addresses the “dimensionality curse” emerging from other conventional manifold learning-based methods. The data embeddings learned by the encoders provide enhanced noise filtering and extrapolation generalization. A local convexity-preserving scheme based on Shepard interpolation is introduced for the data-driven local solution to enhance numerical stability. In this study, an investigation on multiple factors, including data noise, data size, training initialization, and model architectures, is conducted to examine the robustness against noise and convergence properties of the proposed approach. A real-world application to modeling biological tissue is performed to demonstrate the effectiveness of the proposed data-driven computing approach.

16th U.S. National Congress on Computational Mechanics
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Title: Functional Mechanics of the Murine Pulmonary Heart Valve

Author(s): *Xinzeng Feng, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*;

Murine models provide an efficient platform to study heart valve diseases compared to other mammalian animals due to the low maintenance cost and high turn-over rate of mice. Moreover, it is possible to use genetically modified murine models for investigating valvular diseases, and for testing potential therapeutical treatment as well. However, the functional mechanics of murine heart valves is still under-studied due to their small size. To address this gap, we developed an integrated imaging/computational framework to quantify the nonlinear mechanical properties of murine pulmonary valves (PVs) based on μCT-derived geometries. Since each murine PV needs to be fixed before imaging, only one pressure measurement is available per PV. We thus developed representative geometric characteristics from multiple PVs. From the μCT images, we have developed a geometric model of the murine PV at multiple physiological transvalvular pressure levels. In this study, our aim is to extend the work and use mechanical simulation to provide, for the first time, an estimate of the functional elastic parameters for murine PVs and the unloaded shape. We modeled the PV leaflet as a Kirchhoff-Love thin shell, with leaflet-leaflet contact simulated by incorporating a volumetric contact potential. The simulation of PV deformation under hydrostatic pressure was implemented using FEniCS and ShNAPr. We modeled the PV as a Fung-type isotropic hyperelastic material with additional fiber contribution along the circumferential direction consistent. We then developed a geometric model for the unloaded PV mid-surfaces based on the nonuniform rational B-splines (NURBS), which is integrated seamlessly with the finite element solver using the technique of isogeometric analysis. This allowed us to optimize the PV geometry on the fly without remeshing. We used SBPLX to optimize the parameters for both the mechanical and geometric models. The profiles were then compared with the μCT-derived cross sections to obtain the optimal unloaded PV geometry and mechanical parameters. Using our imaging/computational approach, we were able to obtain, for the first time, the functional nonlinear mechanical properties of murine PVs. Our future direction is to combine the numerical method with in vivo imaging techniques (e.g., the high frequency 4D ultrasound imaging) and apply the approach to study aortic valves of diseased mouse models.

16th U.S. National Congress on Computational Mechanics
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Title: Dynamic Fracture Simulation of Rock Using a Rate-Dependent Micropolar Peridynamic Model

Author(s): Haitao Yu, *Tongji University*; *Xizhuo Chen, *Tongji University*;

A novel rate-dependent micropolar peridynamic model is proposed to simulate the dynamic fracture behaviors of rock materials. The governing equations of bonds connecting particles are reformulated from the definition of bond deformation rates, leading to a rate-based expression of mechanical behavior of solid particles. The peridynamic parameters are derived as time-dependent functions with the consistence of the strain energy obtained from the proposed peridynamic model and the continuum mechanics. The damage evolution functions are introduced in the model to capture the loading-rate dependence of rock. Moreover, a new failure criterion is proposed to describe the dynamic fracture progress of rock materials. The proposed model is verified by comparing its results with those from experimental observations. Numerical examples demonstrate that the dynamic fracture behaviors of rock materials under loads with different loading rates are well captured by the proposed model.

16th U.S. National Congress on Computational Mechanics
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Title: A Generalized Kirchhoff-Love Shell Theory with Embedded Fibers and In-Plane Bending

Author(s): *Xuan Thang Duong, *RWTH Aachen University*; Vu Ngoc Khiem, *RWTH Aachen University*; Mikhail Itskov, *RWTH Aachen University*; Roger Sauer, *RWTH Aachen University / Indian Institute of Technology Kanpur / Gdansk University of Technology*;

Fiber reinforced composites are usually modeled from the macroscopic point of view as a shell based on the classical Cauchy continuum. Although this approach is efficient and is capable of predicting the overall behavior of fabrics, it may fail to recover some important local effects. An example is the shear band (or the transition zone of the shear angles [1]) in the bias-extension test. In this case, simulation with finite element shell model based on the Cauchy continuum will fail to converge with mesh refinement to a finite width of the shear band. This is due to the fact that the in-plane bending stiffness of the fibers is not considered in the (shell) Cauchy continuum theory. Similar effects of the in-plane bending stiffness can also be found in heterogeneous and fibrous materials such as textiles, biomaterials and pantographic structures. In this contribution, we extend the classical Kirchhoff-Love shell models to account for the in-plane bending response of the fibers [2]. The theory also extends existing high gradient Kirchhoff-Love shell theory [3] for initially straight fibers to initially curved fibers. I.e.~the kinematics that capture stretching, out-of-plane bending, and in-plane bending is now included at a material point on the mid-surface of the shell. Anisotropic response is allowed for all these kinematics. To describe the in-plane curvature of multiple fiber families, a so-called in-plane curvature tensor is defined for each fiber family. The corresponding moment tensor that causes in-plane bending is then identified from the mechanical power balance. These tensors are all second order and symmetric for general materials. The balance laws are derived with the new kinematics, which results in a fourth order PDE as in the original Kirchhoff-Love shell theory. Therefore, the discretization of the corresponding weak form also requires at least C^1 continuity across shell elements, which can effectively be satisfied e.g.~by the novel isogeometric discretization technique. Several numerical examples are presented to demonstrate the capability of our proposed approach. [1] Boisse, P., Hamila, N., Guzman-Maldonado, E., Madeo, A., Hivet, G., and dell'Isola, F. The bias-extension test for the analysis of in-plane shear properties of textile composite reinforcements and prepregs: a review. Int. J.Mater Form (2017) 10:473-492. [2] Duong, T. X., Khiem, V. N., Itskov, M., and Sauer, R. A. A general theory for anisotropic Kirchhoff-Love shells with embedded fibers and in-plane bending. arXiv:2101.03122 (2021). [3] Steigmann, D. J. Equilibrium of elastic lattice shells. J. Eng. Math (2018) 109:47-61

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Homogenization-Based Optimization of Lattice Structures using Granular Micromechanics Approach

Author(s): *Yahaira Corona, *Tennessee State University*; Ranganathan Parthasarathy, *Tennessee State University*;

With the recent progress in additive manufacturing, lattice structures are being intensively researched for applications such as shock absorption, biomaterial scaffolds, and aerospace structures. They can be considered as structures at the scale of the lattice features, but materials at scales which are orders of magnitude larger. The materials and geometry of lattice structures can be optimized to meet target mechanical properties at the larger scale. In particular, homogenization-based optimization has been extensively studied since it saves computational resources as compared to full-resolution analysis. In this work, we show that the granular micromechanics approach is especially suitable for homogenization-based optimization because of the possibility to obtain closed form relationships between the macro-scale properties and the microstructural features. Effects of inter-nodal stiffness and orientation distribution of the struts on the macro-scale properties are specifically determined. It is demonstrated that the method may be extended in a straightforward manner to optimize chemically active lattice networks.

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Title: Spatiotemporal Atrophy Patterns in Healthy Brain Aging and Alzheimer's Disease

Author(s): *Yana Blinkouskaya, *Stevens Institute of Technology*; Johannes Weickenmeier, *Stevens Institute of Technology*;

Aging and neurodegenerative diseases lead to irreversible changes in brain structure and function. The brain undergoes atrophy, i.e. spatially heterogeneous cell death resulting in tissue volume loss, which manifests in cognitive decline and ultimately death. The objective of the present work is to develop a multiphysics model that predicts the structural shape changes in an anatomically accurate finite element brain model [1]. Specifically, we aim to accurately predict hallmark features of aging including white matter volume loss, cortical thinning, ventricular enlargement, and sulcal widening. In order to differentiate between healthy aging and accelerated aging in neurodegenerative disease, our model couples the AD-related spreading of misfolded proteins, amyloid beta plaques and neurofibrillary tangles, and tissue atrophy. This allows us to differentiate between healthy spatial-temporal pattern of cerebral atrophy in comparison to disease. To that end, we create a finite element model via magnetic resonance image segmentation and differentiate between gray matter, white matter, brain stem, hippocampus, cerebral spinal fluid, and ventricles. We simulate brain aging over the course of four decades and extract classical structural features determined via medical image analysis and widely reported in literature. As such, literature reports increased cerebral atrophy in AD patients in comparison to healthy controls [2]; ventricular enlargement is reported to be twice as pronounced in AD versus healthy aging; the cortex thins more in AD than during normal aging [3]; and the gyrification Index is significantly decreased in aged AD brains in comparison to young healthy brains. Our approach allows for a systematic sensitivity analysis to investigate the role of individual model parameters on structural changes in healthy and accelerated aging. Thus far, we observe that the speed of misfolded protein spreading plays a major role in cerebral atrophy leading to a two- to three-fold increase in volume loss in AD. We qualitatively validate our simulation results via direct comparison with longitudinal imaging data from the Alzheimer's Disease Neuroimaging Study. Using non-rigid image registration, we determine the deformation field between two brain scans and compare the resulting displacement fields with our simulations. References: [1] Weickenmeier et al. PRL 121 (2018) [2] Fox and Schott. The Lancet 31 (2004) [3] Dickerson et al. Neurobiol. Aging 30 (2009)

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Parametric Stitching for Smooth Coupling of Subdomains with Non-Matching Discretizations

Author(s): *Yaxiong Chen, *Purdue University*; Chun-Pei Chen, *Purdue University*; Ganesh Subbarayan, *Purdue University*;

Incompatible parametric subdomains are common in computer-aided design (CAD) and in computer-aided engineering (CAE). We present a unified formulation to smoothly couple non-matching parametric domains for both geometric modeling and analysis of behavior. The key concept used to accomplish the coupling is a “parametric stitching" or p-stitching interface between the incompatible patches. Specifically, p-stitching permits independently varying fields with assured, arbitrary smoothness at the interface between the coupled subdomains. Fundamental to the developed methodology is enriched field approximations. The base approximations in the subdomains are enriched by the interfacial fields constructed as a function of distance from the coupling interfaces. P-stitching relies on building a hierarchy of vertex, edge and face enrichments to couple the patches; it enables modular construction of coupling problems with compatible interfaces as well as the ability to characterize sharp changes in the gradient, as at dissimilar material interfaces. Arbitrary smoothness across the interface or at the vertex is assured by a continuity condition that is easily achieved through an appropriate choice of the weight field value associated with the enrichments. Non-uniform rational B-splines (NURBS) are chosen for discretizing the patches. The method is validated through patch tests on domains with two as well as multiple patches, including those with extraordinary vertices. Several two- and three-dimensional elasto-static as well as heat conduction numerical examples are also solved to illustrate the procedure.

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Title: An Asymptotically Compatible Probabilistic Collocation Method for Randomly Heterogeneous Nonlocal Problems

Author(s): *Yiming Fan, *Lehigh University*; Xiaochuan Tian, *University of California, San Diego*; Xiu Yang, *Lehigh University*; Xingjie Li, *University of North Carolina at Charlotte*; Clayton Webster, *The University of Texas at Austin*; Yue Yu, *Lehigh University*;

In this paper we present an asymptotically compatible method for solving nonlocal equations with stochastic coefficients, describing diffusion in a randomly heterogeneous media. In particular, a probabilistic collocation method (PCM) with sparse grids is used to sample the stochastic process, and the Karhunen-Loeve decomposition is employed to represent material properties. On each sample, the deterministic nonlocal diffusion problem is discretized with an optimization-based meshfree quadrature rule. We present rigorous analysis for proposed approach and demonstrate convergence for a number of benchmark problems, showing that it sustains the asymptotic compatibility spatially and achieves exponential convergence as the number of collocation points in each random dimension grows. Finally, to validate the applicability of this approach we consider a randomly heterogeneous nonlocal problem with large variances, demonstrating that the proposed PCM approach achieves substantial speed-up compared to Monte-Carlo simulations.

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Title: Efficient Nonlinear Manifold Reduced Order Model

Author(s): Youngkyu Kim, *University of California, Berkeley*; *Youngsoo Choi, *Lawrence Livermore National Laboratory*; David Widemann, *Lawrence Livermore National Laboratory*; Tarek Zohdi, *University of California, Berkeley*;

Traditional linear subspace reduced order models (LS-ROMs) are able to accelerate physical simulations, in which the intrinsic solution space falls into a subspace with a small dimension, i.e., the solution space has a small Kolmogorov n-width. However, for physical phenomena not of this type, such as advection-dominated flow phenomena, a low-dimensional linear subspace poorly approximates the solution. To address cases such as these, we have developed an efficient nonlinear manifold ROM (NM-ROM) [1,2], which can better approximate high-fidelity model solutions with a smaller latent space dimension than the LS-ROMs. Our method takes advantage of the existing numerical methods that are used to solve the corresponding full order models (FOMs). The efficiency is achieved by developing a hyper-reduction technique in the context of the NM-ROM. Numerical results show that neural networks can learn a more efficient latent space representation on advection-dominated data from 2D Burgers' equations with a high Reynolds number. A speed-up of up to 11.7 for 2D Burgers' equations is achieved with an appropriate treatment of the nonlinear terms through a hyper-reduction technique. [1] Youngkyu Kim, Youngsoo Choi, David Widemann, Tarek Zohdi, (2020) "A fast and accurate physics-informed neural network reduced order model with shallow masked autoencoder." arXiv preprint, arXiv:2009.11990. [2] Youngkyu Kim, Youngsoo Choi, David Widemann, Tarek Zohdi, (2020) "Efficient nonlinear manifold reduced order model." Workshop on machine learning for engineering modeling, simulation and design, NeurIPS 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Controlling Frontal Polymerization with Phase-Changing Materials

Author(s): *Yuan Gao, *University of Illinois at Urbana-Champaign*; Mason Dearborn, *University of Chicago*; Aditya Kumar, *University of Illinois at Urbana-Champaign*; Sagar Vyas, *University of Illinois at Urbana-Champaign*; Julie Hemmer, *University of Illinois at Urbana-Champaign*; Zhao Wang, *University of Chicago*; Aaron Esser-Kahn, *University of Chicago*; Philippe Geubelle, *University of Illinois at Urbana-Champaign*;

Frontal polymerization (FP), which involves a self-propagating exothermic reaction wave, has been proposed as a rapid, energy-efficient, and environmentally friendly method to manufacture high-performance thermoset polymers and composites. Yet, the further development of this promising manufacturing approach requires a better understanding and control of the stability of the polymerization process. In the proposed research, with the aid of multi-physics finite element analyses based on a reaction-diffusion model of the resin and a phase-transformation/thermal-diffusion model of second-phase particles, we demonstrate that control of FP in dicyclopentadiene (DCPD) and cyclooctadiene (COD) can be achieved by introducing low-melting-point phase-changing polycaprolactone (PCL) macro or nanoparticles placed in the path of the polymerization front. The interaction between the polymerization reaction and the phase transition affects the local cure kinetics and the morphologies of materials produced, providing a feasible way to manufacture polymeric materials with designable, spatially dependent patterns and material properties. With macro-PCL particles, numerical analyses unveil that the significant heat exchange between the exothermic polymerization of DCPD and the endothermic phase transformation influences the front propagation in a controllable manner. By varying the size and the spacing between particles, the front velocity, front temperature, and thermal histories can be effectively tuned according to a predictable trend, determined by the characteristic time lengths of the FP and the melting-thermal diffusion effect. Moreover, the arrangement of the PCL particles opens a design space of thermal patterns, leading to programmable spatially dependent material properties. The numerical findings are validated by experiments with excellent agreements. To model FP in COD with PCL nanoparticles, a homogenized model is proposed. Numerical analyses indicate that the intrinsic thermo-chemical instabilities in the FP of COD can be harnessed by the presence of PCL nanoparticles, leading to four different modes. A parametric study is carried out to investigate systematically the effect of the nanoparticles' concentration and resin initial temperature on the front velocity, temperature, and instability. Good agreement is found between numerical results and theoretical predictions. The proposed work provides a fundamental understanding of FP and its dynamic control via energy competition with either a local or a global endothermic process, which sheds light on the complex, chaotic nature of reaction-diffusion based systems. The results also represent an advance in the one-step fabrication of materials with precisely patterned morphologies and functionalities.

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Title: Recent Advances in Computational FSI: Isogeometric and Meshfree Formulations, Boundary Fitted and Immersed Methods, and Applications

Author(s): *Yuri Bazilevs, *Brown University*;

It is an exciting time to work in computational Fluid-Structure Interaction (FSI). Many methods have matured to the point of being able to robustly handle a wide range of FSI applications. This success is attributable to a new wave of research bringing fresh ideas in the discretization of the stand-alone fluid and solid/structure governing equations and in FSI coupling strategies. The emergence of Isogeometric and Meshfree methods is further advancing the state-of-the-art in FSI and is enlarging the classes of problems that can be handled accurately and robustly. This presentation is focused on highlighting some of these emerging methods and recent innovations in FSI and on showcasing how these methods work for applications that present significant challenges to traditional FSI approaches.

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Title: Estimation of the Magnitude of Deviatoric Stress in the Hypocentral Region of the 2019 Ridgecrest (Eastern California) Earthquakes

Author(s): *Yuri Fialko, *University of California, San Diego*;

There is a long-standing debate in geophysics regarding the level of average shear stress in the Earth's crust. Estimates of earthquake stress drops place a lower bound on shear stress resolved on seismogenic faults on the order of 1-10 MPa. Laboratory measurements of quasi-static rock friction and measurements in deep boreholes in stable intraplate interiors suggest that the brittle upper crust should be able to support much higher deviatoric stresses on the order of the lithostatic pressure (>100 MPa for ~15 km thick seismogenic zone), provided that the pore fluid pressure is approximately hydrostatic. Direct measurements of deviatoric stress at seismogenic depths are limited to a scarce set of observations in deep boreholes. Most of information about the state of stress at depth is derived from seismic data. The most commonly used method relies on the earthquake focal mechanisms to solve for the orientations of principal stress axes that are most consistent with all of the focal mechanisms in a specified volume. This method however is unable to evaluate the magnitude of deviatoric stress. I propose that the magnitude of deviatoric stress can be estimated by quantifying a distribution of fault orientations with respect to one of the principle stress axes, or between sets of conjugate faults activated by a given ambient stress. Precisely relocated seismicity catalogs reveal ubiquitous quasi-linear or quasi-planar clusters of earthquakes that represent active faults. I use machine learning (in particular, unsupervised clustering) algorithms to identify and map the distribution and attitudes of active faults throughout the seismogenic layer. In case of sufficiently localized clusters of micro-earthquakes, fault strikes can be determined with accuracy up to several degrees, an order of magnitude improvement over the individual focal mechanism solutions. Fault orientations (well defined by seismicity lineations), along with the polarity of focal mechanisms, uniquely constrain the sense of slip on the respective faults. A distribution of the dihedral angles formed by conjugate faults carries information about the amplitude and spatial heterogeneity of the deviatoric stress and frictional strength in the seismogenic zone. I illustrate the proposed method using data from the Eastern California Shear Zone that hosted a series of strong earthquakes near the town of Ridgecrest in July of 2019, and provide quantitative estimates on the magnitude of shear stress resolved on seismogenic faults in the Ridgecrest area. The observed distribution of dihedral angles between active conjugate faults suggests the effective coefficient of friction of 0.4-0.6, and depth-averaged shear stress on the order of 25-40 MPa, intermediate between predictions of the "strong" and "weak" fault theories. Combining information about fault orientation provided by interrogation of the precisely located earthquake catalogs with information provided by the earthquake focal mechanisms can improve the accuracy of inversions for the state of stress in seismically active regions.

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Title: Deep Learning of Parameterized Equations with Applications to Uncertainty Quantification

Author(s): Tong Qin, *University of Michigan*; *Zhen Chen, *The Ohio State University*; John Jakeman, *Sandia National Laboratories*; Dongbin Xiu, *The Ohio State University*;

We propose a learning algorithm for discovering unknown parameterized dynamical systems by using observational data of the state variables. Our method is built upon and extends the recent work of discovering unknown dynamical systems, in particular those using deep neural networks (DNN). We propose a DNN structure, largely based upon the residual network (ResNet), to not only learn the unknown form of the governing equation but also take into account the random effect embedded in the system, which is generated by the random parameters. Once the DNN model is successfully constructed, it is able to produce system prediction over longer-term and for arbitrary parameter values. For uncertainty quantification, it allows us to conduct uncertainty analysis by evaluating solution statistics over the parameter space.

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Title: Recent Advances in Image-Based Modeling and Evaluation of Fiber Reinforced Composite Responses to Impact Loading with Integrated Mesh-Based and Particle Methods*

Author(s): *Zhen Chen, *University of Missouri*; A.M. Rajendran, *University of Mississippi*; Robert Moser, *US Army Engineer Research and Development Center*;

Due to the limitation in available experimental techniques, it is very challenging to quantify how the constituent properties and arrangements in fiber reinforced composites (FRC) could affect the impact response involving failure evolution in real time. Recent reports on mesoscopic modeling via the material point method (MPM) for textile-based FRC have demonstrated that the macroscopic residual velocity as obtained with the model-based simulation matches very well with available experimental data for projectile impact/penetration problems, even if all the FRC constituents are modeled as linear elastic ones with the maximum tensile strain failure criterion. A quantitative investigation via the MPM has therefore been performed to explore the effect of constituent modeling and configuration on the textile-based FRC response to impact loading [1]. It appears that the orientation of mesoscopic structure with given fiber geometry and property in FRC, instead of the matrix material, governs the impact response. The matrix material failure could be either brittle or ductile with a trivial effect on the impact response. Since the failure evolution process involves the transition between discontinuity of different degrees, the design of spatial discretization should consider the specific kinematic feature at a given spatial scale [2]. In combination with in-lab experiments, hence, a systematic investigation is being performed to model and evaluate the FRC responses to impact loading with integrated MPM and finite element method (FEM). As both the FEM and MPM are formulated based on the same weak formulation with different mapping procedures, the strengths of both mesh-based and particle methods could thus be combined for image-based precision prediction. In this conference, the recent research results as obtained from this investigation will be presented to demonstrate the potential of the proposed computer test-bed for FRC optimization. *This work was partially supported by the US Army Corp of Engineers Laboratory. [1] Chen, Z., Su, Y., Rajendran, A.M., Su, H., Liu, Y., and Jiang, S., “Study of Constituent Effect on the Failure Response of Fiber Reinforced Composites to Impact Loading with the Material Point Method,” Composite Structures, Vol. 252, No. 112751, 2020. [2] Su, Y., Sewell, T., and Chen, Z., “Comparative Investigation of Shear-Band Evolution Using Discrete and Continuum-Based Particle Methods,” to appear in Acta Geotechnica, 2021.

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Title: Identification of Universal Scaling Laws in Additive Manufacturing with DimensionNet

Author(s): *Zhengtao Gan, *Northwestern University*; Xiaoyu Xie, *Northwestern University*; Wing Liu, *Northwestern University*;

Metal additive manufacturing (AM) has a vast number of parameters with complex interactions and dependencies to be considered when making a component. Universal physical relationships (e.g., scaling laws), which are proven to be valid for different materials, processing conditions, and machines, provide elegant insights into the behavior of this complex system using a minimal set of parameters. This adds simplicity to otherwise highly multivariate or multidimensional systems and helps succinctly guide processes towards parameter optimization, materials development and selection, and real-time process control. We present a data-driven identification approach, called DimensionNet, for searching universal scaling laws from AM experimental or simulation data. It leverages dimensional analysis principles with deep learning neural networks. We demonstrate the methodology by automatically searching for scaling laws from experimental data describing the two problems that are ubiquitous in AM: keyhole dynamics and porosity. Several dimensionless numbers are identified, which controls the defect generation in AM. The reduction of high dimensional parameter space means that fewer experiments will be required to determine optimal processing conditions for new materials, and thus ease the Edisonian burden endemic among current metal AM practitioners. Reference: Gan, Z., Kafka, O., Parab, N., Zhao, C., Fang, L., Heinonen, O., Sun, T. and Liu, W.K., 2020. Universal scaling laws of keyhole stability and porosity in 3D printing of metals. Saha, S., Gan, Z., Cheng, L., Gao, J., Kafka, O. L., Xie, X., ... & Liu, W. K. (2021). Hierarchical Deep Learning Neural Network (HiDeNN): An artificial intelligence (AI) framework for computational science and engineering. Computer Methods in Applied Mechanics and Engineering, 373, 113452.

16th U.S. National Congress on Computational Mechanics
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Title: Computational Models for Simulating Collective Cell Migration in Wound Healing, Cancer Progression, and Gastrulation

Author(s): *Zi Chen, *Brigham and Women's Hospital*; Joseph Sutlive, *Brigham and Women's Hospital / Harvard Medical School*; Catalina Spatarelu, *Dartmouth College*; Wenying Kang, *Harvard T.H. Chan School of Public Health*; Jacopo Ferruzzi, *Harvard T.H. Chan School of Public Health*; Melisa Fuentes, *Dartmouth College*; Hao Zhang, *University of Virginia*; Ziqian Wu, *Dartmouth College*; Ming Guo, *Massachusetts Institute of Technology*; Jeffery Fredberg, *Harvard T.H. Chan School of Public Health*; Bing He, *Dartmouth College*;

Collective cell migration is commonplace in many biological processes with physiological or pathological conditions, including embryonic development and cancer invasion1, 2. The coordinated movement of cells involves the complex interplay of biophysical and biomolecular factors such as the regulation of the intra- and inter-cellular forces1. Here we present a computational framework developed for simulating collective cell migration and present a set of simulation results in conjunction with experiments to identify the roles of physical forces in these biological processes. The computational models illustrate the mechanical basis of gastrulation, wound healing, and cancer cell migration3, as well as how changes in the mechanical properties of cells can lead to significantly different outcomes (e.g., in mutant embryos) in Drosophila. Images from experiments are used for the generation of the computational models and the simulation results are compared with experimental observations of wound healing in embryonic chick embryo tissues, collective migration of cancer cells, and epithelial folding during gastrulation in Drosophila. This work will not only provide new insight into the mechanical basis of pattern formation and evolution in a variety of biological processes, but also shed light on future interventions to aid in applications such as cancer treatment and tissue engineering. Acknowledgement This work was in part supported by the National Science Foundation (award number 2025434) and the National Cancer Institute (grant number U01CA202123); the National Heart Lung and Blood Institute (P01HL120839). Z.C. acknowledges the Branco Weiss - Society in Science Fellowship, administered by ETH Zürich. C.S. acknowledges the Dartmouth University Ph.D. Innovation Fellowship at Thayer School of Engineering. M.G. acknowledges the Sloan Research Fellowship. References 1. K. Duval, et al., Modeling Physiological events in 2D vs. 3D cell culture. Physiology 32 (4), 266, 2017. 2. CP Spatarelu, et al., Biomechanics of Collective Cell Migration in Cancer Progression--Experimental and Computational Methods. ACS Biomater. Sci. Eng. 2019, 5, 8, 3766–3787. 3. W. Kang, et al., Tumor invasion as non-equilibrium phase separation. doi.org/10.1101/2020.04.28.066845.

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Title: A New Peridynamic Framework for Discrete Dislocation Dynamics in 2D Crystal Plasticity

Author(s): *Ziguang Chen, *Huazhong University of Science and Technology*; Wenbo Dong, *Huazhong University of Science and Technology*; Florin Bobaru, *University of Nebraska-Lincoln*; Minsheng Huang, *Huazhong University of Science and Technology*;

Dislocations, common line defects in crystals, are the main carriers of plastic deformation in crystalline materials. Discrete dislocation dynamics (DDD) can track the dynamic evolution of discrete dislocations, including dislocation nucleation and annihilation, dislocation motion, and the interaction between dislocations and other defects/obstacles, which are fundamental to the prediction of plastic deformation in crystalline materials. Compared with atomic dynamics and phenomenological constitutive models, DDD can model a relatively large spatial scale and long time scale while preserves the physical mechanism of plastic formation. DDD simulation is usually realized by combining numerical methods of continuum mechanics to solve the boundary value problems (BVPs). The combination strategies of all existing DDD frameworks can be classified into two categories, i.e. the superposition (SP) scheme and the discrete-continuous (DC) coupling scheme. In this work, we introduce a new SP scheme of discrete dislocation dynamics in the peridynamic framework (DDD-PD) for the elastoplastic deformation of single crystals. The plastic deformation is represented by the slip planes of dislocations, based on which the problems of single dislocation, multiple dislocations, dislocation emitted from the crack tip, the interaction between dislocation and void, and the plastic deformation of single crystal are all analyzed and calculated. The SP scheme for the DDD-PD model is flexible and can be used on arbitrary domains, including those with pre-damage, cracks, or voids of arbitrary shapes. This scheme does not need to derive the displacement field likes the traditional continuum mechanics theory, but only uses the spatial integral equation to solve the mechanical properties of materials, so it has more advantages than other dislocation related methods in solving the discontinuity problem. The accuracy of this scheme is verified by comparing its results with analytical solutions or with numerical results from DDD-FEM and from DC peridynamic approaches. We show that the SP scheme for DDD-PD is more accurate than the DC scheme, especially for the solutions near dislocation cores. The DC scheme is restricted to problems with stagnancy dislocations and in which the dislocations are away from any boundaries, or damage/cracks locations. The stress fields near dislocations' cores calculated with the SP scheme of DDD-PD match well the analytical solution for the infinite domain, while the fields near the boundaries match well with the traction boundary conditions and the results from the DC scheme of DDD-PD. The SP scheme for DDD-PD is also applied to simulate elastoplastic Mode I fracture in a single crystal.

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Title: Parallel Space-Time Multilevel Methods with Application to Electrophysiology

Author(s): *pietro benedusi, *Università della Svizzera italiana*; Patrick Zulian, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*; Carlo Garoni, *Università degli Studi di Roma Tor Vergata*; Stefano Serra-Capizzano, *Università degli studi dell'Insubria*; Michael Minion, *Lawrence Berkeley National Laboratory*;

We present a space-time multilevel method that uses a hierarchy of non-nested meshes, created by semi-geometric coarsening. The "grey box'' multigrid starts from a single fine spatial mesh and automatically generates space-time coarse meshes of any dimension over complex geometries. We consider two model problems: the heat equation, possibly with anisotropy and jumping coefficients and the monodomain equation, a non-linear reaction-diffusion model arising from the study of excitable media such as the myocardium. We use continuous finite elements to discretize in space and, for stability reasons, we adopt discontinuous finite elements (DG) in the time dimension. We analyze the convergence and scaling behaviour of the proposed solution strategies, focusing on the spectral properties and conditioning of the underlying discrete operators that arise from the tensor space-time finite element discretization and the usage parallel block preconditioners. Strong and weak scaling of the multilevel space-time approach is compared to PFASST algorithm (Parallel Full Approximation Scheme in Space and Time), highlighting properties and conceptual and quantitative differences of both approaches.

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Title: Shape Sensitivity Analysis of Linear and Nonlinear Functionals in Structural Topology Optimization: Theory and Practice

Author(s): *Aaron Klein, *University of Toronto*; Prasanth Nair, *University of Toronto*; Masayuki Yano, *University of Toronto*;

In level-set topology optimization methods, shape derivative expressions for objective functions encountered in linear elasticity problems can be formulated in two ways; boundary-based and volumetric shape derivative expressions. The two expressions yield identical results if the domain is smooth and the governing equation is solved exactly; however, the finite element approximation of the expressions for less regular domains yield different results. In this context, we provide theoretical analyses and numerical comparisons of boundary-based and volumetric shape derivative expressions of linear objective functions and nonlinear stress-based objective functions for the optimization of linear elasticity structures. We first review the expressions to demonstrate that the volumetric shape derivative places weaker regularity requirements, which, unlike the requirements for boundary-based shape derivatives, are satisfied in most finite element approximations. We then provide a priori error analysis for the degree-k polynomial finite element approximations of the two expressions for some common objective functions, including nonlinear stress-based functions. This analysis shows that, for sufficiently regular problems, the boundary-based and volumetric shape derivatives provide k-th and 2k-th order accurate approximations, respectively, of the true shape derivative. Finally, using numerical examples, we demonstrate the practical implications of using the volumetric vs boundary-based shape derivatives in topology optimization problems. We demonstrate that methods based on volumetric shape derivatives yield more robust solutions to topology optimization problems, especially for higher-order finite element approximations. In addition, we demonstrate the importance of preserving accurate boundary representations, using e.g. a conforming mesh, for stress minimization problems to accurately resolve local stress concentrations

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Title: "How Sure Are You of That Answer?"

Author(s): *Abani Patra, *Tufts University*;

Most engineering and science translate to answering questions -- ``Will the rocket be safe and lift the payload? How far will the debris flow go? How much will the ice sheet melt?" Our knowledge deployed to answer these questions is often represented by data, models and computer programs that are subject to errors of many types and the intrinsic variabilty of some of these complex systems. Systematic approaches to a) minimize and, b) quantify these errors and uncertainties, is a career long quest. In this talk, I will review the principal ideas of error analysis and reduction strategies and some new developments in better representation of data in models to continue improving our response to the question -- ``How sure are you of the answer"

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Title: Nucleation in the Phase-Field Approach to Brittle Fracture

Author(s): *Aditya Kumar, *University of Illinois at Urbana-Champaign*; Oscar Lopez-Pamies, *University of Illinois at Urbana-Champaign*;

Twenty years in since their introduction, it is now plain that the regularized formulations dubbed as phase-field of the variational theory of brittle fracture of Francfort and Marigo [1] provide a powerful macroscopic theory and computational framework to describe and predict the propagation of cracks in elastic brittle materials under arbitrary quasistatic loading conditions. Over the past ten years, the ability of the phase-field approach to also possibly describe and predict crack nucleation has been under intense investigation. The first objective of this talk is to establish that the existing phase-field approach to fracture at large is fundamentally incomplete to describe and predict crack nucleation. This is because the approach does not properly account for one essentially ingredient: the strength under multi-axial stress states. The second objective is to introduce an amendment, recently presented in [2] and [3], that renders a phase-field theory capable of describing and predicting crack nucleation in general under quasistatic loadings, be it within the bulk, from large pre-existing cracks, small pre-existing cracks, or from smooth and non-smooth boundary points. The central idea is to implicitly account for the presence of the inherent microscopic defects in the material — whose defining macroscopic manifestation is precisely the strength of the material — through the addition of an external driving force in the equation governing the evolution of the phase field. To illustrate its use and showcase its descriptive and predictive capabilities, the proposed theory will be confronted with a variety of experimental results in many different materials. One specific problem that will be discussed is the indentation problem with flat-ended cylindrical indenters in glass for which variational phase-field models in classical form have failed to generate results that are consistent with experimental observations. [1] G.A. Francfort, J.J. Marigo. Revisiting brittle fracture as an energy minimization problem. Journal of the Mechanics and Physics of Solids 46:1319-1342, 1998. [2] A. Kumar, G.A. Francfort, O. Lopez-Pamies. Fracture and healing of elastomers: A phase-transition theory and numerical implementation. Journal of the Mechanics and Physics of Solids, 112, 523—551, 2018. [3] A. Kumar, B. Bourdin, G.A. Francfort, O. Lopez-Pamies. Revisiting nucleation in the phase-field approach to brittle fracture. Journal of the Mechanics and Physics of Solids, 142, 104027.

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Title: A Numerical Method for the Growth of Multiple Fractures in Two Dimensions

Author(s): *Adrian Lew, *Stanford University*; Benjamin Grossman-Ponemon, *Stanford University*;

We introduce a method to simulate the growth of multiple fractures in two dimensions. The method involves three numerical techniques — Universal Meshes to generate conforming triangulations of the evolving cracked domain, the Mapped Finite Element Method to calculate the displacement field with high-order accuracy, and problem-specific interaction integrals to compute stress intensity factors at each crack tip. The evolution of the cracks is governed by a general framework for rate-independent systems, where the equations of crack growth follow from a balance between the crack driving force and the subdifferential of a suitably-defined dissipation potential. We will focus on the discretization of such evolutions in the presence of multiple cracks, and illustrate the method with several numerical examples.

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Title: A Scalable Adaptive Front-Tracking Method for Simulation of Multiphase Flow

Author(s): *Ahmed Basil Kottilingal, *Sorbonne Université*; Stephane Zaleski, *Sorbonne Université*;

This paper presents a scalable Front Tracking code for simulation of multiphase flows in 3D that uses an octree Adaptive Mesh Refinement (AMR) grid. A Front Tracking code involves many communication routines between and among Lagrangian and Eulerian grids. The scalability of a Front Tracking code thus directly depends on the scalability of these communication routines. Parallelization of operations in AMR Eulerian grid is a well-studied subject and is out of this paper's scope. This paper focuses on achieving scalability of communications involving Lagrangian grid which includes communication between Lagrangian and Eulerian grids in a distributed architecture. In parallel AMR simulation, the Eulerian grid is distributed based on the Z-curve, which results in a complex domain decomposition which is modified during mesh refinement. This dynamic nature of the grid distribution makes it difficult to synchronize communications between Lagrangian grid and Eulerian grid. This work utilizes distributed fronts (Lagrangian sub-grids) where Eulerian grid cells store Lagrangian grid entities (points and elements), which gives the capability to maintain a direct mapping between Lagrangian points and Eulerian grid cells. This mapping helps in scaling inter-grid communication routines and reduces the complexity involved in load balancing during refinement. Another requirement of Front Tracking code is front regridding which has to be done periodically to maintain a smooth Lagrangian grid during interface deformation. An associated challenge with distributed Lagrangian sub-grid data structure is the implementation of regrid operations. Therefore, an optimized, scalable algorithm for the regridding of the distributed front is implemented. This paper presents strong and weak scalability tests of some multiphase flow simulations involving a large number of fronts.

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Title: PDE-Constrained Optimization Based Surface Registration for Biological Growth Problems

Author(s): *Aishwarya Pawar, *Purdue University*; David Umulis, *Purdue University*; Adrian Buganza Tepole, *Purdue University*;

We propose a novel PDE-constrained optimization problem for shape registration to capture the deformation of biological tissue from imaging data while satisfying the finite growth framework within continuum mechanics. Shape registration is the process of evaluating optimum alignment between two or more pairs of geometries through a spatial transformation function obtained from minimizing an energy functional. The energy functional typically consists of a distance measure reflecting similarity between the shapes and a regularization term reflecting the geometric regularity of the transformation. Here, we propose a method to constrain the registration problem to satisfy partial differential equations that describe linear momentum balance of growing soft tissues. For the registration framework we start from our previously reported work [1], which uses 3D tensor product B-spline basis functions to interpolate 3D space. The movement of the B-spline control points, composed with an implicit function describing the shape of the tissue, yields the total deformation gradient field. The split into growth and elastic contributions is akin to plasticity. Linear momentum balance is sought, but with the stress being a function of the elastic deformation only. The growth tensor, on the other hand, can be further reduced to a scalar field, with the permanent volume change obeying an ordinary differential equation that is coupled to the elastic deformation. In the proposed method, the weak form of mechanical equilibrium is evaluated using the B-spline basis functions. Our approach follows existing finite element implementations of growing tissue [2], but within the isogeometric analysis framework [3]. We apply the novel shape registration framework to study the growth of biological tissues for two applications: modeling tissue expansion during skin reconstruction surgery and modeling zebrafish embryo growth. Thus, we anticipate that our generalized PDE-constrained shape registration method will improve our understanding of biological and medical problems in which tissues undergo extreme deformations over time. References: [1] A. Pawar, Y. J. Zhang, C. Anitescu, T. Rabczuk. Computers & Mathematics with Applications, 78(10), 3250-3267, 2019. [2] A. M. Zöllner, A. B. Tepole, E. Kuhl. Journal of Theoretical Biology, 297, 166-175, 2012. [3] T. J. Hughes, J. A. Cottrell, Y. Bazilevs. Computer Methods in Applied Mechanics and Engineering, 194(39-41), 4135-4195, 2015.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Computational Budget Allocation in Multi-Fidelity Problems with Bandit Learning

Author(s): Yiming Xu, *The University of Utah*; Vahid Keshavarzzadeh, *The University of Utah*; *Akil Narayan, *The University of Utah*;

Multi-fidelity algorithms stitch together outputs from an ensemble of models in order to attain predictive accuracy that is typically not attainable by any single model alone for the same computational budget. One challenge of applying many multi-fidelity algorithms is the identification of how to allocate computational budget across models. Allocation strategies exist when quantitative relationships between models are available, such as correlations. However, in the absence of such information it is typically a challenging task to decide on budget allocation. We present new strategies for learning quantitative relationships between models through an exploration phase that employs bandit learning algorithms, which use statistical decision paradigms to allocate computational effort. Our particular framework for analysis entails creating a regressor that maps the low-fidelity model(s) to the high-fidelity output. Through this framework we show consistency of the estimator in the limit of infinite budget, and we develop adaptive strategies in an exploration stage that identify which models are useful in regression, and which can be safely discarded. (For example, models that are expensive and uninformative may be safely discarded.) Once quantitative relationships are built between models, then allocation strategies can proceed in an exploitation phase. Examples of multi-fidelity problems in uncertainty quantification show that bandit learning algorithms can successfully be applied in situations with incomplete and limited knowledge about model correlations.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Predicting the Influence of Scanning Strategies and Geometrical Features on Melt Pool Size Variability and Lack of Fusion Porosity During LPBF

Author(s): *Alaa Olleak, *University of Pittsburgh*; Florian Dugast, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

As-built parts manufactured by laser powder bed fusion (L-PBF) suffer from the reduced fatigue strength due to the large pores caused by lack of fusion (LOF) between scan lines. The LOF porosity mainly depends on the melt pool size, which may change based on the geometrical features and scanning strategies, and process parameters. Unlike experimental approaches, numerical-based investigations (e.g. finite element analysis) can help deliver insights on the melt pool morphology, by which LOF porosity can be estimated. To date, finite element part-scale modeling approaches, which can help predict the layer-by-layer LOF porosity formation are very computationally expensive. The current work proposes a framework by which LOF porosity for an entire part can be computed. The computational expense of this problem is overcome by using an efficient adaptive remeshing technique in combination with high performance GPU computing. Two different parts and multiple scanning strategies are considered to show the influence of the scanning strategies and geometrical features (e.g. overhangs). The predictions are validated by experimental results from the literature.

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Title: A Constitutive Structural Parameter for the Work Hardening Behavior of Additively Manufactured Ti-6Al-4V

Author(s): *Alan Jankowski, *Sandia National Laboratory*;

The mechanical behavior of Ti-6Al-4V produced by a laser powder bed fusion process is assessed [1-2] using a Kocks-Mecking-based relationship. A constitutive parameter derived for the microstructure is characteristic of the work hardening behavior determined by the plastic strain between the yield point and ultimate strength. The varied plastic behavior, such as associated with surface and build direction effects, can be evaluated with this approach. Results are presented for the mechanical behavior of Ti-6Al-4V as measured under uniaxial tension. [1] A. Jankowski et al. Int. J. Mater. Res. 110 (2019) 990. doi.org/10.3139/146.111834 [2] A. Jankowski et al. Mater. Des. Proc. Comm. 2 (2020) e96. doi.org/10.1002/mdp2.135

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A methodology for characterizing mechanical parameters of single-layer graphene sheet

Author(s): *Alejandro Pacheco-Sanjuán, *Universidad Técnica Federico Santa María*; Romesh Batra, *Virginia Polytechnic Institute and State University*; Alvaro Tejos, *Universidad Técnica Federico Santa María*;

The macroscale elastic properties of a single layer graphene sheet (SLGS) are typically obtained from experimental indentation load-deflection data fitted to predictions from nonlinear membrane models based on kinematical assumptions in the Föppl-von Karman (FvK) theory. Simplifications of the nonlinear models and a priori assumed value of Poisson's ratio (Nu = 0.165) might overestimate the in-plane Young's modulus, E2D. Based on the experimental data for nanoindentation and bulge tests, we present a four-step methodology to find values of E2D and v by numerically minimizing the difference between the experimental and the computed load-deflection curves. We use numerical results based on the mathematical model that considers all geometric nonlinearities and the St. Venant-Kirchhoff material. This approach gives E2D ~ 225-240 N/m and Nu ~ 0.2-0.3 that, respectively, differ by ~30% and ~40% from the currently accepted values (E2D ~ 340 N/m, Nu ~ 0.165). For the SLGS thickness t ~ 0.335 nm, the predicted value of the 3-D Young's modulus is E3D ~ 0.672-0.716 TPa rather than the literature value of ~ 1.0 TPa.

16th U.S. National Congress on Computational Mechanics
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Title: Affine Similar Trust-Region Method with Application to Phase-Field Models of Brittle Fracture

Author(s): *Alena Kopanicakova, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*;

The numerical simulation of failure mechanism in solids is computationally challenging, as crack-paths with a possibly complex topology have to be resolved. Phase-field models for fracture ease and eventually overcome these difficulties by regularizing the sharp crack interfaces by means of a diffusive damage model. This is computationally challenging due to non-convex nature of the resulting coupled problem, the huge number of unknowns required to resolve the crack zones and the ill-conditioning caused by local changes in the damage variable. As a consequence, the design of an efficient solution method becomes a difficult task. In this talk, we present the affine similar trust-region method (ASTRUM) in order to solve arising minimization problems. This novel solution strategy combines trust-region methods with the pseudo- transient continuation method [1]. The trust-region strategy guarantees global convergence, while the pseudo-transient continuation ensures the convergence to a dynamically stable minimizer. In addition, the pseudo-transient continuation method has a regularization property, which helps to reduce the condition number of the arising linear systems and to speed up the solution process. We will present illustrative numerical examples in order to demonstrate the efficiency of the ASTRUM method. Furthermore, we analyze the convergence behavior of the method and perform a comparison with state-of-the-art nonlinear solvers from the phase-field fracture literature. [1] Deuflhard, P. Newton methods for nonlinear problems: affine invariance and adaptive algorithms. Vol. 35. Springer Science & Business Media, 2011.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Isogeometric/Finite-Difference Approach to Fluid-Structure Interaction of Thin Shells in Incompressible Flows

Author(s): *Alessandro Nitti, *Polytechnic University of Bari*; Josef Kiendl, *Bundeswehr University Munich*; Alessandro Reali, *University of Pavia*; Marco de Tullio, *Polytechnic University of Bari*;

Fluid-structure interaction (FSI) problems involving thin flexible structures are encountered in a broad range of engineering and biologic applications. Modern numerical approaches to FSI problems can play a crucial role for understanding the fundamental physics beyond phenomena and reducing the effort needed for experiments. In the present work a partitioned approach is presented: different discretization schemes are employed for the fluid and structural sub-domains. The fluid motion is resolved in a parallel environment with a pressure projection method on a Cartesian grid, whereas the immersed structure is modeled as a NURBS surface, and the elastic response is obtained through an Isogeometric approach relying on the Kirchhoff-Love shell theory [1]. The interface condition is matched by means of a direct-forcing immersed-boundary method, where the interpolation/spreading of the field variables is performed via moving least squares approximation, which has proven to be very effective for moving boundaries [2]. The combination of these ingredients allows to perform an efficient collocation of the structural (Lagrangian) markers, thus providing an effective enforcement of the fluid-solid interface condition in case of non-uniform Eulerian grid. Furthermore, the method allows for the decoupling of the respective discretization density for fluid and structural solvers, in order to reduce the computational expense. The order of accuracy of the method is verified by refinement analyses, segregating the Eulerian/Lagrangian refinement, which confirm the expected scheme accuracy in space and time. The presented method has successfully been applied to FSI case at low/moderate Reynolds number (from Re ~O(10^0) to Re ~O(10^4)) for energy harvesting and biological applications [3]. REFERENCES [1] Kiendl, J., Bletzinger, K.U., Linhard, J. and Wüchner, R., 2009. Isogeometric shell analysis with Kirchhoff–Love elements. Computer Methods in Applied Mechanics and Engineering, 198(49-52), pp.3902-3914. [2] de Tullio, M.D. and Pascazio, G., 2016. A moving-least-squares immersed boundary method for simulating the fluid–structure interaction of elastic bodies with arbitrary thickness. Journal of Computational Physics, 325, pp.201-225. [3] Nitti, A., Kiendl, J., Reali, A. and de Tullio, M.D., 2020. An immersed-boundary/isogeometric method for fluid–structure interaction involving thin shells. Computer Methods in Applied Mechanics and Engineering, 364, p.112977.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: On the Relation Between 3D Aortic Valve Interstitial Cell Shape and Contractile Behavior

Author(s): *Alex Khang, *The University of Texas at Austin*; Quan Nguyen, *The University of Texas at Austin*; Xinzeng Feng, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*;

Aortic valve interstitial cells (AVICs) reside within all layers of the aortic valve and regulate turnover of the extracellular matrix. AVICs become activated in times of growth and disease and take on a myofibroblast phenotype and increase their contractility. Cell shape is known to correlate closely with stress-fiber geometry and function and is thus a critical feature of cell biophysical state. In this study, we assess the correlation between 3D AVIC shape and contractile behavior using hydrogel matrices to better understand the relation between AVIC shape and local deformation. AVIC contractile behavior was assessed via 3D traction force microscopy [1]. The data was analyzed with a custom software [2] which outputted field displacements and AVIC surface meshes. Field displacements were interpolated onto AVIC surfaces using Gaussian process regression. A surface patch method was used to compute principal curvatures of the AVIC surface meshes to describe local AVIC shape. To describe the global shape, we utilized spherical harmonics (SPHARM) to reconstruct AVIC shapes at a user specified level of detail by tuning the degree of the harmonics used. The resulting SPHARM power spectra was used to describe the complexity of the shape. AVIC contraction produced a complex displacement field with a prominent axis of contraction and expansion in the orthogonal direction. The majority of appreciable displacements occurred within 60 um of the AVIC surface. A significant correlation was observed between curvature and displacement magnitude on the AVIC surface (rho = 0.115, p-value less than 0.001). Regions of higher curvature produced larger displacement magnitudes and were localized at AVIC protrusions. The AVIC shapes were accurately reconstructed using SPHARM. Power spectra analysis showed that larger SPHARM coefficients were required to fit the relaxed AVIC shape than the contracted shape. This suggests that AVIC shape is more spherical while undergoing contraction. Our findings concur with previous 2D studies and suggest that in 3D, AVIC shape and function are correlated. We report that areas of high curvature, such as AVIC protrusions, produce the greatest contractile displacements and that AVIC shape becomes more spherical in a contractile state. This suggests that contraction is mediated by high concentration of stress-fibers localized at cellular protrusions. Future work will involve modeling the sub-cellular components of the AVIC to achieve a mechanistic understanding of the AVIC shape-function relation. [1] Legant et al. Nature Methods, 2010. [2] Lejeune et al. Software X. 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Point-Cloud Deep Learning of Fluid Flow in Porous Media

Author(s): *Ali Kashefi, *Stanford University*; Tapan Mukerji, *Stanford University*;

We present a novel deep learning technique for predicting fluid velocity fields in porous media. The main aim of our neural network is to overcome the challenges of Convolutional Neural Networks (CNNs) used for predicting velocity fields in porous media, which are concisely listed as follows: First, considerable computational resources of CNN frameworks are wasted by masking pixels representing solid grain spaces where no flow occurs. Second, an unreasonable memory size on GPUs is required specifically for high-resolution 3D media. Third, CNNs have shown trouble in identifying the pore versus the grain space during prediction. Specifically for porous media with complicated flow networks and low effective porosities, CNNs predict velocity fields (regardless of the accuracy of its magnitude) in spaces where the flow does not even exist (i.e., in grain spaces). The key idea of designing our neural network comes from the fact that the solution of the governing equations of fluid flow in porous media is a function of the geometry of the grain-pore boundary not the solid grain itself. Accordingly, we take only the pore space of a porous medium (e.g. from high resolution CT-scans) and represent it as a set of points constructing a point cloud. Points on the surface (in 3D) or on the edge (in 2D) of this cloud represent the geometry of grain-pore boundaries. The architecture of our neural network is mainly based on PointNet, which has been widely used for deep learning of point cloud data for classification and segmentation of 3D objects in the area of computer vision. The performance of our neural network is assessed in several ways. First, we explore the accuracy of the predicted velocity fields at different phases of the training procedure. Second, we evaluate the pointwise error of the predicted velocity fields with reference to our numerical solver along with a graphical comparison between the ground truth and prediction for two and three dimensional porous media geometries. Third, we investigate the geometrical features of point clouds with the maximum and minimum pointwise error. Fourth, we compute the speed-up factor obtained by our neural network compared to our conventional numerical solver for flow simulation in pore spaces. Fifth, we evaluate the effect of a range of porosities and spatial correlation lengths of the porous media on the performance of our deep learning framework.

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Title: Microstructural Finite Element Modeling of the Entire Lamina Cribrosa in the Human Optic Nerve Head

Author(s): *Alireza Karimi, *The University of Alabama at Birmingham*; Seyed Mohammadali Rahmati, *Georgia Institute of Technology*; Rafael Grytz, *The University of Alabama at Birmingham*; Christopher Girkin, *The University of Alabama at Birmingham*; J. Crawford Downs, *The University of Alabama at Birmingham*;

The microstructure of the lamina cribrosa (LC), including the size, volume fraction, and orientation of the LC beams likely play a crucial role in protecting the retinal ganglion cell axons passing through the scleral canal. Prior computational models of the LC microstructure have been limited to multiscale approaches, in which a small chunk of the LC microstructure is subjected to displacement boundary conditions predicted from a parent mesoscale model. This regional approach cannot calculate the stresses and strains across the entire LC, and is unable to accurately represent the relatively compliant neural tissues (NT). We developed a finite element (FE) model of posterior pole of the eye, including the LC microstructure that is constructed directly from the binary images of the LC, wherein the LC and interspersed NT were represented as isotropic neo-Hookean materials (Figure). Models of the eyes from three human donors were used to estimate the stresses and strains in the LC and NT under acute IOP elevation, and compared with identical models in which the LC was represented as a single material with either mapped connective tissue volume fraction (CTVF) and anisotropic properties based on local LC beam direction, or homogeneous isotropic neo-Hookean properties. The models were subjected to an IOP elevation to 45 mmHg after pre-stressing from 0 to 10 mmHg, and solved in CalculiX. ONH and LC displacements were matched across the three modeling approaches within each eye, and stresses and strains were compared for the LC and NT combined (continuum material and microstructural), and the LC and NT separately. The regional volumetric average von Mises stress, and 1st, 2nd, and 3rd principal stresses and strains showed that the microstructural model with neo-Hookean properties yielded similar results to our prior approach using an LC continuum representation with mapped CTVF/anisotropy, but the microstructural modeling approach allows analysis of the stresses and strains in the LC and NT separately. In the microstructural models, the LC beams carried most of the IOP load but exhibited less strain, while the encapsulated NT exhibited lower stresses and much higher strains. Strain levels matched prior experimental studies. Microstructural modeling will provide greater insight into the biomechanical factors driving damage to the axons (NT) and connective tissue remodeling of the LC that occur in glaucoma.

16th U.S. National Congress on Computational Mechanics
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Title: Targeting Structure of Water Using Neural Network-Based Force Field

Author(s): *Alireza Moradzadeh, *University of Illinois at Urbana-Champaign*; Amir Taqieddin, *University of Illinois at Urbana-Champaign*; Narayana Aluru, *University of Illinois at Urbana-Champaign*;

In this study, we develop a many-body potential using neural networks to reproduce structural properties of soft molecular systems. We use small neural networks to represent two-and three-body interactions separately, which leads to a reduction in the number of free parameters in the neural network.1 Having separate terms also allows to visualize and assess each term separately, and to understand their contribution to the structural properties.2 To train the networks, instead of the conventional training procedure based on the backpropagation algorithm, we switch to the local search method, a derivative-free method, as structural properties are not directly predicted by the neural networks. We show that by using this method, we can achieve high fidelity results for the radial distribution and angular distribution functions of ab initio water. In particular, we develop two models for ab initio water, one with only two-body interaction and another one with two-and three-body interactions. Our results show that the double-well potential is not representative of water-like interactions and in the presence of three-body interactions the double-well potential vanishes. The absence of double-well potential indicates that a three-body potential is a better representation for water-like behavior in coarse-grained models. 3 (1) Moradzadeh, A.; Aluru, N. R. Transfer-Learning-Based Coarse-Graining Method for Simple Fluids: Toward Deep Inverse Liquid-State Theory. J. Phys. Chem. Lett. 2019, 10 (6), 1242–1250. https://doi.org/10.1021/acs.jpclett.8b03872. (2) Moradzadeh, A.; Aluru, N. R. Molecular Dynamics Properties without the Full Trajectory: A Denoising Autoencoder Network for Properties of Simple Liquids. J. Phys. Chem. Lett. 2019, 7568–7576. https://doi.org/10.1021/acs.jpclett.9b02820. (3) Mashayak, S. Y.; Jochum, M. N.; Koschke, K.; Aluru, N. R.; Rühle, V.; Junghans, C. Relative Entropy and Optimization-Driven Coarse-Graining Methods in VOTCA. PLoS One 2015, 10 (7). https://doi.org/10.1371/journal.pone.0131754.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Free Surface Instabilities During Horizontal Ribbon Growth Solidification Process

Author(s): *Alireza Pirnia, *Clarkson University*; Brian Helenbrook, *Clarkson University*;

Horizontal ribbon growth (HRG) is a novel and efficient technique for growing thin sheets of single-crystal silicon from a molten pool, which are primarily used in solar panels. In this technique, the free surface of the silicon melt is cooled down using a thin jet of non-reactive cooling gas (typically helium), leading to formation of a crystallized ribbon that is continuously and horizontally pulled out. Steady and stable extraction of the ribbon is crucial for commercial purposes, which depends on the interactions between various physical phenomena that occur during the HRG process. These include convective and radiative heat transfer, phase change with a shape-dependent crystal formation (solidification kinetics), and convective and capillary-driven fluid flows. An arbitrary Lagrangian-Eulerian hp-finite element analysis is used in this work to model these physical processes in the three phases of the liquid melt, the solid ribbon, and the surrounding gas. Using a non-dimensional scale analysis, it is shown that capillary-driven flows on the free surface of the melt due to the temperature-dependent surface tension of silicon (namely Marangoni flows) are stronger than convective melt flows with the ribbon pulling speed. At certain conditions, it is observed that Marangoni flows lead to formation of vortices in the melt that results in unsteady and unstable solid-melt interactions. Moreover, the conditions at which the cooling gas jet impinges the free surfaces (liquid-gas and solid-gas interfaces) can further complicate the flow field at the triple junction point position, where the three phases meet. The effect of the jet velocity, position, and impingement angle on the fluid flow during the HRG process and the solidification stability is investigated in this work. The conditions leading to formation of waves on the ribbon surface and the onset of instability are identified, paving way for further understanding of some of earlier experimental observations.

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Title: Towards Patient-Specific Fluid Solid Growth Simulations of Vascular Adaptation and Remodeling

Author(s): *Alison Marsden, *Stanford University*;

Patient-specific modeling and simulation based on medical image data increasingly enables personalized medicine and individualized treatment planning in cardiovascular disease, providing key links between the mechanical environment and subsequent disease progression. It is well known that changes in the vascular mechanical environment impact subsequent growth and remodeling of the vascular wall, impacting cardiovascular disease progression as well as the adaptation of engineered tissues. While substantial progress has been made in our ability to predict changes in morphology and composition of vascular tissues in response to changing loads, models are currently limited to generalized two-dimensional vessel slices. We will discuss our recent progress towards formulating fluid solid growth simulations that interface patient-specific models of hemodynamics with models of vascular growth and remodeling. These developments rely on foundational advances in unified methods for fluid structure interaction simulations that enable handling fully incompressible, viscoelastic tissues. We will discuss our application of these methods in the context of two cardiovascular problems: 1) blood flow simulations of single ventricle patients receiving tissue engineered vascular grafts to assess the impact of stenosis, and 2) arterialization and remodeling of vein grafts following coronary artery bypass graft surgery. We will also provide an overview of our open source SimVascular project, which makes our tools available to the scientific community (www.simvascular.org). Finally, we will provide an outlook on recent successes and challenges of translating modeling tools to the clinic.

16th U.S. National Congress on Computational Mechanics
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Title: Spacetime–Adaptive Simulation of Earthquake Rupture on a Branch Fault System

Author(s): *Amit Madhukar, *University of Illinois at Urbana-Champaign*; Xiao Ma, *University of Illinois at Urbana-Champaign*; Robert Haber, *University of Illinois at Urbana-Champaign*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Space Institute*;

Numerical simulation of earthquake ruptures remains a challenging problem despite recent advances in high performance computing. Earthquakes are multiscale phenomena — faults can extend for hundreds of kilometers and have millimeter-scale rupture process zones. State-of-the art seismic simulation codes are unable to bridge the resulting extreme ranges of spatio-temporal scales, even on today's largest supercomputers. Most seismic codes are nonadaptive, and even those that use adaptive spatial meshing are unable to deliver sufficient dynamic refinement to capture fast-moving rupture process zones at realistic scales. These limitations force numerical analysts to accept under-resolved solutions use or use unrealistic model parameters that artificially increase process zone sizes, either of which undermines the reliability of any quantitative information drawn from a simulation. We review the causal Spacetime Discontinuous Galerkin (cSDG) method as a powerful solution scheme for extreme multiscale problems arising in seismology [1]. The cSDG method features unconditional stability, conservation over every spacetime cell, linear computational complexity, and support for arbitrarily high-order elements. Its most compelling feature, however, is an asynchronous solution scheme that interleaves adaptive unstructured spacetime mesh generation with localized solutions on small `patches' of spacetime elements. There are no synchronous time steps and no global constraints on patch durations, so elements with extremely small spatial and temporal diameters, as required in the vicinity of a rupture tip, do not constrain temporal durations and spatial diameters elsewhere in the mesh. The adaptive meshing is fine-grained, extremely dynamic and able to capture the fine details of earthquake rupture dynamics. We use this powerful tool to study the branch-fault system in the Southern California Earthquake Center TPV14 benchmark. With element diameters ranging from centimeter scale near rupture tips to multiple kilometers in distant regions, and with high-order elements, we explore the physics at the intersection of a main and a branch fault in fine detail. [1] R. Abedi, R. B. Haber and P. L. Clark, Effect of random defects on dynamic fracture in quasi-brittle materials, Int J Fract 208, (2017) pp 241–268.

16th U.S. National Congress on Computational Mechanics
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Title: Enhancing Reduced Order Models for Cardiac Electrophysiology by Machine/Deep Learning Algorithms

Author(s): *Andrea Manzoni, *Politecnico di Milano*; Stefania Fresca, *Politecnico di Milano*; Stefano Pagani, *Politecnico di Milano*;

Projection-based reduced order models (ROM), built through, e.g., the reduced basis method or proper orthogonal decomposition (POD) provide rapid and reliable approximations to parametrized PDEs. ROMs are nowadays essential to enhance the solution to many-query problems such as, e.g., forward UQ, sensitivity analysis, and inverse UQ (parameter estimation and data assimilation) whenever they involve complex physics-based models described in terms of PDEs. Indeed, employing high-fidelity, full order models (FOMs) would make the solution of the aforementioned problem computationally infeasible. Although typically more intrusive to implement, ROMs often yield more accurate approximations than purely data-driven emulators (built, e.g., through Gaussian Process regressions, polynomial chaos expansion, or artificial neural networks) and usually generate more significant computational gains than lower-fidelity models obtained introducing modeling simplifications (e.g., coarser meshes or simplified physics). Nevertheless, building efficient ROMs for nonlinear time-dependent parametrized PDEs could be a difficult task because of the use of expensive hyper-reduction strategies, or the intrinsic difficulty to handle complexity with linear superimpositions of modes. For this reason, we combine classical projection-based ROM techniques with artificial neural networks or deep learning (DL) algorithms, to either make ROMs non-intrusive and overcome the aforementioned difficulties. We show that by performing a prior dimensionality reduction on FOM snapshots through POD, exploiting deep (e.g., feedforward, convolutional, autoencoder) neural networks and relying on a multi-fidelity pretraining stage, the resulting POD-DL-ROMs are extremely efficient at both the testing stage, when evaluating the PDE solution for any new testing-parameter instance in a non-intrusive way, and the training stage, when the ROM is built. On the other hand, to enhance the efficiency of ROMs in order to address variance-based global sensitivity analysis and forward UQ problems, we account for the approximation error with respect to the FOM by means of inexpensive ANN regression models. Compared to a purely data-driven approach consisting of ANN-based models emulating the input-output relationship, the proposed approach provides better results in terms of both accuracy and offline costs. Both strategies are then applied different problems arising from cardiac electrophysiology. 1. S. Fresca, A. Manzoni, L. Dedè, A. Quarteroni. Deep learning-based reduced order models in cardiac electrophysiology. PLOS ONE 15(10): e0239416. 2. S. Fresca, L. Dede', A. Manzoni. A comprehensive deep learning-based approach to reduced order modeling of nonlinear time-dependent parametrized PDEs. arXiv:2001.04001, 2020. 3. S. Pagani, A. Manzoni. Enabling forward uncertainty quantification and sensitivity analysis in cardiac electrophysiology by reduced order modeling and machine learning. Submitted, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Level Set Topology Optimization for Fluid-Structure Interactions

Author(s): *Andreas Neofytou, *Cardiff University*; Feimi Yu, *Rensselaer Polytechnic Institute*; Lucy Zhang, *Rensselaer Polytechnic Institute*; H. Alicia Kim, *University of California, San Diego*;

In this work a level set topology optimization (LSTO) approach is developed for the solution of fluid-structure interaction (FSI) problems. FSI is a challenging class of problems in topology optimization and the literature is very limited as recognized by a recent, extensive review on fluid-based topology optimization [1]. A main challenge in topology optimization for FSI is tracking the interface as the structure undergoes topological changes to correctly apply the loads and coupling conditions. This is addressed here by employing the modified immersed finite element method (mIFEM) [2], [3] in combination with LSTO. The immersed finite element formulation employs an Eulerian background fluid mesh while the Lagrangian solid domain sits on top of the fluid and is free to deform. Since the structure continuously changes throughout the optimization process, remeshing for the solid could become a cumbersome task and the difficulty grows for large deformation problems. In this work we make use of the advantage of mIFEM to allow modularity in the solvers and we employ the reproducing kernel particle method to analyse the solid domain. By using a meshfree method, the crisp structural boundary defined by the level set method is maintained on the computational domain by placing RKPM particles on the boundary thus avoiding the need for re-meshing. The interactions between the solid and the fluid are reflected as tractions on the solid boundary and as body force and no-slip boundary conditions on the overlapping fluid. The coupled equations are then solved on the fluid mesh. Solving the solid dynamics using its own governing equations provides more accurate and realistic coupled solutions. Test cases flows with different Reynolds numbers will be presented examining also higher Reynolds number flows. References [1] Alexandersen J., and Andreasen C. S., “A Review of Topology Optimisation for Fluid-Based Problems,” fluids, Vol. 5, 2020, p. 29. [2] Wang X., and Zhang L. T., “Modified immersed finite element method for fully-coupled fluid–structure interactions,” Computer Methods in, Vol. 267, 2013, pp. 150–169. [3] Cheng J., Yu F., , and Zhang L. T., “Openifem: A high performance modular open-source software of the immersed finite element method for fluidstructure interactions,” CMES, Vol. 119(1), 2019, pp. 91–124.

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Title: Deep Learning Model to Predict Fracture Mechanisms of Graphene and Other Brittle Materials

Author(s): Markus Buehler, *Massachusetts Institute of Technology*; *Andrew Lew, *Massachusetts Institute of Technology*;

Understanding fracture is critical to the design of resilient nanomaterials. Molecular dynamics offers a way to study fracture at an atomistic level, but is computationally expensive with limitations of scalability. In this work, we build upon machine learning approaches for predicting nanoscopic fracture mechanisms including crack instabilities and branching as a function of crystal orientation. We focus on a particular technologically relevant material system, graphene, and apply a novel deep learning method to the study of such nanomaterials and explore the parameter space necessary for calibrating machine learning predictions to physically meaningful results. Our results validate the ability of deep learning methods to quantitatively capture graphene fracture behavior, including its fractal dimension as a function of crystal orientation. Using this model, we further investigate the effect of a grain boundary and how the orientations of the graphene crystal on either side of the boundary affect the fracture path and toughness of the sample, allowing us to quickly map a potential energy surface as a function of crystalline orientations. These results provide promise toward the wider application of deep learning to materials design, opening the potential for other 2D materials.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Reduction of Fluid-Structure-Control Problems and Application to Model Predictive Control

Author(s): *Andrew McClellan, *Stanford University*; Charbel Farhat, *Stanford University*;

Model Predictive Control (MPC) is particularly attractive for many applications including autonomous flight, as it allows imposing constraints on both manipulated and controlled variables as well as operating closer to constraints. It leverages a computational model of the dynamics of a physical system to compute online a control law for this system rather than using a pre-computed counterpart. Hence, for flight systems such as aircraft, and in particular, for aeroservoelastic aircraft systems, the feasibility of MPC hinges on the ability to construct a low-dimensional but accurate computational model for Fluid-Structure-Control Interaction (FSCI) that can perform in real-time. In this sense, Projection-based Model Order Reduction (PMOR) is an enabler for MPC. However, in the context of an aeroservoelastic system, the success of PMOR depends on the ability to construct and train an efficient Reduced-Order Basis (ROB) for the solution of FSCI problems. To this end, this lecture will focus on the linearized setting, which is justified for many aircraft control problems in large portions of the flight envelope, and present an approach with two variants for building an effective, multidisciplinary ROB. The proposed approach is grounded in the three-field, Arbitrary Lagrangian-Eulerian (ALE) formulation of coupled Fluid-Structure Interaction (FSI) problems. It models an aircraft as an unrestrained multibody system with a main body and a number of hinged control surfaces. It introduces the concept of a "Control Surface Mode" (CSM) -- that is, a mode of the entire articulated system where one control surface undergoes a small rotation but the rest of the system is motionless. Then, it constructs a control-aware ROB for the structural subsystem by superposing the CSMs, Rigid Body Modes (RBMs) of the main body, and its natural, Flexible Mode Shapes (FMS)s. It represents the fluid flow around the multibody system using the linearization around an equilibrium position or reference trajectory of any preferred inviscid or viscous CFD model constructed in the ALE setting. In one variant, it constructs and trains a control-aware ROB for the fluid subsystem by computing the response of the linearized FSI subsystem to a perturbation inputted along each CSM, and compressing the resulting solution snapshots. In a computationally lighter variant, it computes instead the response of the linearized fluid subsystem to a perturbation along each CSM, RBM, and FMS. Both variants will be benchmarked in the context of MPC for the automatic landing of an aircraft system and their computational merits will be contrasted.

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Title: Quantification of Margins and Uncertainty using Dakota for a Multi-physics Mechanical Thermal Analysis Workflow

Author(s): *Andrew Murphy, *Sandia National Laboratories, Albuquerque, NM*; Michael Stender, *Sandia National Laboratories, Livermore, CA*; Brent Houchens, *Sandia National Laboratories, Livermore, CA*; Lauren Beghini, *Sandia National Laboratories, Livermore, CA*;

Traditional methods for verification, validation, and uncertainty quantification primarily target scenarios involving only one physics regime (e.g., solid, fluids thermal). However, real-world environments often involve multiple physical phenomena and complex scenarios that require evaluation across multiple physical environments. For example, a mechanical deformation can alter heat transfer paths in a component, resulting in different thermal responses. Traditional multi-physics methods involve a single problem definition and a monolithic mesh used to simulate all physics regimens. This can reduce numerical efficiency and result in suboptimal meshes. In our method, independent model definitions are possible for each physics evaluation. Mapping and reconciliation of the appropriate state variables, as well as evaluation of newly formed radiation enclosures and thermal contact as a result of deformation, is allowed resulting in efficient and targeted models for simulation of multi-physics analyses. These results can then be incorporated into uncertainty quantification analysis for parameters relevant to all considered physics. In this talk, we present an example of a sequential mechanical-thermal problem using the SIERRA software suite for physics analysis and DAKOTA for uncertainty quantification. In our example, a mechanical insult results in an altered thermal response dependent on both mechanical and thermal parameters. Independent models for both solid mechanics and thermal analyses are developed and reconciled into an appropriate and efficient simulation workflow. To quantify margins associated with the thermal response from uncertainties present in the inputs and model parameters, a Latin Hypercube Sampling (LHS) uncertainty quantification analysis is deployed. This LHS study simultaneously considers variations in both mechanical and thermal parameters. The results demonstrate how our proposed approach enables decision making and design optimization under uncertainty for complex physical environments. Results demonstrate how uncertainty propagation can affect design decisions. Future work will target incorporation of additional physics and the integration of material modeling across environments. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: High-Order Time-Stepping Methods for Cut Finite Element Discretizations of Evolving Domain Problems

Author(s): *André Massing, *Norwegian University of Science and Technology, Trondheim, Norway*; Simon Sticko, *Umeå University*; Balázs Kovács, *Universität Regensburg*;

In this talk we present a novel high-order in space and time discretisation approach for the numerical solution of parabolic problems on moving domains. To allow for possibly large deformations of the evolving domain, we consider an Eulerian approach where the discretisation in space is based on high-order cut finite element methods which are rendered geometrically robust by employing so-called ghost-penalties. For the discretisation in time, Backward Difference Formulae (BDF) up to order 5 are employed, extending the ideas in [1-3] where only first and second order BDFs were considered. The time-stepping hinges on implicitly constructed extensions of time-step solutions to sufficiently large neighbourhood band via the use ghost penalties. We provide detailed numerical studies of moving domain and surface problems and demonstrate that the proposed methods achieve high-order convergence (up to order 5) for the fully discretized system. The presentation concludes with a short discussion of current drawbacks and possible extensions to more complicated problems including free boundary problems arising in phase transitions and fluid dynamics. [1] "A stabilized trace finite element method for partial differential equations on evolving surfaces", Lehrenfeld, Christoph and Olshanskii, Maxim A and Xu, Xianmin, SIAM J. NUMER. ANAL. Vol. 56, No. 3, pp. 1643-1672, 2018 [2] "An Eulerian Finite Element Method for PDEs in time-dependent domains", Lehrenfeld, C. and Olshanskii, M., ESAIM: Math. Model. Numer. Anal., 53, 585-614, 2019 [3] "Eulerian time-stepping schemes for the non-stationary Stokes equations on time-dependent domains", Burman, Erik and Frei, Stefan and Massing, André, arXiv:1910.03054, pp.1-42

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Title: A PDE-Constrained Optimization Model for the Material Transport Control in Neurons

Author(s): *Angran Li, *Carnegie Mellon University*; Yongjie Jessica Zhang, *Carnegie Mellon University*;

Neurons exhibit complex geometry in their branched networks of neurites which is essential to the function of individual neuron but also brings challenges to transport a wide variety of essential materials throughout their neurite networks for their survival and function. Many neurodegenerative diseases have been associated with the disruption of the transport. Therefore, it is essential to study how the neurons control the transport process to localize materials to necessary locations. Here, we develop an optimization model to simulate the control mechanism of the material transport in complex neurite networks of neurons. The transport is controlled to avoid traffic jam of the material by minimizing a designed objective function. The optimization of the function subjects to a set of partial differential equations (PDE) that describe the material transport process based on a macroscopic molecular-motor-assisted transport model of intracellular particles. The proposed PDE-constrained optimization model is solved in different geometries such as single-pipe, bifurcation, and tree structures by using isogeometric analysis (IGA). Different simulation parameters are used to introduce traffic jam and study how neurons handle the transport issue. In summary, our model can simulate the material transport process in healthy neurons and predict the formation of a traffic jam in abnormal neurons. Reference: [1] A. Li, X. Chai, G. Yang, Y. J. Zhang. (2019). An Isogeometric Analysis Computational Platform for Material Transport Simulations in Complex Neurite Networks. Molecular & Cellular Biomechanics, 16(2):123-140. [2] A. Li, A. B. Farimani, Y. J. Zhang. (2021). Deep Learning of Material Transport in Complex Neurite Networks. Submitted to Scientific Reports.

16th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification for Random Field Quantities Using Multifidelity Karhunen-Loeve Expansions

Author(s): *Aniket Jivani, *University of Michigan*; Xun Huan, *University of Michigan*; Cosmin Safta, *Sandia National Laboratories*; Beckett Y. Zhou, *Technical University of Kaiserslautern*; Nicolas R. Gauger, *Technical University of Kaiserslautern*;

Uncertainty quantification (UQ) for engineering systems characterized by complex physics and high-fidelity simulations can be computationally prohibitive. One approach to alleviate this cost is through the use of surrogate models. We focus on Karhunen-Loève expansions (KLEs) based on low-rank spectral approximations that are effective surrogate models for characterizing random field quantities. Further, we propose a multifidelity KLE construction to exploit the accuracy-versus-speed tradeoffs between low-fidelity and high-fidelity models. We enable the combining of multiple models by retaining the connection to the physical sources of uncertainty through the use of polynomial chaos expansions inside the KLEs. The resultant multifidelity KLE then allows the generation of surrogate predictions for any particular input parameter value and greatly accelerates the UQ analysis. We demonstrate our method on field quantities from a turbulent round jet application that combines high-fidelity enhanced delayed detached-eddy (EDDES) and low-fidelity Reynolds averaged Navier-Stokes (RANS) simulations. We illustrate advantages of the multifidelity KLE over single-fidelity approaches, particularly with greater accuracy at parameter conditions further away from the existing high-fidelity training data points.

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Title: A Peridynamics Model for Brittle Damage in Solids under Thermomechanical Loading

Author(s): *Anil Pathrikar, *Indian Institute of Science*; Debasish Roy, *Indian Institute of Science*;

We present a fully coupled non-ordinary state-based (NOSB) peridynamics (PD) model for brittle damage in solids undergoing thermomechanical deformation. Due to the full coupling, the thermal field affects the evolution of mechanical deformation and damage, just as each of the latter two fields affects the evolution of the other two. The governing field equations and the associated constitutive relations are obtained consistent with the two laws of thermodynamics. The temperature evolution equation considers the effect of local heat generation at the crack tip and the thermomechanical coupling effect. The heat equation considers heat transfer through conduction and radiation modes. The notion of scalar entropy flux is introduced and the concept of entropy equivalence is exploited in the proposed PD formulation. The constitutive correspondence and entropy equivalence furnish the correspondence relations for the proposed PD model. Numerical simulations of transient heat transfer in a silica tile experiment and Kalthoff's experiment are carried out to validate the model. For further exploration, numerical simulation of a silica tile under fully coupled thermomechanical loading is also carried out.

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Title: Some Numerical Aspects of the Virtual Element Method Applied to the Stokes Problem

Author(s): *Annamaria Mazzia, *University of Padova*; Gianmarco Manzini, *Los Alamos National Laboratory*;

The Stokes problem attracts attention from researchers because the velocity and the pressure variables are coupled in a saddle point system and standard numerical approaches could not work properly if they do not satisfy the inf-sup condition. In this work, we consider three different formulations of the Virtual Element Method (VEM) that generalize the Scott-Vogelius finite element method. The VEM is a finite element method that does not require the explicit knowledge of the basis functions and use of a quadrature formulas to compute the bilinear forms of the Galerkin formulation. This feature allows the construction of the bilinear forms on general polygonal and polyhedral elements through special polynomial projections of the basis functions and their derivatives. Such projections are computable directly from the degrees of freedom of the virtual element functions and ensure the polynomial consistency of the bilinear forms. The three formulations of the VEM that we propose for the solution of the Stokes problem are formulated in the following way: we first consider a straightforward application of the VEM for scalar elliptic problems to the vector case, next we suggest two alternative formulations of the virtual element space for the velocity vector-field. In all formulations, the pressure variable is approximated through discontinuous polynomials. The three formulations are stable and convergent. To obtain optimal convergence rate, we show that it is preferable to use orthonormal basis function not only on the elements of the mesh but also on each edge of the elements. In this way, the observed convergence rates are in accordance with the theoretical expectations on representative families of meshes and benchmark problems. In addition, zero-divergence constraint is always satisfied at the machine precision.

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Title: Numerical Investigation of Healthcare Worker Exposure to Infectious Aerosols in Hospital Isolation Rooms and Extension to Lower Order Compartment Models.

Author(s): *Anthony Perez, *University of South Florida*; Juan Penaloza Gutierrez, *University of South Florida*; Kiesha Pierre, *University of South Florida*; Andres E. Tejada-Martinez, *University of South Florida*;

Aerosol dispersion from a coughing patient in a hospital isolation room is investigated via Reynolds-averaged Navier-Stokes simulation (RANSS). Dispersion in the room is caused by the air circulation driven by the room's ventilation, the cough jet/aerosol generation process, and convective heat transfer. Healthcare worker (HCW) exposure to the aerosol contaminant will be assessed through residence time analysis of the imperfect mixing induced by inflow-outflow channeling (i.e., flow channeling between the supply and exhaust air vents) and dead zone regions in the room. It is observed that dead zones can trap aerosols over periods of time comparable to or greater than the theoretical residence time of the room (approximately ten minutes for typical isolation rooms). Furthermore, increasing the ACH leads to more efficient mixing by weakening dead zones resulting in lower amounts of trapped contaminant. HCW exposure to aerosol contaminant will be quantified as a function of ACH. Finally, the RANSS results will be used to calibrate a less computationally intensive zonal compartment model able to predict average aerosol concentration throughout the room as well as HCW exposure to the infectious aerosols. This zonal compartment model represents the mass transfer between arbitrarily defined regions in space. As it is a mass balance, it leads to a set of ordinary differential equations that can be rapidly solved at greatly reduced computational expense than RANSS. Additionally, these models can be calibrated via RANSS and generalized to many isolation rooms allowing hospitals to rapidly and effectively model aerosol concentrations in their own isolation rooms without having specialized equipment.

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Title: Optimization of Structure Positions in an Acoustic Cavity Using XFEM, Reduced Models and a Gradient-Based Surrogate Model Approach

Author(s): *Antoine Legay, *LMSSC, Conservatoire National des Arts et Métiers*; Luc Laurent, *LMSSC, Conservatoire National des Arts et Métiers, Paris, France*;

Noise reduction for passengers comfort in transport industry, or more generally in an acoustic cavity, is now an important constraint to be taken into account during the design process. The optimization of internal structures positioned according to acoustic of the cavity can lead to the study of several configurations and thus may become prohibitive in terms of computational time. The aim of this work is to be able to efficiently optimize the position of structures in an acoustic cavity. The first idea is to use XFEM in order to take into account the embedded structures, such as seats in a plane cabin [Legay 2013]. These structures are immersed arbitrarily within the acoustic mesh allowing to always use the same acoustic mesh, the acoustic pressure is enriched by a Heaviside function. This makes the parametric study easier since it does not involve a meshing process anymore. The second idea of the proposed approach is to use a surrogate-based optimization in order to furthermore reduce the computational time of the whole optimization process. It is based on the Efficient Global Optimization [Jones 1998]. At least, the use of the XFEM approach enables to easily compute the gradient of the pressure field with respect to the design variables which governed the position of the structure in the cavity. Moreover, a reduced basis [Legay 2015] is used to compute the solution as well as the gradient. Many operators remain indeed independent of the design variables and the main effort consists only of building gradients of the XFEM enrichment operators. These gradients enable to build a more accurate surrogate model [Laurent 2019]. This strategy enable to divide the CPU time by a factor from 2 to 10, depending of the problem complexity. The whole strategy is applied on some 2D and 3D cavities on which the position of a wall is determined in order to minimize the mean quadratic pressure in a control volume. A. Legay. An extended finite element method approach for structural-acoustic problems involving immersed structures at arbitrary positions. International Journal for Numerical Methods in Engineering, 93(4):376-399. 2013 A. Legay. The extended finite element method combined with a modal synthesis approach for vibro-acoustic problems. International Journal for Numerical Methods in Engineering, 101(5):329-350. 2015 L. Laurent, R. Le Riche, B. Soulier and P.-A. Boucard. An Overview of Gradient-Enhanced Metamodels with Applications. Archives of Computational Methods in Engineering, 26(1):61-106. 2019

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Title: Direct Fused Deposition Modeling (FDM) Additive Manufacturing of Voxelized CAD Models

Author(s): *Anushrut Jignasu, *Iowa State University*; Sambit Ghadai, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Abstract: Most additive manufacturing (AM) processes use tessellated CAD models in stereolithography (STL) or virtual reality modeling language (VRML) file format. Tessellated CAD models, in the form of triangle soups, can be easily obtained from generic CAD models, which are usually represented using boundary representation (B-rep) or constructive solid geometry (CSG) modeling of primitives. These tessellated models are further processed or sliced to obtain the layer-by-layer information for AM. However, other data structures representing solids, such as volumetric representations (voxels), point clouds, and medical imaging data (MRI and CT Scans), require complex geometric algorithms to tessellate and represent them as triangular facets. Additionally, developing AM printing strategies for these representations is challenging due to the computational cost of processing these representations at higher fidelity. In this work, we develop an AM strategy that enables direct 3D printing from volumetric representations or multi-level voxel models with higher accuracy and print quality. One of the advantages of using a voxel representation for AM is that the regularity of the voxel grid eliminates the need for explicit slicing, which is a time-consuming process. Slicing CAD models also creates gaps and discontinuities that need further processing to be used for AM. Voxelization alleviates this issue by directly generating a rectilinear occupancy grid conforming to the required layered structure. We present a direct method for the additive manufacturing of multi-level voxelized models that achieves a better surface finish. We have developed a new multi-level marching squares algorithm to identify the boundary of the multi-level voxelized model. We have also developed methods to use the multi-level voxelization to perform the infill operation based on user-defined infill density. We directly generate the GCode that is input to the 3D printer for printing. We show that our method performs well by directly printing test models of multi-level voxel representation of complex CAD geometries, and cardiac CT data. References: 1. Gavin Young, Adarsh Krishnamurthy; GPU-accelerated generation and rendering of multi-level voxel representations of solid models, Computers & Graphics, 75:11–24, 2018.

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Title: Finite Element Based Stabilized Formulation for Hypersonic Flows

Author(s): David Codoni, *University of Calgary*; *Artem Korobenko, *University of Calgary*;

In this talk we present a finite element based numerical framework for hypersonic flows. The fully-implicit formulation is based on Streamline Upwind Petrov-Galerkin (SUPG) method coupled with discontinuity capturing (DC) operator. The robustness, stability, and accuracy of the formulation are shown by solving several benchmark cases for a wide range of Mach numbers and problem complexity, including both reacting and non-reacting flows. The numerical results presented in this work show that the proposed formulation behaves very well in the context of high-speed flows maintaining good accuracy and stability in both steady and unsteady cases. The successful performance of the proposed formulation for high-speed flows sets the stage for the deployment of the techniques developed to more advanced applications such as fluid-thermal-structure interaction modeling for hypersonic vehicles.

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Title: On Development of an Invariant Data-Driven Anisotropic Subgrid Scale Stress Model for Large-Eddy Simulation

Author(s): *Aviral Prakash, *University of Colorado Boulder*; Kenneth Jansen, *University of Colorado Boulder*; John Evans, *University of Colorado Boulder*;

Direct Numerical Simulation (DNS) for turbulent flows is computationally expensive at high Reynolds numbers, and therefore, the use of these simulations is limited to only a few flows at lower Reynolds numbers. At higher Reynolds numbers, Large Eddy Simulations (LES) are often used to obtain turbulent statistics. LES allows us to resolve a vast spectrum of turbulent scales, whereas the interaction of smaller unresolved scales with resolved scales, represented using subgrid scale (SGS) tensor, is modeled. These models use physical and mathematical insights for approximating the SGS tensor. However, these models struggle at high Reynolds number flows and in the presence of walls. In this presentation, we will discuss a data-driven methodology to develop SGS stress closure models. The proposed model relies on an efficient model input and output selection and openly available turbulent flow data. The proposed model by construction satisfies Galilean, time, frame, and dimensional invariance conditions. Unlike previously proposed data-driven SGS closures, the proposed model is also applicable for use with unstructured or anisotropic computational grids. We demonstrate the applicability of the data-driven model by performing a priori and a posteriori tests. We observe that the proposed data-driven model works well with different grid resolutions of computational grids and flow scenarios outside the training dataset.

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Title: InvNet : Physics Informed GANs for Morphology Design

Author(s): *Balaji Sesha Sarath Pokuri, *Iowa State University*; Viraj Shah, *University of Illinois at Urbana Champaign*; Ameya Joshi, *New York University*; Minsu Cho, *New York University*; Soumik Sarkar, *Iowa State University*; Chinmay Hegde, *New York State University*; Baskar Ganapathysubramanian, *Iowa State University*;

An overarching theme of materials research is the design of microstructures that exhibit tailored properties. An associated problem with microstructure-design is the need to reconstruct and quantify microstructures. However, the number of possible microstructures are practically infinite and getting a complete virtual in-stance of a microstructure is non-trivial with limited information. Standard approaches involve generating microstructures that satisfy sets of experimental observations and using the generated microstructures to computationally quantify average case scenario of experimental observations. When the microstructure characterization is limited and the amount of details in the microstructure are large (i.e., a refined representation is required), the number of microstructures required to capture average-case scenario becomes large and simultaneously the task of reconstruction becomes difficult. Hence, several strategies were developed to tackle this problem using both analytical approaches (for simplified characterizations) and optimization approaches (for complicated, multi-faceted characterizations). Traditional approaches, including GRFs, multi-point statistics and layer-by-layer reconstruction are computationally intensive, requiring several compute hours even to simulate just one synthetic example. This reconstruction time increases exponentially with the size of the microstructure. This forms the aim of this work – to assimilate information from both data(implicit physics) as well as the user(explicit physics) for rapid morphology reconstruction. In this work, we intro-duce a novel machine learning technique that use the concept of generative adversarial networks (GANs)to generate microstructures. GANs have a special characteristic of generating data instances on-the-fly with little computational overhead post training. In this work, we propose a systematic extension of GANs that can synthesize data samples obeying pre-specified, analytically defined invariances. We call our new generative models Invariance Networks, or InvNets. We validate our technique using a range of numerical experiments. We show the power of InvNets to learn and generate bi-continuous morphologies, powder-like morphologies and polycrystalline morphologies with multiple domain sizes and orientations. Overall, our results indicate that generative networks coupled with user specified invariances, as presented in this work, have great potential to solve the morphology reconstruction problem with great accuracy.

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Title: Image-Based Bayesian Inference and Patient Specific Prediction of Heterogeneous Tumor Growth

Author(s): *Baoshan Liang, *University at Buffalo*; Jingye Tan, *University at Buffalo*; Luke Lozensk, *Washington University in St. Louis*; David Hormuth, *The University of Texas at Austin*; Thomas Yankeelov, *The University of Texas at Austin*; Umberto Villa, *Washington University in St. Louis*; Danial Faghihi, *University at Buffalo*;

Key Words: Infinite-dimensional Bayesian inference, tumor growth, imaging data, uncertainty quantification Reliable computational prediction of tumor growth using early patient-specific imaging data enables personalized treatment strategies to enhance the efficacy of cancer therapy. Crucial in predictive physics-based modeling of cancer is to capture the morphology, invasiveness, and spatial and temporal heterogeneity of growing tumors. Additionally, the model inadequacy and noise in medical imaging techniques introduce substantial uncertainty in tumor and organ heterogeneity, which translate to uncertainty in model predictions. This contribution develops an image-based predictive model of tumor growth with application to a murine pre-clinical model of glioma (brain tumor). To this end, a high dimensional Bayesian inference framework is proposed for learning spatiotemporal tumor development from magnetic resonance imaging (MRI) data. To characterize the spatial heterogeneity of the brain in a specific rat, an image analytic is developed to register the gray and white matter segmentation provided by digital brain atlases to the MR images of a specific rat. Additionally, a scalable computational method for solving high-dimensional Bayesian inference of the physics-based tumor model is implemented to calibrate the spatially varying model parameters. Furthermore, the reliability of the computational model in the early prediction of tumor morphology in a specific subject is investigated.

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Title: Data Driven RANS Closure with Model Derived Turbulence Variables

Author(s): *Basu Parmar, *University of Colorado Boulder*; Kenneth Jansen, *University of Colorado Boulder*; John Evans, *University of Colorado Boulder*;

Numerical prediction of turbulent flows is critical for the design and analysis of engineered systems. Despite a continued increase in computational power, low fidelity RANS models remain widely used in industrial and academic CFD solvers due to their robustness and low cost. However, the current state of the art RANS models perform poorly for flows exhibiting flow separation, adverse pressure gradients, secondary flows, etc. Recently, there has been a surge in utilizing machine learning techniques to improve turbulence models by leveraging high fidelity data, giving rise to the field of data-driven turbulence modeling. Data-driven RANS models either aim to improve existing models or generate new surrogates for Reynolds stress closure. Many approaches proposed in the literature involve building surrogate models for Reynolds stresses as a function of flow and turbulence variables, such as strain rate, turbulent kinetic energy, dissipation, etc., from a precursor RANS simulation [1]. However, building a data-driven model in such a way leads to fallacious dependencies on problem setup, convergence, etc. Additionally, there is no physical insight gained for developing analytical models, since the surrogate inputs are based on the output from a precursor RANS simulation rather than the output of the trained data-driven model itself. We propose an alternative approach to data-driven RANS modeling that does not suffer from the issues discussed above. In our approach, we first solve the turbulence variable model transport equations given a frozen flow field from high-fidelity simulation data. A neural network is then trained to predict the Reynolds stresses from these model-derived turbulence variables and the high-fidelity flow field. In the final implementation, the mean flow and turbulence model equations are solved simultaneously, with the Reynolds Stresses neural network model a function of the output of the ongoing simulation rather than the output of a precursor RANS simulation. We demonstrate the efficacy of this new data-driven approach by numerical tests on canonical flow cases. References: 1) J.-L. Wu, H. Xiao, E.G. Paterson. “Physics-informed machine learning approach for augmenting turbulence models: A comprehensive framework”, Phys. Rev. Fluids 3, 074602,2020

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Title: Computing Leaky Modes of Optical Fibers using a FEAST Algorithm for Polynomial Eigenproblems

Author(s): *Benjamin Parker, *Portland State University*; Jay Gopalakrishnan, *Portland State University*; Pieter VandenBerge, *Portland State University*;

We present a novel method for computing leaky modes of optical fibers using an adaptation of the FEAST eigensolver. For linear eigenproblems, the FEAST eigensolver uses the spectral projector for the matrix pencil (A,B) to find the desired eigenvalues inside of a simple, closed contour in the complex plane. Our approach seeks to extend this algorithm to handle polynomial eigenvalue problems. A motivating factor for this approach is that the use of Perfectly Matched Layers (PML) for finding leaky modes of optical fibers requires the solution to a nonlinear eigenvalue problem. To solve such a problem, one performs carefully chosen variable substitutions to linearize the polynomial eigenproblem, resulting in a larger, linear eigenproblem. Standard eigensolvers can then be applied to this larger eigenproblem. To prevent potentially costly factorizations during the course of the FEAST algorithm, we take advantage of the structure of the linearization to develop an efficient implementation of the FEAST algorithm. Applications to motivate this approach come from photonics, in which we test our algorithm's efficacy in computing leaky modes of an ytterbium-doped step-index optical fiber and a microstructure fiber.

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Title: Machine Learning Model Development for Additive Manufacturing Process Parameter Optimization

Author(s): *Berkcan Kapusuzoglu, *Vanderbilt University*; Paromita Nath, *Vanderbilt University*; Matthew Sato, *Vanderbilt University*; Sankaran Mahadevan, *Vanderbilt University*; Paul Witherell, *National Institute of Standards and Technology*;

This work develops machine learning models for uncertainty quantification and process optimization in additive manufacturing (AM). With a focus on fused filament fabrication (FFF) AM process, the proposed methodology optimizes the process parameters with two objectives: minimizing the geometric inaccuracy and maximizing the filament bond quality of the manufactured part. First, experiments are conducted to collect data pertaining to the part quality. Then, Bayesian neural network (BNN) models are constructed to predict the geometric inaccuracy and bond quality as functions of the process parameters. Since limited data is generally available, there is insufficient knowledge or information about the model and data (epistemic uncertainty) in the model prediction. BNN is used to describe the epistemic uncertainty caused by the model by placing distributions over the model parameters (neuron weights). The process parameter settings specified by the designer may also fluctuate due to variability in the equipment (aleatory uncertainty). We present a BNN framework that is able to consider both aleatory uncertainty and epistemic uncertainty. Using the stochastic predictions from these models, different robust design optimization formulations are investigated, wherein process parameters such as nozzle temperature, nozzle speed, and layer thickness are optimized under uncertainty for different multi-objective scenarios. Several cases with multiple objectives are considered: minimizing the mean and standard deviation of the bond quality metric, minimizing the mean and standard deviation of part thickness error, minimizing the mean part thickness error and mean bond quality metric, and minimizing the means and standard deviations of both part thickness error and bond quality metric. Uncertainty in the prediction model, input variability, and input uncertainty are considered in the optimization. Finally, Pareto surfaces are constructed using a genetic algorithm to estimate the trade-offs between the objectives. Both the machine learning model and the optimization methodology are validated by manufacturing the parts at multiple settings, including optimal settings.

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Title: Tangled Finite Element Method (TFEM) for Quadrilateral Meshes

Author(s): *Bhagyashree Prabhune, *University of Wisconsin-Madison*; Saketh Sridhara, *University of Wisconsin-Madison*; Krishnan Suresh, *University of Wisconsin-Madison*;

In finite element method (FEM), a mesh is said to be tangled if it contains inverted elements. Tangling can occur, for example, during mesh generation, mesh morphing, shape optimization, and/or large deformation simulation. In standard FEM formulations, tangled meshes can lead to erroneous results, and untangling may not always be possible. The objective of this talk is to introduce a tangled finite element method (TFEM) for 2D quadrilateral meshes. In particular, we consider here implicitly tangled meshes where some of the elements are only partially inverted, i.e., are concave; such meshes are harder to untangle than explicitly tangled meshes where the elements are fully inverted. The proposed TFEM framework fundamentally rests on an unambiguous definition of the field in the tangled region. This definition naturally leads to certain correction terms in the FEM stiffness matrix. Once these corrections and a particular congruence constraint are included, we demonstrate that accurate solutions can be obtained over even severely tangled meshes. Several numerical experiments are carried out to illustrate the robustness of the proposed method.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Data Driven Approach to Improved Exchange-Correlation Functionals in DFT

Author(s): *Bikash Kanungo, *University of Michigan*; Vikram Gavini, *University of Michigan*;

The need for improved exchange-correlation (XC) functionals in density functional theory (DFT) that can provide quantum accuracy can hardly be over-emphasized. To that end, we envisage a data-driven approach to construct XC functionals by using accurate ground-state densities from many-body calculations. The key idea is to use the density and its corresponding XC potential, from multiple molecules, as training data to model the XC functional (i.e., learn a field-to-field map from the density to the XC potential). As a crucial first step, we present an accurate and robust approach to solve the inverse DFT problem of obtaining the exact XC potential from a given density [1]. We remark that the inverse DFT problem had, heretofore, remained an open challenge owing to various numerical instabilities present in the previous attempts at it---incompleteness of the basis employed for discretization and the lack of proper asymptotics in the input density. We resolve these issues using a systematically convergent spectral finite element basis. Furthermore, we employ corrections on the input density and enforce accurate boundary condition on the XC potential to mitigate the effects of the the incorrect asymptotics in the density. As a solution strategy, we cast the inverse problem as a PDE-constrained optimization, with the XC potential as the control variable and the Kohn-Sham eigenvalue problem as the PDE-constraint. We employ limited-memory BFGS (L-BFGS) to solve the resultant non-linear optimization problem. We present the exact XC potential for five molecules---hydrogen molecule at three different bond-lengths, lithium hydride, and water---using accurate ground-state densities from configuration interaction (CI) calculations. Moreover, we present the model XC potentials for the same set of molecules using ground-state densities from DFT calculations with two highly used non-local XC functionals---B3LYP and HSE06. The availability of these exact XC potentials, along with its comparison with model XC potentials, forms the basis of our ongoing efforts at a neural network (NN) based design of XC functionals. [1] Kanungo, B., Zimmerman, P.M., and Gavini, V., Nature Communications, 10, 4497 (2019).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Data-Driven Microstructure Sensitivity Study of Fibrous Paper Materials

Author(s): *Binbin Lin, *Technical University Darmstadt*; Bai-Xiang Xu, *Technical University Darmstadt*;

Sustainable paper materials are versatile with diverse applications. Structure-property relation of such fibrous materials are difficult to access due to its complex structures at fiber, fiber/fiber cross and fiber network scale with high degree of randomness. Our work demonstrates a machine learning based approach to examine the variation in microstructure features on mechanical properties of paper materials. Based on around 2000 computationally generated fiber network samples and the corresponding cohesive zone finite element simulations, the linkage between structural descriptors and mechanical properties including strength, failure strain and effective stiffness is established. We analyse also the derived structural features like fiber-fiber contact morphology and the property sensitivity on both prescribed and derived properties. We found out that “disorderness” represented by standard deviation of fiber network orientation and the mean contact area size as derived properties to be the most dominant influential factors to the mechanical responses, which validate the highly orientation dependance of fibrous materials, the contact contribution to paper strength, as well give new insight to the importance of feature sensitivity as structural parameters.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Quantifying and Modeling of Stress-Driven Short-Circuit in Lithium-Ion Batteries in Electrified Vehicles

Author(s): *Binghe Liu, *Chongqing University*;

Despite the huge expansion of electric vehicle sales in the market, customers are discouraged by the possible catastrophic consequences brought by the safety issues of lithium-ion batteries, such as internal short circuits, especially in crash scenarios. Herein, we reveal the quantitative relation between the deformations of the battery and the internal short circuit. By designing in-situ, ex-situ observation and post-mortem characterization of the component materials, we quantify the stress-driven internal short circuit and failure behavior of the component material. With the aid of the validated numerical computational model as well as the in-situ characterization of the global-field temperature, we successfully identify the minor and major short circuits of the cells upon various mechanical abusive loadings. Finally, we establish the internal short circuit criteria for typical formats of batteries. This discovery also provides a fundamental understanding of both internal and external stress-driven short circuits in a much broader context.

16th U.S. National Congress on Computational Mechanics
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Title: Field Solutions of Parametric PDEs

Author(s): *Biswajit Khara, *Iowa State University*; Aditya Balu, *Iowa State University*; Ameya Joshi, *New York University*; Adarsh Krishnamurthy, *Iowa State University*; Soumik Sarkar, *Iowa State University*; Chinmay Hegde, *New York University*; Baskar Ganapathysubramanian, *Iowa State University*;

We consider mesh based approaches for training neural network to produce field predictions to parametric partial differential equations (PDEs). This is in contrast to current approaches for ``neural PDE solvers`` that employ collocation approaches to make point predictions of PDEs. Our approach has advantages of (a) easier handling of various boundary conditions, and (b) ease of invoking well developed PDE theory -- including analysis of numerical stability and convergence -- on discretized domains. On the other hand, an obvious disadvantage is the network size required for producing field solutions. We explore such a strategy using two loss functions based on (i) Finite Difference Method (FDM) and (ii) Finite Element Method (FEM) on two canonical parametric PDEs. While the FDM loss is closely related to losses used in recent PINN type approaches, the weighted galerkin loss (FEM loss) is akin to an energy functional that produces improved solutions, satisfies a priori mesh convergence, and can easily model Neumann boudary conditions. These results suggest that mesh based neural networks are promising approaches for parametric PDEs.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Crack Evolution in Multilayered 2D Materials Under the Presence of Interlayer Sliding

Author(s): *Bo Ni, *Brown University*; Huajian Gao, *Nanyang Technological University*;

Multilayered 2D materials have found broad applications in fields ranging from flexible electronic devices to reinforced composites. As a stack of homogeneous or heterogeneous 2D material layers, the performance of multilayered 2D materials is influenced by not only the intralayer properties but also the interlayer interactions. Recent progresses in characterizing both the intralayer and interlayer properties in 2D materials have reviled sharp contrasts between these two, which distinguishes multilayered 2D materials from the conventional multilayered composites in macroscale. Thus, it becomes particularly interesting to ask how interlayer interactions affect the fracture process in multilayered 2D materials, given that 2D materials as individual layers often suffer from low fracture resistance. In the present work, we study the toughening effect of the interlayer sliding on crack propagation and the competition between intralayer crack propagation and interlayer crack penetration. Using theoretical analysis and numerical simulations, we derive the energetic driving force for a propagating crack in contact with a neighboring intact layer and demonstrate an enhanced critical fracture strain due to interlayer interaction. The enhancement in the critical strain depends on the sample size, in-plane modulus of the neighboring layer as well as the interlayer shearing stress. Based on that, we further include the strength-controlled failure and provide a phase diagram to predict whether the initial crack will propagate within the layer or penetrate the neighboring layer. Our finding presents a clear fracture mechanics model demonstrating how interlayer sliding can affect intralayer fracture and provide guidance for toughening multilayered 2D materials by choosing suitable sample size and combination of individual layers.

16th U.S. National Congress on Computational Mechanics
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Title: Direct Numerical Simulations of Red Blood Cells in Viscoelastic Fluid Flows

Author(s): *Boon Siong Neo, *Stanford University*; Mehdi Niazi Ardekani, *Stanford University*; Eric Shaqfeh, *Stanford University*;

Suspensions of deformable particles in viscoelastic fluids can be found in a wide range of biological systems. One such model for these particles is that of a capsule: a drop of liquid enclosed in an elastic membrane. The dynamics of a capsule under flow is strongly associated with the shape changes it experiences under different flow conditions, which in turn arises from the stresses the suspending fluid exerts on the capsule. Models of this form have previously been applied to simulating the behavior of cells; in particular, of red blood cells (RBCs) in Newtonian fluid flows[1]. The resultant predictions of RBC shape changes and dynamics are in good agreement with experiments. However, in many systems of interest, the suspending fluid exhibits non-Newtonian viscoelastic behavior; for example, many biologically relevant fluids contain large polymeric molecules. The effect of fluid elasticity on membrane shape changes is hence of biological relevance. In this study, we perform direct numerical simulations of RBCs suspended in non-Newtonian fluids. An immersed boundary algorithm known as the Immersed Finite Element Method (IFEM) is used to accurately determine the internal forces in the solid domain. This scheme does not require costly re-meshing and is able to incorporate non-linear viscoelasticity in the fluid domain. The internal force calculation in the solid domain in the IFEM is coupled with a finite volume based incompressible fluid solver, both of which are massively parallelized for distributed memory architectures. We investigate the effects of viscoelasticity and channel confinement on the deformation and velocity of RBCs in pressure-driven duct flows. For isolated cells, we focus on changes in cell dynamics due to the elasticity of the fluid. We observe fluid elasticity leads to decreased deformation of RBCs in shear flow but increased deformation and velocity in the pressure driven duct flows. We also investigate the effects of fluid elasticity on the collective dynamics of a multiple suspension of red blood cells in duct flow. References: [1] A. Saadat, D. Huyke, D. OyarzunP, . Escobar, I. Øvreeide, E. Shaqfeh, J. Santiago. A system for the high-throughput measurement of the shear modulus distribution of human red blood cells. Lab on a Chip. . . http://dx.doi.org/10.1039/D0LC00283F. 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Time Domain, Intrusive Probabilistic Seismic Risk and Sensitivity Analysis of Nonlinear Earthquake Soil Structure Interaction Systems

Author(s): Hexiang Wang, *University of California, Davis*; Han Yang, *University of California, Davis*; *Boris Jeremic, *University of California, Davis*;

Presented will be a time domain intrusive framework for probabilistic seismic risk analysis of non-linear, inelastic earthquake soil structure interaction (ESSI) systems. Both uncertain seismic motions and uncertain soil-structure inelastic material parameters are characterized as random process and random fields, respectively and modeled using Hermite polynomial chaos expansion. Stochastic Elastic-Plastic Finite Element Method (SEPFEM) is used to calculate full probabilistic results for all displacements, stresses and strains. In addition, sensitivities of probabilistic response to input parameter uncertainties are developed as well. For this purpose use is made of Sobol indices and the polynomial chaos expansion developed within SEPFEM. Stochastic dynamic equations are solved in an intrusive way, circumventing Monte Carlo simulations, thus gaining accuracy and efficiency. Calculated results are used to develop time-evolving probabilistic dynamic response and full-spectrum seismic risk. Examples will be used to illustrate developed framework. Developed framework is readily available within the Real-ESSI Simulator system (http://real-essi.us/).

16th U.S. National Congress on Computational Mechanics
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Title: Orbital Dynamics of Binary Black Hole Systems can be Learned from Gravitational Wave Measurements

Author(s): *Brendan Keith, *Brown University*; Akshay Khadse, *University of Mississippi*; Scott Field, *University of Massachusetts Dartmouth*;

We introduce a gravitational waveform inversion strategy that discovers mechanical models of binary black hole (BBH) systems. We show that only a single time series of (possibly noisy) waveform data is necessary to construct the orbital trajectories and corresponding equations of motion for a BBH system. Starting with a general class of universal differential equations, our strategy involves the construction of a space of plausible mechanical models and a physics-informed constrained optimization within that space to minimize the waveform error. We choose to parameterize the space of models with feed-forward neural networks. This leads to efficient, flexible, and highly accurate algorithms which can be easily implemented with modern software libraries. We apply our method to various BBH systems including extreme and comparable mass ratio systems in eccentric and non-eccentric orbits. We show the resulting differential equations are applicable to time durations larger than the training interval, and a variety of relativistic effects, such as perihelion precession, radiation reaction, and orbital plunge, are automatically accounted for. The methods outlined here provide a new, data-driven approach to studying the dynamics of binary black hole systems. Various applications in gravitational wave astronomy will be discussed as time permits.

16th U.S. National Congress on Computational Mechanics
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Title: Constitutive and Application Modeling of Glass-Ceramic Materials

Author(s): *Brian Lester, *Sandia National Laboratories*; Kevin Long, *Sandia National Laboratories*;

Glass-ceramics are a thermally active material in which inelastic deformations may be induced through temperature excursions. These deformations are associated with the presence of silica polymorphs (cristobalite and/or quartz) in the heterogeneous microstructure of the glass-ceramic that is also comprised of a remnant inorganic glass matrix and thermoelastic phases. Importantly, by varying initial processing steps the content of the silica polymorphs enabling control of the corresponding inelastic deformations producing controllable thermal strain responses. This capability has led to substantial interest in glass-ceramics as hermetic glass-ceramic to metal seals as a way to minimize residual stresses in such applications. However, application of these materials and design or corresponding applications requires appropriate computational models. Previously such efforts were hindered by the lack of appropriate constitutive formulations capable or describing the responses of glass-ceramics. The current work seeks to address the various shortcomings. A novel thermodynamically consistent constitutive model describing the unique phenomenology of glass-ceramics combining reversible phase transformations and viscoelasticity is introduced. A corresponding three-dimensional fully implicit numerical formulation based on a thermoviscoelastic predictor-inelastic corrector is then presented and discussed. The impact of the model and the different mechanisms is investigated by considering a representative seal problem. Different geometric and loading conditions are examined and the impact of the glass-ceramic explored. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: A Surface-Mesh Gradation Tool for Generating Optimized Tetrahedral Meshes of Microstructures with Defects

Author(s): *Brian Phung, *The University of Utah*; Junyan He, *The University of Utah*; Ashley Spear, *The University of Utah*;

A meshing tool for generating tetrahedral meshes of polycrystalline microstructures with an optimal element-size distribution, determined by underlying defects (e.g., cracks and voids), is presented. When simulating defects, a mesh should be refined near regions of interest with high stress gradients and coarsened far from the regions of interest for computational efficiency. Previous work by the authors demonstrated the capability to represent and propagate complex three-dimensional cracks in a realistic microstructure via a voxel-based remeshing method [1]. However, the previous framework was limited in the sense that no mesh-gradation support was implemented, leading to relatively dense and uniform finite-element meshes that were computationally inefficient, and sometimes intractable. Thus, this work addresses this obstacle by providing a framework that adaptively modifies a mesh of a microstructure containing defects, while maintaining a suitable element-size distribution that balances computational cost and simulation accuracy. The meshing tool provides users the capability to tune the element-size distribution, using parameters such as desired edge lengths, and refinement and transition zone radii around defects. As input, the framework utilizes conformal surface meshes of each grain boundary and a point-cloud file to describe the polycrystal and its underlying defects, respectively. Surface meshes can be obtained from image or voxel data generated from tools such as DREAM.3D. The input meshes are preprocessed to remove undesired mesh artifacts. To create a suitable element size distribution informed by the defect structure, elements near the defects are locally refined via edge splitting, while elements far from the defects are coarsened by edge collapsing. A modified version of the edge-collapsing algorithm was developed to handle the complex connectivity near grain-boundary junctions. The quality of the gradated mesh is improved via edge swapping. The modified surface mesh is used in conjunction with a volume mesher to create a gradated volume mesh optimized for the defect(s). The framework is shown to be capable of generating meshes with a sizable improvement in element count and computation time, without a significant impact on stress distributions, even at the crack tip. This tool’s capabilities are demonstrated by three proof-of-concept models: (1) a polycrystalline open-cell foam with intra-ligament voids, (2) an experimentally measured microstructure with an observed fatigue crack, and (3) crack propagation in an additively manufactured polycrystalline microstructure. [1] B. R. Phung, A. D. Spear, A voxel-based remeshing framework for the simulation of arbitrary three-dimensional crack growth in heterogeneous materials, Engineering Fracture Mechanics 209 (2019).

16th U.S. National Congress on Computational Mechanics
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Title: Modeling Crack Nucleation and Propagation in Anisotropic Materials

Author(s): *Bryce Mazurowski, *University of Illinois at Urbana-Champaign*; Patrick O'Hara, *Air Force Research Laboratory*; C. Armando Duarte, *University of Illinois at Urbana-Champaign*;

Anisotropic materials are becoming more and more popular in engineered structures. New materials and manufacturing techniques allow structural scale properties to be tailored in a way that best suits their application. Some popular materials like high-strength aluminum or titanium alloys are typically assumed to behave isotropically, but with desired levels of accuracy increasing and consideration of more extreme design environments, this may not be allowable. Structures designed for these challenging environments and with these cutting edge materials will essentially all develop fractures at some scale. In many structures, the majority of their service life is over the moment a dominant fracture nucleates. There are a number of complex fracture phenomena seen in heavily used materials where the nucleation of new fractures among existing ones is important. In any case, the modeling of fractures in anisotropic materials must consider their anisotropic properties to recover accurate results. The phase-field model of fracture has received significant attention in recent years due to its intrinsic ability to handle complex cracking behavior like branching and coalescence. An extension of the original phase-field model of fracture proposed by Kumar et al. [1] provides an additional term that characterizes the strength of the material. This framework allows crack nucleation to be captured accurately under a variety of loading scenarios while maintaining all of the existing abilities of the phase-field method. In this work, the phase-field method presented in [1] is extended to handle anisotropic materials. Anisotropy of the elastic properties, fracture properties, and material strength are all explored. The effect that these anisotropies have on the nucleation of new fractures, the propagation of existing ones, and the interplay between the two are explored. References: [1] Kumar, A., Bourdin, B., Francfort, G. A., & Lopez-Pamies, O. (2020). Revisiting nucleation in the phase-Field approach to brittle fracture. Journal of the Mechanics and Physics of Solids, 142, 104027.

16th U.S. National Congress on Computational Mechanics
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Title: Learning Based Multi-Scale Method and its Application to Inelastic Impact Problems

Author(s): *Burigede Liu, *California Institute of Technology*; Nikola Kovachki, *California Institute of Technology*; Andrew Stuart, *California Institute of Technology*; Kaushik Bhattacharya, *California Institute of Technology*;

The macroscopic behavior of many materials is complex and the end result of mechanisms that operate across a broad range of disparate scales. Classical stress analysis simplifies the multi-scale problem by postulating a phenomenological constitutive relation so that the computation of large-scale material/structural systems becomes feasible. On the other hand, multi-scale modeling (e.g., FE^2) is capable of capturing the lower-length-scale mechanisms at the expense of high computational cost, therefore only a few hero calculations can be conducted. In the current study, we propose a learning based multi-scale method where the sub-scale mechanisms in a concurrent multi-scale setting are approximated by a function space learning method. By constructing a neural-network in function space, the model is capable of producing constant generalization error regardless of input/output resolution. We demonstrate the applicability of the proposed approach by analyzing the multi-scale impact problem of polycrystalline metals governed by crystal plasticity. We further show that the cost of full-field simulation using learned model is similar to that using the empirical model, and many orders of magnitude smaller than the conventional FE^2 approach.

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Title: Bayesian Inference of a Multiscale Model of Tumor Angiogenesis via Live Cell Imaging, Protein Expression Data, and a 3D Microfluidic Platform

Author(s): *Caleb Phillips, *The University of Texas at Austin*; Manasa Gadde, *The University of Texas at Austin*; Ernesto Lima, *The University of Texas at Austin*; Angela Jarrett, *The University of Texas at Austin*; M. Nichole Rylander, *The University of Texas at Austin*; Thomas Yankeelov, *The University of Texas at Austin*;

Tumor angiogenesis, the process by which new blood vessels are recruited by a developing cancer, is well-recognized as a fundamental mechanism by which tumors can invade and metastasize. Once a tumor grows beyond the capability of the pre-existing blood vessels to sustain growth, hypoxic cancer cells secrete vascular endothelial growth factor (VEGF) that activates endothelial cells on blood vessel walls and causes them to proliferate and migrate toward the tumor, supplying more nutrients to the tumor. In this project, we utilize Bayesian inference to calibrate a hybrid, multiscale model of tumor angiogenesis with experimental data obtained from an in vitro vascularized tumor platform to make and test predictions related to vasculature sprouting. We describe a series of experiments with increasing complexity that isolate key components in the process of angiogenesis and use these data to calibrate model parameters. This sequential approach allows for rigorous investigation of mathematical and experimental systems that builds on the results from each previous subcase. The steps are as follows: 1) calibration of stalk cell growth rate against measurements of angiogenic sprout length, 2) calibration of the secretion and consumption of vascular endothelial growth factor by tumor and endothelial cells, respectively, to VEGF concentration measurements over time, 3) rigorous evaluation of the invertibility of our approach by calibrating the temporal and spatial distribution of vessels using in silico data (i.e., model-generated data), 4) spatiotemporal calibration of the mathematical model of tumor angiogenesis to confocal microscopy data acquired from the 3D microfluidic platform, and 5) testing of the predictive capabilities of the calibrated mathematical model. We assess the fit of the model using the vascular density and report the parameter distributions calculated in step 4. We also report the uncertainty in the model predictions (beyond calibration) in step 5 for multiple regions segmented from our 3D vascularized tumor platform. We conclude that our model, informed from multimodal data sets, can be a useful tool to make predictions of angiogenesis within the 3D microfluidic platform.

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Title: Uncertainty in 3D Image-Based Effective Property Simulations using Bayesian Convolutional Neural Networks

Author(s): *Chance A. Norris, *Purdue University*; Tyler LaBonte, *Sandia National Laboratories*; Carianne Martinez, *Sandia National Laboratories*; Scott A. Roberts, *Sandia National Laboratories*; Partha P. Mukherjee, *Purdue University*;

In recent years there have been great advances in using 3D tomography in battery research, providing the ability to see as-manufactured electrodes at the mesoscale. These structures are then used to find effective properties or perform detailed electrochemical simulations. A key step of this analysis is image segmentation, which differentiates particle and void phases. Image segmentation, however, is meticulous and fraught with subjectiveness. Removing this subjectiveness is paramount in having credible direct numerical simulations to bridge the gap of the computational and experimental regimes. To improve the image segmentation process and quantify its uncertainty, a Bayesian convolutional neural network (BCNN) is implemented to segment greyscale tomograms of graphite electrodes. The use of a BCNN allows for native and explainable uncertainty estimates. Two manually segmented tomograms were used to train the BCNN, which was in turn used to segment an additional seven tomograms. Each tomogram has a different particle morphology and image quality, resulting in varying image segmentation uncertainty. This process was effective in creating high-quality binary stacks, which in some cases presented a subjectively superior segmentation compared to the manual process. Additionally, BCNN-generated uncertainty estimates provide a range of possible image segmentations which in-turn results in a range of possible structures. These nominal and uncertainty ranged structures are propagated through simulations of effective electrical conductivity and pore phase tortuosity, providing both nominal property predictions and geometric uncertainty estimates of those predictions. By using image quality assessments such as Blind/Referenceless Image Spatial Quality Evaluator (BRISQUE) and Otsu inter-variance, we elucidate the influence of tomogram quality has in the geometric uncertainty. Also using structural quantification tools, we find how particular morphologies of particles influence how uncertainties propagate throughout the physics simulations. This work demonstrates a new method for quantifying geometric uncertainty from as-manufactured electrode images and how structural and image characteristics propagate this uncertainty throughout battery-relevant physical phenomena. Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

16th U.S. National Congress on Computational Mechanics
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Title: Self-Consistent Homogenization based Constitutive Model of Composites for High Strain-Rate Deformation with Stress Waves

Author(s): *Chandra Prakash, *Johns Hopkins University*; Somnath Ghosh, *Johns Hopkins University*;

Detailed micromechanical models built to accurately capture the effect of morphology on the dynamic response of composite structure are computationally expensive thus limited to microscale problems. On the other hand, conventional homogenization approaches, that predict the effective dynamic mechanical behavior, neglect the effect of micro-inertia, which has a significant effect under high-frequency loadings. Another issue with the conventional homogenization approaches is that of choosing the appropriate boundary condition. Under conditions of high strain-rate or impact, stress waves evolve and propagate in the composite microstructure, and interact with heterogeneities resulting in reflection and refraction at the interfaces. This stress-wave superposition and annihilation cannot be accurately captured by applying standard boundary conditions, such as periodic boundary conditions, used in conventional homogenization approaches. Alternative forms of boundary conditions are warranted for realizing the effects of stress-wave propagation in the microstructure. To overcome these limitations, a novel self-consistent computational homogenization scheme is developed to predict a Parametrically Homogenized Constitutive Model (PHCM) accounting for micro-inertia. In the proposed framework, an exterior domain is added around the RVE to represent an effective region that accurately captures stress-wave transmission and reflection at the RVE boundaries. The traction and displacement continuity between the RVE and the extended homogeneous region is enforced by the Lagrange multiplier. PHCM parameters are then calibrated using energy equivalence between the RVE and the exterior domain. The homogenized PHCM accounting for micro-inertia is developed for fiber-reinforced composite subjected to high strain rate loading. The micro-inertia effect appears in the form of a non-symmetric dynamic stress field in the equations of motion at the macroscale. The PHCM with micro-inertia effect developed in this work offers a relatively simple tool to analyze the dynamic mechanical response of composite structures subjected to high strain rate loading.

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Title: Hybrid Data-Driven Reduced Order Models for the 3D Turbulent Channel Flow

Author(s): *Changhong Mou, *Virginia Polytechnic Institute and State University*; Honghu Liu, *Virginia Polytechnic Institute and State University*; Leo Rebholz, *Clemson University*; Traian Iliescu, *Virginia Polytechnic Institute and State University*;

We propose a new hybrid reduced order model (ROM) framework for the numerical simulation of fluid flows. This hybrid framework incorporates two closure modeling strategies: (i) A structural closure modeling component that involves the recently proposed data-driven variational multiscale ROM approach, and (ii) A functional closure modeling component that introduces an artificial viscosity technique term. We also utilize physical constraints for the structural ROM operators in order to add robustness to the hybrid ROM. We perform a numerical investigation of the hybrid ROM for the three-dimensional turbulent channel flow at a Reynolds number Re=13,750.

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Title: A Comparative Study of Different J2 Plasticity Models Using a Nonlocal Lattice Particle Method

Author(s): *Changyu Meng, *Arizona State University*; Yongming Liu, *Arizona State University*;

Plasticity is crucial in modern structural analysis, since it is one of common causes of material non-linearity that produce permanent deformation. For ductile materials, plasticity will induce damage evolution and eventually result in the irreversible structural failure. This phenomenon is nonlinear and discontinuous by nature, which makes the traditional continuous simulation approaches like finite element method being unsuitable for modeling the entire failure process. One of the solutions is to use the discrete lattice particle methods for damage and cracking analysis. Recently, a newly developed nonlocal lattice particle method (LPM) has been applied to study the J2 plasticity of isotropic materials. However, this implementation still faces some problems. One is that it utilized the incremental updating method that is similar to explicit rather than implicit integration algorithm, therefore the loading steps should be very small to get an accurate result. This causes the inacceptable time cost to study complex loading when the particle number involved is large. Also, it is hard to directly implement the nonlinear hardening rules in this model. In this work, two new models are proposed to address the above issues. These methods both use the plastic bond stretch as an internal variable and adopted a normality rule in the model formulation. The difference of them comes from whether or not they use the stress tensor to model the normality rule and yield criterion. The stress-based method computes the deviatoric stress tensor from bond force and then apply return mapping algorithm. The force-based method, which does not use stress tensor, directly separates the energy and bond force into distortional and dilatational ones. And it uses distortional bond force to formulate the normality rule. These models are conceptually different from the original incremental updating algorithm of J2 plasticity. The preliminary results show that there is no loading step dependence, and the computational error is small because of implicit integration. This indicates that the proposed methods are more robust than the original one. The nonlinear hardening rules can also be directly added into the current models. Proposed two methods are equivalent to each other in the sense of being consistent with the classical J2 plasticity theory. They paved a way to consider material non-linearity in LPM framework. In the future research, damage behaviors and their associated internal variables will be included. That would provide a powerful tool to study the complex structural failure behavior.

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Title: Passive-Seismic Inversion of an Effective Seismic Force Vector at a DRM Boundary in a 2D Truncated Domain, Subject to Incoming Earthquake Waves, Using Sparsely-Measured Surface Seismic Motions

Author(s): Bruno Guidio, *Central Michigan University*; *Chanseok Jeong, *Central Michigan University*;

There is a need to estimate complex seismic input motions in a near-surface domain, without considering a seismic source at a hypocenter, from limited seismic measurement data. Based on such estimated seismic inputs, engineers can simulate the effect of an earthquake on built environments, including subsurface systems (soil, foundations, and underground structures). In this paper, a new inverse modeling is proposed for reconstructing an SH wave input motion (i.e., its corresponding effective seismic force vector) in a 2D domain that is truncated by a wave-absorbing boundary condition (WABC). The domain reduction method (DRM) is utilized to model seismic input motions coming from the outside domain of the WABC. The partial differential equation (PDE)-constrained optimization method aims at reconstructing a targeted effective seismic force vector, corresponding to targeted incident wavefields, at the DRM boundary. The presented method includes the discretize-then-optimize (DTO) approach, the finite element method (FEM), which is used for solving state and adjoint problems, and the conjugate-gradient scheme, determining the desired search path throughout a minimization process. The numerical results show that an effective force vector at a DRM boundary is reconstructed if a regularization, aimed at suppressing wave energy in an exterior domain outside a DRM boundary, is utilized in an objective functional in conjunction with a typical misfit functional. By using such a regularization term, the presented algorithm can minimize the kinetic energy associated with scattered wave responses outside the DRM boundary and, eventually, improve the inversion performance.

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Title: Hierarchical Deep Learning Neural Network (HiDeNN) for Molecular Simulations

Author(s): *Chanwook Park, *Northwestern University*; Satyajit Mojumder, *Northwestern University*; Sourav Saha, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

In this presentation, we propose a new methodology for parameterizing a coarse-grained molecular dynamics (CGMD) force field using the hierarchical deep learning neural network (HiDeNN) [1]. The key idea is that we train HiDeNN, and then let the HiDeNN find target force field parameter sets. The HiDeNN comprises two feedforward neural networks, hierarchically connected by transfer learning. The first neural network is trained with large data generated from a small CGMD model. It is then transfer learned with small data generated from a big CGMD model. The hierarchical structure shortens the computation time and improves the accuracy of the neural network. We demonstrate this methodology by applying it to practical CGMD systems such as the bulk heterojunction of the photoactive layer in an organic solar cell and polymer/silica nanocomposites. This work suggests a different paradigm to the field of CGMD simulations. The vast majority of the CGMD force field parameterization has solved an optimization problem. However, what frustrates most researchers is that the optimized CGMD force fields are not transferable although they require enormous computation power and labor-intensive processes. Furthermore, a slight change in the problem definition leads to a reparameterization from the scratch. Thus, we need to compromise between the generality (i.e., transferability to various simulation conditions) and the cost required to develop the force field. For instance, if we are to model a CGMD system that requires precise density at different temperatures, we only need a force field that fits well with the experimental density-temperature curve. It does not have to predict the accurate mechanical properties. Given this circumstance, the CGMD force field parameterization is no longer an optimization problem that tries to find a single optimum solution. Instead, we view it as a design problem that can be handled by analyzing and learning from large data. The underlying philosophy is that multiple solutions (i.e., force field parameter sets) exist that accurately predict specific target properties, and any of them are acceptable in the boundary of this specific problem. We anticipate the proposed methodology will ease the burden of developing new CGMD force fields and expand the application of mesoscopic molecular simulations. References [1] S. Saha, Z. Gan, L. Cheng, J. Gao, O. L. Kafka, X. Xie, H. Li, M. Tajdari, A. H. Kim, and W. K. Liu, "Hierarchical Deep Neural Network (HiDeNN): An artificial intelligence (AI) framework for Computational Science and Engineering," special issue on "AI in Computational Mechanics and Engineering Sciences", Comput. Methods Appl. Mech. Engrg. 373 (2021) 113452.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Predicting Wall Shear Stress Using Simulation-Based Imaging

Author(s): *Charles Naudet, *University of Notre Dame*; Matthew Zahr, *University of Notre Dame*;

Three-dimensional, time-resolved, three-directional magnetic resonance flow imaging (4D-flow) is a powerful method for investigation of cardiovascular physiology and pathophysiology. Current 4D-flow acquisition schemes provide comprehensive information on hemodynamics, but the tradeoff between image quality and scan time still limits their utility in clinical studies that require high-resolution images of small systems, such as infants with congenital heart disease. Furthermore, there are also limitations on quantification of physiological parameters, such as wall shear stress, which can be an important biomarker that indicates events such as stroke or blood clot. Recent advances in optimization-driven simulation-based imaging (SBI) have shown promise for applications that require higher resolution, shorter scan times, and accurate quantification of physiological parameters [1]. The SBI method uses a computational fluid dynamics (CFD) simulation to visualize the in vivo flow velocity field and compute relevant quantities of interest. The flow domain is extracted from angiogram images and unknown boundary conditions are determined using adjoint-based optimization to ensure the CFD simulation is consistent with low-resolution 4D flow data. This work aims to establish the ability of SBI to accurately compute quantitative biomarkers, specifically wall shear stress, and quantify the sensitivity of both SBI and conventional magnetic resonance imaging (MRI) postprocessing techniques to noise and Reynolds number. These studies are carried out using a synthetic numerical experiment of steady, viscous, incompressible flow through a two-dimensional idealized stenosis. Wall shear stress predictions based on SBI were up to an order of magnitude more accurate than those based on conventional MRI postprocessing, and were more robust to noise and Reynolds number. [1] Töger, Johannes, et al. “Blood Flow Imaging by Optimal Matching of Computational Fluid Dynamics to 4D?Flow Data.” Magnetic Resonance in Medicine, vol. 84, no. 4, 8 Apr. 2020, pp. 2231–2245., doi:10.1002/mrm.28269.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Operator Learning for Predicting Multiscale Bubble Growth Dynamics

Author(s): *Chensen Lin Lin, *Brown University*; Zhen Li, *Clemson University*; Lu Lu, *Massachusetts Institute of Technology*; Shengze Cai, *Brown University*; Martin Maxey, *Brown University*; George Karniadakis, *Brown University*;

Simulating and predicting multiscale problems that couple multiple physics and dynamics across many orders of spatiotemporal scales is a great challenge that has not been investigated systematically by deep neural networks (DNNs). Herein, we develop a framework based on operator regression, the so-called deep operator network (DeepONet), with the long term objective to simplify multiscale modeling by avoiding the fragile and time-consuming “hand-shaking” interface algorithms for stitching together heterogeneous descriptions of multiscale phenomena. To this end, as a first step, we investigate if a DeepONet can learn the dynamics of different scale regimes, one at the deterministic macroscale and the other at the stochastic microscale regime with inherent thermal fluctuations. Specifically, we test the effectiveness and accuracy of DeepONet in predicting multirate bubble growth dynamics, which is described by a Rayleigh-Plesset (R-P) equation at the macroscale and modeled as a stochastic nucleation and cavitation process at the microscale by dissipative particle dynamics (DPD). First, we generate data using the R-P equation for multirate bubble growth dynamics caused by randomly time-varying liquid pressures drawn from Gaussian random fields (GRF). Our results show that properly trained DeepONets can accurately predict the macroscale bubble growth dynamics and can outperform long short-term memory (LSTM) networks. We also demonstrate that DeepONet can extrapolate accurately outside the input distribution using only very few new measurements. Subsequently, we train the DeepONet with DPD data corresponding to stochastic bubble growth dynamics. Although the DPD data is noisy and we only collect sparse data points on the trajectories, the trained DeepONet model is able to predict accurately the mean bubble dynamics for time-varying GRF pressures. Taken together, our findings demonstrate that DeepONets can be employed to unify the macroscale and microscale models of the multirate bubble growth problem, hence providing new insight into the role of operator regression via DNNs in tackling realistic multiscale problems and in simplifying modeling with heterogeneous descriptions.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Pulsatile Flow Investigation of Flow Pattern in Aortic Aneurysm Under Novel Stent Graft with Various Designs of Slit Perforations

Author(s): *Chi Wei Ong, *Agency for Science, Technology and Research (A*STAR)*; Hwa Liang Leo, *National University of Singapore*; Pei Ho, *National University Health System, Singapore*; Fangsen Cui, *Agency for Science, Technology and Research (A*STAR)*;

Aortic aneurysm can be fatal if left untreated. However, the geometry complexity of the aorta makes it a challenging task on designing effective and personalized treatment of aortic aneurysm. The purpose of this study is to investigate the effect of a novel stent graft with different types of slit perforations to treat the aortic aneurysm in a transient study with the aid of image-based computational fluid dynamics (CFD) method. We designed a stent graft with different types of slit perforations and performed virtual implantation on aortic aneurysms from various CT datasets. To distinguish the flow pattern difference of pre and post-treatment, we modified the geometry of aortic aneurysm through computer-aided design (CAD) to generate the flow pattern throughout the whole cardiac cycle in healthy, pre-treatment and post-treatment geometries. Non-Newtonian Carreau model and realistic boundary conditions were used in the current study to model the realistic blood flow behaviour. Our study showed that the design of slits on the stent graft can alter the hemodynamics of aortic aneurysm. Biomechanical parameters such as vorticity and wall shear stress in both numerical and experimental were analysed qualitatively and quantitatively. Lastly, we demonstrate that the morphology of the slits can change the wall shear stress magnitude that may bring impact to the treatment outcome. The change of wall shear stress also indicates that the stent graft with slits may prevent the aortic aneurysm from rupture. We showed that an image-based CFD can be combined with in-vitro experiment to assist in surgical planning by providing vorticity, pressure and wall shear stress that can be difficult to obtain in vivo. This method can help to evaluate the impact of medical devices virtually with a possibility to reduce the overall design cost of the medical device.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Constitutive Modeling of Magneto-Active Composites with Fibrous and Particulate Terfenol-D Reinforcements

Author(s): You-Shu Zhan, *National Cheng Kung University*; *Chien-hong Lin, *National Cheng Kung University*;

This study presents a micromechanics model to determine the effective magneto-elastic response of magnetostrictive composites. The polymer matrix composites are reinforced by fibrous and particulate Terfenol-D reinforcements. A simplified unit-cell micromechanics model that idealizes the arrangement of reinforcements in a periodic manner is developed for the composites. A microscopically based phenomenological constitutive model is employed for the magnetostrictive fillers. Due to the nature of material nonlinearity of the Terfenol-D reinforcements, the overall magnetostrictive strain and magnetization responses of the composite is nonlinear. The polymer matrix is assumed as a linear elastic solid. In order to obtain the overall nonlinear response, the linearized micromechanical relations are first derived for providing trial solutions following an iterative scheme in order to minimize the error resulted from linearization. For the purpose of comparison, the predictions from the Mori-Tanaka micromechanics model are also presented. The numerical results show that both unit-cell and Mori-Tanaka estimations agree well with experimental measurements. Parametric study reveals that piezomagnetic coefficient and permeability are significantly magnetic?field dependent especially for a high concentration of magneto-active Terfenol?D fillers. In conclusion, the presented micromechanics formulation is useful for studying magnetostrictive Terfenol?D composites, and it can be further used as constitutive law to analyze and design intelligent magneto-active structures.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Tensor-Structured Algorithm for Reduced-Order Scaling Large-Scale Kohn-Sham Density Functional Calculations

Author(s): *Chih-Chuen Lin, *University of Michigan*; Phani Motamarri, *Indian Institute of Science*; Vikram Gavini, *University of Michigan*;

We present a tensor-structured algorithm for efficient large-scale DFT calculations by constructing a Tucker tensor basis that is adapted to the Kohn-Sham Hamiltonian and localized in real-space. The proposed approach uses an additive separable approximation to the Kohn-Sham Hamiltonian and an L1 localization technique to generate the 1-D localized functions that constitute the Tucker tensor basis. The 1-D localized functions span a subspace that represents the eigen-space of the additive separable Hamiltonian. Numerical results show that the resulting Tucker tensor basis exhibits an exponential convergence in the ground-state energy with Tucker rank. Furthermore, our studies reveal that the Tucker basis is more efficient than the plane-wave basis, requiring fewer basis functions to achieve similar accuracy. Our benchmark studies on systems ranging up to 25,000 electrons show that the computational complexity of the Kohn-Sham eigenvalue problem scales sub-quadratically with the system size, owing to the sublinear growth of the number of Tucker basis functions with system-size to achieve chemical accuracy. This reduced-order scaling has resulted in a substantial outperformance of plane-wave DFT implementation for systems containing beyond 5,000 electrons.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Simulation of Interactive Biological Networks: A Phase-field Approach to Slime Molds Development

Author(s): *Christian Peco, *The Pennsylvania State University*; Farshad Ghanbari, *The Pennsylvania State University*; Francesco Costanzo, *The Pennsylvania State University*;

Slime molds develop macroscopic pulsating networks able to modify their structure in response to the environment. Despite their relative simplicity and the lack of a neural system, these organisms can move, solve mazes, sense nutritious or toxic agents at a distance, and even memorize periodic events. Recent studies have revealed that slime mold's pulsating unit — at the small scale — relies more heavily than previously thought on the feedback between the mechanical properties of the membrane, cytoplasm and chemical kinetics. However, the capacity to understand and replicate the emergent behavior at the level of the whole organism remains a challenge. We establish here a theoretical and computational framework to explain, quantify and reproduce how this feedback between macroscopic features and local tuning of mechanical properties determines an emergent coordinated response of the network morphology. These networks have the ability to grow, survive, or die in the presence of different concentrations of nutrients, and to redistribute them thus optimizing its proliferation. We propose a phase-field scalar variable to represent the network matrix evolution, and a diffusive-advective process for the nutrient distribution. This framework enables high fidelity simulations of slime molds in the three-dimensional space, which are challenging due to the coupled physics involved, high-order partial differential equations, and the existence of a highly complex evolving geometry. We support our simulations with experiments on a particular slime mold (Physarum polycephalum). The emergent properties of these organisms are similar in nature to tissues with transport networks, and can play a central role in wound healing, metastasis formation, or embryology. This investigation is a road to the microstructural design of active soft matter, object of interest in many fields of engineering and science.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The Atomic Cluster Expansion

Author(s): *Christoph Ortner, *University of British Columbia*;

I will review the atomic cluster expansion for constructing hybrid mechanistic / data-driven interatomic potentials from ab initio models. The method can be interpreted as a polynomial regression scheme, but despite (or maybe because of) its simplicity it naturally leads to high performance, crystal clear interpretability and remarkable generalisation properties. I will explain the key idea and reason for the excellent performance, show-case some of the features that make it a general and flexible modelling tool, and conclude by show-casing the first practical interatomic potentials (for Cu and Si) based on ACE methodology.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Nonlinear Projection-Based Model Order Reduction in the Presence of Adaptive Mesh Refinement

Author(s): *Clayton Little, *Stanford University*; Charbel Farhat, *Stanford University*;

For many problems in computational mechanics, Adaptive Mesh Refinement (AMR) is desirable as it enhances accuracy for a given computational cost and reduces this cost for a specified accuracy. While it is fairly practiced in the context of high-dimensional, mesh-based computational models, it is in its infancy in that of low-dimensional, generalized-coordinate-based computational models such as Projection-based Reduced-Order Models (PROMs) and Hyperreduced PROMs (HPROMs). This is primarily due to the fact that when AMR is applied at the high-dimensional level, different solution snapshots may be computed on different meshes, which raises two different but related issues: the solution snapshots may have different dimensions, which complicates their collection and compression into a Reduced-Order Basis (ROB); and even if they happen to have the same dimension due to a fortuitous balance between mesh refinement in some regions of the computational domain and mesh coarsening in other regions, they may suffer from some inconsistency due to the fact that their same-index entries may not evaluate the solution at the same spatial location. Most recently, an approach for addressing, to some extent, both aforementioned issues has been proposed by Grassle in the context of the Proper Orthogonal Decomposition (POD) method. Essentially, this approach consists in interpreting all mesh-based computations underlying POD as inner products and computing them in the continuous solution space rather than the semi-discrete counterpart. This talk will present the extension of this approach to hyperreduction, which is indispensable for parametric, Projection-based Model Order Reduction (PMOR) when it is not possible or computationally tractable to pre-compute offline the reduced-order operators and quantities and the computational complexity of their online computation does not scale only with the size of the PROM. In particular, the talk will address how to resolve the difficulties associated with tracking, managing, and approximating the dependencies between mesh adaptation, which is done for one purpose, and mesh sampling or reduction, which is done for a different purpose, in the context of the Energy-Conserving Sampling and Weighting (ECSW) hyperreduction method. Such dependencies give rise to a novel challenge associated with an increased dimensionality in some aspects of the hyperreduction process, which is addressed in this work using the concept of local ROBs. All presented ideas and their significance will be illustrated and highlighted with the solution of nonlinear PMOR problems of relevance to computational mechanics.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Rapid Computation of Thermal Histories for Laser Powder Bed Fusion Additive Manufacturing Processes

Author(s): *Daniel Moser, *Sandia National Laboratories*; Mario Martinez, *Sandia National Laboratories*; Kyle Johnson, *Sandia National Laboratories*; Theron Rodgers, *Sandia National Laboratories*;

Computational modeling of additive manufacturing (AM) processes shows promise as a method for addressing challenges with the use of additive for producing functional parts. Models capable of predicting as-built part properties from process inputs could be used to alleviate some of the experimental workload often required to dial in process settings needed to produce a part that meets functional requirements. AM modeling of laser powder bed fusion (LPBF) has remained computationally expensive, however, due to the large difference in length and time scales between the action of the laser and a full part build. As a result, reduced-order, phenomenological models are generally the only option for predicting the as-built properties of an engineering scale part. This talk describes the development of a physics-based reduced order model of the LPBF process that uses analytical, Green's function solutions to predict the linear temperature response of a workpiece to a laser scan. The nature of the Green's function solution allows independent evaluation at any point in space and time, a highly-parallel computation that is amenable to GPU architectures. Using GPU computing and an adaptive space-time grid, a 72x wall clock speedup is achieved on a benchmark problem as compared to traditional FEM. Also presented are calibration techniques used to address the linearity constraint required by Green's functions as well as comparisons between predictions of microstructure and residual stress using thermal histories computed by FEM and the newly developed Green's function method. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Object Detection in a Through-the-Wall Setting Utilizing Machine Learning

Author(s): *Daniel Pomerico, *Air Force Institute of Technology (USA)*; Aihua Wood, *Air Force Institute of Technology (USA)*;

Abstract Inverse scattering problems have many applications in physics and engineering. A recurring application has been to solve the through-the-wall imaging problem utilizing electromagnetic waves to reconstruct the characteristics of an object such as shape, location, and material properties. In [1], a numerical simulation of a through-the-wall scenario was developed to determine object location in the domain of interest (DOI). This paper continues that work, whereby an object in motion is added to the DOI. To the best of our knowledge, this is the rst time simulated data is used as training data for a machine learning (ML) algorithm for the reconstruction of a moving object in the through-the-wall setting. In particular, we recover the shape and the electric permittivity of an unknown moving object, as well as classifying di erent objects using ML. As in [1], the input data for ML is the numerical solution of Maxwell's Equations. Our model is a square room of size 3m by 3m where all materials are invariant in the z direction. The walls have uniform thickness and permittivity. The object also has uniform relative electric permittivity and is of a convex shape. In order to model the actual physical problem, data is recorded by a series of antenna transmitters/receivers placed outside the room at a set distance. A time series modi cation is utilized to simulate the object in motion. We use K-nearest neighbor (KNN) to baseline the data simulation output. Several Convolutional Neural Network (CNN) schemes are considered for the reconstruction. Our preliminary results show that compared to the case of stationary objects, the KNN yields increased errors in characterizing the object in motion, particularly when the object is relatively small (less than ■10cm in diameter). However, a basic CNN scheme has been able to reconstruct the object shape with accuracy within ■5cm. Work is underway to build a robust CNN scheme that can reconstruct the material parameter of a moving object. References [1] Charnley, M., & Wood, A. (2016). Through-the-wall radar detection analysis via numer-ical modeling of Maxwell's equations. Journal of Computational Physics, 313, 532{548.https://doi.org/10.1016/j.jcp.2016.01.039 [2] Wood, A., Wood, R., & Charnley, M. (2020). Through-the-wall radar detection using machine learning. Results in Applied Mathematics, 7, 1{6. https://doi.org/10.1016/j.rinam.2020.100106

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Hybrid Finite Element – Spectral Boundary Integral Method for 3D Dynamic Fracture Simulation

Author(s): *David Kammer, *ETH Zurich*; Gabriele Albertini, *Cornell University*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*;

Modeling dynamic fracture of a weak interface in a 3D unbounded domain is a useful tool to study fundamental aspects of fracture mechanics related to problems such as the onset of friction and earthquake rupture propagation. Typically, such a simulation involves solving the elasto-dynamic wave equation on a finely discretized domain with an explicit time integration scheme. If the domain is purely elastic and homogeneous, one can apply boundary-element methods [1], which are efficient and limit discretization to the weak interface only. However, if the solid is inelastic or heterogeneous, discretization of the full domain is required and boundaries need to be far enough to approximate an unbounded domain [2]. This results in a very large number of degrees of freedom and thus large computational cost. We propose a hybrid method, which combines the finite-element method with the spectral-boundary-integral method [3]. The discretized finite-element domain describes accurately all non-uniformities near the weak interface. but is truncated and coupled with an infinite boundary condition, which absorbs all incident waves. The infinite boundary condition is provided by the spectral-boundary-integral method, which is based on a semi-analytical solution of the elasto-dynamic impulse response of an infinite elastic half space. The semi-analytical nature provides very accurate wave absorption and the spectral representation provides computational efficiency due to the independent response of each wavelength. We compare the developed hybrid method with full finite-element simulations of established benchmark simulations and determine the potential increase in computational efficiency. REFERENCES [1] Geubelle, P.H., Rice, J.R., 1995. A spectral method for three-dimensional elastodynamic fracture problems. Journal of the Mechanics and Physics of Solids 43, 1791–1824. https://doi.org/10.1016/0022-5096(95)00043-I [2] Albertini, G., Kammer, D.S., 2017. Off-fault heterogeneities promote supershear transition of dynamic mode II cracks. J. Geophys. Res. Solid Earth 122, 2017JB014301. https://doi.org/10.1002/2017JB014301 [3] Ma, X., Hajarolasvadi, S., Albertini, G., Kammer, D.S., Elbanna, A.E., 2019. A hybrid finite element-spectral boundary integral approach: Applications to dynamic rupture modeling in unbounded domains. International Journal for Numerical and Analytical Methods in Geomechanics 43, 317–338. https://doi.org/10.1002/nag.2865

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Construction of an Entropy Stable Discontinuous Galerkin Spectral Element Method for Two-Phase Flows Modeled by an Incompressible Navier-Stokes/Cahn-Hilliard System

Author(s): Juan Manzanero, *Polytechnic University of Madrid*; *David Kopriva, *Florida State University / San Diego State University*; Gonzalo Rubio, *Polytechnic University of Madrid*; Esteban Ferrer, *Polytechnic University of Madrid*; Eusebio Valero, *Polytechnic University of Madrid*;

We develop a robust entropy–stable two–phase incompressible Navier–Stokes/Cahn–Hilliard discontinuous Galerkin (DG) spectral element flow solver method suitable for industrial application. The model uses the Cahn–Hilliard equation as the phase field method, a skew–symmetric form of the momentum equation, and an artificial compressibility method for the pressure. The model satisfies an entropy law, including for free– and no–slip wall boundary conditions with non–zero wall contact angle. The high order Discontinuous Galerkin Spectral Element Method (DGSEM) is discretely entropy conserving with central advective fluxes and the Bassi-Rebay-1 scheme for diffusion, and is entropy stable when an exact Riemann solver is used for the advective numerical flux. The stability proofs hold for three–dimensional unstructured meshes with curvilinear hexahedral elements. The standard discontinuous Galerkin method does not satisfy entropy inequality and is shown to have a 30% probability to fail, whereas the entropy-stable scheme never does. Examples of three-dimensional pipe flow will be presented.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A High-Fidelity 3D Micromechanical Model of Ventricular Myocardium

Author(s): *David Li, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*;

Multiscale computational modeling of the heart has become an important tool for understanding cardiac function. However, there is a need to develop models that are faithful to the microstructure of the myocardium in order to gain insight into the cellular-level mechanical environment, especially to identify mechanisms driving adaptations to structural heart disease. We thus developed a microanatomically realistic finite element model for ventricular myocardium. For this first study, we based our model on a high-resolution 3D imaging dataset from the murine right ventricular free wall to study fiber-specific interactions under planar deformations, with the aim to match the results of our previous tissue-level model. A 3D imaging dataset was acquired from a ~200x200x60-µm section of myocardium via confocal microscopy, with tissue components labeled using antibodies and fluorescent markers. The resulting geometry, including myofibers, ECM, myofibroblasts, and coronary blood vessels, was used to generate a volumetric finite element (FE) layer model consisting of myofiber and ECM elements. The passive behaviors of the myofiber and ECM phases were modeled with nearly incompressible, nonlinear anisotropic materials derived from our previous studies. The myofibers were represented using a locally orthotropic constitutive form, consisting of an isotropic matrix stiffened by mutually orthogonal fiber families in the myofiber (f) and cross-fiber (s) directions within the layer. The stress response FE layer microanatomical model successfully reproduced the tissue-scale structural model prediction. As the FE layer model contained highly aligned myofibers oriented along the f direction, the model showed exponentially stiffening myofiber stress in E_11 with negligible stress along E_22. The ECM exhibited nonlinear stiffening during collagen fiber recruitment, after which fibers were fully recruited and the ECM response became linear, as demonstrated previously. Comparing the stress profiles of the myofiber and ECM phases indicated that total response was governed by myofiber behavior in the low-strain regime. At higher strains, the ECM collagen fibers became the major contributor to the RVFW stress. The fiber axis-focused profile of stress transfer from myofibers to ECM provides insight into possible mechanisms for the coupling interactions hypothesized in previous work. Through this microanatomical approach, exploration of cellular-scale stress transfer between myocytes and their surroundings can be integrated into larger-scale models and used to further probe the effect of micro-level events on organ-level function. Ultimately, our microanatomical model will allow us to investigate fiber-specific remodeling of the cardiac microstructure in response to structural heart disease.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Convergence Studies for Meshfree Peridynamic Simulations of Dynamic Crack Growth

Author(s): *David Littlewood, *Sandia National Laboratories*; Pablo Seleson, *Oak Ridge National Laboratory*; Marco Pasetto, *University of California, San Diego*; Yohan John, *General Electric Global Research*; Jeremy Trageser, *Sandia National Laboratories*;

Meshfree methods are commonly applied to discretize peridynamic models for solid mechanics simulations. Under this approach, the domain is represented by a set of nodal volumes which interact in accordance with the specified material model. Nonlocality results in direct interactions between nodal volumes that are separated by a distance less than or equal to the peridynamic horizon. Previous work by Seleson and Littlewood [1-3] showed that common meshfree methods in peridynamics suffer from accuracy and convergence issues due to the treatment of pairwise interactions as the separation distance between nodal volumes approaches the horizon. Mitigation strategies, including the use of smoothly-decaying influence functions and the so-called partial volume approach, were demonstrated on static simulations and simulations of dynamic wave propagation. In the present study, we extend this prior work to simulations of dynamic crack propagation. Specifically, we investigate mesh convergence for peridynamic simulations of the well-known Kalthoff-Winkler experiment. Numerical studies are conducted using an elastic bond-based material model augmented with a variety of influence functions, and with accurate calculations of the volume of intersection for pairwise interactions. Effectiveness and computational expense are evaluated, with multiple approaches resulting in significant improvement of the convergence behavior. [1] Pablo Seleson. Improved one-point quadrature algorithms for two-dimensional peridynamic models based on analytical calculations. Computer Methods in Applied Mechanics and Engineering, 282:184– 217, 2014. [2] Pablo Seleson and David J. Littlewood. Convergence studies in meshfree peridynamic simulations. Computers and Mathematics with Applications, 71(11):2432–2448, 2016. [3] Pablo Seleson and David J. Littlewood. Numerical tools for effective meshfree discretizations of peridynamic models. In George Z. Voyiadjis, editor, Handbook of Nonlocal Continuum Mechanics for Materials and Structures. Springer, 2019. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2020-14358 A.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Establishing a Data-Driven Deformation Model for Tin Using Symbolic Regression and Genetic Programming

Author(s): *David Montes de Oca Zapiain, *Sandia National Laboratories*; Hojun Lim, *Sandia National Laboratories*; Jay D. Carroll, *Sandia National Laboratories*; Zachary Casias, *Sandia National Laboratories*; Corbett Battaile, *Sandia National Laboratories*; J. Matthew D. Lane, *Sandia National Laboratories*;

Tin (Sn) is a metallic element that exhibits a complex deformation behavior characterized by pressure-dependent structural phase transitions and significant temperature and strain-rate dependent deformation. Consequently, modeling its strength with the associated complex deformation is not trivial. In this work, we present a data-driven strength model for tin valid for the quasi-static regime, high-strain rates and high temperatures. The strength model was developed using genetic programming to perform symbolic regression on Sandia's recent quasi-static experimental results. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND No: SAND2021-1139 A

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Cohesive, Integrated Modeling and Simulation Workflow for Mechanical Response Characterization of Metallic Additively Manufactured Parts

Author(s): *David Najera, *ATA Engineering*; Marc Russell, *ATA Engineering*; Thomas Board, *ATA Engineering*; Eoghan O'Neill, *ATA Engineering*; Johnathan Tran, *ATA Engineering*; Liam Mackin, *ATA Engineering*; Elliot Haag, *ATA Engineering*;

Cost-effective and rapid implementation of additive manufacturing (AM) for complex parts in critical applications is currently impeded by a lack of predictive insights into the physics of AM processes. Individual commercially available modeling and simulation tools have struggled to date with providing cohesive predictive capabilities that span the length scales and physical domains of AM process physics that directly impact the performance and reliability of AM parts. It is clear that, with the maturation of the field, high-fidelity predictive capabilities for AM processes will require an integrated multi-method approach to span the temporal/physical length scales and physics of AM. A complete thermal-mechanical-material modeling and simulation workflow is proposed that uses automated data mapping and translation tools to integrate part-level print simulations, probabilistic grain growth models, and crystal plasticity homogenization techniques to efficiently predict metallic part residual stresses, net shape, and strength. Thermal-mechanical fields during printing are simulated using the finite element analysis code Abaqus. The as-printed grain microstructure is predicted using the kinetic Monte Carlo code SPPARKS from Abaqus thermal history results. The homogenized microstructural response is determined with the crystal plasticity spectral solver DAMASK. Dimensionality reduction is performed by employing a K-means algorithm to cluster regions of similar thermal histories in a part for spatially varying assignment of mechanical properties. Finally, process simulation insights (residual stresses, material properties) are embodied in a part-level finite element model representing the as-built condition. This workflow has been demonstrated and partially validated via prediction of the tensile response of two sets of 316L cylindrical test coupons with varying printing paths and manufactured with a directed energy deposition process, which were presented in Yadollahi et al. [Materials Science and Engineering: A 664, 2015: 171–83]. The results show a path toward a foundational physics-based simulation toolset for part performance characterization that leverages state-of-the-art tools available to industry.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A New Strategy for Automated Tetrahedral Mesh Generation for Producing Credible Discretizations from 3D Image Data

Author(s): *David Noble, *Sandia National Laboratories*; Scott Roberts, *Sandia National Laboratories*; Matthew Staten, *Sandia National Laboratories*; Corey McBride, *Sandia National Laboratories*; C. Riley Wilson, *Sandia National Laboratories*;

Normally, the performance of a part is simulated using a discretized model that conforms to the geometry of the part, as the part was originally designed. However, when there is significant variation from part-to-part, we would like to produce models using the as-manufactured geometry. To this end, we seek to produce credible discretizations using experimentally obtained images of actual parts and microstructures. Previous work has verified the use of the Conformal Decomposition Finite Element Method (CDFEM) for simulating the transport in experimentally imaged domains of multiple materials [1]. However, CDFEM produces poorly conditioned systems of equations when the interfaces come close to the background mesh nodes. Previous work has also shown that incremental mesh improvement algorithms can be used to improve the quality of the discretization produced by CDFEM. In the current work, an entirely new strategy is developed for automated tetrahedral mesh generation, which is more robust and produces higher quality meshes than standard techniques. Like other mesh generators, the first step is to segment the image data for each material domain. Deep learning techniques are employed to improve this segmentation process. The segmented images are then used to generate bounding surface meshes of triangular facets for each domain. This focus of this talk is the novel method that is then used to generate the tetrahedral mesh from the triangular surface meshes for each domain. The basic steps of the new meshing strategy are to generate an overlay mesh with a desired resolution, intersect the overlay mesh with the domain surface meshes, move nodes of the overlay mesh to nearby intersection points, cut the remaining intersection points into the overlay mesh, and then apply incremental mesh improvement to improve the quality of the resulting mesh. These steps are designed and implemented to act on meshes stored in distributed memory. The quality of the resulting discretization is assessed for multiple demonstration problems. The resulting discretization is shown to have much better conditioning and improved mesh quality compared to standard CDFEM discretizations. [1] Roberts, Mendoza, Brunini, and Noble, “A verified conformal decomposition finite element method for implicit, many-material geometries”, Journal of Computational Physics, Volume 375, 2018 *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Towards Predicting the Progression of Osteoarthritis within a Framework of Volumetric Growth and Remodeling

Author(s): Muhammed M. Rahman, *University of Connecticut*; Thomas S. E. Öst, *FOI – Swedish Defense Research Agency*; Corey P. Neu, *University of Colorado Boulder*; *David M. Pierce, *University of Connecticut*;

Osteoarthritis is a disease of the synovial joint, with degeneration and loss of articular cartilage as one hallmark change. Despite the multifactorial nature of osteoarthritis, mechanical stresses play a key role in the destructive evolution of the disease. Both overloading and reduced loading of cartilage induce molecular and microstructural changes that lead to mechanical softening, fibrillation, and erosion. In response to mechanical and chemical stimuli, chondrocytes (the cells within cartilage) express and degrade components of extra-cellular matrix including structural constituents such as collagen, proteoglycan, and other proteins. To facilitate better understanding of the mechanobiology of cartilage and chondrocytes, we established a novel framework to incorporate the evolution of constituents generating volumetric changes in cartilage, i.e., volumetric growth and remodeling (VG&R), by leveraging our established constitutive models of cartilage [1,2]. We proposed generalized multilinear functions for normalized production of proteoglycan and collagen dependent on intra-tissue stretch, and frequency (stretch rate) and duration of loading, and calibrated these using data on cyclic, unconfined compression of cartilage specimens ex vivo. To validate our numerical framework we simulated cartilage undergoing cyclic hydrostatic pressure and predicted both proteoglycan and collagen production over 21 days [3]. Exploiting the very different time scales between daily activities, e.g., walking (sec), and progression of osteoarthritis (days to years), we used iterative rather than simultaneous solutions. We performed our simulations using FEBio (University of Utah). To exercise our novel VG&R framework we successfully predicted the evolution of constituents within articular cartilage under mechanical loading despite differences in the loading modes. We formulated our generalized functions based on experiments under cyclic uniaxial compression, while we predicted the evolution of constituents under cyclic hydrostatic pressure. In predicting the evolution of proteoglycan, our simulations reasonably approximated the experimental results except for day 21. Our predictions of the evolution of collagen followed the trend determined experimentally [3]. Unfortunately, the experimental data available for calibrating our framework were quite sparse. In this light we selected a linear relationship among stretch, frequency, and time. Our framework is the first step towards a new class of computational tools that will facilitate, for the first time, patient-specific modeling of osteoarthritis progression considering the biomechanics and kinetics of extra-cellular matrix turnover and production, both in vitro and in vivo. [1] Pierce et al., Biomech Model Mechanobiol, 15:229-244, 2016. [2] Wang et al., J Mech Behav Biomed Mat, 86:409-422, 2018. [3] Kraft et al., Cartilage, 2:254-264, 2011.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling Continuous Sea Ice Floes with the Discrete Element Method

Author(s): *Devin O'Connor, *Cold Regions Research and Engineering Laboratory*; Brendan West, *Cold Regions Research and Engineering Laboratory*;

The Arctic has undergone significant changes in recent decades due to climate change, with substantial reductions in sea ice extent and multiyear ice, leading to thinner ice that is susceptible to breakup [1]. This so called "New Arctic" presents many challenges including, but not limited to, accurately modeling sea ice dynamics, lead (crack) development, and ridge formation (sea ice floe collision). Particle methods, such as the discrete element method (DEM), can provide detailed descriptions of sea ice dynamics that explicitly model fracture and ridging, which can be difficult with typical continuum sea ice modeling approaches. However, large sea ice floes can deform and break up under external forcing, which presents challenges for the DEM to model these important dynamics accurately. In this talk, we present our current efforts in extending sea ice DEM formulations to be able to model continuous floe mechanics. We will focus on two formulations, (1) a lattice-spring like model called a "cohesive beam" [2], and (2) a novel sea ice peridynamic-DEM hybrid model [3]. We will present results on idealized tests that examine the ability of the models to predict effective continuous sea ice properties including effective stress and strength. Lastly, using our two approaches we discuss results from simulations of sea ice dynamics through the Nares Strait. Realistic particle initial configurations are generated by discretizing MODIS satellite imagery into polygonal floes that are made up of many smaller discrete polygonal particles. The sea ice is forced externally using wind and ocean drag functions in combination with realistic wind and ocean velocities in the Nares Strait region. We compare our simulation results to optical satellite imagery and discuss the models predictive capability. [1] Kohout, A. L., Williams, M. J. M., Dean, S. M., and Meylan, M. H. Storm-induced sea-ice breakup and the implications for ice extent. Nature. (2014) 509(7502), 604. [2] Andre, D., Iordanoff, I., Charles, J. L., and Neauport, J. Discrete element method to simulate continuous material by using the cohesive beam model. Computer methods in applied mechanics and engineering. (2012) 213:113-125. [3] Davis A.D., West B.A., Frisch N.J., O'Connor D.T., and Parno M.D. ParticLS: Object-oriented software for discrete element methods and peridynamics." Computational Particle Mechanics (accepted).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Efficient Model Order Reduction Schemes for Dynamic Contact Problems

Author(s): *Diana Manvelyan, *Siemens AG, Technology*; Bernd Simeon, *Technical University of Kaiserslautern*; Utz Wever, *Siemens AG, Technology*;

Our work proposes an approach for the efficient model order reduction of dynamic contact problems in linear elasticity. We suggest, that for both linear and non-linear contact problems we solve the dual problem of the underlying contact problem. Instead of the augmented Lagrangian method that is commonly used for mechanical contact problems to solve the dual problem, we prefer the Nonlinear Complementary Programming (NCP) method. Since the shape of the contact zone depends strongly on the acting outer forces, the NCP for the Lagrange multipliers must be solved in each time step. In the nonlinear case, however, the node-to-segment condition may be described by a quadratic equation, therefore, the Karush-Kuhn-Tucker condition is still linear in the displacements. The model order reduction scheme, on the other hand, is applied to the large linear system for the displacements and is computed in advance by means of an Arnoldi process. In terms of computational effort, the reduction scheme is very appealing because the contact constraints are fully satisfied, while the reduction acts only on the displacements. For linear contact problems similar approach is applied using Linear Complementary Programming (LCP) method. In both cases, Craig-Bampton method is used to distinguish between the interior nodes and the nodes in the contact zone.

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Title: A New Biomarker for the Assessment of Mechanical Heterogeneity in Biological Tissue

Author(s): *Dieter Klatt, *University of Illinois at Chicago*; Harish Palnitkar, *University of Illinois at Chicago*; Rolf Reiter, *University of Illinois at Chicago*; Shreyan Majumdar, *University of Illinois at Chicago*; Joseph Crutison, *University of Illinois at Chicago*; Shujun Lin, *University of Illinois at Chicago*; Thomas Royston, *University of Illinois at Chicago*;

Magnetic Resonance Elastography (MRE) is a noninvasive diagnostic imaging technique capable of determining the mechanical properties of biological tissues. Conventionally an MRE examination consists of three basic steps: i) introduction of vibrations into the tissue of interest using external mechanical actuators; ii) imaging of time-resolved snapshots of shear wave propagation using phase contrast-based MRI acquisitions; and iii) calculation of mechanical property maps within the tissue using the shear wave images as input for the inversion of the wave equation. The inversion process represents an ill-posed problem and poses a challenge for the demarcation of tissue boundaries in heterogeneous tissues. Furthermore, the use of third order spatial derivatives in the inversion algorithm results in a sevenfold decrease of spatial resolution in the mechanical property maps relative to the MRI images. The presented work uses an alternative approach for the processing of mechanical shear wave images. This approach has the potential to assess the geometry and distribution of tissue inclusions with small dimensions on the order of the inherent MRI resolution. A new biomarker, which we name 1-Norm, is calculated from the frequency components after Fourier analysis of identified shear wave fronts [1]. The presence of inclusions involves wave scattering that implicate higher frequency components on the delineated shear wave fronts and thus increases the 1-Norm. This work presents applications of the new processing approach to inhomogeneous computational and 3D printed phantoms as well as various ex vivo tissue types. One of the observations is that the 1-Norm values increase with the presence of pathological changes in a mouse model of Alzheimer’s Disease. We believe that the 1-Norm can serve as a diagnostic marker for diseases that change the degree of mechanical inhomogeneity in biological tissues. Reference: [1] Palnitkar H, Reiter RO, Majumdar S, Lewis P, Hammersley M, Shah RN, Royston TJ, Klatt D. An investigation into the relationship between inhomogeneity and wave shapes in phantoms and ex vivo skeletal muscle using Magnetic Resonance Elastography and Finite Element Analysis. Journal of the Mechanical Behavior of Biomedical Materials 2019; 98 (October): 108-120.

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Chicago, IL, July 25-29. 2021

Title: Interpretation of Intragranular Strain Fields in High-Energy Synchrotron X-Ray Experiments via Finite Element Simulations and Analysis of Incompatible Deformation

Author(s): *Diwakar Naragani, *University of Dayton Research Institute*; Paul Shade, *Air Force Research Laboratory*; Armand Beaudoin, *Cornell University*; Mark Obstalecki, *Air Force Research Laboratory*; William Musinski, *Air Force Research Laboratory*; Darren Pagan, *Cornell University*; Joel Bernier, *Lawrence Livermore National Laboratory*; Donald Boyce, *Cornell University*;

A finite element framework is developed to resolve the intragranular fields of incompatible deformation generated intrinsically in response to applied deformation, through linear elasticity complemented by the theory of continuous distribution of dislocations and experimental grain-scale observations. Discrete grain-averaged lattice strains, characterized along with grain orientations via X-ray diffraction microscopy, enable high fidelity continuous solutions anchored to measured response while satisfying boundary conditions, equilibrium and compatibility through a finite element model. A continuous distribution of strain fields in a nickel-based superalloy, evaluated periodically during R = 0 cyclic loading, exposes the fundamental heterogeneity in polycrystalline response which creates localization of high stress gradients and potential sites of failure. Incompatibility correction is shown to be an increasingly effective measure in representing the accumulation of plasticity with loading particularly at twin and high angle grain boundaries. Furthermore, incompatible deformation is shown, through both specific examples and statistically, to be predominantly preserved upon elastic recovery improving our understanding of the history dependence of residual stresses. Locations of change in incompatibility, upon unloading, are analyzed to reveal the positive correlation between residual stress and incompatible deformation. The saturation of material response or shakedown in response to cyclic loading is also captured after a few cycles. The scalability and compatibility of the framework with experiments at multiple length scales and opportunities therein are briefly discussed.

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Title: Bayesian Optimization of Spatial Phase Modulation for Programmable Localization in Plasmonic Metasurface

Author(s): *Doksoo Lee, *Northwestern University*; Shizhou Jiang, *Northwestern University*; Oluwaseyi Balogun, *Northwestern University*; Wei Chen, *Northwestern University*;

Electromagnetic metasurfaces (EMMs) are artificially engineered ultrathin structures that are capable of manipulating optical properties of light propagation with subwavelength building blocks. In pursuit of shaping electromagnetic responses at will, EMM design leverages rich design freedom that resides in geometry, material constituents, and incident conditions, often followed by aperiodic bottom-up synthesis of the building blocks. While there is a plethora of existing works that investigate the behavior of EMM on geometric variation under periodic boundary conditions, design optimization on aperiodic incident conditions has rarely been reported to the best knowledge of the authors. Spatial phase modulation is such an example in that it relies on spatially aperiodic phase lags of incident wave to tailor energy localization in a geometrically periodic EMM. Tailoring localization patterns that are essential for advanced photonics applications can be achieved by formulating and solving an inverse problem on spatial phase modulation. A few existing works on this topic area address the inverse design on phase modulation [1] but largely resort to physics- or intuition-based trial-and-error, leaving room for improvements in terms of spatial selectivity and diversity of localization patterns. In this study, Bayesian optimization (BO) based inverse design on spatial phase modulation is proposed to achieve dynamic on-demand localization on a stationary plasmonic metasurface. Derivative-free search using BO enables the identification of global optima over a highly nonlinear design space, which saves the calls to the electromagnetic solver significantly compared to the exhaustive approaches. To reduce the high dimensionality of both design input (phase distribution) and performance output (electric field), the spatial harmonic phase representation and a localization metric are proposed, respectively. A response matrix comprising the localization metrics is scored and treated as an objective function of BO for achieving various target patterns. As a proof-of-concept, multiple high-contrast patterns over a static metasurface are set as the design objective. The optimization results show that diverse high-contrast responses can be dynamically controlled at will on the plasmonic metasurface using the proposed BO approach. This study shows that BO could expedite inverse design on incident conditions to realize system-level target responses at will. [1] T. S. Kao, E. T. F. Rogers, J. Y. Ou, and N. I. Zheludev, "'Digitally' addressable focusing of light into a subwavelength hot spot," Nano Lett., vol. 12, no. 6, pp. 2728–2731, 2012.

16th U.S. National Congress on Computational Mechanics
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Title: A Quadrilateral Mesh Generation Technique with Application to Shallow Water Modeling

Author(s): *Dominik Mattioli, *The University of Iowa*; Ethan Kubatko, *The Ohio State University*; Dylan Wood, *University of Notre Dame*;

Quadrilateral elements/cells are extensively used in finite element and finite volume methods for both solid and fluid mechanics applications. In some applications, it has been found that quadrilaterals offer advantages over triangles in terms of computational efficiency, accuracy, and robustness. Specifically, in coastal ocean/shallow water modeling contexts, it has been shown that quadrilateral elements yield higher computational efficiency in terms of computational cost required to achieve a given error level compared to triangular elements (Wirasaet et al., 2010). Further, quadrilateral elements do not suffer from spurious numerical solution modes exhibited by triangular cells in finite volume formulations (Androsov et al., 2019). However, use of quadrilateral elements tends to reduce the average element quality of the mesh in comparison to fully triangular meshes, diminishing the advantages offered by the element type. This issue can become pronounced for domains with complex boundary geometry, where triangular elements would be more efficacious than quadrilaterals. In coastal ocean/shallow water computational applications, there is a continued need for mesh generation techniques that produce high quality meshes and robust numerical solutions with minimal user input. Our previous work on an automatic mesh generator of high quality triangular meshes for shallow water domains (Conroy et al., 2012) has been continued to include a relatively simple post-processing approach to create quadrilateral elements from the original triangular elements. We present the new technique and discuss how we leverage the advantages of both quadrilateral and triangular elements while maintaining the sizing and high quality of the original triangular mesh. Results demonstrate the effectiveness of the approach for several shallow water domains by comparing numeric results obtained for an original triangular mesh, a corresponding quadrilateral mesh, and a mixed-element mesh.

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Title: Image Segmentation for FIB-SEM Serial Sectioning of a Si/C–Graphite Composite Anode Microstructure Based on Preprocessing and Global Thresholding

Author(s): *Dongjae Kim, *Seoul National University*; Jaewook Nam, *Seoul National University*;

The choice of materials that constitute electrodes and the way they are interconnected, i.e., the microstructure, influences the performance of lithium-ion batteries. For batteries with high energy and power densities, the microstructure of the electrodes must be controlled during their manufacturing process. Moreover, understanding the microstructure helps in designing a high-performance, yet low-cost battery. In this study, we propose a systematic algorithm workflow for the images of the microstructure of anodes obtained from a focused ion beam scanning electron microscope (FIB-SEM). Here, we discuss the typical issues that arise in the raw FIB-SEM images and the corresponding preprocessing methods that resolve them. Next, we propose a Fourier transform-based filter that effectively reduces curtain artifacts. Also, we propose a simple, yet an effective, global-thresholding method to identify active materials and pores in the microstructure. Finally, we reconstruct the three-dimensional structures by concatenating the segmented images. The whole algorithm workflow used in this study is not fully automated and requires user interactions such as choosing the values of parameters and removing shine-through artifacts manually. However, it should be emphasized that the proposed global-thresholding method is deterministic and stable, which results in high segmentation performance for all sectioning images.

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Title: Reliability-Based Shape Design Optimization under Dependent Random Variables by a Generalized Polynomial Chaos Expansion

Author(s): *Dongjin Lee, *The University of Iowa*; Sharif Rahman, *The University of Iowa*;

A new computational method was developed for reliability-based design optimization (RBDO) of complex mechanical systems in the presence of input random variables with arbitrary, dependent probability distributions. The method involves (1) a generalized polynomial chaos expansion (GPCE), introduced by the authors [1], for component or system reliability analysis subject to dependent input random variables; (2) a new blended method exploiting GPCE for reliability analysis and score functions for design sensitivity analysis; and (3) a standard optimization algorithm, establishing a multi-point, single-step design process. When coupled with score functions, the GPCE method yields analytical formulae for calculating the failure probability and its design sensitivities simultaneously. Through collaboration with the multi-point, single-step framework, the proposed method allows one to solve industrial-scale RBDO problems. Numerical results from a mathematical problem affirm that the new method developed is theoretically convergent and provides computationally efficient design solutions. Finally, the shape design of a 14-dimensional turbine blade root was successfully conducted, demonstrating the ability of the proposed method to address practical RBDO problems. Reference: [1] Lee D, Rahman S (2020) Practical Uncertainty Quantification Analysis Involving Statistically Dependent Random Variables. Applied Mathematical Modelling 84:324–356.

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Title: An Interface-Enriched Generalized Finite Element Formulation for Locking-Free Coupling of Non-Conforming Discretizations and Contact

Author(s): *Dongyu Liu, *Delft University of Technology*; Sanne J. van den Boom, *Delft University of Technology*; Alejandro M. Aragón, *Delft University of Technology*; Angelo Simone, *Delft University of Technology / University of Padova*;

In this presentation we propose an enriched finite element formulation that addresses the computational modeling of contact problems [1]. The displacement field is augmented by enriched terms that are associated with generalized degrees of freedom collocated along non-conforming interfaces or contact surfaces. We illustrate, by means of several numerical examples, the method's ability to ensure continuity of the displacement field in coupling problems and to accurately transfer tractions at contact interfaces, without the need for stabilization terms. In addition, we show that the formulation is stable with respect to the condition number of the stiffness matrix. References [1] Liu, D., van den Boom, S.J., Simone, A. and Aragón, A.M. An interface-enriched generalized finite element formulation for locking-free coupling of non-conforming discretizations and contact. Comput. Methods Appl. Mech. Engrg. (submitted, 2021).

16th U.S. National Congress on Computational Mechanics
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Title: A Sharp Interface Lagrangian-Eulerian Fluid-Structure Interaction Approach for Simulating the Migration and Trapping of Deformable Blood Clots

Author(s): *Ebrahim Kolahoduz, *University of North Carolina at Chapel Hill*; Kenneth Aycock, *US Food & Drug Administration*; Brent Craven, *US Food & Drug Administration*; Boyce Griffith, *University of North Carolina at Chapel Hill*;

Modeling the transport dynamics and fluid-structure interaction (FSI) of flexible blood clots in the venous vasculature is critical to predicting the performance of embolic protection devices like inferior vena cava (IVC) blood clot filters. IVC filters are metallic medical devices that are implanted in the IVC, a large vein in the abdomen through which blood returns to the heart from the lower extremities, to capture clots before they can migrate to the lungs and cause a potentially fatal pulmonary embolism. In this work, we are developing an FSI framework to simulate the migration and trapping of blood clots in the IVC, which is especially challenging due to the relatively large size of the clots that affects the local fluid dynamics, the large deformations that are generated, and the occurrence of contact between the clots, the vein wall, and the implanted device. We use a sharp interface immersed Lagrangian-Eulerian (ILE) method that combines a partitioned approach to FSI with an immersed coupling strategy. Like other partitioned formulations, the ILE approach uses distinct momentum equations for the fluid and solid regions. Unlike body-fitted arbitrary Lagrangian-Eulerian methods, our approach uses a non-conforming discretization of the dynamic fluid-structure interface that is “immersed” in the surrounding fluid and does not require any grid regeneration or mesh morphing to treat large structural deformations. Blood is modeled as a Newtonian fluid and the blood clot is modeled with a non-linear finite element model and hyperelastic material behavior. Fluid-structure interaction is mediated by a coupling approach that uses the immersed interface method that accounts for both dynamic and kinematic coupling conditions between the fluid and structure. A penalty approach is used to relax the kinematic constraint. Specifically, the penalty formulation uses two representations of the fluid-structure interface, including a thin surface mesh and a bulk volumetric mesh, that are connected by forces that impose kinematic and dynamic interface conditions. The dynamics of the volumetric mesh are driven by the accurate exterior fluid traction obtained from the sharp interface approach. Simulation of clot transport and IVC filter trapping are presented. Verification and validation of the simulations is underway and will be performed by comparing with in vitro experimental measurements.

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Title: Viscoplastic Material with Shear Bands Effect

Author(s): *Eligiusz Postek, *Institute of Fundamental Technological Research Polish Academy of Sciences*; Zdzis?aw Nowak, *Institute of Fundamental Technological Research Polish Academy of Sciences*; Ryszard P?cherski, *Institute of Fundamental Technological Research Polish Academy of Sciences*;

The paper‘s subject is the formulation accounting for shear bands in fine-grained metals [1] in terms of peridynamics. The formulation stands for an extension of the viscoplasticity model [2]. Several experimental investigations prove that plastic deformation's main mechanism is developing shear bands in prevailing cases. An influence of the rapid shear banding generation on the cumulated plastic strain field is investigated. The model is valid for finite strains. The primary interest is focused on impact analysis. The numerical models of Taylor bar are shown. A complex structure, such as copper open-cell foam, was presented in [3]. The numerical examples given in [3] are enriched with the newly developed formulation. References 1) Nowak Z, Perzyna P, P?cherski RB (2007) Description of viscoplastic flow accounting for shear banding. Arch Metall Mater 52(2):217-222 2) Foster JT, Silling SA, Chen WW (2010) Viscoplasticity using peridynamics. Int J Numer Meth Eng 81(1):1242-1258 3) Postek E, P?cherski RB, Nowak Z (2019) Peridynamic simulation of crushing process in copper open-cell foam. Arch Metall Mater 64(4):1603-1610

16th U.S. National Congress on Computational Mechanics
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Title: A Graph Theoretic Approach to Reduced Order Models in Coronary Blood Flow

Author(s): *Elizabeth Livingston, *University of Michigan*; Alberto Figueroa, *University of Michigan*; Krishna Garikipati, *University of Michigan*;

Coronary artery disease is characterized by a narrowing or stenosis in the coronary arteries. Fractional flow reserve (FFR) is the pressure gradient across a stenosis and is measured by clinicians by a catherization procedure that is technically difficult and invasive. Developing computational methods to estimate the FFR could avoid risks associated with these procedures. High-fidelity (3D) models are computationally expensive and impractical for real-time diagnosis. Low fidelity models based on 1D nonlinear theory are computationally inexpensive[1] but cannot fully characterize the complexities of the flow across a stenosis. In this project, we aim to develop a reduced order model (ROM) of blood flow using a graph theoretic framework, capable of accurately describing the complexities of flow across a coronary stenosis in a computationally efficient manner. We mapped a large ensemble of 3D incompressible flow simulations to a graph and used nonlocal calculus on finite weighted graphs to derive corrections to a 1D nonlinear blood flow model. Each simulation may be defined by a low dimensional state vector of quantities of interest (QOI) such as geometric variables, inflow and outflow boundary conditions, etc., all of which were treated as input parameters. Other QOI include model outputs such as velocity and pressure profiles. Graph vertices are defined by the state vector and variations of the vector quantities define graph edges[2]. Nonlocal calculus on graphs was then used to define multiple differential operators to infer a ROM for velocity and pressure profiles via system inference techniques such as stepwise regression[3]. In this work, we utilized graph theoretic approaches to blood flow modeling using simplified geometries and explored the effect of varying degrees of stenosis on blood flow in a single idealized coronary artery. High (3D) and low (1D) fidelity models were run for each geometry resulting in a graph that was constructed for each ensemble of simulations and correction terms for the 1D model were estimated. The suitability of selected differential operators to infer the ROM will be presented and discussed. 1) N. Xiao, J. Alastruey, and C. A. Figueroa, Int. J. Numer. Meth. Biomed. Engng., (2013). 2) R. Banerjee, K. Sagiyama, G.H. Teichert, K. Garikipati, Comput. Methods Appl. Mech. Engrg., 351 (July 2019), pp. 501-530. 3) G. Gilboa and S. Osher, Multiscale Model. Simul., 7.3 (2008) pp. 1005-1028.

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Title: Estimation of Regional Structure-Function Relationship in the Infarcted Left Ventricle

Author(s): *Emilio Mendiola, *Texas A&M University*; Hamed Babaei, *Texas A&M University*; Samer Merchant, *The University of Utah*; Qian Xiang, *Texas Heart Institute*; Edward Hsu, *University of Utah*; Peter Vanderslice, *Texas Heart Institute*; Reza Avazmohammadi, *Texas A&M University*;

Myocardial infarction (MI) results in cardiac myocyte death and the formation of a fibrotic scar in the left ventricular free wall (LVFW). In the days and weeks that follow an acute MI, LVFW remodeling takes place consists of several alterations in the structure and properties of cellular and extracellular components with a heterogeneous pattern across the LVFW. The normal function of a heart is strongly influenced by the passive and active biomechanical behavior of the LVFW, and progressive myocardial structural remodeling can have a detrimental effect on both diastolic and systolic functions of the LV leading to heart failure. Despite significant advances in understating LVFW remodeling in the setting of MI [1-3], the relationship between LVFW regional mechanics, heterogenous remodeling in the LVFW architecture, and organ-level LV function remains understudied. We hypothesize that the image-based cardiac modeling can effectively address this gap and bridge between fiber-level regional LVFW remodeling and organ-level cardiac function. We have developed high-fidelity finite-element (FE) heart models of MI using extensive longitudinal datasets from MI rat hearts representing the heart remodeling from one-week to four-week MI. We have developed a pipeline that integrates a meshed geometry from a high-resolution image of the rat heart, detailed imaging data on the fiber structure of the same heart, and semi-automated identification of infarct zone using late gadolinium enhancement done prior to terminal measurements and magnetic-resonance imaging. Our pipeline accounts for image-based characterizations of the heterogenous remodeling of the architecture in the LVFW and allows us to study the effect of this remodeling on the organ-level function as MI proceeds from early-stage scarring to late-stage remodeling. We use our model to understand the effect of timewise alterations in LVFW architecture on the regional and organ-level function in the LV. Remodeling of fiber architecture in LVFW during healing is expected to serve as a key mechanism in producing a heterogenous contractile behavior in the LVFW. The detailed description of regional remodeling patterns can replace the traditional measures of LV anatomy and function that often lead to gross and limited information on cardiac performance. Ultimately, the development and implementation of our model in patient-specific organ-level simulations will allow the investigation of individualized prognosis and interventions for MI. References [1] Holmes, JW et al, Annu Rev Biomed, 7:223-53, 2007. [2] Fomovsky, GM et al, Am J Physiol Heart Ci 298:221-8, 2010. [3] Sirry, MS et al, J Mech Beh Biomed Mat, 63:252-64, 2016.

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Title: Tricuspid Valve Parameterization, Geometric Modeling, and Isogeometric Analysis

Author(s): *Emily Johnson, *Iowa State University*; Devin Laurence, *University of Oklahoma*; Fei Xu, *Ansys, Inc.*; Caroline Crisp, *Iowa State University*; Chung-Hao Lee, *University of Oklahoma*; Ming-Chen Hsu, *Iowa State University*;

Approximately 1.6 million patients in the US are affected by tricuspid valve regurgitation, which occurs when the tricuspid valve does not close properly to prevent backward blood flow into the right atrium. Despite its critical role in proper cardiac function, the tricuspid valve has received limited research attention compared to the mitral and aortic heart valves on the left side of the heart. As a result, proper valvular function and the pathologies that may cause dysfunction remain poorly understood. To promote further study of the tricuspid valve behavior and its biomechanical response, this work establishes a parameter-based approach that provides a template for tricuspid valve modeling and simulation. The developed tricuspid valve parameterization includes a comprehensive description of the leaflet surface and the complex chordae tendineae. The proposed simulation framework provides a practical procedure for modeling generalized tricuspid valves and offers a robust, flexible method to analyze the performance and effectiveness of various valve configurations using isogeometric analysis. The proposed parametric valve model and simulation methods are applied to optimize the design of tricuspid valve prosthetics with less intricate structures and equivalent or better performance compared to native tricuspid valves.

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Title: Towards Application Driven Computational Models of Human Induced Pluripotent Stem Cell-Derived Cardiomyocytes

Author(s): *Emma Lejeune, *Boston University*; Bill Zhao, *Boston University*;

A better fundamental understanding of human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs) has the potential to advance both drug discovery and cardiac repair. Automated quantitative analysis of beating hiPSC-CMs is an important and fast developing component of the hiPSC-CM research pipeline. Here we introduce ``Sarc-Graph,'' a computational framework to segment, track, and analyze sarcomeres in hiPSC-CMs with fluorescently tagged striations. Our framework includes functions to segment z-discs and sarcomeres, track z-discs and sarcomeres in beating cells, and perform automated spatiotemporal analysis and data visualization. In addition to reporting good performance for sarcomere segmentation and tracking with no manual parameter tuning and a short runtime, we introduce two novel analysis approaches. First, we construct spatial graphs where z-discs correspond to nodes and sarcomeres correspond to edges. Second, we treat tracked and segmented components as fiducial markers and use them to compute the approximate deformation gradient of the entire tracked population. This represents a new quantitative descriptor of hiPSC-CM function. Then, we conclude with an outlook on how we plan to transition this work towards predictive modeling. For more information, please see: https://arxiv.org/abs/2102.02412

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Simulating the Emergent Dynamics of Hydrodynamically-Coupled Active Particles

Author(s): *Enkeleida Lushi, *New Jersey Institute of Technology*;

The field of Active and Living Matter has seen a plethora of studies on the collective dynamics of "dry" active particles. However many micro-scale units such studies model, eg. bacteria microalgae and colloids, exist and move in fluid. As such, hydrodynamic interactions with other units affect their dynamics near boundaries and collective organization. I will describe new advances made in the coupling the dynamics of the fluid to that of the self-propelling or driven particles in it, and show how the emergent behavior is affected. I will illustrate the method by showing examples of individual and collective dynamics of bacteria and spinning colloids.

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Title: Refinement of Polygonal Grids Using Convolutional Neural Networks with Applications to Polygonal Discontinous Galerkin and Virtual Element Methods

Author(s): *Enrico Manuzzi, *Politecnico di Milano*; Paola Francesca Antonietti, *Politecnico di Milano*;

We propose new strategies to handle polygonal grids refinement based on Convolutional Neural Networks (CNNs). We show that CNNs can be successfully employed to identify correctly the "shape" of a polygonal element so as to design suitable refinement criteria to be possibly empoyed within adaptive refinement strategies. We propose two refinement strategies that exploit the use of CNNs to classify elements' shape, at a low computational cost. We test the proposed idea considering two families of finite element methods that support arbitrarily shaped polygonal elements, namely polygonal discontinuous Galerkin methods and Virtual Element methods. We demonstrate that the proposed algorithms can greatly improve the performance of the discretization schemes both in terms of accuracy and quality of the underlying grids. Moreover, since the training phase is performed off line and is problem independent the overall computational costs are kept low.

16th U.S. National Congress on Computational Mechanics
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Title: A Coupled Peridynamic and Finite Element Approach in ANSYS Framework for Fatigue Life Prediction Based on the Kinetic Theory of Fracture

Author(s): Yanan Zhang, *University of Arizona / Central South University, China*; *Erdogan Madenci, *University of Arizona*;

Fatigue is one of the primary reasons for engineering structures to fail. Prediction of fatigue life and crack propagation path still poses challenges due to the complex nature of cracking and loading cycles. Many fatigue life prediction criteria provide acceptable options; however, they rely on empirical parameters. These criteria along with simulation tools are valuable for predicting fatigue life and crack propagation in order to minimize time to collect experimental data and cost. The finite element method (FEM) and its modified versions in conjunction with a fatigue life prediction criterion provide the framework for the existing simulation tools. However, the FEM faces challenges because of its fundamental assumptions arising from the classical continuum mechanics in the presence of cracks. The peridynamic (PD) theory removes these challenges, and it is suitable for simulating the process of crack initiation, propagation, bifurcation, and coalescence without special procedures. The PD equilibrium equations do not involve partial derivatives of the displacement field and can be solved by employing simple integration techniques. This study introduces a new coupled PD and FE approach in ANSYS framework for simulating the process of failure under cyclic loading based on the kinetic theory of fracture (KTF). The PD governing equations are constructed by using MATRIX27 element in the ANSYS framework and solved by employing an implicit method. The PD interactions are considered in the region of potential failure sites; otherwise, traditional finite elements are employed in the discretization of the domain. The coupling between the MATRIX27 elements and traditional finite elements are achieved through the coupled degrees of freedom (DOF) command available in the ANSYS framework. The verification of the coupled PD-FE approach is demonstrated by comparison against the FE prediction of displacement fields in a plate with and without a hole under tension. Its validity for predicting crack growth is established by simulating compact tension experiments under cyclic loading. The breakage of the PD element depends on the evolution of damage state variable in KTF and the visibility criteria. This coupled approach successfully simulates the Mode-I and mixed-mode fatigue failure under cyclic loading for crack initiation, propagation path and final fatigue life based on the S-N and Mode I fracture data. The predictions capture experimental measurements for self-similar and non-self-similar crack propagation paths as well as the number of cycles to failure.

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Title: Phase-Field Modeling of Deformation Twinning in Polycrystalline Solids

Author(s): *Eric Ocegueda, *California Institute of Technology*; Kaushik Bhattacharya, *California Institute of Technology*;

Mechanical twinning is a form of permanent deformation that occurs in various crystalline solids, especially in low symmetry crystals, such as hexagonal close-packed (HCP) metals. The presence and formation of twins have been shown to have drastic effects on the strength and ductility of materials. With recent increased interest in using HCP metals, such as magnesium, in structural, automotive, and armor applications due to their high strength to weight ratio, there is a need for comprehensive modeling of deformation twinning to understand the material's response to various loading conditions. Past studies on mechanical twinning have taken either a microscopic or macroscopic approach to the phenomenon. Microscopic approaches have utilized density functional theory or molecular dynamic simulations to explore the underlying physics in twins at the sub-grain scale; while macroscopic approaches have used crystal plasticity to model twins as a "pseudo-slip", ignoring length scale effects, to obtain bulk responses. However, twins form collectively across multiple grains with complex local morphology propagating into bulk behavior. These mesoscale aspects have been less studied and so is the focus of the current work. We propose a mesoscale model where twinning is treated using a phase-field approach and dislocation slip is considered using crystal plasticity. Lattice reorientation, length-scale effects, interactions between dislocations and twin boundaries, as well as twin and slip interactions with grain boundaries are all carefully accounted for within the model. We present the model, the implementation using a novel approach of accelerated computational micromechanics, and demonstrate it using simulations on polycrystalline materials. We summarize the insights gained from these studies and the implications on the macroscale behavior of HCP materials.

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Title: A Probabilistic Model-Free Data-Driven Solver Scheme

Author(s): *Erik Prume, *RWTH Aachen University*; Robert Eggersmann, *RWTH Aachen University*; Stefanie Reese, *RWTH Aachen University*; Michael Ortiz, *California Institute of Technology*;

The data-driven solution of mechanical boundary value problems with uncertainties in material data as proposed in [1] is further extended in order to infer additional information from stochastic systems. These uncertainties can stem from measurement issues, but also from intrinsic randomness of material properties on lower scales influencing the macroscopic material state. In particular, the latter issue may result in data sets with non-standard noise distributions. For such cases, approaches with particular models for the probability distribution describing the noise are prone to fail and are thus avoided in this approach. Together with the absence of a material model itself the goal is to infer the probability distribution of a quantity of interest in a material model-free manner. Central concepts to be defined are the definition of a likelihood measure for the mechanical system and a carefully chosen quenching schedule. The numerical scheme to tackle this cost-intensive computation will be discussed. Furthermore, numerical examples will be presented to provide further insights into the method and related questions. [1] Kirchdoerfer, Trenton, and Michael Ortiz. "Data driven computing with noisy material data sets." Computer Methods in Applied Mechanics and Engineering 326 (2017): 622-641.

16th U.S. National Congress on Computational Mechanics
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Title: The Mechanical Loading of the Human Uterus and Cervix in Pregnancy Based on Ultrasound-Derived Finite Element Models

Author(s): *Erin Louwagie, *Columbia University*; Joy Vink, *Columbia University Irving Medical Center*; Helen Feltovich, *Intermountain Health*; Kristin Myers, *Columbia University*;

In 2019, 1 in 10 babies born in the United States were born prematurely, with preterm birth (PTB) being defined as birth before 37 weeks gestation. Infants born preterm are at an increased risk of numerous short- and long-term health complications. However, there is currently no accurate method of predicting PTB nor an impactful strategy to prevent it. A significant barrier to improving PTB prediction and prevention is a lack of knowledge on the normal function of the human uterus and cervix throughout gestation, making it difficult to determine a patient's risk for PTB. To study the mechanics of the gravid environment on the population level and their effects on PTB rates, a patient-specific framework for capturing maternal anatomy that is easily implementable into current clinical workflows are necessary. Therefore, we propose using patient-specific parametric computational models from 2D ultrasound to investigate how maternal anatomy affects uterine and cervical loading throughout gestation. Trained sonographers took ultrasound images of healthy pregnant patients at four gestational ages (8-14, 14-16, 22-24, 32-34 weeks). We built parametric solid models of the uterus and cervix using an automated design-table driven framework. A simplified model of the pregnant anatomy was created for finite element analysis (FEA) by separating the cervix from the uterus and adding a fetal membrane and supporting abdomen. The models were discretized into finite elements and prepared for computational analysis by adding tissue material properties derived from literature and inverse FEA, assigning physiologically relevant boundary conditions and contact between parts, and applying a gestationally determined intrauterine pressure to the fetal membrane. We investigate how patterns of stress and stretch in the uterus and cervix evolve with increasing gestational age, identify maximum stretch and stress locations, and draw comparisons between maternal geometry and their associated FEA results. This research marks a significant advancement in the fields of women's healthcare and computational biomechanics. The results of this study will aid in establishing an understanding of normal mechanical loading of the uterus and cervix during pregnancies that do not result in preterm birth. Furthermore, it introduces a clinically implementable framework for other researchers to build and analyze patient-specific pregnant geometry using widespread commercial and open-source software, enabling further computational work in pregnancy biomechanics.

16th U.S. National Congress on Computational Mechanics
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Title: Development, Calibration, and Treatment Optimization of a Breast Cancer Model

Author(s): *Ernesto A. B. F. Lima, *The University of Texas at Austin*; Reid Wyde, *The University of Texas at Austin*; Anna G. Sorace, *The University of Alabama at Birmingham*; Thomas E. Yankeelov, *The University of Texas at Austin*;

In the United States, breast cancer is the second most common type of cancer in women. If breast cancer cells overexpress the human epidermal growth factor receptor 2 (HER2) protein, the tumor is identified as HER2+. This type of cancer can be treated with drugs that target the HER2 receptor, such as trastuzumab, in combination with chemotherapy. Trastuzumab binds with the HER2 receptor, downregulating the HER2 protein and reduces cell proliferation. Doxorubicin is a commonly used chemotherapy treatment that is given in combination with other drugs for the treatment of breast cancer. In [1], the authors quantified the output of different treatment protocols of trastuzumab and doxorubicin in a murine model of human HER2+ breast cancer. The authors confirmed that administering trastuzumab prior to doxorubicin improved the treatment outcome. In this work, we aim to find the optimal treatment protocol for HER2+ breast cancer using trastuzumab-doxorubicin combination therapy. Using different assumptions for the drug-tumor interactions, we hypothesize ten different models to characterize the system dynamics, including the relationship between tumor volume and drug bioavailability and drug-drug interaction. Using the Occam Plausibility Algorithm [2], each of these models are calibrated to the dataset available in [1]. The most plausible model is selected to represent the system. We apply optimal control theory (OCT) to the selected model to derive the optimal treatment protocol. We consider uncertainty in the biological system model parameters when applying OCT. Values of the parameters are sampled from the posterior obtained during the model calibration, and OCT is applied to each set of parameters. We set the maximum dosage for doxorubicin and trastuzumab in the optimal treatment protocol to the maximum dose delivered experimentally in [1]. Our results indicate that the optimal combination of these two drugs would be to deliver the maximum trastuzumab dose during the first 48 hours, followed by the maximum doxorubicin dose during the following 48 hours. Compared to the experimental tumor volume at day 68, our model indicates a tumor volume reduction of 98.92% under this treatment protocol. [1] Sorace, Anna G., et al. Trastuzumab improves tumor perfusion and vascular delivery of cytotoxic therapy in a murine model of HER2+ breast cancer: preliminary results. Breast cancer research and treatment 155.2 (2016): 273-284. [2] Farrell, Kathryn, J. Tinsley Oden, and Danial Faghihi. A Bayesian framework for adaptive selection, calibration, and validation of coarse-grained models of atomistic systems. Journal of Computational Physics 295 (2015): 189-208.

16th U.S. National Congress on Computational Mechanics
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Title: The Effects of CYGNSS-Enhanced Parametric Wind Fields on Storm Surge Modeling

Author(s): *Ethan Kubatko, *The Ohio State University*; Younghun Kang, *The Ohio State University*; Mohammad Al-Khaldi, *University Corporation for Atmospheric Research*; Joel Johnson, *The Ohio State University*;

A key factor in obtaining accurate simulations of hurricane storm surge from hydrodynamic models is the input of accurate meteorological (wind and pressure) fields. While meteorological fields could be obtained from large-scale atmospheric models, most operational storm surge models, such as the ADCIRC (ADvanced CIRCulation) finite element model, generally make use of relatively simple parametric storm models that generate wind (and pressure) fields based on only a small number of key storm parameters (e.g., storm track, maximum winds, and radius of maximum winds). Obviously, the success of this approach requires accurate retrieval of the parameters from available storm data. A new NASA mission, the Cyclone Global Navigation Satellite System (CYGNSS), offers potential opportunities to improve the estimation of these key storm parameters, and thereby to improve storm surge calculations, through its ability to provide accurate measurements of ocean surface winds in and near the eye of the storm throughout the lifecycle of tropical cyclones. To assess this potential benefit, in this study, we examine the effects of CYGNSS-based parametric wind fields on ADCIRC storm surge calculations through validation studies of a select set of storms from recent hurricane seasons. We provide a brief overview of the retrieval algorithms used to obtain the storm parameters from CYGNSS data and present results obtained using the CYGNSS-based winds compared to storm surge results using other wind field sources. Model results are validated against observations obtained from several agencies, including the National Oceanic and Atmospheric Administration (NOAA) and the Federal Emergency Management Agency (FEMA).

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Title: LVIRA+, an Extension of the Least Squares Volume-of-Fluid Interface Reconstruction Algorithm for Domains with Three and More Materials

Author(s): *Eugene Kikinzon, *Los Alamos National Laboratory*; Portage Team, *Los Alamos National Laboratory*;

We present LVIRA+, a method to reconstruct interfaces between materials inside multi-material cells based on their volume fractions, which improves accuracy over previous methods on domains with three and more materials. The standard LVIRA [1] is often used to perform interface reconstruction on two-material domains, where it's second-order accurate while requiring the same material data as Youngs'/Volume-Of-Fluid methods. This is achieved by solving an optimization problem to determine the orientation of the material interface instead of simply using the gradient of material's volumetric distribution. However, when employed in the context of the nested dissections algorithm for cells with three and more materials, it can demonstrate the results that are no better than those of the Youngs' method. Moreover, the reduced accuracy can be observed even in two-material cells when some of their neighbors contain non-cell materials. LVIRA+ is an extension of the original algorithm which is designed to address those issues and improve accuracy on domains with many materials. It employs a modified objective function designed to be used with material order permutations. When used in the nested dissections algorithm for cells with three and more materials, it is material order independent and generally provides better accuracy than the standard algorithm. Other modifications to the objective function reduce or eliminate reconstruction errors due to the presence of non-cell materials in its stencil. This is achieved through weighting the error contributions from the neighboring cells and employing material order permutations in conjunction with grouping of cell and non-cell materials in the cell's stencil. As the result, even when geometries of material interfaces violate the assumptions that are fundamental to the LVIRA and therefore cannot be recovered exactly, the presented algorithm still demonstrates a qualitative improvement in the reconstruction accuracy compared to the direct application of the original method. When interface reconstruction is performed for cells with only two materials in their LVIRA stencil, the new method falls back to the standard algorithm to optimize performance. LVIRA+ has been implemented and tested both in 2D and 3D on domains with three and more materials. We will demonstrate test results for three and four-material 2D domains that showcase the differences between the LVIRA and LVIRA+.
[1] Pilliod Jr, J.E. and Puckett, E.G., 2004. Second-order accurate volume-of-fluid algorithms for tracking material interfaces. Journal of Computational Physics, 199(2), pp.465-502.

16th U.S. National Congress on Computational Mechanics
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Title: Imposing Local Boundary Conditions for Peridynamics Equation of Motion in Arbitrary Domains by a Generalized Fictitious Nodes Method

Author(s): *Farzaneh Mousavi, *University of Nebrask-Lincoln*; Jiangming Zhao, *University of Nebrask-Lincoln*; Siavash Jafarzadeh, *University of Nebrask-Lincoln*; Florin Bobaru, *University of Nebrask-Lincoln*;

Peridynamics (PD) is a nonlocal reformulation of continuum mechanics which uses integrals instead of derivatives in its governing equations. This makes the PD models capable of capturing discontinuities such as cracks. Along with the many advantages that PD offers come a few challenges. Enforcing local boundary conditions in PD nonlocal setting is one of these challenges. The PD surface/skin effect is another issue produced by nonlocality where the material response differs in its outer layer due to lower stiffness at the surface. Different approaches have been proposed so far to reduce the surface effect and to approximate local boundary conditions in PD settings. One popular group of such approaches are the Fictitious nodes methods (FNM), where the body is extended by a layer of nodes with certain prescribed values to effectively enforce the desired local boundary conditions [1,2]. Surface effect can be addressed if free surfaces are viewed as a special natural BC (e.g. traction free in mechanics) and therefore can be addressed by FNM. However, FNMs are limited to simple geometries (straight edges without kinks, curves), and also produce large errors at the corners [1]. A generalized version of mirror-based FNM is introduced in [2] for diffusion problems and has been shown capable in handling complex geometries and works well at the corners or cracks surfaces. In this study, we extend this method to the PD equation of motion and provide the formulation for both Dirichlet and Neumann local boundary conditions. The method is general and independent of the material model. We verify the method with 2D examples for elastic and elasto-plastic deformations [3] by comparing the results against Abaqus finite element solutions. References: [1] Le, Q. V., & Bobaru, F. (2018). Surface corrections for peridynamic models in elasticity and fracture. Computational Mechanics, 61(4), 499-518. [2] Zhao, J., Jafarzadeh, S., Chen, Z., & Bobaru, F. (2020). An algorithm for imposing local boundary conditions in peridynamic models on arbitrary domains. engrXiv Preprints (https://doi.org/10.31224/osf.io/7z8qr) [3] Mousavi, F., Jafarzadeh, S., & Bobaru, F. (2020). An ordinary state-based peridynamic elastoplastic 2D model consistent with J2 plasticity. arXiv preprint arXiv:2010.08043.

16th U.S. National Congress on Computational Mechanics
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Title: On the Solution of Statistical Inverse Problems Using Machine Learning Methods Based on Artificial Neural Networks

Author(s): *Florent Pled, *Université Gustave Eiffel*; Christophe Desceliers, *Université Gustave Eiffel*;

This work adresses the solution of a statistical inverse problem in computational elastodynamics using machine learning based on artificial neural networks (ANNs). The stochastic computational model (SCM) corresponds to a simplified random elasto-acoustic multilayer model of a biological system that is representative of the axial transmission technique for the ultrasonic characterization of cortical bone properties from experimental velocity measurements. The three-layer biological system consists of a random heterogeneous damaged/weaken elastic solid layer (cortical bone layer) sandwiched between two deterministic homogeneous acoustic fluid layers (soft tissues and marrow bone layers) and excited by an acoustic line source [1]. Such SCM is parameterized by two geometrical parameters, corresponding to the thicknesses of the "healthy” and “damaged” elastic solid parts, a dispersion parameter controlling the level of statistical fluctuations of the random elasticity field, and a spatial correlation length characterizing the spatial correlation structure of the random elasticity field . An innovative ANN-based identification methodology has been recently proposed in [2] and applied to multiscale computational mechanics. In this work, the proposed methodology is extended to linear elastodynamics for the statistical inverse identification of the four aforementioned hyperparameters from fourteen quantities of interest of the SCM, corresponding to the scattered acoustic energy stored at fourteen receivers located in the soft tissues layer. It consists in (i) constructing of a synthetic database generated from the SCM and consisting of network input data (quantities of interest) and target data (hyperparameters), (ii) postprocessing this initial database by conditioning the network input data with respect to the network target data using kernel density estimation methods to improve the ANN performance, (iii) designing an efficient ANN trained using the processed database to identify the optimal hyperparameters corresponding to given expected quantities of interest, (iv) constructing a probabilistic model of the network input random vector to take into account the uncertainties on the input quantities of interest, and (v) designing another ANN trained using the initial and processed input data to identify the probabilistic model of the network input random vector from given observed quantities of interest. [1] C. Desceliers, C. Soize, S. Naili, G. Haiat. Probabilistic model of the human cortical bone with mechanical alterations in ultrasonic range. Mechanical Systems and Signal Processing, 32:170–177, 2012. [2] F. Pled, C. Desceliers, T. Zhang. A robust solution of a statistical inverse problem in multiscale computational mechanics using an artificial neural network. Computer Methods in Applied Mechanics and Engineering, 373:113540, 2021.

16th U.S. National Congress on Computational Mechanics
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Title: Analysis of Ocean-Atmosphere Coupling from the Point of View of Domain Decomposition Methods

Author(s): *Florian Lemarié, *Inria*;

In this talk, we address the ocean-atmosphere coupling problem from the point of view of domain decomposition methods. We show that present coupling methods used in realistic ocean-atmosphere coupled models can be written in the formalism of Schwarz iterative algorithms, and correspond to methods that are not pushed to convergence, which may lead to imperfect coupling. We discuss the objective of achieving a mathematically and physically consistent ocean-atmosphere coupling and we show that using improved coupling algorithms (like Schwarz methods) can impact the solution of a realistic climate model quite significantly (Marti et al., 2020). Finally, we conclude by summarizing some challenges in the numerical formulation of climate models (e.g. Lauritzen et al. 2021). References: Marti, O., Nguyen, S., Braconnot, P., Valcke, S., Lemarié, F., and Blayo, E.: A Schwarz iterative method to evaluate ocean- atmosphere coupling schemes. Implementation and diagnostics in IPSL-CM6-SW-VLR, Geosci. Model Dev., https://doi.org/10.5194/gmd-2020-307, 2020. Clément, S., Lemarié, F., and Blayo, E.: Discrete analysis of Schwarz waveform relaxation for a diffusion reaction problem with discontinuous coefficients, BIT Numerical Mathematics, under review, 2021 Lauritzen, P., Kevlahan, N., Donahue, A., Dubos, T., Eldred C., Gassmann, A., Harrop, B. Herrington, A., Jablonowski, C., Large, W., Larsson, V., Lemarié, F., Rasch, P., Shipway, B., Tailleux, R., Wan, H.: Reconciling and improving formulations for thermodynamics and conservation principles in Earth system models, J. Adv. Model. Earth Syst., in preparation, 2021

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Title: A Computational Model of Fiber Networks: From Blood Clots to Asthmatic Airways

Author(s): *Francesco Pancaldi, *University of California, Riverside*; Samuel Britton, *University of California, Riverside*; Mark Alber, *University of California, Riverside*; Qixuan Wang, *University of California, Riverside*; Mona Eskandari, *University of California, Riverside*;

Many biomaterials have one or more components consisting of a network of biopolymer fibers. These structures act as scaffolds for other components and are important mechanical components during dynamic changes due to external or environmental forces. Two examples of such biomaterials are blood clots and respiratory airways. Blood clots are composed of many constituents but one of the most important structural components is the fibrin network regulating the shape and elastic properties of the clot [1]. Analogously, respiratory airways have a layer of mixed fiber networks composed of both elastin and collagen, responsible for both structural and mechanical regulation [2]. Pathologies affecting blood clots and respiratory airways alter the composition of these structural networks, ultimately impeding their normal function. In order to better understand these structures and the impact of these abnormalities, we have developed a multi-scale computational model for fiber network mechanics to simulate these biomaterials [3]. Here we will present the development and fundamental aspects of the model initially formulated to study in-vitro and in-vivo blood clot fibrin networks, adapted to include contraction dynamics due to platelets and the forces exerted by their filopodia, and extended to represent the complex elastin and collagen networks in asthmatic airways. Our simulation results have hemodynamic and pulmonary clinical implications and can be applied to similar pathologies impacting the fiber network. References [1] Kim, Oleg V., Rustem I. Litvinov, Mark S. Alber, and John W. Weisel. "Quantitative structural mechanobiology of platelet-driven blood clot contraction." Nature communications 8, no. 1 (2017): 1-10. [2] Eskandari, Mona, Tara M. Nordgren, and Grace D. O’Connell. "Mechanics of pulmonary airways: linking structure to function through constitutive modeling, biochemistry, and histology." Acta biomaterialia 97 (2019): 513-523. [3] Britton, Samuel, Oleg Kim, Francesco Pancaldi, Zhiliang Xu, Rustem I. Litvinov, John W. Weisel, and Mark Alber. "Contribution of nascent cohesive fiber-fiber interactions to the non-linear elasticity of fibrin networks under tensile load." Acta biomaterialia 94 (2019): 514-523.

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Title: DG Discretizations of the INS Equations, Which Features Matter the most?

Author(s): Lorenzo Botti, *University of Bergamo*; *Francesco Carlo Massa, *University of Bergamo*;

Discontinuous Galerkin (DG) methods are widely employed in the CFD field because of their robustness in convection dominated flow regimes and their favourable dispersion and dissipation properties in undersolved turbulent flows computations. From the numerical viewpoint a) their construction is independent from the space dimension, b) they provide the ability to deal with arbitrarily shaped polytopic elements meshes, c) the order of approximation can be selected according to the expected or estimated regularity of the exact solution, d) upwinding can be introduced based on the Godunov flux approach. Recently, hybrid versions of DG methods, namely Hybridizable Discontinuous Galerkin (HDG) methods and Hybrid High-Oder (HHO) methods, have been gaining increased popularity in the CFD community. HHO and HDG methods are based on degrees of freedom that are broken polynomials on the mesh and on its skeleton. Since, by design, only skeletal DOFs are globally coupled, the leading block size of the global Jacobian matrix grows as the dimension of polynomial spaces in d?1 variables when considering a d-dimensional problem. Accordingly, with respect to DG methods, the global matrix is smaller and sparser when high-order polynomials are employed. Besides computational efficiency, HHO and HDG seek to enhance DG with: 1) local (element-by-element) conservation of physical quantities, 2) increased convergence rates thanks to higher-order stabilization terms penalizing face residuals, 3) increased robustness with respect to mesh distortion and mesh anisotropy. While these features have been demonstrated in the diffusion-dominated flow regime, extensions to the convection-dominated regime are still missing. We remark that, up to the authors' knowledge, there is no analogue to the Godunov approach in the context of hybridized formulations. In this work artificial-compressibility DG formulations [1], robust in the inviscid limit, will be compared with HDG and HHO featuring kinetic energy preservation [2] and pressure robustness [3] tackling challenging benchmark test cases. [1] F. Bassi, A. Crivellini, D.A. Di Pietro and S. Rebay (2006). An artificial compressibility flux for the discontinuous Galerkin solution of the incompressible Navier–Stokes equations, Journal of Computational Physics, 218:2, pp 794-815. [2] L. Botti and D. Di Pietro and J. Droniou (2019). A Hybrid High-Order method for the incompressible Navier--Stokes equations based on Temam's device. Journal of Computational Physics 376, pp 786-816. [3] S. Rhebergen and G. N. Wells (2018). A hybridizable discontinuous Galerkin method for the Navier–Stokes equations with pointwise divergence-free velocity field. Journal of Scientific Computing 76(3):1484-1501.

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Title: Numerical Homogenization and the Arlequin Method

Author(s): *Frederic Legoll, *Ecole des Ponts ParisTech / Inria*;

We numerically investigate, and improve upon a computational approach originally introduced by R. Cottereau in [Cottereau, IJNME 2013] which aims at evaluating the effective coefficient of a medium modelled by a highly oscillatory coefficient. This computational approach is based on a Arlequin type coupling. It combines the original fine-scale description of the medium (modelled by an oscillatory coefficient) with an effective description (modelled by a constant coefficient) and optimizes upon the coefficient of the effective medium to best fit the response of the actual heterogeneous medium using a purely homogeneous medium. The approach can thus be regarded as a way to extract the effective coefficient of a heterogeneous medium without using the standard ingredients of homogenization (computation on large RVEs, ...), and which can also be applied in the case of moderate scale separation. We present various improvements of the algorithms, in order to obtain a procedure as efficient as possible. Representative numerical results, both for deterministic and random heterogeneous models, demonstrate the added value of our approach in comparison to the original approach. Joint work with O. Gorynina and C. Le Bris (ENPC and Inria).

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Title: Multilevel Estimators for Measures of Robustness in Optimization Under Uncertainty

Author(s): *Friedrich Menhorn, *Technical University of Munich*; Gianluca Geraci, *Sandia National Laboratories*; Daniel T. Seidl, *Sandia National Laboratories*; Michael S. Eldred, *Sandia National Laboratories*; Hans-Joachim Bungartz, *Technical University of Munich*; Youssef M. Marzouk, *Massachusetts Institute of Technology*;

Optimization under uncertainty (OUU) deals with the solution of stochastic optimization problems. Here, we are interested in finding a robust and/or reliable optimal design for a stochastic objective restricted by stochastic constraints. The uncertainty in the problem is the result of uncertain conditions which can, e.g., stem from inaccurate measurements or inexact models. To be able to tackle such problems, measures of robustness and reliability are employed. Common examples are the expectation and the standard deviation of the underlying problem. A typical formulation consist in maximizing the expectation of a quantity of interest while minimizing its standard deviation. These measures can then be evaluated by using a sampling based approach, namely Monte Carlo (MC) methods. Hence, we have as an outer loop an optimization problem over a deterministic design space where we solve a stochastic problem at each optimization step to evaluate the measure of robustness. Since MC methods show slow convergence, multilevel Monte Carlo (MLMC) methods have gained popularity in recent years. Here, the main idea is to leverage a hierarchy of discretization levels by using an optimal allocation of samples over the levels. To find this optimal allocation, we solve an optimization problem with respect to a prescribed measure of robustness. For the expected value, this optimization problem can be solved analytically as done in [2]. In this work, we show that it is crucial to formulate a MLMC allocation problem by targeting the specific robustness measure used in the OUU formulation [3]. We present MLMC estimators for the standard deviation and also for the combination of mean and standard deviation. We show that these estimators show improved performance, within the OUU problem, with respect to the standard MLMC estimator targeting the mean. Furthermore, we show that we get similar performance to MC for lower computational cost. To solve the OUU problem, we also present the derivative-free stochastic optimization method SNOWPAC [1]. We showcase these results on a variety of benchmark problems. [1] Augustin, F. and Marzouk., Y.M. A trust-region method for derivative-free nonlinear constrained stochastic optimization. arXiv:1703.04156 (2017) [2] M.B. Giles, Multi-level Monte Carlo path simulation. Operations Research, 56(3):607-617 (2008) [3] Menhorn, F. , Eldred, M. S. , Geraci, F., King, R. N., Bungartz, H.-J. and Marzouk, Y. M. Higher moment multilevel estimators for optimization under uncertainty applied to wind plant design. AIAA 2020-1952 (2020) SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Accurate Artificial Boundary Conditions for the Semi-Discretized One-Dimensional Peridynamics

Author(s): *Gang Pang, *Beihang University*; Songsong Ji, *Peking University*; Jiwei Zhang, *Wuhan University*;

The peridynamic theory reformulates the equations of continuum mechanics in terms of integro■differential equations instead of partial differential equations. It is not trivial to directly apply naive approach in artificial boundary conditions for continua to peridynamics modeling, because it usually involves semi-discretization scheme. In this talk, we present a new way to construct accurate boundary conditions for semi-discretized peridynamics using kernel functions. Specially, the kernel functions that represent the Green functions with single source are combined to construct the accurate boundary conditions. The recursive relationships between the kernel functions are proposed, therefore the kernel functions can be computed through a differential and integral system with high precision. The numerical results demonstrate the efficiency of the boundary conditions. The proposed method can be applied to modeling of wave propagation for other nonlocal theories and high dimensional cases.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analysis of the Crack-Band Approach for Modelling Cracking in Concrete with Continuous Damage Models

Author(s): *Gelacio Juarez Luna, *Universidad Autónoma Metropolitana*; Gustavo Ayala Milián, *Universidad Nacional Autónoma de México*;

An analysis of the crack bandwidth approach to overcome the problem of mesh dependency for modelling cracking in concrete with continuous damage models is presented. The practical recommendations to estimate the crack bandwidth, h, given in the literature and in commercial software are described and evaluated (Bazant and Oh, 1983; ?ervenka, 1995; Rots et al., 1985; Rots 1988; ?ervenka et al. 1995). The problem of mesh dependency affects the sensitivity of the load-displacement results and the mesh objectivity in such a way that energy dissipation of the fracture process cannot be guaranteed. Two solutions suggested to overcome this deficiency are developed: i) modifying the fracture energy per unit volume and keeping the crack bandwidth as the length of the element and ii) computing a modified crack bandwidth, hmod. These solutions are based on a rational analysis of the kinematics of the classical continuous damage model and on the fracture energy per unit area, which has to be dissipated into a volume by a fully developed crack. It is analytically shown that the relationship, gfh=Gf, between the fracture energy per unit area, Gf and fracture energy per unit volume, gf, is only valid if the cracking area is the same than the reference cross-sectional area of the element. The non-linear behaviour of concrete is described by continuous constitutive models, which include linear and exponential softening. Numerical examples validate the proposed hmod for modelling cracking in concrete, which guarantee the correctness of the energy dissipation during the fracture process. These numerical examples were modelled with 1D, 2D and 3D elements with full integration scheme.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An hp-HDG Approach for Anisotropic Diffusions

Author(s): *Geonyeong Lee, *The University of Texas at Austin*; Jau-Uei Chen, *The University of Texas at Austin*; Tan Bui-Thanh, *The University of Texas at Austin*;

We propose a high-order hp-Hybridized Discontinuous Galerkin (HDG) approach with mortar-based interpolation operator for solving anisotropic diffusion problems numerically. We show that the proposed HDG method is well-posed for h-, p- and hp-nonconforming cases by using the energy method with the aid of interpolation operator. By interpolating every computation onto the mortar, the HDG method facilitates the coupling of fluxes from neighboring elements which have distinct polynomial orders or non-matching interfaces. This mortar-based technique simplifies both analysis and implementation. We also present several numerical results to demonstrate high-order capacity of HDG method which reduces numerical pollution induced by misaligned meshes where mortar has directions difference from the principal axes of transport. The oscillations due to the high-order capacity can be alleviated by hp-adaptivity even in the region where sharp gradient exits. Also, the influence of singularity or discontinuity in the solutions can be indeed confined within the smaller region as hp-adaptation is performed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Feasibility of Vascular Remodeling Parameter Estimation for Assessing Hypertensive Pregnancy Disorders

Author(s): *Georgios Kissas, *University of Pennsylvania*; Eileen Hwuang, *University of Pennsylvania*; Nadav Schwartz, *University of Pennsylvania*; Walter R. Witschey, *University of Pennsylvania*; John A. Detre, *University of Pennsylvania*; Paris Perdikaris, *University of Pennsylvania*;

Hypertensive pregnancy disorders, such as preeclampsia, are leading sources of both maternal and fetal morbidity in pregnancy. Non-invasive advanced imaging, such as ultrasound and magnetic resonance imaging (MRI), can be an important tool in predicting and monitoring these high risk pregnancies. While imaging can measure hemodynamic parameters, such as UtA pulsatility and resistivity indices, the interpretation of such metrics for disease assessment rely on ad hoc standards which are not strictly defined and provide limited insight to the physical mechanisms underlying the emergence of hypertensive pregnancy disorders, such as preeclampsia. To provide meaningful interpretation of measured hemodynamic data in patients, advances in computational fluid dynamics can be brought to bear. In this presentation, we will present the a patient specific computational framework that combines Bayesian inference with a reduced order Navier-Stokes model to infer remodeling parameters, such as vascular resistance, compliance and vessel cross-sectional area, known to be related to the development of hypertension. The proposed framework also enables the prediction of hemodynamic quantities of interest, such as pressure and velocity, directly from sparse and noisy MRI measurements. We illustrate the effectiveness of this approach in two systemic arterial network geometries: an aorta with carotid and a maternal pelvic arterial network. For both cases, the model can reconstruct the provided measurements and infer parameters of interest. In the case of the maternal pelvic arteries, the model can make a distinction between the pregnancies destined to develop hypertension and those that remain normotensive, expressed through the value range of the predicted absolute pressure.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The Arbitrary-Order Virtual Element Method for Linear Elastodynamics Models

Author(s): *Gianmarco Manzini, *Los Alamos National Laboratory*; Paola Antonietti, *Politecnico di Milano*; Ilario Mazzieri, *Politecnico di Milano*; Hashem Mourad, *Los Alamos National Laboratory*; Marco Verani, *Politecnico di Milano*;

We present the conforming virtual element method for the numerical approximation of the two dimensional elastodynamic problems. For the scheme, we prove stability and convergence of the semi-discrete approximation and derive optimal error estimates under h-refinement in both the energy and the L^2 norms, and optimal error estimates under p-refinement in the energy norm. The performance of this virtual element method is assessed on a set of different computational meshes, including non-convex cells up to order four in the h-refinement setting. Exponential convergence is experimentally observed under p-refinement.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Structure-Based Multi-Scale Modeling of the Intervertebral Disc

Author(s): *Grace O'Connell, *University of California, Berkeley*; Minhao Zhou, *University of California, Berkeley*; Benjamin Werbner, *University of California, Berkeley*;

Intervertebral disc research aims to develop a deeper understanding of spine biomechanics, the complex relationship between disc health and back pain, and mechanisms of injury and repair. Many researchers have focused on characterizing tissue-level properties of the disc, where the roles of tissue subcomponents can be more systematically investigated. Unfortunately, experimental challenges often limit the ability to measure important disc tissue- and subtissue-level behaviors, including fiber-matrix interactions, transient nutrient and electrolyte transport, and damage propagation. Constitutive modeling approaches for biological tissues relies on hyperelastic descriptions, where parameters do not represent physical features of the tissue, limiting conclusions that can be drawn. Moreover, models calibrated for one loading condition (e.g., uniaxial tension) often have poor predictive power for other loading conditions (e.g., planar biaxial tension), and calibrating model parameters to multiple loading phenomena simultaneously results in poor fits to some loading conditions. We recently developed a structure-based multi-scale model of the annulus fibrosus (AF) and intervertebral disc where model parameters were determined using known values for subtissue properties, such as proteoglycan content (i.e., fixed charge density) and fiber stiffness. Triphasic mixture theory was used to describe tissue swelling behavior and link model parameters to proteoglycan content or fixed charge density. This approach for model development resulted in a robust model that was capable of predicting both tissue- and joint-level mechanics under multiple loading phenomenon. At the tissue-scale, the model accurately predicted linearity of the stress-stretch response and stiffness under uniaxial tension, biaxial tension, and shear. We then used this model to elucidate relationships between specimen geometry and modulus, Poisson’s ratio, tissue stress–strain distributions, and fiber reorientation. It was observed that AF tensile properties and stress transmission mechanisms were dependent on specimen geometry, partially explaining large variations noted in experimental data based on changes in sample preparation. The model also demonstrated that the contribution of fiber–matrix interactions to tissue mechanical response was dependent on the specimen size- and fiber orientation with respect to the loading direction. At the joint-level, model parameters related to proteoglycan content were altered to simulate early and moderate degeneration by decreasing fixed charge density in the nucleus pulposus or the nucleus pulposus and AF, respectively. A decrease in fixed charge density resulted in alterations in disc morphology and mechanical behavior that have been observed with degenerated discs, including a decrease in disc height, increased stress distribution to the AF and buckling of the AF.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Image-Based Computational Modeling of Prostate Cancer Growth to Assist Clinical Decision-Making

Author(s): *Guillermo Lorenzo, *The University of Texas at Austin / University of Pavia*; Thomas J. R. Hughes, *The University of Texas at Austin*; Alessandro Reali, *University of Pavia*; Hector Gomez, *Purdue University*; Thomas E. Yankeelov, *The University of Texas at Austin / MD Anderson Cancer Center*;

Prostate cancer (PCa) is a major pathology among ageing men worldwide. Currently, most prostatic tumors are detected at an early stage. However, the limited individualization of monitoring and treatment strategies have led to significant rates of overtreatment and undertreatment. Computational modeling of PCa growth has the potential to overcome these issues by providing personalized predictions of tumor growth that can assist physicians in clinical decision-making. In this context, pathological forecasting relies on computer simulations based on a system of partial differential equations that describes the key mechanisms involved in tumor growth and that is parameterized using readily available clinical and imaging data. Here, we present our current efforts to model the growth of organ-confined PCa. Our simulations leverage Isogeometric Analysis to address the computational challenges of this problem. The patient-specific mesh of the prostate is built from the segmented anatomy of the organ via magnetic resonance images. Our simulations recapitulate many of the clinical manifestations of PCa and provide new insights in tumor evolution and monitoring with direct implications in the clinical management of this disease. REFERENCES [1] Lorenzo G, Scott MA, Tew K, Hughes TJR, Zhang YJ, Liu L, Vilanova G, and Gomez H. Tissue-scale, personalized modeling and simulation of prostate cancer growth, Proc Natl Acad Sci USA (2016) 113(48):E7663-E7671. [2] Lorenzo G, Hughes TJR, Dominguez-Frojan P, Reali A, and Gomez H. Computer simulations suggest that prostate enlargement due to benign prostatic hyperplasia mechanically impedes prostate cancer growth. Proc Natl Acad Sci USA (2019) 116(4):1152-61. [3] Lorenzo G, Hughes TJR, Reali A., Gomez H. A numerical simulation study of the dual role of -reductase inhibitors on tumor growth in prostates enlarged by benign prostatic hyperplasia via stress relaxation and apoptosis upregulation. Comp Methods Appl Mech Engrg (2020) 362: 112843.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Objective Molecular Dynamics (OMD) Simulation of Dislocation Dynamics

Author(s): *Gunjan Pahlani, *University of Minnesota*; Ananya Renuka Balakrishna, *University of Southern California*; Richard James, *University of Minnesota*;

Objective Molecular Dynamics (OMD) is a generalization of periodic molecular dynamics which exploits the invariance of the equations of MD and the underlying potential energy hypersurface [1]. This relatively new method addresses the time scale limitation of atomic simulations by using the long-range symmetries in bulk crystalline materials under external loads. We apply this modeling technique to investigate the dynamics of dislocations. Specifically, we explore the dynamics of a screw dislocation when it leaves its primary crystallographic plane and glides into a conjugate "cross-slip" plane---this motion is known to cause plastic deformation, however, the precise mechanism of dislocation evolution is not well understood. In this work, we study the cross-slip mechanism and report on the dislocation pathways and stacking fault widths in a material as a function of the different loading conditions. Additionally, we investigate how different strain rates affect a material's stress–strain response and its dislocation mechanism. For example, we observe two different mechanism, variant of Friedal-Escaig and Fleisher mechanism for cross-slipping and the critical shear stress is shown to have a strong dependence on strain rate. More broadly, we show how OMD methods can be applied to provide insights into dislocation dynamics. Reference 1. Dayal, K. and James, R.D., 2010. Nonequilibrium molecular dynamics for bulk materials and nanostructures. Journal of the Mechanics and Physics of Solids, 58(2), pp.145-163.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Explicit Semi-Lagrangian Discontinous Spectral Element Method for Solution of Stochastic Differential Equations

Author(s): *Gustaaf Jacobs, *San Diego State University*; Hareshram Natarajan, *San Diego State University*; Pavel Popov, *San Diego State University*;

An explicit semi-Lagrangian method method is developed for the solution of stochastic differential equations that is consistent with Discontinuous Spectral Element Method (DSEM) approximations of Eulerian conservation laws. The method extends the favorable properties of DSEM that include its high-order accuracy, its local and boundary fitted properties and its high performance on parallel platforms for the concurrent Monte-Carlo, semi-Lagrangian and Eulerian solution of a class of time-dependent problems that can be described by coupled Eulerian-Lagrangian formulations. The method is shown to be consistent with solutions of the Fokker-Planck equations. Several tests verify the spectral accuracy of the method.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Characterizing the Polycrystalline Materials' Microstructure Resulting from Atomistic Simulations of Solidification: Methods, Algorithms, and Applications

Author(s): *Hang Li, *Iowa State University*; Yipeng Peng, *Iowa State University*; Ji Rigelesaiyin, *Iowa State University*; Thanh Phan, *Iowa State University*; Liming Xiong, *Iowa State University*;

In this work, we present an in-house computer software and its applications in determining the key microstructure features, including grain sizes, disorientation angles, crystal structures, phase volume fractions, and among several others, in polycrystalline materials obtained from molecular dynamics (MD) simulations of solidifications. Taking polycrystalline ice resulting from water freezing and Ti-alloys resulting from additive manufacturing as model materials, this software's applicability will be demonstrated through: (i) resolving the evolution of the grain orientations evolution during the solidification process; (ii) characterizing the grain size and grain disorientation distributions; (iii) differentiating the cubic and hexagonal phases; and (iv) quantifying the effects of the cooling rates, chemical compositions, as well as the substrate's roughness on the microstructures resulting from solidification. This software provides researchers with a high-fidelity high-resolution vehicle to quantitatively analyze the complex microstructures of a variety of polycrystalline materials resulting from solidification. A utilization of this platform together with the gained knowledge in guiding the setup the higher length scale computer models for polycrystalline materials with microstructure complexities will be also discussed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Role of Mitral Valve Leaflet Pre-Strain in an Integrated Left Ventricle-Mitral Valve Model

Author(s): *Hao Liu, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*;

When strain is relieved when an organ is excised from the body, it is defined as a form of residual or pre-strain. Along these lines, we discovered mitral valve tissues also exhibited pre-strain in a novel in-vivo study. We determined that a unit square of leaflet's area decreased by 17% when heart was excised from the body, and by 43% when MV leaflets were excised from the heart. However, this effect has never been explored as part of LV function. The goals of the present study were to 1) investigate the role of MV leaflet prestrain on model predictions and 2) study the role of regional myocardial infarction patterns on MV function and strain. A biventricular LV/MV ovine model was developed, with all data collected in a single living heart to facilitate model integration of the various model components. With respect to mitral valve, we processed real-time 3D echocardiographic (rt-3DE) images of another animal to obtain geometry of leaflets and the MV plane. Finally, we used functionally equivalent chordal structure [9] to capture the native chordal behavior. After the LV-MV computational model was established, we moved on to next step of looking into pre-strain of mitral valve leaflets. Adding pre-strain into MV leaflets was performed by updating deformation matrix F^new=F^old F^(pre-strain) where the amount of pre-strain applied in circumferential and radial direction were introduced. First trial has been made with uniform pre-strain applied on MV leaflets. Then, actual in-vivo pre-strain measured from sonocrystal study of MV was obtained and it was used as input for in-silico model. We then compared the open and close state of MV geometries from LV-MV in-silico model to this result, using various pre-strain values. When compared to the in-vivo strain maps, some differences have been observed including less compression (?<1) along free edge in circumferential direction and larger fiber extension (?>1) in radial direction. Uniform prestrain as ?_1= ?_2=0.9 was prescribed in the MV leaflets which results in strain increase while uniform pre-strain of ?_1= ?_2=1.1 leads to strain reduction due to material stiffening. Interestingly, when the actual observed in-vivo pre-strain was used, the strain maps agreed most closely. This study established a connection between MV in-vivo functional state and in-vitro reference state through applying pre-strain. The importance of this role has been emphasized by comparing with in-vivo stain mapping and it should be included in the future LV-MV modeling.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multigrid and Saddle-Point Preconditioners for Unfitted Finite Element Modeling of Inclusions

Author(s): *Hardik Kothari, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*;

In real-world modeling of the materials, discontinuities are omnipresent. We consider the modeling of weak discontinuities such as inclusions using the unfitted finite element methods. In the unfitted methods, structured background meshes are used and only the underlying finite element space has to be modified to incorporate the discontinuities. Hence, the unfitted methods are more flexible to model the problems with multiple inclusions in a domain. We employ the method of Lagrange multipliers for enforcing the interface conditions weakly, as the method does not depend on any additional stabilization parameters as compared to Nitsche's method. The downside of this method is the arising linear system is of saddle point type. We use the Uzawa method for solving the saddle point problem and propose some preconditioning strategies for primal and dual systems. For the dual systems, we review and compare the preconditioning strategies that are developed for solving the saddle point system that arises in FETI and SIMPLE methods. While for the primal system, we employ a tailored multigrid method developed for the unfitted meshes. For the transfer operator, we use pseudo-L2- projection-based prolongation and restriction operators to transfer the information between the mesh hierarchies. In this work, the robustness and the efficiency of the proposed preconditioners will be demonstrated using numerical experiments. REFERENCES [1] H.Kothari, R. Krause. A Multigrid Method for a Nitsche-based Extended Finite Element Method, arXiv:1912.00496 [cs, math], (2019) [2] A. Klawonn and O. Widlund. FETI and Neumann-Neumann iterative substructuring methods: Connections and new results, Communications on Pure and Applied Mathematics, 54(1):57–90, (2001) [3] E. Béchet, N. Moes, and B. Wohlmuth. A stable Lagrange multiplier space for stiff interface conditions within the extended finite element method, International Journal for Numerical Methods in Engineering, 78(8):931–954, (2009)

16th U.S. National Congress on Computational Mechanics
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Title: A Stable Immersed Discontinuous Galerkin Method for Wave Propagation in Heterogeneous Acoustic Elastic Media

Author(s): Slimane Adjerid, *Virginia Polytechnic Institute and State University*; *Haroun Meghaichi, *Virginia Polytechnic Institute and State University*;

Immersed finite element methods are applied to solve interface problems on interface-independent meshes that allow interface elements that are cut by the interface. Here we propose an immersed discontinuous Galerkin (DG) method to solve acoustic-acoustic, elastic-elastic and acoustic-elastic interface problems on Cartesian meshes with interface elements that consist of more than one fluid, more than one solid or a combination of fluids and solids separated by interfaces. These problems are modeled by either the same PDE system with discontinuous coefficients as is the case for acoustic-acoustic and elastic-elastic interface problems or by different PDE systems as for acoustic-elastic interface problems. These PDE systems are coupled by jump conditions across the interfaces. We present a stable weak DG formulation combined with a piecewise polynomial immersed finite element (IFE) space. The IFE space is such that on each interface element we use a piecewise polynomial space satisfying the interface jump conditions while on non-interface elements we use standard polynomial spaces. We discuss the stability of the method and a time-marching algorithm. We conclude with several numerical examples showing the performance of our method by solving problems of wave propagation in heterogeneous elastic acoustic media.

16th U.S. National Congress on Computational Mechanics
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Title: Tempered Fractional Laplacian in the Nonlocal Framework

Author(s): *Hayley Olson, *University of Nebraska-Lincoln*; Mikil Foss, *University of Nebraska-Lincoln*; Petronela Radu, *University of Nebraska-Lincoln*; Marta D'Elia, *Sandia National Laboratories*; Mamikon Gulian, *Sandia National Laboratories*;

Tempered fractional operators provide models with effects that cannot be captured by standard partial differential equations -- such as superdiffusion and subdiffusion -- and have applications in fields such as geoscience and hydrology. The tempered fractional Laplacian can be integrated into the nonlocal vector calculus framework and viewed as a special case of the nonlocal operators from the recently developed unified nonlocal calculus. The tempered fractional Laplacian is a computationally expensive operator, so there is desire to find a computationally cheaper alternative. In this work, we compare it to the computationally cheaper truncated fractional Laplacian. In particular, we show the equivalence of the tempered and truncated energies. Then, we investigate choices in parameters that can make the tempered and truncated fractional Laplacian operators act equivalently.

16th U.S. National Congress on Computational Mechanics
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Title: Hierarchical Deep-Learning Neural Networks for Physics Discovery and Mechanical Design

Author(s): *Hengyang Li, *Northwestern University*; Abdullah Amin, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

In this work, we are introducing a novel Hierarchical Deep-Learning Neural Networks (HiDeNN) approach for physics discovery and mechanical design. The ability of the deep learning neural networks (DNNs) to handle nonlinearity and universal approximation has been demonstrated to computationally solve physics equations and partial differential equations (PDEs). However, problems with higher degrees of freedom yield a large number of input variables for a DNN, making it challenging and computationally expensive as the advantages are diminished over conventional computational methods. In the current approach, the knowledge of finite element is transferred to a HiDeNN framework in the form of a predefined neural block structure to assist in solving PDEs to maintain the computational advantage. By predefining the neural network structure, HiDeNN reduces the number of required design variables significantly and offers built-in mesh adaptivity to improve accuracy in the local region compared to conventional finite element methods. The first part of this talk introduces the theory of HiDeNN and shows the advantage over conventional FEA. The second part of this talk demonstrates its extensions in multiphysics discovery and topology optimization.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Programmable Lattices via Geometry Projection

Author(s): *Hesaneh Kazemi, *University of California, San Diego*; Julián Norato, *University of Connecticut*;

This work presents a topology optimization method for design of programmable lattices. In programmable lattices, each strut can be activated or deactivated via some actuation mechanism. This actuation mechanism can be through the use of electromagnetic (EM) joints, or hollow struts that can be filled with a magnetorheological fluid. The program of the lattice refers to the open or closed state of the struts. The proposed method designs the unit cell of a periodic material to obtain different properties for different programs. Our technique simultaneously optimizes the spatial layout of the struts within unit cell and determines the open/closed state for each strut in each program to achieve different effective properties. A state variable per program is assigned to each strut to represent its open/closed state. The struts are in the lattice are represented as bar primitives, specifically as the offset surface of the bar's medial axis. The lattice design corresponds to the combination of these bar primitives. This representation ensures an open cell design that facilitates fabrication with additive manufacturing techniques, as the open cell configuration allows for removal of sacrificial support material. The geometry projection method is used to map the high-level geometric description of the struts onto a density field. This density is used to interpolate material properties and perform the analysis on a fixed finite element mesh upon design changes as in density-based topology optimization methods. The geometry projection mapping is differentiable; therefore, design sensitivities can be obtained, and efficient gradient-based optimization methods can be used for the design. The proposed method allows the imposition of desired material symmetries by defining the struts only in a reference region of symmetry and reflecting the projected density field with respect to appropriate symmetry planes. To ensure that the state variables are either 0 or 1 in the optimal design, a discreteness constraint is enforced. A no-cut constraint ensures the struts are not partially cut by the unit cell faces or the boundaries of the symmetry reference region in order to render the struts whole and facilitate manufacturing. We demonstrate the effectiveness of the proposed method via numerical examples that design a programmable lattice to minimize the lattice weight and attain two and three desired effective properties for different actuation programs.

16th U.S. National Congress on Computational Mechanics
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Title: Singular Patch and Patch Superposition Method in IGA for Linear Fracture Mechanics Analysis

Author(s): Rino Watanabe, *Tokyo University of Science*; Daichi Nakahara, *Tokyo University of Science*; Omar Tabaza, *Tokyo University of Science*; Yuto Otoguro, *Tokyo University of Science*; *Hiroshi Okada, *Tokyo University of Science*;

In this investigation, we developed a patch superposition method for linear fracture mechanics analysis. The patch superposition method is based on Isogeometric analysis (IGA) [1]. In this method, two kinds of IGA patches are adopted to model a solid with a crack. One is called the “global patch” which represents the structure without the crack. The other is the “local singular patch” representing the crack with stress singularity. The concept of the patch superposition method is analogous to that of the s-version FEM (see [2] for example). Three kinds of stiffness matrices are generated. They are the stiffness matrices for the global and the local patches and the matrix that couples them. Also, a generalized version of auxiliary mapping [3] for IGA is adopted in building the local-singular patch. By this method, the square root stress singularity in a desired span from the crack tip can be reproduced. For example, the span of an entire singular patch may have the singular behavior. Or the span of the singular behavior may be confined in the immediate vicinity of the crack tip. The singular behavior can be controlled by appropriately setting the locations of control points. The method is similar to the Barsoum’s singular element [4] in the context of the finite element method. For the evaluation of the stress intensity factor, the domain integral method is adopted. In the presentation, we will discuss i) the singular patch method, ii) improvement on the accuracy due to the adoption of the singular patch method, iii) the patch super position method and its numerical implementation and iv) some numerical demonstrations for the proposed scheme. It will be demonstrated that linear fracture mechanics analysis can be performed very accurately while its IGA modeling remains to be very simple and tractable. References [1] T.J.R. Hughes, J.A. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, Comput. Methods Appl. Mech. 194 (2005), pp.4135-4195. [2]H. Okada, S. Endoh, M. Kikuchi, On fracture analysis using an element overlay technique, Engrg Fract. Mech. 72 (2005), pp. 773-789. [3] J.W. Jeong, H.-S. Oh, S. Kang, H. Kim, Mapping techniques for isogeometric analysis of elliptic boundary value problems containing singularities, Comput. Methods Appl. Mech. Engrg. 254 (2013), pp. 334–352. [4] R.S. Barsoum, On the use of isoparametric finite elements in linear fracture mechancis, Int. J. Num. Meth. Engrg. 10 (1976), pp. 25-37.

16th U.S. National Congress on Computational Mechanics
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Title: Human Lamina Cribrosa Material Properties Using Inverse Finite Element Approach

Author(s): *Hirut Kollech, *University of Pittsburgh*; Reza Behkam, *University of Pittsburgh*; Jonathan Vande Geest, *University of Pittsburgh*;

The biomechanics of the optic nerve head region including the lamina cribrosa (LC) and sclera is fundamental for the development and progression of glaucoma. The main risk factors include age, race, and elevated intraocular pressure. Even though there are several studies showing that eyes of African Descent (AD) and Hispanic Ethnicity (HE) donors exhibit LC microstructure and biomechanical response that are significantly different than European Descent (ED) [1,2], the material properties across racioethnic groups have not been studied. Therefore, the purpose of this work is to investigate the biomechanical properties of the LC across the racioethnic groups. Non-glaucomatous human eyes from the three groups were imaged using a multiphoton microscope during a pressure inflation experiment (AD; n=6, ED; n=5, HE; n=6). Second-harmonic generation images were collected and utilized to generate 3D geometry meshes and to calculate the displacement field using digital volume correlation (DVC). The DVC results were applied as boundary conditions and to check the computational displacement in the finite element simulation. Segmented images were used to identify the collagenous region of the LC. The Holzapfel material model was used for this part to account for the anisotropic and hyperelastic behavior and Neo-Hookean was used for the non-collagenous (nerve tissue) region. Since the full LC mesh is computationally expensive, several small subdomain regions were created for the optimization. In each simulation, displacement on interior nodes was output to calculate the error. The objective function is described as the sum of the square of the residuals between the experimental displacement and computational displacement at different pressure steps. A particle swarm optimization with multi-start was used for the inverse Finite Element simulation. Our preliminary results collected from 4 samples shows optimized C10 values for the ED samples were 263 kPa and 76.1 kPa with a displacement percent error of 9.76 x 10-6 and 4.52 x 10-6 (w.r.t DVC displacement). For HE; these values were 79.5 kPa and 77.0 kPa with 1.75 x 10-6 and 1.3 x 10-6 error respectively. Although this preliminary analysis shows that C10 values are bigger in one of the ED samples while HE samples had smaller stiffness values, this is ongoing work with a total of 17 samples. The final results from the rest of the samples will be critical to report a comprehensive statistical analysis across these groups. Reference: [1] Tamimi E et al., IOVS, 58(10):4235-4246, 2017. [2] Behkam R et al., Acta Biomaterialia, 88:131-140, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Nonlocal Fracture Model for Cohesive-Frictional Materials via a Volume Averaging Approach

Author(s): *Hojjat Mohammadi, *McMaster University*; SeonHong Na, *McMaster University*;

The onset of cracks and their propagation is an important issue of the mechanical behaviour in cohesive-frictional materials, such as rocks. In this study, a nonlocal fracture model is presented based on the volume averaging approach [Pietruszczak, 1999], which is a homogenization technique for a domain having both an intact region and a localized deformation. In this method, the post-localization response is formulated, including a characteristic dimension defined by the ratio of the area of the fractured plane to the given referential volume, which introduces mesh-independence. We develop a new return mapping algorithm, i.e., the general return mapping, for both compression and tension loading conditions. Coulomb criterion is used as a failure criterion that triggers the onset of crack under compression loading condition. For the tensional regime, a cohesive-crack model is adopted for the onset and propagation of the crack. The direction of a new crack under compression is defined based on the Mohr-Coulomb criterion, while the tensional crack propagates along with the eigenvector of the maximum principal stress. The softening behaviour is captured via an exponential decay function that includes a constant parameter governing the softening rate. A stress-point calculation is performed to validate the constitutive behaviour followed by boundary value problems to demonstrate the robustness of the proposed return mapping algorithms and the nonlocal effect of the volume averaging approach.

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Title: Interfacial Multiphysics Using an ALE Interface-Tracking Method

Author(s): *Holger Marschall, *Technical University Darmstadt*; Heba Alkafri, *Technical University Darmstadt*; Chiara Pesci, *ESI Engineering System International GmbH*; Andre Weiner, *Technical University of Braunschweig*; Dieter Bothe, *Technical University Darmstadt*;

We have enhanced a finite-volume based Arbitrary Lagrangian-Eulerian (ALE) Interface-Tracking method (cp. doi:10.1016/j.compfluid.2011.11.003 and doi:10.1016/j.compfluid.2014.06.030) and developed a comprehensive framework for numerical modeling of interfacial transport of soluble and insoluble surfactants (doi:10.1017/jfm.2018.723) to cope with interfacial multiphysics at fluid interfaces. Transport equations are solved via collocated Finite Volume and Finite Area Method (FVM/FAM) on unstructured meshes of general topology, i.e. polyhedral/polygonal meshes, with moving mesh support. This talk will set out the continuum model as well as details regarding the numerical method development and implementation within the OpenFOAM C++ library. Emphasis will be put on Dirichlet-Neumann coupling of interfacial transmission and jump conditions and the critical role of an accurate, finite-area based and force-balanced numerical discretisation of surface tension. We will further detail on the treatment of surfactant mixtures on the interface and in the bulk, the transport of which is coupled via sorption processes resulting in a multi-equation/multi-region coupling problem. In particular, we will focus on numerical modeling of the two limiting sorption regimes, namely diffusion-controlled (fast) and kinetically-controlled (slow) adsorption, which necessitate substantially different numerical treatments. Verification and validation results are provided for a selection of test cases. Application relevance is exemplified for a single bubbles rising in quiescent liquid under the influence of surfactants.

16th U.S. National Congress on Computational Mechanics
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Title: Coupled Mechanical-Electrochemical-Thermal Simulation for Short-Circuit Prediction of Lithium-Ion Batteries Under Mechanical Abuse

Author(s): *Honggang Li, *Northwestern Polytechnical University, China*; Chao Zhang, *Northwestern Polytechnical University, China*;

Lithium-ion batteries (LIBs) are currently the state-of-the-art power sources for a variety of applications, due to their high energy density, high voltage and low self-discharge rate, from consumer electronic devices to electric-drive vehicles (EDVs). However, the safety behavior of LIBs under external mechanical abuse is increasingly severe. The failure mechanism and coupled propagation behavior for mechanical abuse induced internal short circuit (ISC) are complicated, depending on the layered architecture, electrochemical activity, thermal performance, and state of charge et al. In this work, a simultaneously coupled mechanical-electrochemical-thermal model was developed based on a commercial ?nite element software COMSOL Multiphysics to simulate the short-circuit behavior of LIBs under mechanical abuse. A multi-layer (anode-separator-cathode) unit cell model was established and correlated against the experimental mechanical and charge-discharging results. The stress-strain curves of component materials (anode, cathode and separator) under compression were verified against uniform compression test results and validated against indentation tests. A 2D electrochemical-thermal model of LIB based on Newman model was introduced to simulate the electrical-electrochemical-thermal behavior. A maximum-strain criterion is proposed to determine the onset of internal short circuit due to the mechanical crash. The resistance of separator first changes slowly and linearly with through-thickness strain, and decreases sharply once the through-thickness strain goes below a threshold value, which corresponds to the failure of separator and occurrence of electric contact between anode and cathode. The presented model provides a technique to study the relationship between mechanical failure and electrical-thermal responses. Numerical case studies are conducted to investigate the propagation of internal electrical and thermal failure crossing different unit cell elements, which provides insights on preventing catastrophic failure of a battery pack or module. The simultaneously coupled modeling methodology will be especially useful for the crashworthiness design of electric vehicles. References [1]. H. Li, B. Liu, D. Zhou, C. Zhang*, Coupled mechanical–electrochemical –thermal study on the short-circuit mechanism of lithium-ion batteries under mechanical abuse, Journal of the Electrochemistry Society, 2020, 167: 120501. [2]. H. Li, D. Zhou, C. Du, C. Zhang*, Parametric study on the safety behavior of mechanically induced short circuit for lithium-ion pouch batteries, Journal of Electrochemical Energy Conversion and Storage, 2021, 18: 020904. [3]. C. Zhang, S. Santhanagopalan, M. A. Sprague, A. A. Pesaran, Coupled mechanical-electrical -thermal modeling for short-circuit prediction in a lithium-ion cell under mechanical abuse, J. Power Sources, 2015, 290: 102–113.

16th U.S. National Congress on Computational Mechanics
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Title: On Learning/Solving Differential Equations with Kernels

Author(s): *Houman Owhadi, *California Institute of Technology*;

There is a growing interest in solving differential equations as learning problems. Popular approaches can be divided into (1) Kernel methods, and (2) methods based on variants of Artificial Neural Networks. We illustrate the importance of using adapted kernels in kernel methods and discuss methods for learning the kernel from data. We show how ANN methods can be formulated as kernel methods with warping kernels learned from data. We show how kernel methods can be generalized to nonlinear differential equations.

16th U.S. National Congress on Computational Mechanics
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Title: Sharp Interface Isogeometric Solution to Reaction-Diffusion Problems

Author(s): *Huanyu Liao, *Purdue University*; Pavan Kumar Vaitheeswaran, *Intel Corporation*; Ganesh Subbarayan, *Purdue University*;

Abstract: Reaction-Diffusion problems are challenging to model due to complex multi-physics interactions, and complex thermodynamic conditions governing the moving interfaces. Commonly, these class of problems are solved using methods that implicitize the interface geometry such as the phase field or level set methods. In this talk, we describe the development of general sharp interface governing equations for reaction-diffusion problems as well as an explicit interface enriched isogeometric analysis (EIGA) computational procedure for tracking the moving interfaces. The interface governing equations for reaction-diffusion systems are developed using the fundamental interface balance laws and thermodynamic principles, including bulk diffusion, interface evolution phase growth condition and appropriate constitutive relations. The EIGA computational procedure relies on generating Algebraic Level Sets (ALS) from explicitly defined parametric boundaries using the Dixon resultant. A significant challenge in isogeometric analysis is classification of points as lying inside or outside a given region. This challenge is overcome naturally in the present solution method since ALS provide a measure of signed distance from a Bezier surface, and allow algebraic Boolean operations on Bezier surfaces to obtain a composed signed distance measure from a NURBS surface. The sign of the ALS naturally classifies any point in the domain. The developed theory and the computational procedure are demonstrated through two- and three-dimensional simulations of important phenomenon observed in microelectronic devices. First, two- and three-dimensional simulations of void growth in circuit lines under high current density is carried out and compared against experimental observations. Next, growth of Cu-Sn intermetallic compound in a microscale solder interconnect under elevated temperature is simulated and compared against experimental observations. Keywords: reaction-diffusion problems, sharp interface model, algebraic level sets, enriched isogeometric analysis

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Title: Dislocation Transmission Across Sigma 3 {112} Incoherent Twin Boundary: Combined Atomistic and Phase-Field Study

Author(s): *Hyojung Kim, *Los Alamos National Laboratory*; Tengfei Ma, *University of Nevada, Reno*; Nithin Mathew, *Los Alamos National Laboratory*; Darby J. Luscher, *Los Alamos National Laboratory*; Lei Cao, *University of Nevada, Reno*; Abigail Hunter, *Los Alamos National Laboratory*;

We perform atomistic and mesoscale simulations to study the interaction between a dislocation and grain boundary (GB), and specifically the transmission behavior of dislocation across the GB. GBs, which are the boundary between two differently oriented atomic arrangements, play a significant role in plastic deformation at low temperatures as pinning or nucleation sources for dislocations. However, it is challenging to observe the interaction and determine the critical stress of dislocation transmission through experiments. In this study, we perform molecular statics (MS) simulations to compute the generalized stacking fault energy of Cu and structural parameters to inform the mesoscale model called phase field dislocation dynamics (PFDD). Using PFDD, we construct the Sigma 3 {112} incoherent twin boundary for Cu, which consists of a repetition of three partial dislocation arrays, and compute the interaction between glide dislocations and the GB. The PFDD-computed transmission plane across the GB matches well with the results from MS modeling. The critical stress of dislocation transmission is comparable to the MS results, while we attribute the differences to the other slip behaviors, such as glide within the GB, which we did not incorporate for the present PFDD modeling. We also provide theoretical analysis on transmission behavior to understand the computational results and discuss the effect of anisotropic elasticity on the transmission behavior.

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Title: Virtual Element Method on Curved Geometries for Acoustic Wave Propagation Analysis

Author(s): *Ilario Mazzieri, *Politecnico di Milano*; Alessio Fumagalli, *Politecnico di Milano*; Franco Dassi, *Università degli Studi di Milano Bicocca*;

Simulations for underground study often present critical aspects related to the difficulty to directly access data and their intrinsic complexity. Highly heterogeneous materials with several horizons and fractures dominate the simulation outcome, and the numerical schemes need to be flexible enough to provide accurate solutions in a reasonable amount of time. We focus on the wave equation on geometries that might include curved internal interfaces or boundaries. To avoid spurious phenomena, we extend the virtual element method to represent the computational domain exactly. A new virtual space is thus introduced along with a suitable projection operator. On the curved edges, a computable mapping is given to preserve the expected convergence rate. Applications of the proposed approach are the seismic exploration of the underground. Simulations and analysis will show the effectiveness of the proposed approach.

16th U.S. National Congress on Computational Mechanics
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Title: The Coupled Momentum Method Revisited: Formulation, Higher-Order Elements, Solver Technology, and Verification

Author(s): *Ingrid Lan, *Stanford University*; Ju Liu, *Southern University of Science and Technology*; Weiguang Yang, *Stanford University*; Alison Marsden, *Stanford University*;

Key Words: Fluid-Structure Interaction, Coupled Momentum Method, Variational Multiscale Formulation, Generalized-alpha Method, Nested Block Preconditioning. Compared to the arbitrary Lagrangian-Eulerian (ALE) method, the coupled momentum method (CMM) [1] offers a computationally efficient approach for modeling fluid-structure interaction, which is critical for capturing wave propagation phenomena in three dimensional cardiovascular simulations. In brief, CMM keeps the fluid mesh fixed and models the vessel wall as a transverse-shear-enhanced linear membrane whose degrees of freedom are strongly coupled to those of the fluid boundary. Given recent advances in computational methods, we propose to enhance the original method in aspects including the spatiotemporal discretization, membrane dynamics, preconditioner design for the resulting linear system, and use of higher-order elements. In particular, we employ the residual-based variational multiscale formulation for stabilized spatial discretization rather than the classical Streamline Upwind Petrov-Galerkin method. In addition, contrary to the ubiquitous approach of collocating pressure at time step t_{n+1}, we evaluate pressure at the intermediate time step in the generalized-alpha method to achieve second-order temporal accuracy of pressure [2]. To introduce numerical damping at high frequency modes, we compute the membrane displacement from its velocity via the generalized-alpha method rather than the Newmark-beta method. Combined with the nested block preconditioner [3] and quadratic tetrahedral elements, our proposed methodology offers improved performance and higher-order accuracy for clinically significant quantities, including pressure and wall shear stress. Verification of the method against the analytical solution to Womersley's deformable wall theory will be presented for both linear and quadratic elements. REFERENCES [1] C.A. Figueroa, I.E. Vignon-Clementel, K.E. Jansen, T.J.R. Hughes, C.A. Taylor. A coupled momentum method for modeling blood flow in three-dimensional deformable arteries. Comput. Methods App. Mech. Eng. 195:5685-5706, 2006. [2] J. Liu, I.S. Lan, O.Z. Tikenogullari, A.L. Marsden. A note on the accuracy of the generalized-alpha method for the incompressible Navier-Stokes equations. Int. J. Numer. Meth. Eng. 122(2):638-651, 2021. [3] J. Liu and A.L. Marsden. A robust and efficient iterative method for hyper-elastodynamics with nested block preconditioning. J. Comput. Phys. 383:72-93, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Fracture Modeling of the Reissener-Mindlin Shell in Peridynamics

Author(s): *Sai Li, *Wuhan University of Technology*; Xin Lai, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*;

In current work, dynamic analysis and fracture are modelled and implemented in Reissener-Mindlin shell by Peridynamics. Peridynamic Reissener-Mindlin shell theory is adopted here to provide the discretization of the shell, in which the shell is described and represented by material points that stands in mean-plane of the shell structure with its drilling rotation ignored in the kinematic assumption. The fracture properties of the material is realized by adopting the Mohr-Coulomb failure criterion. The crack path is simulated by series of geometric algorithm. This approach of fracture modeling will direct maneuver the initialization and simulate the spontaneous growth and branching of the cracks. To improve the numerical accuracy, the stress-point integration method is utilized to eliminate numerical instability induced by the zero-energy mode and rank-deficiency. Several numerical examples are presented to validate the modeling and implementation of the shell, and also demonstrate the capability if proposed model on predicting the brittle fracture in finite deformation.

16th U.S. National Congress on Computational Mechanics
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Title: Space-Time Simulation of a Heaving and Pitching Foil with Time Periodicity

Author(s): *Jacob Lotz, *Delft University of Technology*; Marco ten Eikelder, *Delft University of Technology*; Ido Akkerman, *Delft University of Technology*;

The interest in hydrofoils has been renewed in recent years. To improve their stability, the effect of the orbital motion of waves on hydrofoils and their actuators has to be studied. The result is an unsteady inflow which can be characterized as a combined heave and pitch motion. These motions are periodic in time. In this talk we present residual-based variational multiscale (RBVMS) turbulence model- ing in a time-periodic space-time formulation for the simulation of submerged hydrofoils. We apply NURBS-based isogeometric analysis [1] for the spatial discretization. This pro- vides a better representation of both the curvature at the leading edge of the hydrofoil and of the prescribed mesh motion. The no-slip boundary conditions of the moving body are enforced weakly. We employ a second-order periodic NURBS C-mesh which is C1-continuous in the interior temporal domain. [1] T. J.R. Hughes, J. A. Cottrell, and Y. Bazilevs. “Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement”. In: Computer Methods in Applied Mechanics and Engineering 194.39 (2005), pp. 4135–4195.

16th U.S. National Congress on Computational Mechanics
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Title: A Thresholding Method for the Kobayashi-Warren-Carter Grain Boundary Model with General Mobilities

Author(s): *Jaekwang Kim, *University of Illinois at Urbana-Champaign*; Matt Jacobs, *University of California, Los Angeles*; Nikhil Admal, *University of Illinois at Urbana-Champaign*;

In this work, we develop a lightweight numerical model to describebgrain boundary (GB) evolution under anisotropic misorientation-dependent GB energies and mobilities. The Kobayashi--Warren--Carter (KWC) model is a dual phase field approach, which was originally developed to describe two-dimensional Read--Shockley-type misorientation-dependent grain boundary energies. The main advantage of the KWC model is that it only uses two order parameters to describe GB evolution: one for structural order, and the other for crystal orientation. The elegance of the KWC model is offset by the severe restriction to Read--Shockley-type grain boundary energy and enormous computational costs resulting from the singular diffusive nature of the governing equation. To address the above limitations, in our recent work, we generalized the KWC model to describe general grain boundary energies that respect the crystal symmetry, and developed a highly efficient thresholding method to simulate the stiff equations of the original KWC model. Our formulation, which combines features of diffuse-interface (for the structural order parameter) and sharp-interface (for the crystal orientation parameter), are shown to be orders of magnitude faster than the finite element method. However, its implementation was restricted to grain boundary mobility equal to the inverse of grain boundary energy. In this talk, we present our thresholding algorithm, and current work on extending it to include general mobilities. The computational cost of the algorithm remains O(N log N), where N is the number of grid points. It is envisaged that the extension of our algorithm will enable us to explore the role of grain boundary energy and mobility in a statistical study on large ensembles of polycrystals.

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Title: Computational and Experimental Analyses of Blade Coating

Author(s): Hyungjoo Yim, *Seoul National University*; Junmo Lee, *Seoul National University*; *Jaewook Nam, *Seoul National University*;

Blade coating is a simple method to apply a uniform thin liquid film on moving substrate, where an excess of the coating liquid is metered by a narrow channel formed between a blade and the substrate. It is widely used from large-scale productions in the paper industry to laboratory scale experiments for fabricating functional films. For high-speed operations in commercial productions, where the viscous force is dominant, a simple hydrodynamic model without considering of capillary force is adequate to describe the system and to predict the wet film thickness. However, the model cannot explain the low-speed blade coating operations in laboratory scale experiments, where the capillary and viscous forces compete with comparable order of magnitudes. In this study, we attempt to analyze the impact of the capillary force around the gas-liquid interface on the low-speed blade coating of non-evaporative Newtonian fluids. A simple asymptotic visco-capillary model was derived to predict the wet thickness. Numerical computations using the Galerkin finite element method (G/FEM) was also performed for verification. The momentum balance is solved simultaneously with the mesh generation equation such that the unknown positions of the liquid-air interface are obtained together with the velocity and pressure fields. The model shows fairly reasonable agreements with visualization experiments and numerical computations.

16th U.S. National Congress on Computational Mechanics
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Title: Thermomechanical-Electromagnetic Coupling in Micromorphic Medium

Author(s): *James Lee, *George Washington University*; Jiaoyan Li, *University at Buffalo*;

This work presents a systematic and rational formulation of the electromagnetic theory of deformable micromorphic medium. Finite element formulation and numerical solutions of sample problems are also included. To begin with, we present Maxwell's equations in both fixed and moving frames of reference. Lorentz transformation will be discussed. To establish the thermomechanical-electromagnetic (TM-EM) interactions, the basic laws for mass, microinertia, linear momentum, moment of momentum, energy, and entropy in micromorphic theory, including electromagnetic force, couple, and energy, will be presented and discussed in detail. We rigorously formulate the integrated constitutive theory for thermo-visco-elastic-plastic-electromagnetic materials. In this constitutive theory, one clearly sees (I) the dependence of stresses and heat flux on electric and magnetic fields, (II) the dependence of polarization, magnetization, and current on strains, strain rates, and temperature gradients. Correspondingly, we perform a rigorous finite element formulation. It is noticed that, from Maxwell's equations, the electric field and the magnetic field are not mutually independent; instead they can be derived from a scalar potential and a vector potential. Therefore, in the finite element analysis, each node has 17 degrees of freedom, i.e. one for temperature, three for displacements, nine for micromotions, one for scalar potential, and three for vector potential. A few sample problems have been solved. Numerical solutions will be presented and discussed.

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Title: Quadrature for Implicitly-Defined Finite Element Functions on Curvilinear Polygonal Meshes

Author(s): *Jeffrey Ovall, *Portland State University*; Samuel Reynolds, *Portland State University*;

H1-conforming Galerkin methods on polygonal meshes such as VEM, BEM-FEM and Trefftz-FEM employ local finite element functions that are implicitly defined as solutions of Poisson problems having polynomial source and boundary data. Recently, such methods have been extended to allow for mesh cells that are curvilinear polygons. Such extensions present new challenges for determining suitable quadratures. After reviewing results for Trefftz-FEM, we describe an approach for integrating products of these implicitly defined functions, as well as products of their gradients, that reduces integrals on cells to integrals along their boundaries. The methods and assertions will be illustrated numerically.

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Title: Non-Diffusive Volume Advection with A High Order Interface Reconstruction Method

Author(s): Jin Yao, *Lawrence Livermore National Laboratory*; *Jerry Liu, *Lawrence Livermore National Laboratory / Duke University*;

We show that non-diffusive volume advection in two-dimensions is achieved with several bench-mark problems using a newly developed high order volume of fluids interface reconstruction method. 1. A new VOF (volume of fluids) interface reconstruct method using circular/corner facets We create a circular interface facet in each mixed zone by matching neighbor zone partial volumes with a Newton's method and the local solution is final. If the partial volumes are consistent with the geometry of a polygon with boundary faces of arcs (a straight line is a degenerated case of an arc), the interface reconstructed with our new scheme would exactly recover such an input polygon. In the general case, the new VOF interface reconstruction has 3rd order of accuracy and can be easily made seamless. This is to say the new method fixed some intrinsic issues with the Youngs method such as gaps between interface facets in the case of a curved interface, and inability to define curvature nor identify corners. 2. A non-diffusive volume advection scheme In an ALE advection step, a well-defined interface can be carried over through a Lagrange step and used to compute volume distribution into a relaxed mesh. Then, an interface reconstruction step is performed to redefine the interface in the relaxed mesh. We must point out that the interface carried over is also a solution of interface reconstruction because all the partial volumes in the relaxed mesh are naturally matched. In this sense interface-reconstruction and interface-tracking are not distinguishable. This prior geometrical info seems not utilized in existing advection methods using Youngs interface reconstruction because reconstructed faces are disjointed by using linear facets. With the new interface reconstruction method, we can create a seamless, curved interface with possible corners. it is granted to use the prior info as initial guess to obtain quick convergence. As a result, we are able to treat double facets inside a single mixed cell and obtain highly accurate, non-diffusive solution for advection problems with rather coarse meshes. We will show our solutions for two-dimensional incompressible flows with two materials with a) the X + O diagonal translation; b) the Zalesak rotational test; and 3) the single vortex spiral test. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Jerry Liu is partially supported by LLNL's HEDP summer intern fund and SDOT development fund.

16th U.S. National Congress on Computational Mechanics
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Title: A Locally L^p-DPG Method for the Convection-Diffusion Problem

Author(s): *Jiaqi Li, *The University of Texas at Austin*; Leszek Demkowicz, *The University of Texas at Austin*;

In the finite element community, Discontinuous Petrov-Galerkin (DPG) method is a recently developed technology that offers many desirable properties: symmetric positive-definite stiffness matrix, guaranteed ability for well-posed problems, built-in a posteriori error estimator, etc. The original DPG method is based on Hilbert spaces. Following Houston et al. [1], we generalize DPG method to the Banach spaces [2], and present numerical results showing that the Gibbs phenomena can be eliminated. In this talk, we will discuss a modification to our L^p-DPG method, which only resort to Banach space locally where necessary. The exponent p delineating the energy space, is set as a variable across elements. In those elements where residual is large, we raise the local p. This method is an improvement to the L^p-DPG method, and has the advantage of saving computational cost as well as reducing conditional number. Theory is proposed and 2D numerical results will be presented. References [1] P. Houston, S. Roggendorf, and K. G. van der Zee, Eliminating Gibbs phenomena: A non-linear Petrov–Galerkin method for the convection–diffusion–reaction equation, Computers & Mathematics with Applications, 80 (2020), pp. 851–873. [2] J. Li, L. Demkowicz, An Lp-DPG method for the convection–diffusion problem, Computers & Mathematics with Applications (2020), in press.

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Title: Extended DeepILST: Data-Driven Coarse-Graining of Multi-Atom Molecules at Various Thermodynamic States

Author(s): *Jinu Jeong, *University of Illinois at Urbana-Champaign*; Alireza Moradzadeh, *University of Illinois at Urbana-Champaign*; Narayana Aluru, *University of Illinois at Urbana-Champaign*;

Molecular dynamics simulation is widely used to understand molecular phenomena and to compute the physical properties of microscopic systems. Despite its versatility and accuracy, MD simulation requires a substantial computational effort when the target system is composed of millions of atoms. Many coarse-grained modeling approaches have been developed, based on various techniques such as the relative entropy method [1], integral equation theory [2], etc. While these methods provide computational efficiency, they lack transferability and are limited to specific thermodynamic states. Recently, data-driven and machine learning approaches have been attempted for coarse-grained modeling of molecular systems. In this study, we expand the range of thermodynamic states used for training of DeepILST [3], a deep learning framework for solving the inverse problem of liquid-state theory. We also assess DeepILST's coarse-graining performance for multi-atom molecules and find the target molecule characteristics affecting the coarse-graining performance of DeepILST. References [1] A. Moradzadeh, M. H. Motevaselian, S. Y. Mashayak, and N. R. Aluru, "Coarse-Grained Force Field for Imidazolium-Based Ionic Liquids," J. Chem. Theory Comput., vol. 14, no. 6, pp. 3252–3261, Jun. 2018. [2] S. Y. Mashayak, L. Miao, and N. R. Aluru, "Integral equation theory based direct and accelerated systematic coarse-graining approaches," J. Chem. Phys., vol. 148, no. 21, p. 214105, Jun. 2018. [3] A. Moradzadeh and N. R. Aluru, "Transfer-Learning-Based Coarse-Graining Method for Simple Fluids: Toward Deep Inverse Liquid-State Theory," J. Phys. Chem. Lett., vol. 10, no. 6, pp. 1242–1250, Mar. 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Coupling Hemodynamics with Mechanobiology in Patient-Specific Computational Models of Ascending Thoracic Aortic Aneurysms

Author(s): *Joan Laubrie, *Mines Saint-Etienne - Université de Lyon*; Jamal Mousavi, *Mines Saint-Etienne - Université de Lyon*; Raja Jayendiran, *Mines Saint-Etienne - Université de Lyon*; Stéphane Avril, *Mines Saint-Etienne - Université de Lyon*;

Background and Objective. The prevention of ascending thoracic aortic aneurysms (ATAAs), which affect thousands of persons every year worldwide, remains a major issue. ATAAs may be caused by anything that weakens the aortic wall. Altered hemodynamics, which concerns a majority of patients with bicuspid aortic valves, has been shown to be related to such weakening and to contribute to ATAA development and progression. However the underlying mechanisms remain unclear and computational modeling in this field could help significantly to elucidate how hemodynamics and mechanobiology interact in ATAAs. Methods. Accordingly, we propose a numerical framework combining computational fluid dynamics and 4D flow magnetic resonance imaging (MRI) coupled with finite element (FE) analyses to simulate growth and remodeling (G&R) occurring in patient-specific aortas in relation with altered hemodynamics. The geometries and the blood velocities obtained from 4D flow MRI are used as boundary conditions for CFD simulations. CFD simulations provide an estimation of the wall shear stress (WSS) and relative residence time (RRT) distribution across the luminal surface of the wall. An initial insult is then applied to the FE model of the aortic wall, assuming that the magnitude of the insult correlates spatially with the normalized RRT distribution obtained from CFD simulations. G&R simulations are then performed. The material behavior of each Gauss point in these FE models is evolved continuously to compensate for the deviation of the actual wall stress distribution from the homeostatic state after the initial insult. The whole approach has been applied on a cohort of healthy and diseased subjects. The G&R parameters are calibrated against previously established statistical models of ATAA growth rates. Results. Among the variety of results provided by G&R simulations, the analysis will focus especially on the evolution of the wall stiffness, which was shown to be a major risk factor for ATAAs. It is shown that the normalized RRT distribution plays a less critical role than parameters related to the G&R response, as for instance the rate of collagen production or cell mechanosensitivity. Conclusions. The findings obtained with the G&R computational framework show that patient-specific modeling coupling hemodynamics with mechanobiology is a promising approach to explore aneurysm progression.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Machine Learning Model for Phase-Field Informed Crystal Plasticity Shape Memory Alloy Effect

Author(s): *Jobin Joy, *Texas A&M University*; Pawan Chaugule, *Texas A&M University*; Rajendran Harikrishnan, *Texas A&M University*; Jean-Briac le Graverend, *Texas A&M University*; Dimitris Lagoudas, *Texas A&M University*;

In recent years, advancements in machine learning (ML) have provided promising tools for understanding and predicting material behaviors. In this work, we build an ML framework that will learn the coupling between different mechanisms in Shape Memory Alloy (SMA) behavior. As the first step, based on the aging conditions, statistical volume elements (SVEs) were generated from the phase-field model. The data used for ML training were then generated using these realistic phase-field microstructures in a finite-element crystal plasticity model, which is composed of slip and transformation systems to predict the plastic behavior in both the austenite and martensite phases and during phase transformation. The ML model was built using an architecture of artificial neural networks (ANNs). The uncertainty quantification is performed through multiple training of the data and analyzing the variability in the predictions. The developed ML framework can provide reasonable predictions for different microstructures, crystal orientations, and loading conditions by training with the crystal plasticity model results.

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Title: Towards full Eulerian Framework for Fluid-Solid-Heat Treatment

Author(s): *Joe Khalil, *Mines ParisTech - CFL - CEMEF*; Ramy Nemer, *Mines ParisTech - CFL - CEMEF*; Aurelien Larcher, *Mines ParisTech - CFL - CEMEF*; Rudy Valette, *Mines ParisTech - CFL - CEMEF*; Elisabeth Massoni, *Mines ParisTech - CFL - CEMEF*; Elie Hachem, *Mines ParisTech - CFL - CEMEF*;

Quenching is a very important cooling process adopted nowadays by most of the industries, in particular automotive, aerospace and nuclear industries. The importance of this process comes from its ability to control the microstructure, to have better thermal and mechanical properties, and to release residual stresses. Nevertheless, it is a very complex process since it includes several physical phenomena on both the fluid (quenchant) and the solid. On the fluid level, because of the direct contact with a hot surface, the fluid will evaporate and reach the boiling point. On the solid level it exists stresses, deformations that changes the piece shape, and phase transformation which will generate latent heat [1]. Khalloufi et al. [2] proposed an adaptive Eulerian framework to simulate evaporation and boiling at the same time. It was shown that this approach is efficient for multi-phase flows. This model, includes all the physical phenomena that exist on the interface during quenching. Its importance is its ability to give a real description of the heat transfer happening between the solid and the fluid. The temperature change in the solid will affect both the phase transformation and the mechanical response of the piece. In this work, a new hybrid model is developed to solve the boiling and evaporation, at the same time phase transformation parameters and the mechanical response. In a fluid-solid domain, Navier-Stokes coupled with the heat equation is solved to give a temperature distribution in the solid. In a solid domain only, the phase transformation parameters along with the stresses and deformations using a thermo-elastic solver [3] are calculated based on the temperature distribution transported from the fluid-solid domain. The novelty of this model, is the ability to work and interact with two domains simultaneously while using the same solver. Many test cases were done and validated through both experimental and numerical results. [1] S.-H. Kang and Y.-T. Im, “Three-dimensional thermo-elastic–plastic finite element modeling of quenchingprocess of plain-carbon steel in couple with phase transformation,”International Journal of MechanicalSciences, vol. 49, no. 4, pp. 423–439, 2007 [2] M. Khalloufi, R. Valette, and E. Hachem, “Adaptive eulerian framework for boiling and evaporation,”Journal of Computational Physics, vol. 401, p. 109 030, 2020,issn: 0021-9991 [3] R. Nemer, A. Larcher, T. Coupez, & E. Hachem (2021). “Stabilized finite element method for incompressible solid dynamics using an updated Lagrangian formulation.” arXiv preprint arXiv:2101.07057.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Porosity Growth and Plasticity Model for Under-Dense Material Subject to Extreme Loadings

Author(s): *John Moore, *Marquette University*; Nathan Barton, *Lawrence Livermore National Laboratory*;

With the advent of additive manufacturing (i.e., 3D-priting), under-dense materials have become versatile and controllable components of applications requiring high stiffness materials with low densities. Under-dense materials have high porosities and include: foams, lattice structured materials, triply periodic minimal surface materials, and a wide array on complex meta-materials. Applications range from bone replacements to energy absorbers. However, traditional porosity models are not generally built for such high porosities. Under-dense materials subject to extreme loadings from impacts and explosions show dramatic reductions in porosity and can become fully dense from compression. Many traditional porosity growth models also cannot address this large range of porosities. The proposed work extends the Cocks-Ashby porosity growth model [1] to address high initial porosities and large ranges in porosity values. The model also incorporates the effects of micro-inertia specially formatted for under-dense material [2]. The model's results are compared to direct numerical simulations of under-dense material during high velocity impacts. The ability of the model to address such complex extreme loadings and associated calibration procedures are highlighted. This work was performed, in part, under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Release number LLNL-ABS-818519. [1] Cocks, A. C. F., and M. F. Ashby. "On creep fracture by void growth." Progress in materials science 27, no. 3-4 (1982): 189-244. [2] Barthélémy, Romain, Nicolas Jacques, Steven Kerampran, and Fabrice Vermeersch. "Modelling of micro-inertia effects in closed-cell foams with application to acoustic and shock wave propagation." International Journal of Solids and Structures 97 (2016): 445-457.

16th U.S. National Congress on Computational Mechanics
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Title: Accelerating Real-Space Electronic Structure Methods by Discontinuous Projection

Author(s): *John Pask, *Lawrence Livermore National Laboratory*;

By virtue of multiple advances over the past two decades, real-space electronic structure methods have surpassed planewave methods in large-scale calculations of isolated and extended systems alike. Combining advances in both finite-difference and finite-element methods, we discuss a new approach to accelerate real-space methods further still, while retaining the simplicity, systematic convergence, and parallelizability inherent in the methodology. The key idea is to compress the large, sparse real-space Hamiltonian by projection in a strictly local, systematically improvable, discontinuous basis spanning the occupied subspace. We show how this basis can be constructed and employed to reduce the dimension of the real-space Hamiltonian by up to three orders of magnitude. Molecular dynamics step times of a few minutes for systems containing thousands of atoms demonstrate the scalability of the methodology in a discontinuous Galerkin formulation. Results for 1D, 2D, and 3D systems demonstrate the additional advantages afforded by the new projection formulation [1]. [1] J. Chem. Phys. 149, 094104 (2018). This work was performed, in part, under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Reduced-Order Modeling of the Circulation During Cardiovascular Stress

Author(s): *Joseph Muskat, *Purdue University*; Vitaliy Rayz, *Purdue University*; Craig Goergen, *Purdue University*; Charles Babbs, *Purdue University*;

Utilizing reduced-order models based upon an electrical transmission line analogy, we simulated blood flow in the major systemic vessels of the trunk, limbs, and head to investigate the hemodynamic effects of two states of cardiovascular stress (i.e., fear and aerobic exercise). We based blood vessel dimensions on modern high-resolution anatomical datasets obtained from medical imaging (taken from 2010 – present) with a focus on young, active humans. Wave propagation is initialized by a pressure-controlled pump mimicking the myocardial contraction of the left ventricle. The vasculature is modeled with a network of lumped elements (0.5 cm or smaller arterial segments) together with peripheral three-element Windkessel boundaries which are connected to the pump via a lumped venous compartment to form a closed-loop system. The transmission line equations are numerically integrated, using the explicit Euler method, to determine instantaneous changes in flow rates (i.e., electrical current) and pressures (i.e., electrical voltage) in all segments. We compared simulated time domain waveforms of diameter (D) and flow velocity (U) in the common carotid and femoral arteries to published experimental recordings (1–3). As indicated in (2), local wave speed may be described by the linear relationship between lnD and U. Carotid and femoral lnDU-loops demonstrate physiologically realistic increases in pulse wave velocities within anticipated ranges for rest (400 – 650 cm/s), fear (650 – 800 cm/s), and exercise (700–1200 cm/s) simulations. The developed model is useful in studying the effects of cardiovascular stress on pulse waveforms of the peripheral vasculature, such as in the cerebral circulation. In particular, model predictions indicate bi-directional shunting through communicating arteries of the circle of Willis increases with cardiovascular stress. Our updated anatomical dataset is available for public access and allows for patient-specific assessment of hemodynamics in the human circulatory system. These computationally efficient models may also be coupled with the one-dimensional transport equations to predict the propagation of various agents through the vascular system. 1. A Borlotti et al. J Appl Physiol 113: 727–735, 2012. 2. Feng J, Khir AW. J Biomech 43: 455–462, 2010. 3. N Pomella et al. Am J Physiol - Hear Circ Physiol 315: H233–H241, 2018.

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Title: Computational Models for Fluid-to-Solid Transitions in Yield Stress Fluids

Author(s): *Josh McConnell, *Sandia National Laboratories*; Weston Ortiz, *University of New Mexico*; Anne Grillet, *Sandia National Laboratories*; Pania Newell, *The University of Utah*; Rekha Rao, *Sandia National Laboratories*;

Materials that behave as both fluids and solids can be seen in a wide variety of applications from pouring concrete to lava flows and food processing. Yield stress is a useful concept for developing models that demonstrate both fluid and solid behavior depending on the local state of the fluid. In this talk, we will discuss an ongoing project to use elastoviscoplastic models to understand the complex flow profiles of a model yield stress fluid, Carbopol, as it evolves in time in a free surface flow. We use a Saramito model to describe the rheology of the fluid (Saramito, "A new constitutive equation for elastoviscoplastic fluid flows." Journal of Non-Newtonian Fluid Mechanics 145.1 (2007): 1-14). This model describes the material as a Maxwell fluid above yield and an elastic solid below yield, with a yield criterion based on the von Mises stress. Conservation equations for momentum and mass and the Saramito constitutive equations for stress are solved using the finite element method coupled to a free-surface moving mesh algorithm. We verify our implementation by comparing our results to benchmarks in the literature such as flow past a sphere and a ball falling in a tube full of yield stress fluid. Furthermore, we compare results from mold filling simulations to validation flow visualization experiments in a quasi-two-dimensional flow where fluid fills a thin gap between transparent plates. The experiments show regions of low strain where the fluid displaces as a solid body and high strain regions where the Carbopol is fluidized. The computational model matches qualitatively for the yield stress fluid. Future work with include a thixotropic component to the model to improve predictions. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: A Solution Strategy for Fluid-Structure Interaction Using the Unified Continuum Formulation, Quasi-Direct Coupling, and Nested Block Preconditioning

Author(s): *Ju Liu, *Southern University of Science and Technology*;

In this work, we first review the unified continuum modeling framework for viscous fluids and hyperelastic solids using the Gibbs free energy as the thermodynamic potential, which was originally proposed in [1]. This framework naturally leads to a pressure primitive variable formulation for the continuum body, which is well-behaved in both compressible and incompressible regimes. We perform a variational multiscale (VMS) analysis for this general continuum model, and the resulting formulation recovers the residual-based VMS formulation for the Navier-Stokes equations. For hyperelastic materials, this VMS formulation provides a mechanism to circumvent the inf-sup condition for low-order tetrahedral elements. For the fully discrete problem, a block factorization is performed for the consistent tangent matrix, which reduces the linear algebra problem to a simpler one with a two-by-two block structure. This naturally leads to the quasi-direct coupling method for fluid-structure interaction (FSI) problems, which is amenable to implementation within existing software framework. As a generalization of the conventional block preconditioners, a three-level nested block preconditioner using Schur complement reduction is introduced to attain a better representation of the Schur complement, which plays a key role in the overall algorithm robustness and efficiency [2,3]. This approach provides a flexible, algorithmic way to represent the Schur complement for problems involving multiscale and multiphysics coupling. The robustness, efficiency, and parallel scalability of the proposed technique are then examined in several settings, including the tensile test of an incompressible anisotropic hyperelastic arterial wall model, moderately high Reynolds number flows, vortex induced beam vibration, and physiological flows with strong resistance effect due to the downstream vasculature model. [1] J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. Computer Methods in Applied Mechanics and Engineering, 337:549--597, 2018. [2] J. Liu and A.L. Marsden. A robust and efficient iterative method for hyper-elastodynamics with nested block preconditioning. Journal of Computational Physics, 383:72-93, 2019. [3] J. Liu, W. Yang, M. Dong, and A.L. Marsden. The nested block preconditioning technique for the incompressible Navier-Stokes equations with emphasis on hemodynamic simulations. Computer Methods in Applied Mechanics and Engineering, 367:113122, 2020.

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Title: A DPG-Based Time-Marching-Scheme for Linear Transient Problems

Author(s): *Judit Muñoz-Matute, *The University of Texas at Austin*; David Pardo, *University of the Basque Country*; Leszek Demkowicz, *The University of Texas at Austin*;

The Discontinuous Petrov-Galerkin (DPG) method with optimal test functions is a well stablished method to approximate the solution of Partial Diff erential Equations (PDEs). The main idea of this method is to select optimal test functions that guarantee the discrete stability of non-coercive problems. For that, we employ test functions that realize the supremum in the inf-sup condition. It has been previously applied to transient problems in the context of space-time formulations or together with fi nite differences in time. In this work, we follow the approach of applying the DPG method only in the time variable in order to obtain a DPG-based time-marching scheme for linear transient PDEs. We fi rst semidiscretize in space by a classical Bubnov-Galerkin method and we consider an ultraweak variational formulation of the resulting system of Ordinary Diff erential Equations (ODEs). Then, we calculate the optimal test functions analytically employing the adjoint norm. The optimal test functions are in this case exponential-related functions of the stiff ness matrix. Finally, we substitute the optimal test functions into the ultraweak variational formulation and we obtain the DPG-based time-marching scheme. Here, we obtain an independent formula for the trace variables and a system to locally compute the interiors of the elements. The equation we obtain for the trace variables is called variation-of-constants formula and it is the starting point of the so-called of exponential integrators for solving systems of ODEs. In these type of methods, it is necessary to approximate the exponential of the stiff ness matrix and related functions called phi-functions. Although the theory of exponential integrators is classical, they have recently gained popularity due to the rise of the available software and efficient algorithms to compute the action of function matrices over vectors. We express the DPG-based time-marching scheme in terms of the phi-functions in order to employ the software available from the exponential integrators community. We show the performance of our method for 2D/3D+time parabolic and hyperbolic problems. References: 1.- J. Muñoz-Matute, D. Pardo, and L. Demkowicz. A DPG-based time-marching scheme for linear hyperbolic problems. Computer Methods in Applied Mechanics and Engineering, 373:113539, 2020. 2.- J. Muñoz-Matute, D. Pardo, and L. Demkowicz. Equivalence between the DPG method and the Exponential Integrators for linear parabolic problems. Journal of Computational Physics, in press, 2020.

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Title: Data-Driven Learning of Effective Coefficients from Multiscale Data

Author(s): *Jun Sur Park, *University of Iowa*; Xueyu Zhu, *University of Iowa*;

Multiscale equations with scale separation can be approximated by corresponding homogenized equations with slowly varying effective (homogenized) coefficients. Recovering the homogenized model from multiscale data measurement is a difficult task as it is typically ill-posed. In this work, we develop an efficient Physics-informed neural networks (PINNs) algorithm for recovering the effective coefficients given (noisy) multiscale solution data. We demonstrated that our approach could produce desirable approximations to the effective coefficients and, consequently, homogenized solutions via a small amount of data. Besides, we demonstrate the robustness of our method via several benchmark examples with both noise-free and noisy solution data.

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Title: Multi-Physics Modeling of Electrochemical Deposition

Author(s): *Justin Kauffman, *Virginia Tech*; John Gilbert, *Virginia Tech*; Eric Paterson, *Virginia Tech*;

Electrochemical deposition (ECD) is a common method used in the field of microelectronics to grow metallic coatings on an electrode. The deposition process occurs in an electrolyte bath where dissolved ions of the depositing material are suspended in an acid while an electric current is applied to the electrodes. The proposed computational model utilizes the finite volume method and the finite area method to predict copper growth on the plating surface without the use of a level set method or deforming mesh because the amount of copper layer growth is not expected to impact the fluid motion. The finite area method enables the solver to track the growth of the copper layer and utilizes the current density as a forcing function for an electric potential field on the plating surface. The current density at the electrolyte-plating surface interface is converged within each PISO (Pressure Implicit with Splitting Operator) loop iteration and incorporates the variance of the electrical resistance that occurs via the growth of the copper layer. This presentation will demonstrate the application of the finite area method for an ECD problem and additionally incorporates coupling between fluid mechanics, ionic diffusion, and electrochemistry for a strongly coupled multi-physics simulation.

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Title: A Physics-Based Crystal Plasticity Model for the Prediction of the Microstructural Evolutions as well as GND and SSD Densities in Metals and Alloys.

Author(s): *Juyoung Jeong, *Louisiana State University*; George Z. Voyiadjis, *Louisiana State University*;

A physics-based crystal plasticity model is developed to address the dislocation motion in metals. The model encompasses the heterogeneous deformation in the microstructure and its evolution expressed through the geometrically necessary dislocation (GND) densities and statistically stored dislocations (SSD) densities. The description of the SSD densities contributes to the dislocation densities evolutions including generation, annihilation, and interactions as metals are hardened. The evolution laws are expressed by coupling between mobile and immobile SSD dislocations. The main feature of this work is that not only GND densities but mobile/immobile SSD densities are also incorporated in the evolution of microstructure serving the strain hardening stages of metals and alloys. We perform a wedge indentation simulation for a nickel single crystal by comparing computational simulation results are compared with the released experiment (Kysar et al. 2010) in terms of predicts GND densities and non-zero Nye dislocation density tensor. The nonlocal model clarifies the accurate prediction of the complex microstructural evolutions as well as GND and SSD densities in metals and alloys.

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Title: The Shifted Fracture Method

Author(s): *Kangan Li, *Duke University*; Nabil Atallah, *Duke University*; Antonio Rodr ??guez-Ferran, *Universitat Polite`cnica de Catalunya*; Guglielmo Scovazzi, *Duke University*;

We propose a new framework for fracture mechanics, based on the idea of an approximate fracture geometry representation combined with approximate interface conditions. Our approach evolves from the shifted interface method, and introduces the concept of an approximate fracture surface composed of the full edges/faces of an underlying grid that are geometrically close to the true fracture geometry. The original interface conditions are then modified on the surrogate fracture, by way of Taylor expansions, to achieve a prescribed level of accuracy. The shifted fracture method does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with specific integrals on the approximate fracture. Furthermore, the energetics of the true fracture are represented within the prescribed level of accuracy and independently of the grid topology. The computational framework is presented here in its generality and then applied in the specific context of cohesive zone models, with an extensive set of numerical experiments in both 2D and 3D.

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Title: Dynamic Brittle Fracture of Thin Shell Structures based on a High-Order Phase Field Approach

Author(s): *Karsten Paul, *RWTH Aachen University*; Thomas J.R. Hughes, *The University of Texas at Austin*; Chad M. Landis, *The University of Texas at Austin*; Roger A. Sauer, *RWTH Aachen University*;

During the previous decade, phase field approaches for fracture prediction have gained popularity because they do not require interface tracking or the definition of ad hoc criteria. In the present work, brittle fracture of thin shell structures is investigated. The shell theory is formulated within a curvilinear coordinate system and kinematics follow from Kirchhoff-Love theory [1]. The phase field framework for dynamic brittle fracture is also formulated in the convective coordinate system and the membrane and bending energies are decomposed separately into a part that contributes to fracture, and a part that does not. The required higher continuity is obtained by means of an isogeometric discretization and Locally Refinable (LR) splines are used for the adaptive local refinement in space [2]. Numerical examples show complex fracture patterns on single- and multi-patch geometries. For the latter, continuity constraints are employed to enforce the higher continuity required across patch interfaces [3]. [1] T.X. Duong, F. Roohbakhshan, R.A. Sauer, A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries, Comput. Methods Appl. Mech. Engrg. 316, 2017 [2] K.Paul, C. Zimmermann, K.K. Mandadapu, T.J.R. Hughes, C.M. Landis, R.A. Sauer, An adaptive space-time phase field formulation for dynamic fracture of brittle shells based on LR NURBS, Comp. Mech. 65, 2020 [3] K. Paul, C. Zimmermann, T.X. Duong, R.A. Sauer, Isogeometric continuity constraints for multi-patch shells governed by fourth-order deformation and phase field models, Comput. Methods Appl. Mech. Engrg. 370, 2020

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Title: Multi-Output Surrogate Construction for Fusion Simulations

Author(s): *Kathryn Maupin, *Sandia National Laboratories*; Anh Tran, *Sandia National Laboratories*;

As the third pillar of science, computational simulation has allowed scientists to explore, observe, and test physical regimes previously thought to be unattainable. High-fidelity models are derived from physical principles and calibrated to experimental data. However, missing or unknown physics and measurement, experimental, and numerical errors give rise to uncertainties in model form and parameter values in even the most trustworthy models. Thus, uncertainty quantification plays a crucial role in computational modeling. Bayesian analysis provides a natural framework for incorporating the uncertainties that undeniably exist in computational modeling. However, the ability to perform quality Bayesian and uncertainty analyses is often limited by the computational expense of first-principles physics models. In the absence of a reliable low-fidelity physics model, phenomenological surrogate models can be used to mitigate the expense of performing Bayesian analysis and uncertainty quantification; however, phenomenological models may not adhere to known physics or properties. Furthermore, the interactions of complex physics in high-fidelity codes lead to dependencies between quantities of interest (QoIs) that are difficult to quantify and capture when individual surrogates are used for each observable. In applications that consider multiple QoIs simultaneously, separate Gaussian Processes (GPs) are constructed for each QoI. This results in a loss of valuable information regarding the correlated behavior of QoIs, which is detrimental to calibration efforts for which data is limited. Predicting multiple QoIs with a single GP preserves valuable insights regarding the correlated behavior of the target observables and maximizes the information gained from available data. We present a method of constructing GPs that emulate multiple QoIs simultaneously. As an exemplar, we consider Magnetized Linear Inertial Fusion, a fusion concept that relies on the direct compression of magnetized, laser-heated fuel by a metal liner to achieve thermonuclear ignition. Plasma physicists rely on diagnostic metrics to infer the state of the fuel, as direct observation of the physical system is not possible. However, the calibration of these metrics is complicated by sparse experimental data and expensive high-fidelity neutron transport models. The use of a surrogate is therefore warranted, the development of which raises long-standing issues in modeling and simulation, including calibration, validation, and uncertainty quantification. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell In- ternational Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: Control Informed Fully Resolved Multiphase Simulations of Wave Energy Converters

Author(s): *Kaustubh Khedkar, *San Diego State University*; Amneet Bhalla, *San Diego State University*;

A significant amount of modeling accuracy can be achieved by solving the non-linear incompressible Navier-Stokes equations to simulate the wave energy converter (WEC) dynamics and to test different types of controllers in a more realistic setting. Simulating WEC devices involves complex fluid-structure interactions. We make use of the fictitious domain Brinkman penalization (FD/BP) technique which is found to be computationally more efficient when compared to the body-conforming grid techniques. The FD/BP technique involves solving fluid equations in the entire domain including the solid domain. To enforce the rigidity of the solid body, an additional penalization force term is included in the fluid equations. To track the solid, liquid, and gas phases, two-level set functions are defined. A multiphase flow solver that is robust, second-order accurate, and preserves stability in the case of high-density ratio flows is implemented on adaptive and locally refined Cartesian grids. We simulate fully resolved multiphase simulations of a vertical heaving cylinder at the air-water interface in a numerical wave tank (NWT) for regular and irregular sea waves. The model predictive control (MPC) with a receding horizon strategy is used to optimize the performance of the vertical heaving cylinder type WEC. The objective function is to maximize the mechanical energy absorption by the power take-off (PTO) system over a moving time horizon. The Auto-regressive model is used to predict the future wave elevations from the past data collected by a sensor located at a pre-calculated distance in front of the body. Path constraints on the displacement, velocity, and control input are implemented. To reduce the aggressiveness of the controller and to limit two-way power flow at the PTO system, penalty terms are added to the objective function. Results show that the fully resolved multiphase simulations are closer to reality than the boundary element method (BEM) based linear potential flow theory model that overpredicts the WEC dynamics.

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Title: Noise Evaluation System Based on Fast Multipole Boundary Element Method and VR Technology

Author(s): *Kazuo Kashiyama, *Chuo University*; Makoto Shoji, *Chuo University*; Kazushi Fukazawa, *Chuo University*; Hitoshi Yoshikawa, *Kyoto University*;

The evaluation of noise is very important for planning and designing of various construction works in an urban area. There have been presented a number of evaluation methods for noise simulation. Based on the frame of reference used, those methods can be classified into two categories: 1) Methods based on the geometrical acoustic theory and 2) Methods based on acoustic wave theory. Both methods have advantages and disadvantages. For the methods based on the geometrical acoustic theory, the CPU time is very short but the numerical accuracy is low comparing with the methods based on the acoustic wave theory. On the other hand, the method based on the acoustic wave theory gives accurate solution but the simulation becomes a large scale simulation. In the conventional studies, the computed noise level is described by the visualization using computer graphic such as iso-surface. Although the visualization is a powerful tool to understand the distribution of noise, it is difficult to recognize the noise level intuitively. In this presentation, an experience based noise evaluation system using virtual reality technology is presented. The fast multipole boundary element method is employed for the system based on the wave acoustic theory. The system exposes to the users the computed noise level with both the auditory information using sound source signal and the visual information using CG image. In order to investigate the validity and efficiency of the method, we performed the observation of construction noise. The present system is useful for planning and designing tools for various constructions works in an urban area, and also for consensus building for designers and the local residents.

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Title: Continuum Modeling of Thromboembolism: Embolization of Formed Clots in a Sudden Expansion

Author(s): Nick Tobin, *The Pennsylvania State University*; *Keefe Manning, *The Pennsylvania State University*;

Simulations are presented of the breakdown and embolization of a blood clot in a cylindrical geometry with a sudden expansion. Thrombosis and thromboembolism are major risk factors in blood-contacting medical devices such as stents, prosthetic valves, grafts, and pumps, and investigating the mechanics of embolization is challenging. Clots are modeled with a modified Phan-Thien-Tanner [1] viscoelastic model that solves separate evolution equations for a cohesive link density, and a cohesive stress, which couples clot behavior to the fluid flow [2]. A clot grows for 15 minutes of simulated time at conditions matching previous MRI experiments [3]. These MRI results are also used to fit the growth and decay functions in the viscoelastic model. After the clot is formed, the flow rate through the domain is increased to encourage thromboembolization. At modestly higher laminar flow rates, the clot adjusts to the change in flow conditions by changing shape over several minutes and breaks down slowly without significant macro-embolization. In contrast, at transitional and turbulent Reynolds numbers, the shape of the clot is significantly disturbed and portions embolize in the span of several seconds. These results highlight the risk of rapidly changing flow conditions in the progression from thrombosis to thromboembolism. Future work will focus on evaluating the predictive value of this model in identifying embolism risk factors in blood-contacting medical devices. [1] Thien, Nhan Phan, and Roger I. Tanner. "A new constitutive equation derived from network theory." Journal of Non-Newtonian Fluid Mechanics 2.4 (1977): 353-365. [2] Fogelson, Aaron L., and Robert D. Guy. "Immersed-boundary-type models of intravascular platelet aggregation." Computer methods in applied mechanics and engineering 197.25-28 (2008): 2087-2104. [3] Yang, Ling, Thomas Neuberger, and Keefe B. Manning. "In vitro real-time magnetic resonance imaging for quantification of thrombosis." Magnetic Resonance Materials in Physics, Biology and Medicine (2020): 1-11.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Manifold-Based Optimization for Constrained Trajectories

Author(s): Cosmin Safta, *Sandia National Laboratories*; *Kelli McCoy, *University of Southern California*; Roger Ghanem, *University of Southern California*;

We demonstrate the Probabilistic Learning on Manifolds (PLoM) on the problem of constrained path planning of autonomous aerial vehicles. The task at hand is to anticipate the remaining path, having traversed a portion of an actual trajectory, and having trained on a particular multi-fidelity set of trajectories. The problem of one of conditional estimation, which typically requires a very large training set as it involves estimation in high-dimensional space. We leverage a hierarchy of model fidelities, with the manifold structure determined by low-fidelity model solutions augmented with a subset of higher fidelity models. We are then in a position to cast the constrained optimization task as a problem of conditional estimation. We are aided in this task by an projected MCMC algorithm for augmenting the training set, constrained to the instrinsic structure, as required by statistical tolerances.

16th U.S. National Congress on Computational Mechanics
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Title: Scale Resolving Simulations of a Bump with Strong Favorable and Adverse Pressure Gradients

Author(s): *Kenneth Jansen, *University of Colorado Boulder*; Riccardo Balin, *University of Colorado Boulder*; James Wright, *University of Colorado Boulder*; John Evans, *University of Colorado Boulder*;

The turbulent boundary layer over a Gaussian shaped bump is computed by direct numerical simulation (DNS), wall resolved large eddy simulation (WRLES), wall modeled large eddy simulation (WMLES), and Reynolds averaged Navier-Stokes (RANS) simulations. The two-dimensional bump causes strong and rapidly switching pressure gradients. At the inflow, the momentum thickness Reynolds number is approximately $1,000$ and the boundary layer thickness is $1/8$ of the bump height. The DNS results show that the strong favorable pressure gradient (FPG) causes the boundary layer to enter a relaminarization process. The near-wall turbulence is significantly weakened and becomes intermittent, however relaminarization is incomplete. The streamwise velocity profiles deviate above the standard logarithmic law and the Reynolds shear stress is reduced. The strong acceleration also suppresses the wall-shear normalized turbulent kinetic energy production rate. Ahead of the bump peak, the FPG switches to an adverse gradient (APG) causing a sudden enhancement of turbulence much like a transition process. The result is a new highly energized internal layer which is therefore much more resilient to the strong APG and only produces incipient flow separation on the downstream side of the bump. The near-wall region responds to the pressure gradients and determines the skin friction. These conditions provide very difficult challenges to both forms of LES and for RANS. Results from all SRS and RANS simulations of the bump are also discussed and clearly show the lack of predictive capacity of the near-wall pressure gradient effects on the mean flow.

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Title: An Algorithm for Temporal Scale-bridging of Chemistry in a Multiscale Model of a Reacting Energetic Material

Author(s): *Kenneth Leiter, *CCDC US Army Research Laboratory*; James Larentzos, *CCDC US Army Research Laboratory*; Brian Barnes, *CCDC US Army Research Laboratory*; Richard Becker, *CCDC US Army Research Laboratory*; Jaroslaw Knap, *CCDC US Army Research Laboratory*;

In models of energetic materials, capturing the coupling between deformation and chemistry is crucial to obtain accurate predictions of material behavior. Multiscale modeling promises to enable the development of models which capture the coupling between deformation and chemistry through the incorporation of individual models that explicitly resolve both processes at their appropriate scales, but challenges remain to bridge the scales due to the vastly different time scales present. In this talk, we introduce a multiscale model of the energetic material 1,3,5-trinitrohexahydro-s-triazine (RDX) which incorporates chemical kinetics. The multiscale model consists of two at-scale models: a macroscale continuum finite element model of a deforming body and a microscale dissipative particle dynamics model that includes chemical reactivity (DPD-RX). The macroscale model propagates its solution forward in time using a multiscale integration scheme that requires the evaluation of the microscale model under two distinct conditions: 1) at constant energy, density, and material composition to obtain the equation of state of the material at equilibrium; 2) under a prescribed energy input and volume change to obtain the instantaneous rates of change of the chemical composition. We will discuss challenges associated with obtaining accurate quantities from the DPD-RX model and discuss how the rates of change of the chemical composition are incorporated into the macroscale model and the material composition propagated forward in time. We will utilize the model to perform several simulations of RDX decomposition including simulations of a plate impact experiment and a scaled thermal explosion (STEX) experiment.

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Title: Human Mobility and the Outbreak Dynamics of COVID-19

Author(s): *Kevin Linka, *Stanford University*; Mathias Peirlinck, *Stanford University*; Ellen Kuhl, *Stanford University*;

The spreading of infectious diseases including COVID-19 depends on human interactions. In an environment where behavioral patterns and physical contacts are constantly evolving according to new governmental regulations, measuring these interactions is a major challenge. Mobility has emerged as an indicator for human activity and, implicitly, for human interactions. Here, we study the coupling between mobility and COVID-19 dynamics and show that variations in global air traffic and local driving mobility can be used to stratify different disease phases [1]. We propose a dynamic SEIR epidemiology model with a time-varying reproduction number, which we identify using machine learning. We found a strong correlation between passenger air travel, driving, walking, and transit mobility and the effective reproduction number with a time lag of 17.2 ± 2.0 days. Our findings suggest that trends in local mobility allow us to forecast the outbreak dynamics of COVID-19 for a window of two weeks and adjust local control strategies in real time [2]. Moreover, our new dynamic SEIR model provides the flexibility to simulate various outbreak control and exit strategies to inform political decision making and identify safe solutions in the benefit of global health. [1] Linka, K., Goriely, A. & Kuhl, E., Global and local mobility as a barometer for COVID-19 dynamics. Biomech Model Mechanobiol (2021). https://doi.org/10.1007/s10237-020-01408-2 [2] Linka, K., Peirlinck, M. & Kuhl, E. The reproduction number of COVID-19 and its correlation with public health interventions. Comput Mech 66, 1035–1050 (2020). https://doi.org/10.1007/s00466-020-01880-8

16th U.S. National Congress on Computational Mechanics
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Title: An Optimally Convergent Partition-of-Unity B-spline Construction for Unstructured Quadrilateral and Hexahedral Meshes

Author(s): *Kim Jie Koh, *University of Cambridge*; Eky Febrianto, *University of Cambridge*; Deepesh Toshniwal, *Delft University of Technology*; Fehmi Cirak, *University of Cambridge*;

The construction of optimally convergent B-splines for unstructured quadrilateral and hexahedral meshes is still an open challenge in isogeometric analysis. We present an optimally convergent partition-of-unity B-spline construction which is applicable both to unstructured quadrilateral and hexahedral meshes. We blend B-splines with a set of enrichment functions to yield smooth basis functions around extraordinary vertices and edges in the mesh. Similar to the construction of manifold-based basis functions for unstructured quadrilateral meshes (Majeed and Cirak, 2017; Zhang and Cirak, 2020), the partition-of-unity method is used for constructing the new basis functions. In contrast to the manifold-based constructions, our proposed construction is conceptually simpler and generalises to unstructured hexahedral meshes. We show that the weight functions required for the blending can be defined directly using B-splines. As a result, the resulting basis functions are polynomials of relatively low degree so that they can be efficiently numerically integrated. The proposed method is particularly appealing for unstructured meshes with only a few extraordinary features (Wei et al., 2018). In summary, we obtain optimally convergent basis functions in closed form that are smooth around extraordinary vertices and edges, linearly independent, non-negative and low in polynomial degree. Majeed, M., and Cirak, F. (2017). Isogeometric analysis using manifold-based smooth basis functions. Computer Methods in Applied Mechanics and Engineering, 316, 547-567. Wei, X., Zhang, Y. J., Toshniwal, D., Speleers, H., Li, X., Manni, C., Evans, J. A., and Hughes, T. J. (2018). Blended B-spline construction on unstructured quadrilateral and hexahedral meshes with optimal convergence rates in isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 341, 609-639. Zhang, Q., and Cirak, F. (2020). Manifold-based isogeometric analysis basis functions with prescribed sharp features. Computer Methods in Applied Mechanics and Engineering, 359, 112659.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling Analysis of UNSM's Effect on Residual Stress in Laser Directed Energy Deposition

Author(s): *Kishore Mysore Nagaraja, *The University of Texas at Dallas*; Wei Li, *The University of Texas at Dallas*; Youngsik Pyun, *Sunmoon University*; Dong Qian, *The University of Texas at Dallas*;

Laser Directed Energy Deposition (L-DED) is an advanced additive manufacturing process in which a high-power laser beam coaxially aligned with the flow of powder particles is irradiated onto a substrate forming a local melting pool. Like many other AM processes, DED can lead to residual stresses that critically affect the service life of AMed parts/products. While post-processing techniques such as heat treatment, laser shock peening, and others have been developed, these techniques only address residual stress at the surface level approximately up to 20 microns depth. In this work, we present computational studies on an innovative in-situ surface engineering approach called Ultrasonic Nanocrystal Surface Modification (UNSM). By generating severe plastic deformation using an ultrasonic vibration mechanism, UNSM not only converts the tensile stress into compressive but also refines the microstructure locally which improves the wear resistance. To study the effect of UNSM on the DED components, two different computational modeling techniques have been developed. Firstly, a combined discrete element method/computational fluid dynamics approach has been employed to capture the DED process. Based on an Eulerian-to-Lagrangian mesh coupling scheme, the simulation results obtained from the DED simulation serve as the inputs for FEM in predicting the effects of UNSM. We show that the developed computational approach can well capture the surface geometry and roughness, defects, precise laser modeling, and layer characteristics from DED. Furthermore, the computational study shows that UNSM treatment over the DED component effectively shifts the tensile residual stresses into compressive ones for each layer that is deposited. The computational predictions are also validated with the experimental results published in the literature. Keywords: Direct Energy Deposition, Ultrasonic Nanocrystal Surface Modification, Residual Stress, Laser Directed Additive Manufacturing Process.

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Title: Randomized Multilevel Monte Carlo Methods for Inference

Author(s): *Kody Law, *University of Manchester*; Ajay Jasra, *King Abdullah University of Science and Technology*;

Multilevel Monte Carlo (MLMC) methods have recently gained a lot of attention as an option for the solution of Bayesian inverse problems. An attractive alternative is randomized MLMC (rMLMC) where one samples from an appropriate distribution on the integers with corresponding decreasing schedule of samples, instead of utilizing a fixed finite hierarchy. Through a double application of this technology we are able to achieve unbiased estimation for Bayesian inverse problems. Benefits include that (i) this bypasses cumbersome tuning related to bias, (ii) such i.i.d. sampling is `embarrassingly parallel', and (iii) unbiased estimates are preferable in the context of stochastic gradient descent methods. The approach will be illustrated for estimating the gradient of the log (marginal) likelihood with multilevel sequential Monte Carlo (MLSMC) samplers and applied within stochastic gradient descent for maximum a posteriori estimation of (hyper)parameters. Time permitting, I will summarize analogous results for unbiased online particle filtering and unbiased Markov chain Monte Carlo.

16th U.S. National Congress on Computational Mechanics
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Title: Semi-Implicit Eulerian Formulation Using Marker Particles with a Reference Map for Fluid-Structure Interaction Problems

Author(s): *Koji Nishiguchi, *Nagoya University*; Tokimasa Shimada, *Kobe University*; Hiroya Hoshiba, *Nagoya University*; Junji Kato, *Nagoya University*;

The authors have been developing a full Eulerian scheme for nonlinear solid dynamics [1] and a full Eulerian fluid-structure interaction (FSI) scheme using a fixed hierarchical Cartesian mesh suitable for large-scale parallel computing [2]. However, a full Eulerian method cannot avoid the numerical dissipation of material interfaces and history-dependent solid variables due to the advection. Due to this problem, full Eulerian methods cannot accurately compute geometrically complex structures or solid with many history-dependent variables. Given the background mentioned above, in this work, we propose an Eulerian fluid-structure interaction scheme using marker particles with a reference map, which is the initial position vectors of the solid region. To avoid numerical dissipation of material interfaces and history-dependent variables of solid, marker particles represent the solid region and carry history-dependent variables. We propose a novel semi-implicit scheme using a fourth-order Jacobian tensor to relax time-step size limitation in the present method. To verify the current approach, we will demonstrate several numerical examples in the presentation. [1] Nishiguchi K, Okazawa S, Tsubokura M. Multimaterial Eulerian finite element formulation for pressure-sensitive adhesives. International Journal for Numerical Methods in Engineering 2018; 114:1368-1388. https://doi.org/10.1002/nme.5790 [2] Nishiguchi K, Bale R, Okazawa S, Tsubokura M. Full Eulerian deformable solid-fluid interaction scheme based on building-cube method for large-scale parallel computing. International Journal for Numerical Methods in Engineering 2019; 117:221-248. https://doi.org/10.1002/nme.5954

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Title: A Nonlinear Fibrous Viscoelastic Model Describes the Experimental Tensile Behavior of Human Cervix

Author(s): Lei Shi, *Columbia University*; Joy Vink, *Columbia University Irving Medical Center*; Ronald Wapner, *Columbia University Irving Medical Center*; *Kristin Myers, *Columbia University*;

Cervical remodeling during pregnancy is characterized by a dramatic softening of the cervical tissue to allow for the safe passage of the fetus. The cervix is a soft tissue mainly composed of cross-linked collagen fibers embedded in a compressive groundsubstance formed by the negatively charged proteoglycans and glycosaminoglycans [1]. Cervical tissue exhibits complex material properties such as anisotropy and viscoelasticity, due to its hydrated biological composition. Cervical viscoelasticity is an important factor in pregnancy because the tissue must be viscoelastic so it does not break under large deformation. The cervical viscoelasticity evolves significantly in cervical remodeling as shown in mouse mechanical studies [2]. The aim of this work is to describe the viscoelastic behavior of the human cervix under uniaxial tensile tests by proposing a nonlinear continuous fibrous viscoelastic constitutive model. Four non-pregnant and three pregnant human cervices were obtained from consented hysterectomy patients at Columbia University Irving Medical Center. Multiple-level load-hold and load-unload uniaxial tensile experiments, coupled with video extensometry, were conducted on human cervical strip samples from different anatomical locations. The constitutive model was established based on the Bergstrom-Boyce flow rate law [3] in a continuous fibrous framework with a von-Mises distribution to account for anisotropy. The constitutive model was coded as a plugin of FEBio (V2.9.1, url: febio.org) and the FEA analysis was done in FEBio to simulate the experiments. Inverse finite element analysis (IFEA) was utilized to fit the fibrous viscoelastic constitutive model to tensile force responses, and the best-fit material parameters were obtained. Differences in material properties between pregnant and nonpregnant samples were analyzed. The material behavior is found sensitive to loading rate. The preliminary result shows the constitutive model fits the experimental data well. The cervix remodels to relax more and faster during pregnancy and could be reflected by the change of the microstructure-inspired material parameters. Next, we will run an automatic IFEA of all remaining tensile force data and validate the model by predicting the shape changes obtained from the images captured during the experiments. We will also fit the model to the indentation experimental data. The final goal will be to describe the material behavior of the human cervix under both the tensile and indentation tests. REFERENCES [1] House, M et al., 2009, S. Perinatol, 33, 300-307. [2] Yoshida, K , et al., 2019, Interface focus 9.5. [3] Bergstrom, B., & Boyce, C.M., 1998, J. Mech. Phys. Sdids.

16th U.S. National Congress on Computational Mechanics
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Title: Predicting Mechanical Performance in Additive Manufacturing Components Using Deep Learning

Author(s): *Kyle Johnson, *Sandia National Laboratories*; John Emery, *Sandia National Laboratories*; Demitri Maestas, *Sandia National Laboratories*; Matthew Smith, *Sandia National Laboratories*; Carianne Martinez, *Sandia National Laboratories*; Mircea Grigoriu, *Cornell University*;

Across a range of disciplines, Deep Learning has shown tremendous success in detecting features and patterns within input data by detecting potentially unknown structures and hierarchies. This talk will present results of a recent effort to utilize Deep Learning algorithms to predict microstructure-dependent mechanical performance in synthetic metal coupons representative of additively manufactured material. To train the Deep Learning network, a large database of synthetic simulation responses was developed based on physical material measurements of AlSi10Mg tensile bars. First, fine-scale finite element models of tensile specimens containing explicitly represented voids were generated. Voids found in AM material through high-resolution uCT characterization were used to form statistical distributions for size and spacing. These distributions were then sampled and used to inform meshes of representative tensile samples. The samples were then loaded in tension, with different pore distributions leading to strain localization in different regions over a range of peak loads. The resulting data was used to train a 3D Convolutional Neural Network to predict mechanical properties in different stress states and specimen geometries. Progress to date will be discussed, along with challenges and future work. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: Embedding Structures that are not Grid Aligned in Shallow Water Flow

Author(s): *Kyle Mandli, *Columbia University*; Chanyang Ryoo, *Columbia University*; Jiao Li, *Columbia University*;

The shallow water equations provide the basic modeling equations for a number of coastal flooding hazards, such as tsunamis and storm surge. In realistic scenarios there are often structures important to these flows that have a large extent but small width, including sea-walls, berms and harbor barriers. Explicit time stepping schemes, most often used for the shallow water equations, can then suffer from time step restrictions due to the CFL condition. In this talk we will introduce a couple of related approaches that side-steps these issues be allowing barriers to have zero-width and to cut a cell arbitrarily without suffering from CFL restrictions. This is done by supplementing existing Riemann solvers and leveraging cut-cell methods such as h-box and state redistribution methods. These methods preserve the properties of the Riemann solver and add negligible cost to the original solvers.

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Title: Computation of Stress Intensity Factor for Arbitrary and Low Quality Meshes

Author(s): *Kyoungsoo Park, *Yonsei University*; Habeun Choi, *Yonsei University*; Hui-Ru Cui, *Army Engineering University of PLA*;

To accurately compute the stress intensity factor (SIF) for arbitrary and low quality meshes, the present study proposes a simple and effective method in conjunction with the virtual grid-based stress recovery technique (VGSR) (Choi et al., 2021). The VGSR computes the accurate stress fields even with low quality meshes (Choi and Park, 2019), and the accuracy of VGSR is demonstrated for both 2D and 3D examples. Based on a virtual grid along the crack front, the SIFs are evaluated using the equivalent domain integral method. The computational results demonstrate that SIFs obtained from unstructured and low quality meshes is as accurate as SIFs obtained from structured and high quality meshes. Furthermore, the VGSR is considered as a post-processing techniques, and thus SIFs can be also evaluated using other energy-based methods such as the interaction integral method, the contour integral method, etc.

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Title: Machine Learning Based Interactive Geometry Modeling of Human Organ in 3D Medical Images for Computational Biomechanics

Author(s): *Liang Liang, *University of Miami*; Minliang Liu, *Georgia Institute of Technology*; Wei Sun, *Georgia Institute of Technology*;

For realistic computational modeling of a human organ on a patient-specific level, the 3D geometry of the organ can be obtained from 3D medical images. The geometry reconstruction is usually performed by (1) manually labeling the pixels of the organ in an image editing software, and (2) generating an ad-hoc mesh through the marching cubes algorithm, and (3) converting the ad-hoc mesh into a finite element mesh suitable for computational analyses, e.g., finite element analysis (FEA), where the step (3) still needs human inputs to edit the mesh. The geometry modeling process may take hours or even days, which has prevented population-scale computational analyses. Automatic geometry modeling methods have been proposed by utilizing machine learning (ML) techniques. However, ML suffers a known fundamental problem: if the input (e.g., an image) to an ML model is very different from the training data, which is called out of distribution, then the ML model output will become unreliable. A solution could be combining ML and human inputs in an interactive manner. In this study, we developed an ML-based interactive geometry modeling method and demonstrated it for aortic valve geometry modeling from 3D clinical CT images, which takes 10~20mins to generate a finite element mesh model of the aortic valve ready for FEA simulations. Given an input image, the user draws the leaflet boundary curve and the upper and lower planes, which are used to initialize the ML algorithm. Then, the algorithm will automatically reconstruct the geometries of the three leaflets and the aortic wall by using a dictionary of aortic valve shapes that have been trained offline. Another algorithm for automatic mesh processing will stitch the geometries of the four parts together and remesh the combined geometry with quadrilateral and tetrahedral elements, which are then ready for finite element simulation. If the user is not satisfied with the output, then the user can give additional inputs to the algorithm by placing an unlimited number (from 1 to many) of fiducial markers to specify the location of a piece of the aortic valve. Given the fiducial markers along with the initial inputs, the algorithm will compute a displacement field that will deform the geometry towards the fiducial markers. We have used the method to create 3D aortic valve geometries of 190 patients, which enables a large-scale analysis of geometries and stresses.

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Title: Moving Mesh Finite Element Models of BMP Signaling Network in Developing Zebrafish Embryos with Dynamic Cell Imaging Data

Author(s): *Linlin Li, *Purdue University*; Adrian Buganza-Tepole, *Purdue University*; David Umulis, *Purdue University*;

Embryonic development is a complicated phenomenon that combines cellular signaling, gene regulation, and cellular movement to form structures and tissues that presage adult physiology. Morphogens mediate the cell fate decision by their time-varying spatial distribution. Numerous morphogens are secreted and transported around the zebrafish embryo to drive fate specification and organize processes involved in gastrulation. In zebrafish, patterns of gene expression along the dorsal-ventral (DV) body axis are regulated by Bone Morphogenetic Proteins (BMPs)(Tucker et al. 2008). Throughout gastrulation, the cell layers of the blastoderm begin to thin as the cells spread toward the vegetal pole of the embryo and surround the central yolk until the entire embryo is covered by a thin cell layer. This process is called epiboly. The cell proliferation and movement during epiboly lead to a growth-like cell flow in the system. Such systems are often considered on a growing domain and many have incorporated domain growth into models of pattern formation (Crampin et al. 1999). In our work, we are interested in how the cellular movements impact the formation of gradients by contributing an advective term whereby the morphogens are swept with the moving cells as they move vegetally(Li et al. 2020). We developed an integrated, moving-mesh finite element model whereby the cell velocities directly inform the mesh movement, providing a realistic domain for computing pattern formation. To handle the extreme deformation during epiboly we use the updated Lagrangian (UL) formulation to model the growth. By only tracking the previous configuration of the stress-free state throughout the deformation, we are able to handle the extreme deformations. Our goal is to develop a complete advection-diffusion-reaction model that incorporates all stages of zebrafish embryonic development data to investigate the mechanism in underlining BMP driven DV patterning during epiboly. We evaluated the accuracy of the mesh updating compare to the advection caused by cell movement and its role in embryonic patterning. Reference Crampin E, Gaffney EA, Maini PK (1999) Reaction and Diffusion on Growing Domains: Scenarios for Robust Pattern Formation. Bull Math Biol 61:1093–1120. doi: 10.1006/bulm.1999.0131 Li L, Wang X, Mullins MC, Umulis DM (2020) Evaluation of BMP-mediated patterning in a 3D mathematical model of the zebrafish blastula embryo. J Math Biol 80:505–520. doi: 10.1007/s00285-019-01449-x Tucker JA, Mintzer KA, Mullins MC (2008) The BMP Signaling Gradient Patterns Dorsoventral Tissues in a Temporally Progressive Manner along the Anteroposterior Axis. Dev Cell 14:108–119. doi: 10.1016/j.devcel.2007.11.004

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Title: XIGA: an eXtended IsoGeometric Analysis Framework for Multi-Phase Interface Problems.

Author(s): *Lise Noel, *Delft University of Technology*; Mathias Schmidt, *University of Colorado Boulder*; Keenan Doble, *University of Colorado Boulder*; John A. Evans, *University of Colorado Boulder*; Kurt Maute, *University of Colorado Boulder*;

Interface problems play an important role in a broad range of applications. However, such problems often exhibit complex geometries, intricate material arrangements, or thin features along with physical responses presenting large gradients or discontinuities. In these cases, providing body-fitted meshes to perform classical finite element analysis and obtaining accurate numerical solutions remain challenging tasks. Immersed boundary techniques, such as the eXtended Finite Element Method (XFEM), provide elegant solutions for the problems characterized above. Enrichment techniques alleviate the need for generating conforming meshes by capturing singular and discontinuous behaviors within mesh elements. From an analysis point of view, increased accuracy of the physical responses and the geometry description can also be achieved by using smooth and higher-order interpolation bases. B-splines or NURBS as basis functions have become an increasingly popular approach, along with the development of IsoGeometric Analysis (IGA). In this work, we propose a so-called eXtended IsoGeometric Analysis (XIGA) framework to predict the physical responses in multi-phase interface problems. The geometry of the boundaries and interfaces are described implicitly by one or multiple level set functions. The finite element approximations are extended by a generalized Heaviside enrichment strategy with multiple enrichment levels. Higher-order B-spline shape functions (linear to cubic) are used for both the geometry representation and the analysis. Boundary and interface conditions are enforced weakly, namely with Nitsche’s method. Additionally, the face-oriented ghost stabilization is used to mitigate numerical instabilities associated with small phase subdomains. In this talk, different features of the proposed XIGA framework are explained. Numerical experiments are performed to validate the approach. In particular, two and three dimensional canonical problems focusing on heat transfer and elasticity are studied in details. Specific aspects of the analysis method are studied: considering multiple phases, with higher-order interpolations and associated stabilization. Finally, the developed XIGA framework is used to tackle problems characterized by complex geometries, including sharp-edged interfaces, intricate phase arrangements, and multi-phase junctions, for heat transfer and elasticity problems in two and three dimensions.

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Title: Multiscale DNN for Stationary Navier Stokes Equations with Oscillatory Solutions

Author(s): *Lizuo Liu, *Southern Methodist University*; Wei Cai, *Southern Methodist University*; Bo Wang, *Hunan National University*;

In this talk, we develop new multi-scale deep neural network to compute oscillatory flows for stationary Navier-Stokes equation in complex domains. The multiscale neural network is the structure that can convert the high frequency components in target to low frequency components thus accelerate the convergence of training of neural network. Navier Stokes flow with high frequency components in 2-D domain are learned by the multiscale deep neural network. The results show that the new multiscale deep neural network can be trained fast and accurate. Joint work with Bo Wang, Wei Cai.

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Title: Recent Developments in Recovery-based Discontinuous Galerkin

Author(s): *Loc Khieu, *University of Michigan*; Philip Johnson, *University of Michigan*; Eric Johnsen, *University of Michigan*;

The recovery concept for DG discretization was first developed by Nomura & Van Leer in 2005, for linear diffusion equation. It was subsequently expanded by Lo & Van Leer in 2011 to nonlinear diffusion–shear terms as appeared in Navier–Stokes equations, albeit the work was concentrated mostly on Cartesian meshes. In this approach, the ambiguities at an arbitrary element interface caused by the discontinuous nature of DG are removed by constructing a higher-degree polynomial aptly named recovery function, which spans the union of two elements abutting the interface. The recovery function is constructed in such a way that its least-square projections are indistinguishable from the original piecewise numerical solution. The resulting schemes—named Recovery-based DG or RDG—exhibit superior accuracy and stability characteristics, albeit the computational stencil might necessarily be non-compact. In recognition of all good pedigrees embedded in the recovery concept—namely accuracy and stability—we have been actively developing it further, in both depth and width, with the objective of exploring new paradigms for very large-scale simulations. In one direction, realizing the overall accuracy of advection–diffusion DG discretization is now hamstrung by upwind DG, we follow the MUSCL-approach by using recovery to enrich the Riemann inputs. In another direction concerning just diffusion–shear problems, we apply the recovery concept to the more popular first-order-system formulation of diffusion, successfully maintain a compact stencil. Lastly, we also expand to triangular meshes, limited to structured ones for now, but with tensor-product basis.

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Title: Stiffness Mapping for Early Detection of Breast Cancer: Combined Force and Displacement Data

Author(s): *Lorraine Olson, *Rose-Hulman Institute of Technology*; Robert Throne, *Rose-Hulman Institute of Technology*;

Early detection of breast cancer is crucial for improving patient survival rates. Manual breast exams and mammograms are currently the most effective and widely used early detection techniques. Manual breast exams depend on tissue stiffness but are limited in their ability to detect tumors. Mammograms, while effective, expose the patient to radiation. In addition, mammograms are sensitive to tissue density rather than stiffness, so identifying cancerous sites in the half of women over 40 with dense breasts can be challenging. Our ultimate goal is to develop a system that automates/refines the manual breast exam process to detect the roughly 10x stiffness difference between healthy and cancerous tissues. An electro-mechanical device will gently indent the tissue surface in various locations, recording the forces required and the tissue surface deflections on the remainder of the surface. This force and deflection data will be used with inverse techniques involving finite element methods and genetic algorithms to provide detailed 3D maps of the elastic modulus of the interior of the breast tissue. These 3D maps could be used to identify any suspicious sites and would provide quantitative values for comparing baseline data with data taken on subsequent visits. We have developed 3D mapping algorithms and have conducted experiments on tissue phantoms to validate a displacement-only approach and a force-only approach. The displacement-only approach indents the surface and measures only surface displacements while the force-only approach measures only the force required to perform the indentation. In the displacement-only approach we tested 12 tumor-free samples and 14 tumor-containing samples. In all cases, the algorithm correctly identified the presence or absence of a tumor. In the force-only approach we conducted 16 tumor-free tests and 16 tests on phantoms with tumors. This resulted in one false positive and the correct identification of the remaining 31/32 samples. We will present preliminary results which demonstrate that the combination of displacement and force measurements yields a more robust method than either measurement alone. Results on two tumor-free phantoms and four tumor-containing phantoms allowed us to correctly identify all samples with the combined measurements even when one measurement modality failed to give correct identifications. We also present a displacement-acquisition technique using a structured light scanner which costs less than one-tenth as much as the original digital image correlation system.

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Title: Crystalline Order of Colloids on a Curved and Deformable Elastic Membrane

Author(s): *Luigi Perotti, *University of Central Florida*; Shah Wasif Sazzad, *University of Central Florida*; Sanjay Dharmavaram, *Bucknell University*;

Interacting colloids have been employed to model complex material systems, such as shaping of elastic nanotubes - where colloids represent nanoparticles - or shape changes of viral shells - where colloids represent proteins and capsomers. The equilibrium configuration of a system of attractive colloids depends not only on the temperature of the system and their interaction potential, but also on the curvature of the underlying surface on which the colloids are deposited [1]. The local curvature directly affects the state of stress in the local packing, for example promoting the formation of pentagonal (heptagonal) defects in regions of positive (negative) Gauss curvature. Several studies have investigated the arrangement of interacting colloids on rigid surfaces, but the interaction between colloids and their elastic substrate is often neglected. In this work we investigate the competition between surface curvature and surface elasticity in colloidal packing. Representing the motion of interacting colloids on an elastic substrate requires a challenging, strongly coupled computational model. As the colloids move on the surface, they affect the substrate configuration, which in turns affects the colloidal interactions. We have recently proposed a new method [2] where particle positions are described in the reference configuration using a "pull-back" operator. This step guarantees that the particles are automatically on the deformable medium without needing any additional artificial constraint. In order to investigate the colloids crystalline order on the elastic substrate, this Lagrangian scheme is coupled with the basin hopping energy minimization method, combining Monte Carlo and gradient minimization steps. We will apply our scheme to a colloidal system partially covering surfaces with positive (sphere) and mixed (torus) Gauss curvature. The colloidal arrangement and the phase transition from liquid to solid is investigated as a function of temperature, range of interaction potential and surface curvature. These results are compared with the rigid substrate case in order to understand if substrate elasticity is sufficient to eliminate lines of defects (pleats and/or scars) that plague colloidal assemblies on rigid interfaces. In future work, these results can be used to program deformable shapes and colloidal arrangements based on substrate elasticity and colloidal interaction potential. [1] Law J.O., Dean J.M., Miller M.A., and Kusumaatmaja H.: "Phase transitions on non-uniformly curved surfaces: coupling between phase and location." Soft Matter, 16(34), pp.8069-8077, 2020. [2] Dharmavaram S. and Perotti L.E.: "A Lagrangian formulation for interacting particles on a deformable medium." Comput. Methods Appl. Mech. Eng., 364, p.112949, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Hybrid FEA/IGA Vehicle Crash Simulations in LS-DYNA

Author(s): *Lukas Leidinger, *DYNAmore GmbH*; Stefan Hartmann, *DYNAmore GmbH*; David Benson, *ANSYS LST*; Attila Nagy, *ANSYS LST*; Lambros Rorris, *BETA CAE Systems*; Ioannis Chalkidis, *BETA CAE Systems*; Frank Bauer, *BMW Group*;

In the last few years, Isogeometric Analysis (IGA) in LS-DYNA has gained increasing attention from (automotive) industry. One reason is certainly the rapid progress in the IGA capabilities of LS-DYNA itself, especially in explicit dynamic analysis of NURBS-based shell structures including coupling and stabilization of trimmed patches [1,2]. Another reason is the increasing availability of preprocessing capabilities for IGA, in particular from ANSA [3]. These novel IGA capabilities in ANSA now enable an efficient generation of trimmed NURBS-based multi-patch shell structures for the analysis in LS-DYNA. The basis for the communication between ANSA and LS-DYNA is the new, jointly developed IGA keyword format including topology information as in B-Rep CAD models. A third reason for the attractiveness of IGA in LS-DYNA is the possibility to simulate hybrid models, i.e. models consisting of both, IGA and conventional FEA components. First head impact simulations on a hybrid FEA/IGA engine hood model for pedestrian safety have already shown promising results. In this contribution we present our attempts to extend the capabilities of LS-DYNA towards hybrid full vehicle crash simulations with certain FEA components replaced by their IGA counterparts. The focus of this endeavor with BMW is to enable a one-by-one substitution of the FEA component without any additional model modifications, to make industrial tests and comparisons with IGA components as easy as possible. Here, the challenge is not only to consider all the IGA-specific aspects for crash like analysis-suitable modeling, time step size, mass scaling, coupling of trimmed patches or stabilization of trimmed elements, but also to support all the various FEA connection technologies such as spotwelds, tied contact or attached rigid bodies for IGA components. We show hybrid FEA/IGA vehicle crash simulations with LS-DYNA and discuss the encountered issues as well as our latest developments in this regard. [1] D. J. Benson, A. P. Nagy, L. Li, S. Hartmann, Recent developments in isogeometric analysis for LS-DYNA, in: Proceedings of the 15th International LS-DYNA Users Conference, Detroit, Michigan, USA, 2018. [2] L. F. Leidinger, M. Breitenberger, A. M. Bauer, S. Hartmann, R. Wüchner, K.-U. Bletzinger, F. Duddeck, L. Song, Explicit dynamic isogeometric B-Rep analysis of penalty-coupled trimmed NURBS shells, Computer Methods in Applied Mechanics and Engineering 351 (2019) 891-927. [3] L. Rorris, A. Nagy, S. Hartmann, I. Chalkidis, A. Vafeidis, The ANSA / LS-DYNA approach for IGA Simulations, in: Proceedings of the 12th European LS-DYNA Conference 2019, Koblenz, Germany, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Utilizing the Cellular Automata Finite Element Model to Simulate Thin Wall Microstructures of 3D Printed Metals

Author(s): *Lukasz Kuna, *National Research Council*; Kirubel Teferra, *US Naval Research Laboratory*;

The rise of additive manufacturing (AM) technologies has allowed for the creation of lighter, more complex designs that are otherwise too difficult or expensive to build using traditional methods (i.e. dies, molds, and machining). As opposed to traditional methods, AM builds undergo highly localized rapid thermally-driven phase change giving rise to unique challenges that must be overcome to properly manufacture a part. Specifically, the microstructural properties are determined by the nature of the phase change and must be well understood to properly engineer mechanical properties. To examine and better understand the microstructures of AM builds, the cellular automata finite element (CAFE) approach has been developed and used to simulate the AM process in large domain sizes. The AM CAFE code is capable of simulating the solidification process and the resulting microstructure, but up until now, has only been able to handle bulk material. In this work, the AM CAFE model has been extended to include the model of Steuben et al.[1] enabling the consideration of free surfaces via an enriched analytical solution. These enrichments to the analytical solution specifically include the handling of strong nonlinear variations in material properties due to their dependence on temperature and behavior of heat sources very near domain boundaries. With these enhancements, the AM CAFE code has been utilized to study thin wall structures and how various laser parameters influence the resulting microstructure and also the mechanical properties. In contrast to bulk sections, the outline, or “contour”, pass produces a distinctly different grain structure and texture on wall surfaces where nucleation occurs off the surrounding powder and growth follows the curved surface of the melt pool (as opposed to the tail). As the thickness of a structure approaches the width of the melt pool, the surface grain morphology constitutes an increasingly large fraction of the structure resulting in mechanical properties that differ from what is known about bulk sections. Structures of various thicknesses, some as small as the width of a melt pool, have been investigated, specifically for their unique surface features and grain morphology. [1] Steuben, John C., et al. "Enriched analytical solutions for additive manufacturing modeling and simulation."?Additive Manufacturing?25 (2019): 437-447.

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Title: Lumbar Spine Mechanics During Vehicle Impact into Road Safety Barrier

Author(s): *Lukasz Pachocki, *Gdansk University of Technology*; Karol Daszkiewicz, *Gdansk University of Technology*; Piotr Luczkiewicz, *Medical University of Gdansk*; Wojciech Witkowski, *Gdansk University of Technology*;

There are many types of injuries of occupants during vehicle crashes with road safety equipment and some of the injuries concern specific sections of a spine. Research of frontal impacts of vehicles [1,2] suggested that lumbar spine fractures were more frequent in late model vehicles than early ones. It could be beneficial to find a reason for this phenomenon so to help prevent it from happening. Hence, this research aimed to investigate the mechanics of a lumbar spine during a vehicle crash with a road safety barrier. To do that, two simulations were prepared, a global simulation and a local simulation. The global simulation concerned an occupied vehicle crash into a road safety barrier under specified initial conditions. In that simulation, specific displacements of a lumbar spine part from a Human Body Model (HBM) were extracted. Then, those displacements were imposed as boundary conditions to a detailed lumbar spine model in the local simulation. The vehicle model that was used was a 2014 Honda Accord mid-size sedan as it was a relatively new and common vehicle. The HBM was the 50th female and was located on a passenger seat with all relevant passive safety systems. The chosen road safety barrier was a concrete system which was a relatively stiff structure. The detailed model of a lumbar spine was acquired from Ref. [3] and enhanced for the current application. All mentioned models were validated separately against experiments. The global simulation was successfully conducted, and the relevant boundary conditions were extracted. Then the mechanics of the detailed lumbar spine model were investigated. REFERENCES [1] J. Zheng, L. Tang, J. Hu, A Numerical Investigation of Risk Factors Affecting Lumbar Spine Injuries Using a Detailed Lumbar Model, Appl. Bionics Biomech. 2018 (2018) 1–8. doi:10.1155/2018/8626102. [2] R.P. Kaufman, R.P. Ching, M.M. Willis, C.D. Mack, J.A. Gross, E.M. Bulger, Burst fractures of the lumbar spine in frontal crashes, Accid. Anal. Prev. 59 (2013) 153–163. doi:10.1016/j.aap.2013.05.023. [3] S.M. Finley, D.S. Brodke, N.T. Spina, C.A. DeDen, B.J. Ellis, FEBio finite element models of the human lumbar spine, Comput. Methods Biomech. Biomed. Engin. 21 (2018) 444–452. doi:10.1080/10255842.2018.1478967.

16th U.S. National Congress on Computational Mechanics
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Title: Supporting the Metal Additive Manufacturing Simulation Community Through Validation Measurements

Author(s): *Lyle Levine, *National Institute of Standards and Technology*; Brandon Lane, *National Institute of Standards and Technology*; Thien Phan, *National Institute of Standards and Technology*; Fan Zhang, *National Institute of Standards and Technology*; Mark Stoudt, *National Institute of Standards and Technology*; Brian Simonds, *National Institute of Standards and Technology*; David Deisenroth, *National Institute of Standards and Technology*;

Additive manufacturing (AM) is a transformative technology that provides game-changing new capabilities across a wide range of material systems and applications. Metal AM enables production of three-dimensional parts with geometries that can be too costly, difficult, or in some cases, impossible to produce using traditional manufacturing processes. In many cases, however, difficulties persist regarding throughput, reliability, and the properties of the printed parts. Quantitative modeling is critical for predicting and understanding these issues, but model validation requires community access to extensive high-quality test data [1]. As just a few examples, validation measurements are needed for models of heat transport and cooling rates, melt-pool geometry [2], microstructure evolution during solidification and subsequent post-build processing, residual stress [3], part distortion, and mechanical behavior. Ideally, such measurements should build upon each other in a hierarchical fashion to provide seamless data sets from feedstock characterization to mechanical behavior. I will describe some of NIST's measurements that specifically target model validation for metal AM, including in situ and ex situ synchrotron X-ray and neutron measurements. I will also describe the important role that the Additive Manufacturing Benchmark Series (AM-Bench) plays in AM model validation. AM-Bench includes extensive in situ and ex situ measurements by NIST and several partner organizations, simulation challenges for the AM modeling community, and a corresponding conference series. [1] L.E. Levine, et al., "Outcomes and Conclusions from the 2018 AM-Bench Measurements, Challenge Problems, Modeling Submissions, and Conference," Integr Mater Manuf Innov 9, 1–15 (2020) [2] B. Lane, et al., "Measurements of Melt Pool Geometry and Cooling Rates of Individual Laser Traces on IN625 Bare Plates," Integr Mater Manuf Innov 9, 16–30 (2020) [3] T.Q. Phan, et al., "Elastic residual strain and stress measurements and corresponding part deflections of 3D additive manufacturing builds of IN625 AM-Bench artifacts using neutron diffraction, synchrotron X-ray diffraction, and contour method," Integr Mater Manuf Innov, 8, 318-334 (2019)

16th U.S. National Congress on Computational Mechanics
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Title: Sensitivity of Void Mediated Failure to Geometric Design Features of Porous Metals

Author(s): G.H. Teichert, *University of Michigan*; *M. Khalil, *Sandia National Laboratories*; C. Alleman, *Sandia National Laboratories*; K. Garikipati, *University of Michigan*; R.E. Jones, *Sandia National Laboratories*;

Material produced by current metal additive manufacturing processes is susceptible to variable performance due to imprecise control of internal porosity, surface roughness, and conformity to designed geometry. Using a double U-notched specimen, we investigate the interplay of nominal geometry and porosity in determining ductile failure characteristics during monotonic tensile loading. We simulate the effects of distributed porosity on plasticity and damage using a statistical model based on observed populations of pores visible in computed tomography scans and additional sub-threshold voids required to match experimental observations of deformation and failure. We used a Karhunen–Loève expansion to model the porous media as a 3-dimensional random process, calibrated with aforementioned computed tomography scans. Statistical models of the probability of failure near stress concentrations are constructed, in the form of calibrated beta mixture models. These mixture models are intrinsically interpretable models with the components capturing different causes of failure (e.g. porosity vs geometry), allowing us to interpret the results from a physical viewpoint. We provide guidance for designs where material defects could cause unexpected failures depending on the relative importance of these defects with respect to features of the nominal geometry.

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Title: Isogeometric Residual Minimization Method for Time-Dependent Maxwell Problem

Author(s): *Maciej Paszynski, *AGH University of Science and Technology*; Marcin ?o?, *AGH University of Science and Technology*; Luis Garcia-Castillo, *University Carlos III of Madrid*;

In this paper, we introduce a computational paradigm for a stable, accurate solution of time-dependent Maxwell equations, using the implicit scheme, which we call Isogeometric Residual Minimization (iGRM), with the following unique combination of features (1) Linear computational cost O(N) of the direct solver solution (2) Unconditional stability of the implicit time integration scheme (3) Unconditional stability in the spatial domain. We believe this new paradigm may have an impact on the way the computational mechanics community runs simulations. It mixes the benefits of the state-of-the-art modern methods, namely the Residual Minimization (RM) [1], the Isogeometric Finite Element Method (IGA-FEM), and Alternating Direction Implicit solvers (ADI) [2]. We have previously applied this methodology for non-stationary advection-dominated diffusion and Navier-Stokes problems [3]. In this paper, we focus on the non-stationary Maxwell problem that requires special stabilization effort. We focus on non-stationary Maxwell equations defined on a regular patch of elements as considered in the isogeometric analysis. We apply the time-integration scheme following the ideas developed by the Finite-difference community [1] to derive a weak formulation resulting in discretization with Kronecker product matrices. Going further, we investigate the application of the residual minimization (RM) method for stabilization of the Maxwell equations within the isogeometric analysis setup. The residual minimization method is introduced in every time step of the implicit time integration scheme. We introduce the RM in such a way that we preserve the Kronecker product structure of the matrix. We take the tensor product structure of the computational patch of elements from the IGA framework as an advantage, allowing for linear computational cost factorization in every step, with the RM method's automatic stabilization. Thus, we have proposed a new computational paradigm for ultra-fast, stable, and accurate time-dependent Maxwell equations using an implicit time-integration scheme. The iGRM method delivers a linear computational cost O(N) solver, unconditional stability in time, offered by the implicit time integration scheme, and the unconditional stability in space, as delivered by the RM method. [1] J. Chan, J. A. Evans, A Minimum-Residual Finite Element Method for the Convection-Diffusion Equations, ICES-Report 13-12 (2013). [2] M. Hochbruck, T. Jahnke, R. Schnaubelt, Convergence of an ADI splitting for Maxwell's equations, Numerishe Mathematik, 129 (2015) 535-561. [3] M. ?o?, I.Muga, J.Muñoz-Matute, M.Paszynski, Isogeometric residual minimization (iGRM) for non-stationary Stokes and Navier–Stokes problems, Computers & Mathematics with Applications, https://doi.org/10.1016/j.camwa.2020.11.013 The work is supported by National Science Centre, Poland, grant no. 2017/26/M/ ST1/ 00281

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Title: Projection Based Energy Stable Methods for Thermodynamically Consistent, Coupled Cahn-Hilliard Navier-Stokes Framework for Two Phase Flows

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We report on two phase flow simulations with high density contrasts(1:1000), particularly for buoyancy driven flows and for Rayleigh Taylor instabilities. We use a diffuse interface approach, which utilizes a thermodynamically consistent set of coupled Cahn Hilliard Navier-Stokes equations. We present three second order numerical time integration schemes and prove that they are energy stable in the semi-discrete form, we also discuss existence and uniqueness for these methods. Two of these methods use a pressure projection method instead of the fully coupled Pressure Stabilised Petrov-Galerkin (PSPG) method. We compare the efficiency and scalability of the three methods. We use a residual based variational multi-scale method to discretize the momentum and advective Cahn-Hilliard equations. Using the Cahn-Hilliard equation for tracking the interface also allows to maintain explicit mass conservation on the continuous form, and this property is seamlessly inherited in the discretized form. The length scales which need to be resolved for correct interfacial dynamics (governed by CH) and the associated velocity scales(governed by NS) are disparate, and call for a fast adaptive meshing framework. To solve this problem, we use linear continuous Galerkin finite elements on octree based meshing strategy, which makes the framework massively parallel and fast, potentially providing a leeway into simulating multiple/bubbles droplets and interfacial instabilities. We present several numerical experiments to validate the framework against experimental datasets, and to illustrate the properties of the numerical scheme.

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Title: Planar Domain Parameterization with Hierarchical B-Splines

Author(s): *Maodong Pan, *University of Science and Technology of China*; Falai Chen, *University of Science and Technology of China*;

Constructing a high-quality parameterization of a given planar domain is a fundamental research problem in isogeometric analysis, which has been well investigated so far. However, most of the current approaches employ non-uniform rational B-splines (NURBS) to describe the geometry of the physical domain. Obviously, the use of such splines induces redundant degrees of freedom due to the tensor-product structure. In this paper, we use hierarchical B-splines that possess local refinement abilities for the parameterization, and employ the quasi-conformal map as the framework. Firstly, an initial parameterization is obtained by solving a quadratic optimization model which characterizes the smoothness and fairness of a map. Secondly, a quasi-conformal map represented by hierarchical B-splines is modeled as a non-linear optimization problem. We present an efficient algorithm to compute the quasi-conformal map by solving two quadratic optimization problems alternatively. Then the hierarchical B-splines are updated based on the injectivity and distortion of the computed parameterization. The above procedure is repeated until a bijective map with low distortion is achieved. Several examples are demonstrated to verity the effectiveness and advantages of the proposed approach

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Title: A Reproducing Kernel Enhanced Approach for Peridynamic Solutions

Author(s): *Marco Pasetto, *University of California, San Diego*; Yu Leng, *Purdue University*; Jiun-Shyan Chen, *University of California, San Diego*; John Foster, *The University of Texas at Austin*; Pablo Seleson, *Oak Ridge National Laboratory*;

Peridynamics is a nonlocal reformulation of continuum mechanics in which balance laws are computed through integration rather than differentiation [1]. For this reason, the peridynamic theory does not require any assumptions on the spatial differentiability of the displacement fields and remains valid in the presence of displacement discontinuities. Peridynamics is thus directly applicable to problems involving material failure and damage. The most common discretization method for peridynamic models used in engineering problems is the node-based meshfree approach. This method discretizes peridynamic domains by a set of nodes, each associated with a nodal cell with a characteristic volume, leading to a particle-based description of continuum systems. The behavior of each particle is then considered representative of its cell. This limits the convergence rate to the first order [2]. This work proposes the use of a meshfree Reproducing Kernel (RK) approximation [3] to the field variables in the peridynamic equations in order to increase the order of convergence of peridynamic numerical solutions. In this work, the peridynamic framework and the RK approximations are reviewed, the proposed approach is presented and the improved convergence rates in static peridynamic problems obtained using the proposed method is shown through numerical examples. References [1] Silling, S.A., “Reformulation of elasticity theory for discontinuities and long-range forces”, Journal of the Mechanics and Physics of Solids, 48, 175-209, 2000. [2] Seleson, P., Littlewood, D.J., "Convergence studies in Meshfree Peridynamics", Computers and Mathematics with Applications, 71, 2432-2448, 2016. [3] Chen, J. S., Pan, C., Wu, C. T., and Liu, W. K., "Reproducing Kernel Particle Methods for Large Deformation Analysis of Nonlinear Structures", Computer Methods in Applied Mechanics and Engineering, 139, 195-227, 1996.

16th U.S. National Congress on Computational Mechanics
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Title: High Order Multiscale Finite Element Method for Thermoelasticity Problems

Author(s): *Marek Klimczak, *Cracow University of Technology*; Witold Cecot, *Cracow University of Technology*;

The multiscale finite element method (MsFEM) [1] enables performing a coarse mesh analysis that accounts for the micro-scale phenomena without an extremely fine discretization. To increase the efficiency of MsFEM, we use the high order approximation at the coarse-scale level. The application of this framework combined with the hp-adaptivity was presented in [2] for the viscoelasticity problem and non-periodic materials. In this paper, we apply high order MsFEM to the thermoelasticity problem using a novel improvement of the solution accuracy by the implicit residual error estimate. A posteriori error estimation for upscaling techniques was already tackled, e.g. in [3]. Herein, we use the error estimate to enhance the upscaling results for the steady-state of weakly coupled temperature and displacement fields. However, the whole framework is general, and it also can be used for the transient, fully coupled analysis. Special prolongation operators for both fields are constructed independently to capture in the coarse-scale analysis the spatial distribution of the constituents of the underlying microstructure. Due to its complex performance, we selected asphalt concrete (AC) as a test material to verify the argued framework. The difficulty of the analysis lies in two main aspects: (i) the large disproportion in coefficients of thermal expansion for AC constituents, and (ii) substantial decrease of the Young modulus for the asphalt binder in higher temperatures. The obtained results are compared with the overkill mesh solutions. The p-convergence plots in both L2 and energy norms confirm the reliability of the presented methodology. A significant improvement due to the applied correction term can be observed, particularly for the fluxes and stresses. [1] Y. Efendiev and T.Y. Hou. Multiscale Finite Element Methods for Porous Media Flows and Their Applications. Applied Numerical Mathematics, 57:577-596, 2007. [2] M. Klimczak and W. Cecot. An Adaptive MsFEM for Non Periodic Viscoelastic Composites. International Journal for Numerical Methods in Engineering, 114(8):861-881, 2018. [3] O. Duran, P. Devloo, S. Gomes, F. Valentin. A multiscale hybrid method for Darcy’s problems using mixed finite element local solvers. Computer Methods in Applied Mechanics and Engineering, 354:213-244, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Fully Coupled Dynamic Simulations of Bioprosthetic Aortic Valves based on an Embedded Strategy for Fluid-Structure Interaction

Author(s): *Maria Giuseppina Chiara Nestola, *Institute of Computational Science,USI /Inst. für Geochemie und Petrologie, ETHZ*; Barna Becsek, *University of Bern*; Pascal Corso, *University of Bern*; Patrick Zulian, *Institute of Computational Science,USI*; Dominik Obrist, *University of Bern*; Rolf Krause, *Institute of Computational Science,USI*;

Bioprosthetic Aortic valves (BAVs) are prone to structural valve deterioration and expose patients to the risk of re-intervention after 10-15 years. In vitro testing shows that structural deterioration is a multifactorial process that may be promoted by high mechanical stress concentration and abnormal hemodynamic patterns close to the leaflets of the BAV. Computational models can describe the complex and nonlinear interaction of blood flow and structure dynamics occurring at the level of the BAV leaflet. Thus, they play a crucial role in the attempt to optimize the durability of BAVs. In this work, we present an embedded approach for the numerical solution of fluid-structure problems. This approach is designed to simulate the full dynamics of a BAV and can be used to analyze its mechanical and hemodynamic performances. The key elements of the proposed fluid-structure interaction framework are 1) the solution of elastodynamics equations for the structure, 2) the use of a high-order Navier-Stokes solver for the flow, and 3) the variational transfer for coupling the solid and fluid physics. The computational models presented in this work allow for the analysis of the fluid flow and the spatial distribution of the mechanical stresses in a BAV, and could be employed for the optimization of the leaflet and stent design.

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Title: Prediction of Residual Stress States Using an Eulerian Plasticity Model

Author(s): *Martin Kroon, *Linnaeus University*; Miles Rubin, *Technion - Israel Institute of Technology*; Per Lindström, *Linnaeus University*;

Solidification processes play an important role in several industrial processes, such as welding and additive manufacturing, and the resulting residual stress state is often critical for the structural integrity of the material. A thermomechanical model was developed for the analysis and prediction of such solidification processes. The approach is based on a model proposed by Rubin (Int. J. Eng. Sci. 25, 1175-1191, 1987). This plasticity model was formulated for finite strains using an Eulerian evolution equation for a unimodular elastic distortional deformation tensor. This evolution equation automatically ensures thermodynamic consistency and preservation of incompressibility of inelastic deformations. The model incorporates work hardening as well as softening due to annealing at high temperatures. The thermomechanical model was calibrated using experimental data from the literature. Two types of problems were analyzed: a 1D problem in the form of a circular disc under plane stress, and a 2D problem in the form of a butt weld joint. The main outcome from the analyses were the residual strain and stress distributions. In the case of the welding simulations, the results could be compared to experimental data from the literature. A parametric study was performed, illustrating the influence on the residual strains and stresses of different model parameters.

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Title: Tensor Random Fields with Fractal and Hurst Effects

Author(s): *Martin Ostoja-Starzewski, *University of Illinois at Urbana-Champaign*;

A wide range of natural phenomena (geological formations, material structures, living systems, turbulence…) possess fractal and Hurst (long-memory) characteristics [1,2]. While the conventional stochastic models are scalar-valued, motivated by the mechanics/physics of heterogeneous media, we continue to develop tensor-valued random fields (TRFs) [3]. The primary focus is on statistically homogeneous and isotropic TRFs with arbitrary local anisotropy modeling dependent fields or constitutive responses. Various examples, including the treatment of boundary value problems, come from elastodynamics, conductivity, and damage mechanics. In this talk, a cellular automata (CA) model is used to find the transient dynamic responses of anti-plane shear Lamb's problems on random media described by random media with fractal and Hurst effects. Both Cauchy and Dagum random field models are employed to capture the combined effects of spatial randomness in both mass density and stiffness tensor fields. With a dyadic representation, we formulate a second-rank anti-plane stiffness TRF. Through parametric studies for both Cauchy and Dagum TRFs, the sensitivity of wave propagation on random fields is assessed for a wide range of fractal and Hurst parameters. In general, the mean response amplitude is lowered by introduced randomness, and the Hurst parameter in the anti-persistent case is found to have a stronger influence than the fractal dimension on the response. The results are compared with two simpler random fields: (i) randomness is present only in the mass density field; (ii) randomness is present in the mass density field and a locally isotropic stiffness tensor field. Overall, the results show that a second-rank anti-plane stiffness TRF with full anisotropy leads to a stronger fluctuation in displacement responses than a locally isotropic (i.e., scalar-valued) RF model.

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Title: Comparison of Meshfree Approach Based on Peridynamic Formulation and Meshless Local B-Spline Collocation Method for Heterogeneous Heat Conduction in Multi-Medium Materials

Author(s): *Mas Irfan P. Hidayat, *Institut Teknologi Sepuluh Nopember*;

Comparison of Meshfree Approach Based on Peridynamic Formulation and Meshless Local B-spline Collocation Method for Heterogeneous Heat Conduction in Multi-medium Materials Mas Irfan P. Hidayat Laboratory of Materials Innovation, Department of Materials and Metallurgical Engineering, FT-IRS Institut Teknologi Sepuluh Nopember Surabaya Email: irfan@mat-eng.its.ac.id Abstract – Peridynamics is an integro-differential nonlocal reformulation of the classical theory of continuum mechanics, which has attracted great interest and been widely applied for solving engineering science problems recently. The most common and widely used discretization method for peridynamic models is the node-based meshfree approach. It is hence of great interest to evaluate performance of meshfree implementation of peridynamics in comparison to available classes of meshless methods. It is noted that reports concerning this aspect are only a few and still limited in literature. In this paper, comparison of meshfree approach based on the peridynamic formulation and meshless local B-spline collocation method (MLBCM) for solving heterogeneous heat conduction in multi-medium materials is presented. In contrast to the meshfree implementation of peridynamics employing quadrature for the integral form, the MLBCM employs differential quadrature technique to discretize the governing equations. In the later, unknown field variables are approximated by using B-spline basis functions within overlapping support domains covering the geometry of materials. In this study, implementation and treatment aspects in handling material discontinuities for both approaches are particularly highlighted. Effect of such material discontinuities treatment to the accuracy and efficiency of the methods is emphasized. Furthermore, numerical performance in terms of accuracy and efficiency for both methods in solving the heat conduction problems involving multi-medium materials are presented and elucidated. Several numerical examples of 2D heterogeneous heat conduction problems are chosen to show the evaluation and comparison study. Simulation results are compared with solutions from analytical or other numerical methods available in literature. Keywords: meshfree; peridynamics; B-splines; heterogeneous heat conduction; multi-medium materials References: 1. Silling, S. A. and Askari, E. (2005), “A meshfree method based on the peridynamic model of solid mechanics”, Computers and Structures, 83, pp. 1526–1535. 2. Madenci, E. and Oterkus, E. (2014), Peridynamic Theory and Its Applications, Springer-Verlag New York. 3. Hidayat, M.I.P. (2019), “Meshless local B-spline collocation method for heterogeneous heat conduction problems”, Engineering Analysis with Boundary Elements, 101, pp. 76–88.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Parameter Influence of Supervised/Unsupervised use of Convolutional Neural Networks for Fluid Flow Analyses

Author(s): *Masaki Morimoto, *Keio University*; Kai Fukami, *University of California, Los Angeles / Keio University*; Kai Zhang, *Rutgers University*; Aditya G. Nair, *University of Nevada, Reno*; Koji Fukagata, *Keio University*;

Convolutional neural networks (CNNs) have recently been applied to a wide range of fluid flow problems[1]. The filter operation inside CNN enables us to handle fluid flows in a computationally efficient manner. Since there are massive choices of hyper parameters inside CNN, clarification of influence on various parameters can promote the efficient and practical uses of CNN for fluid flow analyses. We here investigate the dependence of CNN performance for fluid flow problems on various parameter choices[2]. We consider two types of CNN for metamodeling and low-dimensionalization purposes, respectively. As for the CNN-based metamodeling, we consider two types of laminar flows; a flow around two side-by-side cylinders and a flow over a flat plate. The present CNN here attempts to estimate drag and lift coefficients from the vorticity input with the assist of supplemental scalar values which characterize the flow field. Although it is a commonly used technique, the input placements of the scalar values are often determined as a user's like. Hence, we seek the optimal placements of the scalar inputs among a CNN training pipeline. The scalar inputs at the layers closer to the input basically help the estimation effectively, while it highly relies on the flow fields users handle. The CNN autoencoder (CNN-AE) with isotropic homogeneous decaying turbulence is also employed to investigate the influence of various parameters and operations inside CNN. The use of various padding operations which can account for boundary condition of flow fields is also exhibited. Furthermore, we investigate the performance of several dimensional reduction/extension methods through the CNN-AE. Based on the findings thorough the present study, we will also provide considerable outlooks of CNN and fluid dynamics in the talk. [1] K. Fukami, K. Fukagata, and K. Taira, ``Assessment of supervised machine learning for fluid flows," Theor. Comput. Fluid Dyn., 34 (2020), pp.497-519. [2] M. Morimoto, K. Fukami, K. Zhang, A. G. Nair, and K. Fukagata, "Convolutional neural networks for fluid flow analysis: toward effective metamodeling and low-dimensionalization," arXiv:2101.02535.

16th U.S. National Congress on Computational Mechanics
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Title: Using Multiscale Data-Driven Modeling to Characterize Sex Differences in Drug Development

Author(s): *Mathias Peirlinck, *Stanford University*; Francisco Sahli Costabal, *Pontificia Universidad Católica de Chile*; Ellen Kuhl, *Stanford University*;

For both men and women, drugs often have undesired side effects. By interacting with specific ionic channels in the heart, they can induce arrhythmias such as Torsades de Pointes, associated with potentially lethal ventricular fibrillation. Therefore, pro-arrhythmic risk assessment is mandatory before a drug can enter the market. The high cost and poor specificity of gold-standard experimental procedures assessing the pro-arrhythmic risk of new compounds currently hinders potentially useful drugs to reach the market. Computational modeling can form an interesting initiative to address these limitations through predictive mechanistic assessments of the multiscale effects that subcellular ion channel blocks can have on the cell, tissue and organ level behavior. Studies have shown that female sex is a determinant to Torsades de Pointes arrhythmias [1]. It is becoming increasingly clear that one model does not fit all, and regulations should account for sex-specific population differences in cardiac electrophysiology. With this in mind, we created a multiscale computational model that predicts the pro-arrhythmic potential of drugs [2] and discriminates between sex-specific arrhythmic drug sensitivities. Specifically, we coupled protein-level ion channel expression to subcellular ion channel activity, to cellular action potential evolution, to the spatiotemporal activation profile and the electrocardiogram at the tissue and organ levels. To keep our analysis computationally tractable, we combine high-performance computing with machine learning techniques, including multifidelity Gaussian process classification and active learning, and create sex-specific risk assessments diagrams for male and female hearts. References: [1] James, A. F., Choisy, S. C., and Hancox, J. C. Recent advances in understanding sex differences in cardiac repolarization. Progress in Biophysics and Molecular Biology 94, 3 (2007), 265-319. [2] Sahli Costabal, F., Yao, J., Sher, A., and Kuhl, E. Predicting critical drug concentrations and torsadogenic risk using a multiscale exposure-response simulator. Progress in Biophysics and Molecular Biology 144 (2019), 61-76.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: MatCal: A Specialized Dakota Tool to Assist in Advanced Material Model Calibration

Author(s): *Matthew Kury, *Sandia National Laboratories*; Kyle Karlson, *Sandia National Laboratories*;

Physics and engineering simulation tools are becoming more prevalent in decision making processes. Accurately simulating a physical system requires accurately modelling the response of the materials that the system contains. The representation of a material's response to physical effects is captured in an analyst's choice of material model. Material models contain a set of equations and parameters governing a material's behavior under a given set of conditions. For nonlinear material models with several parameters, determination of the modelling parameters can be a difficult task. In this talk we will discuss how our python software tool, MatCal, provides a specialized interface to Dakota [1] for material model calibration. MatCal's specialization aims to simplify the calibration process for higher fidelity material models, and to provide access to standardized calibration workflows. MatCal provides data pre/post-processing, simulation management and objective function evaluation for common material calibration purposes. It also provides standard models that are used for comparison to standardized material characterization tests such as the uniaxial tension test. By providing these features in an easy to use python package, the burden on the analyst for material calibration is significantly reduced. In addition to standard material calibration workflows, MatCal serves as a test bed for developing and standardizing calibration methods that use advanced full-field data sources such as digital image correlation (DIC) and thermal imaging. MatCal implements two methods for calibration to full-field data: (1) the virtual fields method [2] and (2) an image decomposition method based on Alpert tree-wavelets [3]. Enabling calibrations to full-field data provides more data sufficiency in calibrating material models with many model parameters. [1] Dakota, a multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis: Version 6.7 users manual. Technical Report SAND2014-4633, Sandia National Laboratories, Albuquerque, NM, Updated November 2018. Available online from http://dakota.sandia.gov/documentation.html [2] Jones, EMC, Karlson, KN, Reu, PL. Investigation of assumptions and approximations in the virtual fields method for a viscoplastic material model. Strain. 2019; 55:e12309. https://doi.org/10.1111/str.12309 [3] M. Salloum, et al., Systematic Comparison off Experimental and Simulation Data Fields using Compressive Alpert Multiwavelets for Model Validation and Calibration. ASME Verification and Validation Symposium, Minneapolis, MN - 16 May 2018 Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2021-0264 A

16th U.S. National Congress on Computational Mechanics
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Title: Distributed Time-Parallel Solution of Transient Problems with MGRIT and p-Multigrid Methods

Author(s): *Matthias Möller, *Delft University of Technology*; Roel Tielen, *Delft University of Technology*;

In a series of publications, we have developed an efficient p-multigrid approach for solving the linear systems of equations that result from the discretization of steady-state convection-diffusion problems by higher-order B-Spline basis functions (https://doi.org/10.1016/j.cma.2020.113347, https://doi.org/10.1007/978-3-030-49836-8_10). The key idea is to first perform coarsening in the spline degree p and solve the residual equation on the coarsest p-level by means of a standard h-multigrid method, which is known to be efficient for low-order discretizations. As it is known that the performance of classical smoothers like Gauss–Seidel being applied in the context of IGA deteriorates as the spline degree p increases, we perform (block-)ILUT smoothing at the high-order level, which leads to a solution algorithm that is robust in h and p, and in the number of patches in a multi-patch IGA formulation. In this talk we extend our previous work to transient problems by combining our p-multigrid approach with a multigrid-reduction-in-time (MGRIT) method to enable parallelization over the temporal dimension. The key idea is to successively coarsen in the temporal direction, solve the intermediate space-time slabs in parallel and synchronize them on the coarsest temporal level with the aid of a sequentially performed time integrator. Preliminary results indicate that the combination of MGRIT and our p-multigrid method for solving the linear systems of equations at each time instance (and on the coarser time multigrid levels) yields an overall efficient solution algorithm. Our implementation is based on the two open-source software libraries G+Smo (Geometry + Simulation Modules, https://github.com/gismo/gismo) and XBraid (https://github.com/XBraid/xbraid). Next to the theoretical analysis of the interplay of the various multigrid components, the focus of this talk is on the computational efficiency and parallel scalability of our solution approach.

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Title: Learning Interaction Laws in Particle- and Agent-Based Systems

Author(s): *Mauro Maggioni, *Johns Hopkins University*; Fei Lu, *Johns Hopkins University*; Jason Miller, *Johns Hopkins University*; Sui Tang, *University California, Santa Barbara*; Ming Zhong, *Johns Hopkins University*;

Interacting agent-based systems are ubiquitous in science, from modeling of particles in Physics to prey-predator and colony models in Biology, to opinion dynamics in economics and social sciences. Oftentimes the laws of interactions between the agents are quite simple, for example they depend only on pairwise interactions, and only on pairwise distance in each interaction. We consider the following inference problem for a system of interacting particles or agents: given only observed trajectories of the agents in the system, can we learn what the laws of interactions are? We would like to do this without assuming any particular form for the interaction laws, i.e. they might be “any” function of pairwise distances. We consider this problem both the mean-field limit (i.e. the number of particles going to infinity) and in the case of a finite number of agents, with an increasing number of observations, albeit in this talk we will mostly focus on the latter case. We cast this as an inverse problem, and study it in the case where the interaction is governed by an (unknown) function of pairwise distances. We discuss when this problem is well-posed, and we construct estimators for the interaction kernels with provably good statistically and computational properties. We measure their performance on various examples, that include extensions to agent systems with different types of agents, second-order systems, and families of systems with parametric interaction kernels. We also conduct numerical experiments to test the large time behavior of these systems, especially in the cases where they exhibit emergent behavior. This is joint work with F. Lu, J.Miller, S. Tang and M. Zhong.

16th U.S. National Congress on Computational Mechanics
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Title: Development of High-Order, Super-Convergent Elements for Fluid Mechanics

Author(s): *Mayuresh Patil, *Georgia Institute of Technology*;

Finite element method (FEM) has been a workhorse tool for analysis and design of structures for the past five decades and is becoming more common in fluid applications over the past two decades. FEM was originally developed for solid mechanics and was based on equilibrium equations. Over time, a variational derivation and significant mathematical foundation led to error estimation. For self-adjoint problems like elasticity, the Galerkin approach leads to an energy minimization problem and symmetric matrices. For non-self-adjoint problems, FEM had to be modified – using sometimes ad hoc and sometimes mathematically rigorous methods. For saddle-point problems, mixed discretization satisfying the Brezzi-Babuska are used. For convective systems various stabilization approaches are used, e.g., streamline upwind Petrov-Galerkin (SUPG). This paper presents an alternate approach to SUPG-FEM by using a non-conformal Petrov-Galerkin (ncPG) formulation. The focus of the approach is to use local solutions, homogeneous and non-homogeneous, of the differential equations to represent the solution over an element. The local solutions then are written in terms of nodal variables and thus automatically guarantee nodal continuity but do not guarantee inter-element continuity. Non-conformal trial as well as test functions cannot be used in an FEM formulation and thus, we have to couple conformal test functions to the non-conformal trial functions. The primary requirement of the test function is to impose coercivity. This leads to a Petrov-Galerkin approximation. Since only the solutions of the linear (linearized) differential equations are used as trial function, the approximation is super-convergent, i.e., for a given level of discretization, a higher-order approximation can be used as compared to typical Galerkin or SUPG or Taylor-Hood FEM. Furthermore, using the divergence theorem, the interior weighted residual equation can be transformed to a boundary equation and thus parametric shape functions are not required. Finally, since the integration over the element interior is minimized, the accuracy of the method is not dependent on the choice of integration points (again the requirement is only the imposition of coercivity). ncPG-FEM is most similar to hybridized discontinuous Galerkin (HDG) method. The ncPG-FEM approach is applied to the linear, scalar, 2D convection-diffusion equation and linear, 2D Stokes flow. In both cases the stability and order of super-convergence of rectangular elements will be verified using benchmark validation test cases. Based on these results, the method will be extended to Navier-Stokes equations in the future.

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Title: Simulation of Injection-Induced Seismicity Using Hybrid Finite Element-Spectral Boundary Integral Scheme

Author(s): *Md Shumon Mia, *University of Illinois at Urbana-Champaign*; Mohamed Abdelmeguid, *University of Illinois at Urbana-Champaign*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*;

Induced seismicity is a man-made hazard which can arise from industrial waste-water injection or CO2 sequestration. Modelling injection-induced seismicity is computationally challenging as it requires resolving space-time evolution of pore pressure along with diverse spaciotemporal scales related to slow aseismic slip and rapid dynamic rupture. In this study, simulation of sequence of earthquake cycles with evolving pore pressure is carried out for an anti-plane fault using a hybrid finite element-boundary integral method. We employ an alternating quasidynamic and fully dynamic scheme which enables simulating both interseismic deformation with approximation of inertia by radiation damping, and rapid seismic slip with full inertia effects. Spectral Boundary Integral (SBI) scheme is coupled at the boundary of a narrow FEM domain. This hybrid scheme allows to reduce the computational domain by replacing the half-space with boundary integral equation. We consider a vertical fault embedded at depth within a linear elastic half-space and governed by a regularized rate and state friction law. Fluid is assumed to be injected directly to the fault core and pore pressure diffusion is assumed to be constrained to the fault parallel direction. The evolution of the effective stress is determined analytically with modification for free surface boundary condition by including image source and allowing intermittent injection. We have investigated the effect of injection on seismicity pattern by varying injection pressure. In absence of injection, the fault generates periodic system spanning events. Fluid injection leads to aperiodicity and space time clustering of the events. Injection reduces inter seismic event time and leads to accelerated slip accumulation. After stopping injection, we observe a delay to recover the original pre-injection state. A period of seismic quiescence is observed after injection shut off, followed by a larger seismic event. Higher injection pressure is found to generate more frequent seismic events during injection. We also discuss how off-fault inelastic deformation and fault dynamic weakening may affect these findings. These results are useful for addressing the risk of injection-induced seismicity.

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Title: Multiscale Computational Hemodynamic Predictions in the Pulmonary Vasculature

Author(s): *Mette S Olufsen, *North Carolina State University*; Michelle Bartolo, *North Carolina State University*; Naomi Chesler, *University of California, Irvine*;

Left heart failure (LHF) impacts nearly 5.9 million adults and contributes to 1 out of every 9 deaths in the United States. Pulmonary hypertension due to LHF (PH-LHF) is a progressive disease that occurs in 60-80% of these patients. PH-LHF begins as a passive process termed isolated post-capillary PH (Ipc-PH), diagnosed by elevated mean pulmonary artery pressure (mPAP) with normal pulmonary vascular resistance (PVR), but significantly increases mortality once Ipc-PH transitions to combined pre-/post-capillary PH (Cpc-PH). Clinical and experimental hypotheses suggest that pathological shear stress and cyclic stretch are critical regulators of pulmonary vasoconstriction and remodeling, yet the exact mechanical stimuli of PH-LHF are unknown. We propose an in-silico computational one-dimensional fluid dynamics including large and small pulmonary arteries and veins as well as capillaries to predict shear stress and cyclic stretch in networks representing a healthy control and a PH-LHF patient. Large vessel hemodynamics are predicted in a geometry reconstructed from computed tomography imaging [1], while small vessel predictions occur in an empirically driven, bifurcating fractal tree [2]. The arterial and venous trees are connected by pulmonary capillaries whose network geometry is characterized by a sheet of fluid placed between two membranes [3]. This multiscale model predicts dynamic blood pressure, blood flow, and area deformation throughout the pulmonary circulation. Preliminary numerical results in the healthy network show that in the large vessels, the shear stress increases coincide with larger flow and pressure, while in the microvasculature, we find that as vessel radius decreases, shear stress increases and flow decreases. In arterioles, this corresponds with lower pressures; however, in venules, smaller vessels have higher pressure. For this study, we will discuss the impact of including capillaries in the model and how PH-LHF affects these results. Our model will be embedded in a novel tool and used to analyze and investigate hypotheses related to understanding the physiological mechanisms underlying the progression of pulmonary diseases. References 1] Chambers, MJ et al., Structural and hemodynamic properties of murine pulmonary arterial networks under hypoxia-induced pulmonary hypertension, J Eng Med, 234: 1312-1329, 2020. [2] Qureshi, MU et al., Numerical simulation of blood flow and pressure drop in the pulmonary arterial and venous circulation, Biomech Model Mechan, 13: 1137-1154, 2014. [3] Fung, YC et al., Theory of sheet flow in lung alveoli. J Appl Physiol, 26: 472-488, 1969.

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Title: Quantifying the Unknown: Impact of Segmentation Uncertainty on Image-Based Simulations

Author(s): *Michael Krygier, *Sandia National Laboratories*; Tyler LaBonte, *Sandia National Laboratories*; Carianne Martinez, *Sandia National Laboratories*; Chance Norris, *Purdue University*; Krish Sharma, *Sandia National Laboratories*; Lincoln Collins, *Sandia National Laboratories*; Partha Mukherjee, *Purdue University*; Scott Roberts, *Sandia National Laboratories*;

Image-based simulation, the use of 3D images to calculate physical quantities, relies on image segmentation for geometry creation. However, this process introduces image segmentation uncertainty because different segmentation tools (both manual and machine-learning-based) will each produce a unique and valid segmentation. First, we demonstrate that these variations propagate into the physics simulations, compromising the resulting physics quantities. Second, we propose a general framework for rapidly quantifying segmentation uncertainty. Through the creation and sampling of segmentation uncertainty probability maps, we systematically and objectively create uncertainty distributions of the physics quantities. We show that physics quantity uncertainty distributions can follow a Normal distribution, but, in more complicated physics simulations, the resulting uncertainty distribution can be surprisingly nontrivial. We establish that bounding the uncertainty can fail in these nontrivial situations. While our work does not eliminate segmentation uncertainty, it improves simulation credibility by making visible the previously unrecognized uncertainty plaguing image-based simulation.

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Title: Global Sensitivity Analysis via Hybrid MLMC PCE

Author(s): *Michael Merritt, *North Carolina State University*; Gianluca Geraci, *Sandia National Laboratories*; Michael Eldred, *Sandia National Laboratories*; Teresa Portone, *Sandia National Laboratories*;

Sensitivity Analysis supports the development of mathematical models by studying how the variability of a model's output can be assigned to the different sources of uncertainty in the model's input [1]. Unfortunately, in the context of high-fidelity computer simulations, Global Sensitivity Analysis (GSA) requires several evaluations of a computer code and its computational cost is often prohibitively large. In the context of Uncertainty Quantification, to tackle this issue, it has been demonstrated that a prescribed accuracy for the statistics can be reached by leveraging a large number of lower accuracy evaluations with only a limited number of high-fidelity simulations. Approaches that fuse information from several sources, e.g. models with a varying discretization, are often referred to as multifidelity strategies and are, in general, more efficient than their single fidelity counterparts. In this contribution we show how Multilevel Monte Carlo (MLMC) [2] can be used to accelerate the GSA workflow. This work is based on the recently proposed hybrid method [3] that combines a Polynomial Chaos Expansion (PCE), which provides a convenient way of performing GSA, based on Sobol' variance decomposition, with MLMC, which provides a framework for deriving an optimal sample allocation among models. In particular, the sample allocation of the MLMC-PCE method is derived as an optimal solution, which minimizes the overall computational cost while satisfying a prescribed accuracy for a set of sensitivity indices. We plan to present several numerical results based on verification problems and more complex applications such as wind energy, geological waste repository and chemical systems. [1] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, S. Tarantola, Global Sensitivity Analysis. The Primer. John Wiley & Sons, 2008. [2] M. Giles, Multilevel Monte Carlo methods, Acta Numerica (24), 2015. [3] M. Merritt, G. Geraci, M. Eldred, T. Portone, Hybrid multilevel Monte Carlo - polynomial chaos method for global sensitivity analysis, SAND2020-12580R, 2020. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
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Title: nPINNs: Nonlocal Physics-Informed Neural Networks

Author(s): Goufei Pang, *Brown University*; Marta D'Elia, *Sandia National Laboratories*; *Michael Parks, *Sandia National Laboratories*; George Karniadakis, *Brown University*;

Physics-informed neural networks (PINNs) have proven effective in solving inverse problems based on differential equations with sparse data by incorporating governing equations (reflecting physical laws) into the loss function. In this talk, we introduce nonlocal PINNS (nPINNS), an extension of PINNs to parameter and function inference for nonlocal models. We propose a parameterized nonlocal Laplace operator for which the classical Laplacian and fractional Laplacian are special cases, and which thus has the potential to fit a broad spectrum of data sets. We demonstrate nPINNs on this nonlocal Laplace operator by estimating its model parameters and characterizing the kernel of the operator, showing that nPINNs can correctly infer classical, fractional, and general nonlocal Laplacians from data. Lastly, we propose another nonlocal operator with spatially variable order which is more suitable for modeling turbulent Couette flow. Our results show that nPINNs can jointly infer this function as well as the nonlocal interaction distance. These parameters exhibit a universal behavior with respect to the Reynolds number, a finding that contributes to our understanding of nonlocal interactions in wall-bounded turbulence.

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Title: An Immersed Method for Finite Elements and Particles in an ALE Background Mesh with Contact

Author(s): *Michael Puso, *Lawrence Livermore National Laboratory*; Paul Tsuji, *Lawrence Livermore National Laboratory*;

A Lagrange multiplier type immersed boundary approach for foreground finite elements superposed on an ALE background mesh was developed in [1] and [2] and extended to treat foreground particle discretizations such as SPH in [3]. In this presentation a review of [1] and [2] is given along with the additional details required for the particle implementation of [3]. In addition, a focus on how unilateral contact and friction is handled for foreground bodies interacting with the background material (e.g. skin friction) and surface-to-surface contact between impacting foreground bodies. Details regarding the implementation and parallel performance for large scale production problems is presented. Finally, some new validation problems are presented that include penetration, blast effects and damage. [1] Puso M., Sanders J., Settgast R., Liu B. An embedded mesh method in a multiple material ALE Comput. Methods Appl. Mech. Engrg., 245 (2012) [2] Puso M., Kokko E., Settgast R., Sanders J., Simpkins B., Liu B. An embedded mesh method using piecewise constant multipliers with stabilization: mathematical and numerical aspects Internat. J. Numer. Methods Engrg., 104 (7) (2015) [3] P. Tsuji, M. Puso, C.W. Spangler, J.M. Owen, D. Goto, T. Orzechowski, Embedded smoothed particle hydrodynamics Comput. Methods Appl. Mech. Engrg., 366 (2020)

16th U.S. National Congress on Computational Mechanics
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Title: CutFEM Approach for Handling Non-Stationary Interfaces in Large-Deformation Solid Mechanics: Application to Fracture

Author(s): *Mikhail Poluektov, *University of Warwick*; Lukasz Figiel, *University of Warwick*;

There is a variety of numerical methods to handle problems with interfaces in solid mechanics. Most methods can be classified into two groups: the diffuse-interface methods and the sharp-interface methods. There is an important class of methods within the latter group – the fictitious domain methods, to which the CutFEM approach belongs. This class of methods allow the interface to cut through the elements and to avoid any kind of mesh generation that conforms to the mesh. This is extremely convenient from the practical point of view when non-stationary interfaces are considered, as the interfaces can move independently of the mesh. Initially, the CutFEM method has been proposed for linear PDEs [1,2]. Recently, a generalisation of the CutFEM method to large deformations and arbitrary constitutive behaviour of materials in solid mechanics has been performed [3]. In this talk, the results of [3] are further generalised to cases when the interface represents a more complex physical behaviour – fracture, i.e. separation of the interface, and contact between the separated surfaces. The starting point is the case of the simple solid-solid phase boundary (e.g. a discontinuity in material behaviour), which is first generalised to fracture (crack opening), then generalised to contact. The contact case is considered separately and provides an additional challenge because the contact points might not coincide in the reference configuration of the material. From the numerical point of view, two goals are addressed here. The first goal is to ensure that any incremental generalisation of the approach contains a prior approach as a particular case, i.e. the phase boundary problem is a particular case of the fracture problem, while the latter can become a particular case of the contact problem under certain specific conditions. The second goal is to ensure that the weak form obtained for the contact problem is symmetric with respect to the choice of the contact surfaces for the integration. The presentation of the method is followed by a number of numerical examples highlighting the applicability of the approach. [1] P.Hansbo, GAMM-Mitt. (2005) 28(2):183-206 [2] E.Burman, P.Hansbo, Appl. Numer. Math. (2012) 62(4):328–341 [3] M.Poluektov, L.Figiel, Comput.Mech. (2019) 63:885-911

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Title: Coupling Free-Flow and Porous Medium with preCICE -- and Other Use Cases

Author(s): *Miriam Mehl, *University of Stuttgart*; Alexander Jaust, *University of Stuttgart*; Benjamin Uekermann, *University of Stuttgart*;

The open source coupling library preCICE that we develop in a cooperation of the University of Stuttgart and the Technical University of Munich has been established throughout the last years as a highly flexible, powerful and efficient tool to couple different components of multi-physics and multi-scale simulations in a highly modular and scalable way. In this presentation, we show results for various applications in the context of environmental engineering. We show how the three main components offered by preCICE can be optimally configured and used in this context: (i) point-to-point data communication between several executables via MPI or sockets, (ii) data mapping between non-matching grids or - more general - different sets of data points, and (iii) convergence acceleration by means of quasi-Newton schemes (also known as Anderson acceleration or generalized Broyden) for the outer iterative domain-decomposition-based solver. Our two concrete scenarios are the following: (i) a partitioned simulation at the REV scale of free-flow and porous-medium Darcy flow, (ii) hybrid-dimensional coupling of flow and porous medium for hydromechanical fracture opening in a poro-elastic material as introduced in [1]. For (i), we show how novel interface coupling conditions [2] developed within the collaborative research center CRC1313 (https://www.sfb1313.uni-stuttgart.de/) could be integrated in a minimally-invasive way in a setting with DuMux (https://dumux.org/) as simulation tool for both free-flow (Navier-Stokes) and porous medium (Darcy flow). (ii) is a good example for the coupling of different dimensional models - a reduced-dimensional 2D flow equation in the fractures and a full 3D flow and material model for the surrounding porous matrix. As simulation codes for this application, we use Fenics (https://fenicsproject.org/). In addition to these two showcases and the respective numerical and communication methods, we will present an outlook on future development plans for the coupling library preCICE, in particular improved and more flexible data mapping, volume coupling, and multi-scale coupling that might be of importance to enable further efficient and modular simulation environments in the context of environmental system, weather and climate. [1] Steeb, H., & Renner, J. (2019). Mechanics of Poro-Elastic Media: A Review with Emphasis on Foundational State Variables. Transport in Porous Media. https://doi.org/10.1007/s11242-019-01319-6 [2] Eggenweiler, E. & Rybak, I., “Effective coupling conditions for arbitrary flows in Stokes-Darcy systems,” Multiscale Model. Simul. (in press), 2021. Available: http://arxiv.org/abs/2006.12096.

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Title: Developing Pulmonary Biomechanics Models Using Digital Image Correlation: an Inverse Finite Element Analysis of Ex-Vivo Porcine Specimens

Author(s): *Mohammad Maghsoudi-Ganjeh, *University of California, Riverside*; Crystal Mariano, *University of California, Riverside*; Samaneh Sattari, *University of California, Riverside*; Mona Eskandari, *University of California, Riverside*;

Worldwide, pulmonary diseases are the top cause of morbidity and mortality. Computational biomechanical models of the respiratory system, informed and validated by experimental data, can serve as powerful tools to investigate underlying mechanisms of various lung diseases and to predict disease progression [1]. To date, computational respiratory models have relied heavily on computer tomography (CT) or magnetic resonance imaging (MRI) modalities to construct model geometry and motion, and done so primarily to optimize radiation therapy outcomes. However, the deformable image registration step needed for these models is a tedious task, and difficult to validate due to the lack of universal standards [2]; this often necessitates the need for expert-determined landmark identification, which may be inaccessible. Moreover, the in-vivo nature of such imaging limits applicability, not supporting invasive yet highly insightful ventilation modes to evaluate the effect of respiratory parameters, such as volume and rate, in a controlled and continuous manner. To address this issue, here we present a simple biophysical model of the lung using 3D digital image correlation (DIC) synchronized with a validated in-house pressure-volume apparatus [3] to experimentally characterize global and local lung kinetics. We generate a finite element (FE) model of the visceral pleura layer discretized by 3D membrane elements subjected to experimentally collected pressure loading data during inflation. Various constitutive models including isotropic hyperelasticity, anisotropic hyperelasticity, and heterogeneous linear elasticity are examined. By implementing a fully automated inverse FEA framework, we predict the set of optimal material parameters using two classes of derivate-based and gradient-free optimization algorithms to minimize the displacement error between simulation and experiment. The compound material properties predicted by the inverse model accounts for the effective response of parenchyma, airways, and visceral pleura. Furthermore, we find the spatial pattern of strain to demonstrate anisotropy and heterogeneity, similar to the experimental profiles. The innovative image-based framework, established for pulmonary macromechanics for the first time, can be readily applied to investigate the impact of various ventilation modes on local pulmonary force and stretch distributions and to further explore how diseased states may alter the load-bearing material behavior of the lung. References [1] Eskandari, M et al., Acta Biomater., 97: 513-523, 2019 [2] Li, P et al., Phys. Med. Biol, 53:4621-4637, 2008 [3] Sattari, S et al., Front. Bioeng. Biotechnol, 8:1183, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: SimNet: A Neural Framework for Physics Simulations

Author(s): Oliver Hennigh, *Nvidia*; Susheela Narasimhan, *Nvidia*; *Mohammad Amin Nabian, *Nvidia*; Akshay Subramaniam, *Nvidia*; Kaustubh Tangsali, *Nvidia*; Max Rietmann, *Nvidia*; Jose del Aguila Ferrandis, *Massachusetts Institute of Technology*; Wonmin Byeon, *Nvidia*; Zhiwei Fang, *Nvidia*; Sanjay Choudhry, *Nvidia*;

Simulations are pervasive in every domain of science and engineering. However, they become computationally expensive as either the complexity of the geometry and physics or the number of design parameters increases. Although supervised deep learning offers a path to overcome this constraint, generating data can be expensive and very time consuming. Moreover, trained models may not obey the governing physics of the problem, involve extrapolation and generalization errors, and provide unreliable results. In comparison with the traditional solvers, physics-driven neural network solvers can not only do parametrized simulations in a single run, but also address problems not solvable using traditional solvers and data-driven models. Although the existing research studies played a crucial role in advancing the neural network solvers, attempted examples are mostly limited to simple 1D or 2D cases with straightforward governing physics, and these solvers still struggle to solve real-world applications that involve complex 3D geometries and multi-physics systems due to the gradients, singularities and discontinuities introduced by complex geometries or physics. We present SimNet, an end-to-end physics based neural framework for simulations that aims at addressing these computational challenges by offering several novel features, including signed distance functions for loss weighting, integral continuity planes for flow simulation, advanced neural network architectures that are optimized for high-performance GPU computing, point cloud generation for real world geometries using constructive geometry and STL modules, and parameterization of both geometry and physics. Additionally, for the first time to our knowledge, we solve high Reynolds number turbulent flow in industrial applications without using any training data. SimNet offers fast turnaround time by enabling parameterized system representation that solves for multiple configurations simultaneously, and offers scalable performance for multi-GPU/multi-node implementation with accelerated linear algebra as well as FP32, FP64 and TF32 computations. Through several numerical examples, we show that SimNet addresses use cases across four major areas in computational science and engineering, that are, inverse and data assimilation problems, real time simulations, improved physics and predictions, and digital design and manufacturing. The examples include data assimilation in patient-specific intracranial aneurysm, digital twin of damage accumulation in an aircraft fuselage, wave propagation with layered velocity, and design space exploration of NVSwitch heat sink in Nvidia DGX A100. We also present extensive accuracy and efficiency comparisons of SimNet with open source and commercial solvers. The SimNet source code is available at https://developer.nvidia.com/simnet.

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Title: Using Predictive Simulations to Uncover the Effects of Ring-Based Annuloplasty on the Human Tricuspid Valve

Author(s): *Mrudang Mathur, *The University of Texas at Austin*; William Meador, *The University of Texas at Austin*; Marcin Malinowski, *Medical University of Silesia School of Medicine in Katowice*; Tomasz Timek, *Spectrum Health*; Manuel Rausch, *The University of Texas at Austin*;

Functional tricuspid regurgitation (FTR) is closely associated with left-heart pathologies such as dilated or ischemic cardiomyopathy and affects 30-50% of patients with severe mitral regurgitation. Currently, suture- or ring-based annuloplasty remains the common repair strategy for treating FTR. Unfortunately, these procedures have a low success rate with recurrent FTR in 30% of cases and a mortality rate of 37% associated with reoperations. A first critical step toward improving these suboptimal outcomes is to understand and characterize the effects of annuloplasty on tricuspid valve mechanics. To achieve this goal, we will virtually implant commercially available annuloplasty devices into patient-specific finite element models of the tricuspid valve. To create patient-specific tricuspid valve models, we first reperfused beating healthy donor hearts in an organ preservation system. We simultaneously recorded tricuspid annulus dynamics using sonomicrometry over multiple cardiac cycles, in addition to hemodynamics, on a loaded right ventricle. Upon arresting the hearts, we then excised the tricuspid valve complex, imaged the leaflets, and digitized their geometry. Next, we recreated the 3D annulus from sonomicrometry data onto which we non-rigidly transformed the leaflet geometries. Subsequently, we used imaging data to assign chordal insertions and rebuild the valve in-silico. Additionally, we characterized material properties and microstructural information of the leaflets and chordae through in-vitro planar biaxial and uniaxial testing, respectively, and 2-Photon microscopy. We then imposed boundary conditions through annular displacement fields and transvalvular pressure gradients as measured in the beating hearts. Finally, we simulated the dynamics of the tricuspid valve over one full cardiac cycle in Abaqus/Explicit. The tricuspid valve models faithfully capture leaflet geometry and coaptation as validated against 2D echo scans of the same beating hearts. In these validated models, we will then asymmetrically dilate the tricuspid annulus and displace the papillary muscles to recreate the effects of FTR. Furthermore, we will stiffen the stress-strain behavior of the tricuspid valve leaflets to incorporate their maladaptive fibrotic response in FTR [1]. Upon successfully creating regurgitant tricuspid valves, we will implant 6 previously digitized [2] tricuspid annuloplasty rings in our valve models and simulate the dynamics of the repaired valve. We hypothesize that tricuspid annuloplasty generates unphysiological stress concentrations within the valve and will use this modeling pipeline to delineate the effects of annuloplasty ring implantation on the tricuspid valve annulus and leaflets. [1] Meador WD et al. eLife, 2020. [2] Mathur M et al. The Annals of Thoracic Surgery, 2020.

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Title: Application of Transfer Learning in Multi-Fidelity Surrogate Model for Design Optimization

Author(s): *Mushi Li, *Shanghai Jiao Tong University*; Zhao Liu, *Shanghai Jiao Tong University*; Yang Li, *Ford Motor Company*; Ping Zhu, *Shanghai Jiao Tong University*; Guosong Li, *Ford Motor Company*; Zhenyan Gao, *Ford Motor Company*;

The design optimization of complex engineering applications often requires a great number of evaluations of time-consuming computer-aided engineering (CAE) simulations. Surrogate modeling based on various types of algorithms has been widely used to improve the efficiency. However, training the surrogate models has proved to be challenging for complex engineering problems with high dimensionality and strong nonlinearity [1]. To ensure the accuracy of the surrogate models, tremendous amount of training data has to be collected. Multi-fidelity surrogate modeling has been explored as a promising solution in this scenario, in which data obtained from testing or CAE with lower fidelity yet much easier access can be leveraged to enrich the training set [2]. However, most of the existing multi-fidelity approaches heavily relies on high fidelity data in the original training set, which limits its value in real-life applications. To address this issue, we propose a new multi-fidelity surrogate modeling approach, multi-fidelity output regression neural network, which is inspired from the transfer learning method in the field of deep learning [3]. The transfer learning method is used to extract general features between high and low fidelity data in this approach, thereby reducing the reliance of modeling on high fidelity data. The hidden layers of this neural network consist of a group of general feature layers and two groups of different specific feature layers connected in parallel. In order to maximize the accuracy and robustness of this neural network, a new loss function and a new neural network training process are developed. In addition, before training, Gradient Boosting Machine (GBM) is used to enhance the low-fidelity data in the case where low-fidelity training data needs expansion. Bayesian optimization method is applied to adaptively adjust the hyper-parameters of the model during training, e.g., the number of neuron layers and the number of neurons in each layer. It is shown that the developed methodology in this study shows significantly lower dependence on amount of high-fidelity data in validation problems. Keywords: Multi-fidelity data, surrogate modeling, transfer learning [1] Haftka, Raphael T.; Villanueva, Diane; Chaudhuri, Anirban (2016). Parallel surrogate-assisted global optimization with expensive functions – a survey. Structural and Multidisciplinary Optimization, 54(1), 3–13. [2] Peherstorfer, Benjamin; Willcox, Karen; Gunzburger, Max (2018). Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization. SIAM Review, 60(3), 550–591. [3] Pan, Sinno Jialin; Yang, Qiang (2010). A Survey on Transfer Learning. IEEE Transactions on Knowledge and Data Engineering, 22(10), 1345–1359.

16th U.S. National Congress on Computational Mechanics
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Title: High-Accuracy and High-Efficiency 3D Crack Propagation Analysis Based on S-Version Finite Element Strategy

Author(s): *Naoki Morita, *University of Tsukuba*; Kouta Kishi, *The University of Tokyo*; Naoto Mitsume, *University of Tsukuba*; Kazuki Shibanuma, *The University of Tokyo*;

We propose a three-dimensional analysis method based on the local fracture stress criterion and the s-version finite element (s-FE) strategy for crack propagation. The local fracture stress criterion states that a crack propagates when the local stress near the crack tip reaches the fracture stress [1]. This criterion has been validated as a fracture criterion for brittle crack propagation in steel. When the standard finite element method (FEM) is used to calculate this criterion, it is difficult to represent the curved crack front and huge computational cost is required to evaluate the local stress in detail. On the other hand, The s-FE strategy achieves high local-accuracy while reducing computational cost of the FEM by superimposing a global mesh that represents the behavior of the entire domain and a local mesh that represents the detailed behavior of the region of interest. By combining these methods, this study proposes a three-dimensional crack analysis method that is both highly-accurate and highly-efficient. The accuracy of proposed method is verified for a three-dimensional elastic analysis. [1] F. Yanagimoto, K. Shibanuma, K. Suzuki, T. Matsumoto, S. Aihara, Mater. Des., 144 (2018) 361–373.

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Title: Particle-Based Free-Surface Flow Analysis with Bottom Boundary-Fitted Coordinate Transformation

Author(s): *Naoto Mitsume, *University of Tsukuba*; Kyuya Matsumoto, *University of Tsukuba*; Yusuke Imoto, *Kyoto University*; Mitsuteru Asai, *Kyushu University*;

We propose an effective numerical method for simulating ocean waves based on a mesh-free particle method with a bottom boundary-fitted coordinate transformation. While particle methods such as the smoothed particle hydrodynamics (SPH) and the moving particle semi-implicit/simulation (MPS) method have been applied to simulations of free-surface flows including tsunamis [1, 2], they have difficulty in handling curved boundary such as seabed. Though an existing study has proposed the curvilinear SPH [3], which adopts a coordinate transformation corresponding to bottom boundaries, the curvilinear SPH has mainly focused on simulation of inviscid flow ignoring the viscous term. This study proposes a bottom boundary-fitted coordinate transformation for the Navier–Stokes equations considering the viscous term. We adopt the explicit MPS method as a mesh-free particle method, where pressure field is explicitly computed instead of solving the pressure Poisson equation. We derive a mixed derivative model of the MPS method since the coordinate transformation of viscous term generates the mixed partial derivatives. Our proposed method including the derivative model is verified by the simulation of a hydrostatic pressure problem with round-shaped bottom. [1] Asai, M., Miyagawa, Y., Idris, N. A., Muhari, A., Imamura, F.: Coupled tsunami simulations based on a 2D shallow-water equation-based finite difference method and 3D incompressible smoothed particle hydrodynamics. Journal of Earthquake and Tsunami, 10(05), 1640019 (2016) [2] Zheng, H., Shioya, R., Mitsume, N.: Large-scale parallel simulation of coastal structures loaded by tsunami wave using FEM and MPS method. Journal of Advanced Simulation in Science and Engineering, 5(1), 1–16 (2018) [3] Tavakkol, S., Zarrati, A. R., Khanpour, M.: Curvilinear smoothed particle hydrodynamics. International Journal for Numerical Methods in Fluids, 83(2), 115–131 (2016)

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Title: Fluid-Shell Interactions Using Non-Intrusive Coupling Based on the Immersed Finite Element Method

Author(s): *Narendra Nanal, *Rensselaer Polytechnic Institute*; Lucy Zhang, *Rensselaer Polytechnic Institute*; Scott Miller, *Sandia National Laboratories*; Jesse Thomas, *Sandia National Laboratories*;

This study presents a computational framework for simulating the interaction of a shell structure with a fluid flow. Simulating complex movement patterns of a thin solid in the fluid flow is a challenging problem. Most of the existing studies for fluid-shell interaction are based on immersed boundary method where solids do not occupy volume, thus cannot replicate the thickness of the thin structure. In the immersed computational framework, the shell structure can be explicitly represented with its own governing equations and formulations. We use the modified immersed finite element method (mIFEM) [1], where structures are represented with volumes. In this work, we used OpenIFEM [2], a high performance and modularly built open-source software for the coupling of fluid and shell structures. An external solid solver [3] based on the Kirchhoff-Love thin shell theory is coupled with OpenIFEM. The shell structure is projected into a volumetric space along the directions normal to the shell surface based on a given thickness. The mid-surface solution obtained from the shell solver is extrapolated onto the volume, which allows the background fluid domain to identify the solid location. The forcing acting on the shell structure from the fluid is first calculated on the boundaries of the projected volume which is then used to calculate the equivalent nodal forces and moments acting on the shell surface. The fluid-shell coupling algorithm is validated using three test cases: fluid interacting with a deformable thin elastic wall, a thin cantilever beam represented by shells, and an L-shaped shell. This study also demonstrates the versatility of the mIFEM algorithm as it can accurately capture solid dynamics for general 3D solids as well as thin shells. This work is supported by Sandia National Laboratories. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. References [1] Xingshi Wang and Lucy T. Zhang. Modified immersed finite element method for fully-coupled fluid-structure interactions.Computer Methods in Applied Mechanics and Engineering, 267:150–169, 2013. [2] Jie Cheng, Yu Feimi, and Lucy T Zhang. OpenIFEM: A high performance modular open-source software of the immersed finite element method for fluid-structure interactions. Computer Methods of Engineering and Sciences, 119:91–124, 2019. [3] Stephan Herb. Fem code for fluid-structure coupling - structure solver implementing flat shell elements.https://github.com/precice/fem-shell, 2016.

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Title: A General Method to Evaluate Bond Micromoduli for Anisotropic Bond-Based Peridynamics Models

Author(s): *Naveen Prakash, *Corning Incorporated*;

Peridynamics has evolved into a powerful method for computational modeling of materials. Peridynamics has been used for a variety of applications ranging from dynamic fracture in glass and fiber reinforced composites to hydraulic fracturing, piezoresistivity in nanocomposites, functionally graded materials, polycrystalline fracture and corrosion. Although a couple of different options are available for material modeling in peridynamics, namely bond-based and state-based models, bond-based models have in general received more attention because of its straightforward implementation. While anisotropic bond-based material models have received some attention, mostly for transversely isotropic materials such as fiber reinforced composites, there still remains a gap in literature with regards to modeling general anisotropic Cauchy materials. In nearly all cases, parameters for bond-based peridynamics material models such as the micromodulus of bonds are evaluated using analytical expression based on the principle of strain energy equivalence to classical continuum mechanics expression. Prakash1 recently proposed a numerical method for the calibration of bond micromoduli based on the equivalence of the peridynamic and classical material stiffness tensors. This method poses the calibration step as a system of equations which is solved in a least-squares sense to evaluate a discrete distribution of bond micromoduli. Preliminary results of this method for general anisotropic Cauchy materials are promising and show that this method may be effectively used for the calibration of many different material classes using the same approach. Examples of all eight material symmetry classes – from triclinic to isotropic will be shown. The proposed method is also able to find solutions with a variety of horizon sizes, horizon shapes and influence functions. Moreover, since this is a discrete approach, an added advantage is that volume correction is inherently accounted for and removes the need for additional computations for volume corrections. References 1. Prakash, Naveen. "A Novel Numerical Method for Modeling Anisotropy in Discretized Bond-Based Peridynamics." arXiv preprint arXiv:2011.08013 (2020).

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Title: Implicit Discontinuous Galerkin Methods for High-Speed Turbulent Flows on Graphics Processors

Author(s): *Ngoc-Cuong Nguyen, *Massachusetts Institute of Technology*; Jaime Peraire, *Massachusetts Institute of Technology*; Sebastien Terrana, *Massachusetts Institute of Technology*;

We present an implicit matrix-free discontinuous Galerkin method for numerical computation of turbulent flows at high Reynolds numbers. The method is implemented using CUDA C++ with MPI-based parallelization to harness the computing power of GPUs and available as an open-source code at https://github.com/exapde/Exasim. Our method is used to to predict transonic buffet phenomena over the OAT15A supercritical airfoil at Reynolds number 3 millions and transitional hypersonic flows over the Purdue's flared cone at Reynolds number 10.8 millions. The method can capture various turbulence phenomena such as periodical low-frequency oscillations of shock wave in the streamwise direction, strong shear layer, shock wave boundary layer interaction, small scale structures broken down by the shear layer instability in the transition region, and shock-induced flow separation. The pressure coefficient, the root mean square of fluctuating pressure and streamwise range of shock wave oscillation are in good agreement with the experimental data. Our simulation results show that hypersonic boundary layer transition is sensitive to freestream disturbances resulting in the development and growth of the second-mode waves and the subsequent breakdown of the Görtler vortices. The good agreement between the computed heat transfer and the experimental data before the peak of the heat transfer coefficient suggests that the natural transition observed in the experiments is initiated by the receptivity of boundary layers to freestream disturbances.

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Title: Overlay Grid Mesh Adaptation Using Discrete Interface Reconstruction

Author(s): *Nicolas Le Goff, *French Alternative Energies and Atomic Energy Commission*; Franck Ledoux, *French Alternative Energies and Atomic Energy Commission*; Jean-Christophe Janodet, *Université d'Évry-Val-d'Essonne, Paris-Saclay*;

Some overlay grid methods provide mesh adaptation capabilities relying on the principle that when the base mesh, usually a grid, would not give satisfactory results it is adapted to better fit the CAD model, for example when capturing small details is relevant. On the other hand, a few of the overlay grid methods [1] take instead a mesh carrying materials volume fraction data as an input and produce a mesh with pure cells as an output. As those methods start from the input mesh and its carried volume fractions we are not at liberty to change the mesh resolution or refine it locally to capture some details of the CAD – which we actually do not have. Nevertheless, we propose to mimic this capability by use of a voxel-based interface reconstruction [2] that allows the transfer of volume fractions between two meshes. We obtain a different mesh with corresponding volume fractions on which the overlay grid method can then be run again. We show how introducing a user-guided bias during the interface reconstruction can be used to help accommodate meeting some requirements on the output mesh, for example in preserving thin layers. We also combine this procedure with some criteria that detects where the mesh should be locally refined in order to refeature the obtained mesh. [1] S. J. Owen, M. L. Staten and M. C. Sorensen. Parallel hex meshing from volume fractions, Engineering with Computers 30 (2014). [2] N. Le Goff, F. Ledoux, J.-C. Janodet and S. J. Owen. Guaranteed quality-driven hexahedral overlay grid method, Proceedings of the 28th International Meshing Roundtable (2019)

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Title: Hemodynamics and Bio-Mechanics of Model Saccular Aneurysms of Basilar Artery Using Fluid Structure Interaction Simulations.

Author(s): *Nimmy Thankom Philip, *Indian Institute of Technology Madras*; B. S. V. Patnaik, *Indian Institute of Technology Madras*; Sudhir B. J., *SCTIMST, Trivandrum*;

Hemodynamics under pulsatile conditions plays an important role in the growth, rupture, and surgical treatment of intracranial aneurysms (ICA). Wall shear stress (WSS) and its spatial and temporal variants are hypothesized to be correlated with the continuous expansion and eventual rupture of the ICAs. Another hypothesis is that aneurysm rupture mechanism is also dependent on the progressive wall remodeling happening due to the cyclic fluid stresses, which can lead to plastic deformation under fatigue like conditions. Also, an understanding of the velocity field and the stress patterns in the aneurysm dome and neck is helpful in the correct placement of endovascular coils/clips. This work attempts to describes the flow dynamics and bio-mechanics of an idealized saccular aneurysm of circular shape located at the basilar artery (BA) bifurcation with fluid flow under Newtonian fluid and linear elastic vessel wall approximation. The geometry, inlet/outlet boundary conditions are adopted from the Computational fluid dynamics (CFD) study carried out by Valencia et al. [1] with the two posterior cerebral arteries (PCA) having different diameters. FSI based simulations are carried out for the BA aneurysm providing valuable insight into the WSS, pressure, vessel wall stress/deformation, when subjected to physiologically realistic pulsatile loads. A comparative assessment of the flow features obtained from the present FSI simulation with the results reported by Valencia et al. [1] under rigid wall assumptions are reported. References 1. Valencia AA, Guzmán AM, Finol EA, et al. Blood flow dynamics in saccular aneurysm models of the basilar artery. J Biomech Eng 2006; 128: 516–526.

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Title: An Image-Based Numerical Workflow for the Analysis of Additively Manufactured Lattice Structures

Author(s): *Nina Korshunova, *Technical University of Munich*; Gianluca Alaimo, *University of Pavia*; Iason Papaioannou, *Technical University of Munich*; Seyyed Bahram Hosseini, *Aalto University*; Massimo Carraturo, *University of Pavia*; Alessandro Reali, *University of Pavia*; Jarkko Niiranen, *Aalto University*; Daniel Straub, *Technical University of Munich*; Ferdinando Auricchio, *University of Pavia*; Ernst Rank, *Technical University of Munich*; Stefan Kollmannsberger, *Technical University of Munich*;

Recent developments in additive manufacturing (AM) have allowed for producing lightweight metal lattice structures. However, the manufacturing process's complexity puts a significant uncertainty on the final product's confidence levels. This is due to the fact that metal AM processes introduce geometrical defects, which mainly result in deviations from the nominal geometry. These geometrical and topological process-induced defects are among the primary causes of the gap between the as-designed and as-manufactured mechanical behavior of AM products. Thus, incorporating as-manufactured geometries into the numerical analysis is crucial for a reliable estimation of their mechanical behavior. The most common way to acquire the printed geometrical shape is through a Computed tomography (CT). However, CT-based numerical analysis is computationally challenging. In this presentation, an immersed image-to-material-characterization numerical workflow is proposed. The core of the proposed methodology is the high-order Finite Cell Method (FCM). It provides a powerful numerical tool to perform an analysis of the complete AM parts via direct numerical testing or via numerical homogenization. To this extent, we will validate the numerical model for the case of 3D printed octet-truss structures ([1],[2]). Furthermore, the effect of the randomness of the geometry on the performance of the structure is evaluated. To this end, we will introduce a novel CT-based binary random field model. This model is then combined with the validated numerical results to predict the mean and variance of lattice structures' elastic properties. 1. Korshunova, N., Alaimo, G., Hosseini, S.B., Carraturo, M., Reali, A., Niiranen, J., Auricchio, F., Rank, E., and Kollmannsberger, S. (2020). A CT-based numerical characterization of tensile behavior of additively manufactured octet-truss structures and its experimental validation. Preprint submitted to Additive Manufacturing, https://arxiv.org/abs/2012.07452. 2. Korshunova, N., Alaimo, G., Hosseini, S.B., Carraturo, M., Reali, A., Niiranen, J., Auricchio, F., Rank, E., Kollmannsberger, S. (2021). Bending behavior of additively manufactured lattice structures: numerical characterization and experimental validation. Preprint submitted to Materials & Design, https://arxiv.org/abs/2101.09034.

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Title: Blended Isogeometric Kirchhoff-Love and Continuum Shells with Application to Aircraft Horizontal Stabilizer Analysis

Author(s): *Ning Liu, *Global Engineering and Materials, Inc.*; Emily Johnson, *Iowa State university*; Manoj Rajanna, *Iowa State university*; Jim Lua, *Global Engineering and Materials, Inc.*; Nam Phan, *Naval Air Systems Command*; Ming-Chen Hsu, *Iowa State university*;

The computational modeling of thin-walled structures based on isogeometric analysis (IGA) and Kirchhoff-Love (KL) shell formulation has attracted significant research attention in recent years. While these methods offer numerous benefits, including exact representation of the geometry, naturally satisfied high-order continuity, and computationally efficient rotation-free formulations, they also present a number of challenges in modeling real-world engineering structures of considerable complexity. Specifically, these models are usually comprised of numerous patches, with discontinuous derivatives, non-conforming discretizations, and non-watertight connections at their interfaces. Moreover, the analysis of such structures often requires the full stress and strain tensors (i.e., including the transverse normal and shear components) for subsequent failure analysis and remaining life prediction. Despite the efficiency provided by the KL shell, the formulation cannot accurately predict the response in the transverse directions due to its kinematic assumptions. In this work, a penalty-based formulation for the blended coupling of KL and continuum shells is presented. The proposed approach embraces both the computational efficiency of KL shells and the availability of the full-scale stress/strain tensors of continuum shells where needed by modeling critical structural components using continuum shells and other components using KL shells. The proposed method enforces the displacement and rotational continuities in a variational manner and is applicable to non-conforming and non-smooth interfaces. The efficacy of the developed method is demonstrated through a number of benchmark studies with a variety of analysis configurations, including linear and nonlinear analyses, matching and non-matching discretizations, and isotropic and composite materials. Finally, an aircraft horizontal stabilizer is considered to demonstrate the applicability of the proposed blended shells to real-world engineering structures of significant complexity.

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Title: Comparison of Membrane, Shell, and 3D Solid Formulations for Vascular Biomechanics

Author(s): *Nitesh Nama, *University of Michigan*; Miquel Aguirre, *Université Lyon*; Rogelio Ortigosa, *Technical University of Cartagena*; Antonio J. Gil, *Swansea University*; Jay D. Humphrey, *Yale University*; C. Alberto Figueroa, *University of Michigan*;

Computational techniques to simulate cardiovascular biomechanics in three-dimensional models of arteries have attracted significant interest owing to their applications in disease research, medical device design, and surgical planning [1]. Typically, the arterial wall is modelled, with increasing degree of detail, as either as a membrane, a shell, or a 3D solid element. Each of these formulations has its own advantages and disadvantages concerning accuracy, ease of implementation, and computational costs and the choice of optimal formulation must be made depending on the desired numerical accuracy and computational cost for a specific application. However, despite the widespread use of these formulations for cardiovascular applications, there is little information concerning the impact of this choice on numerical accuracy. Consequently, the decision regarding the optimal choice often relies on intuition or previous experience, with unclear consequences of choosing one approach over the other. In this work, we present a systematic comparison between four different vessel wall models: (i) a nonlinear incompressible membrane model, (ii) a rotation-free incompressible shell model with only displacement degrees of freedom, (iii) a 3D solid model with linear prismatic elements, and (iv) a 3D solid model with quadratic prismatic elements. We use both the idealized and patient-specific geometries to compare the accuracy and efficiency of these approaches. For the idealized geometries, we will present a comparison of these formulations against the well-known axisymmetric solution for cylindrical geometries. Subsequently, we will discuss the performance of these approaches for subject-specific geometries with fiber-based constitutive models to provide a general guideline for choosing the adequate approach. Lastly, we will present the extension of rotation-free shell formulation to develop a computationally efficient fluid-structure interaction framework for vascular biomechanics. REFERENCES [1] C. A. Taylor and C. A. Figueroa, Annu Rev Biomed Eng, Vol. 11, pp. 109-134, 2009.

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Title: OpenFOAM Based Modeling and Simulation of Aluminium Smelting Process

Author(s): *Nithin Panicker, *Oak Ridge National Laboratory*; Rajneesh Chaudhary, *Alcoa Corporation*; Prashant Jain, *Oak Ridge National Laboratory*; Vivek Rao, *Oak Ridge National Laboratory*; Marc Delchini, *Oak Ridge National Laboratory*;

Aluminium smelting process is used to produce aluminium from alumina. Smelting occurs in an electrolytic cell filled with an electrolyte subjected to Direct current (DC). Alumina powder fed into the cell dissolves into the electrolyte and is reduced to aluminium metal on cathode. Flow modeling and simulation of smelting process is challenging due to the coupled multi-physics involved in the process. To ensure optimum productivity and energy efficiency of the cells, a distinct understanding of flow physics inside the cell is required, involving multiphase momentum, heat and mass transfer, along with magneto hydrodynamics. A Computational Fluid Dynamics (CFD) model based on multi-fluid Eulerian-Eulerian approach to model the smelting physics is discussed. The CFD model accounts for multiple physics involving, 1) Multiphase gas driven electrolyte flow; 2) alumina dissolution, diffusion and consumption in electrolyte; 3) magneto-hydrodynamics further impacting gas driven electrolyte flow; 4) thermal energy evolution as alumina dissolves. CFD simulations are performed using the multiphaseEulerFoam solver in OpenFOAM (an open source CFD code). The predictions of various multi-physics obtained from the open source solver are discussed. The results are compared with the commercial CFD Siemen’s code StarCCM+ and validated with experiments.

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Title: A Neural Ordinary Differential Equations Approach to Modeling Chemical Kinetics

Author(s): *Opeoluwa Owoyele, *Argonne National Laboratory*; Pinaki Pal, *Argonne National Laboratory*;

Computational fluid dynamics (CFD) simulations of practical combustors often employ simplified models due to the prohibitive cost of solving for a large number of chemical species in space and time. Emerging as a promising way to incorporate detailed chemistry into CFD simulations of reactive flow systems, machine learning models have increasingly been applied to predict chemical source terms as functions of the thermochemical states in recent years. In this approach, data containing various thermochemical states and their corresponding reaction rates are generated by running simplified simulations. Machine learning models, often artificial neural networks are then trained to minimize a loss function that measures the differences between the actual and predicted chemical source terms. However, combustion is a highly nonlinear phenomenon, leading to divergence from the true solution when the neural network-predicted source terms are integrated in time. In this work, a neural ordinary differential equations approach to modeling chemical kinetics is developed to address this issue. In this approach, a neural network is trained to predict the chemical source terms that lead to accurate temporal evolution of the chemical species. By backpropagating errors through the ordinary differential equations (ODE) solver and the neural network layers, the neural network's parameters are adjusted to minimize the difference between the predicted and actual ODE solutions. It is shown that even when the dimensionality of the thermochemical manifold is trimmed to remove redundant species, the proposed approach accurately captures the correct physical behavior and reproduces the results obtained using the full chemical mechanism.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Geomiso DNL: A Cloud-Based Software for Non-Linear Inelastic Dynamic Isogeometric Analysis

Author(s): *Panagiotis Karakitsios, *Geomiso Company*; Konstantinos Margaronis, *Geomiso Company*; Elektra Theloura, *Geomiso Company*;

This paper presents Geomiso DNL (www.geomiso.com), a new hybrid software for applications on non-linear inelastic dynamic isogeometric analysis and 3D design with NURBS and T-splines, which satisfies the rising industrial need for seamless integration of computer-aided design and computer-aided analysis. The isogeometric method has attracted increasing attention in both academia and industry, while modern T-splines overcome limitations inherent to NURBS, permit local refinement and ensure higher-order continuity across patches. Geomiso DNL is not just a plug-in, but a both stand-alone and cloud-based program, which enables engineers to simulate dynamic phenomena, whose impact on products and structures in real-world environments can be more efficiently evaluated. This new software fully integrates the industrial design of any geometry with its computational real-time testing by facilitating the geometry modeling within analysis. Its hybrid graphical user interface offers an innovative way to merge geometric design with mesh generation into a single procedure and preserves the exact geometry at all refinement levels in contrast with finite element programs. Applications to dynamic analysis are demonstrated with a comparison between Geomiso DNL and finite element software. We compare the matrix assembly and solver time, as well as the accuracy of the numerical results, for typical examples arisen in structural dynamics. We also conduct parametric investigations on the effects of control point number, element number and polynomial order of basis functions. This software appears to be preferable to finite element software packages, as it represents major improvements, such as higher accuracy, robustness, and stability level, combined with significantly reduced computational cost. This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T2EDK-00338). Keywords: Isogeometric analysis, Finite element analysis, Computational structural dynamics, Inelastic analysis, T-splines, NURBS, Accuracy, Computational cost, Software, Cloud Rererences [1] P. Karakitsios, G. Karaiskos, A. Leontaris, P. Kolios, Geomiso TNL: A software for non-linear static T-spline-based isogeometric analysis of complex multi-patch structures, 14th World Congress in Computational Mechanics (WCCM), ECCOMAS Congress (2020). [2] A. Karatarakis, P. Karakitsios, M. Papadrakakis, GPU accelerated computation of the isogeometric analysis stiffness matrix, Comput. Methods Appl. Mech. Engrg., 269 (2014) 334-355. [3] A. Idesman, D. Pham, J.R. Foley, M. Schmidt, Accurate solutions of wave propagation problems under impact loading by the standard, spectral and isogeometric high-order finite elements. Comparative study of accuracy of different space-discretization techniques, Finite Elements in Analysis and Design, 88 (2018) 208-240.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Chemically-Driven Fracture in Porous Media: A Phase-Filed Fracture Study

Author(s): *Pania Newell, *The University of Utah*; Louis Schuler, *ENS Paris-Saclay*;

Predicting and controlling fractures in porous materials has posed many challenges in understanding the long-term performance of such complex systems. Geological systems such as CO2 sequestration, geothermal, waste repositories, oil and gas recoveries, are examples of natural porous materials, where fracture and damage play significant roles. In many of these systems, chemical alterations lead to change in the properties of fracture as well as the mechanics of the intact porous material. This presentation focuses on fracture initiation and propagation and shows how the state-of-the-art phase-field fracture can be used to model chemically-driven fracture in porous systems. We introduce a chemical damage parameter that is coupled with the mechanical damage parameter obtained from the phase-field equation. The chemical damage parameter is also coupled with the change in porosity due to dissolution occurring in the porous material. We will demonstrate how this coupled formulation enables us to understand fracture behavior in various geological porous systems. We also discuss how chemical dissolution impacts the crack speed and directionality.

16th U.S. National Congress on Computational Mechanics
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Title: Physics-Informed Deep Learning for 4D-Flow MRI

Author(s): *Paris Perdikaris, *University of Pennsylvania*; Sifan Wang, *University of Pennsylvania*; Georgios Kissas, *University of Pennsylvania*; Xinling Yu, *University of Pennsylvania*;

Because of its noninvasive nature and the ability to provide a range of structural and physiological contrasts, magnetic resonance imaging (MRI) has become an indispensable tool for quantitative in-vivo assessment of blood flow and vascular function in patients with cardiac and cardiovascular disease. However, MRI measurements of the vasculature are often limited by insufficient spatial resolution and are corrupted by complex noise processes, leading to ad hoc workflows for reconstructing vascular topologies and associated flow conditions. Here we leverage recent developments on physics-informed deep learning to enhance the resolution and information content of current MRI technologies, with a specific focus on 4D flow MRI. We develop deep neural network algorithms that are constrained by the Navier-Stokes equations to effectively de-noise MRI data and yield physically consistent reconstructions of the underlying velocity and pressure fields that ensure conservation of mass and momentum at an arbitrarily high spatio-temporal resolution. Moreover, the filtered velocity fields can be employed to identify regions of no-slip flow, from which we are able to estimate the geometry of the arterial wall, as well as infer important quantities such as wall shear stresses, kinetic energy and dissipation. Taken together, the proposed methods can significantly advance the capabilities of MRI technologies for probing vascular structure and function in both clinical and research scenarios.

16th U.S. National Congress on Computational Mechanics
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Title: Multi-fidelity Methods for Uncertainty Quantification of Nonlocal Diffusion Model

Author(s): *Parisa Khodabakhshi, *The University of Texas at Austin*; Max Gunzburger, *Florida State University*; Karen Willcox, *The University of Texas at Austin*;

Nonlocal models are useful at describing certain physical phenomena for which conventional PDEs fail to describe the behavior. In nonlocal models, distant interactions are considered between points that are less than a finite length scale (usually referred to as the horizon) apart from each other. As a result of distant interactions, nonlocal models are generally computationally more expensive than their local counterparts due to the reduced sparsity. The higher computational cost of nonlocal models might inhibit the implementation of an outer-loop application (e.g., uncertainty quantification, optimization, inference, control) where multiple model evaluations are required. Employing a multi-fidelity method for nonlocal models that combines surrogate models of lower fidelity with the high-fidelity model can help eliminate this constraint. In this study, we propose a multi-fidelity approach for a nonlocal diffusion model to be used in an uncertainty quantification setting. The surrogate models are built by reducing the mesh refinement, the horizon, or both. The multi-fidelity method achieves the speed-up in Monte Carlo estimations of the quantity of interest by allocating most model evaluations to the cheap surrogate models while keeping high-fidelity model evaluations at a relatively low number. It is shown that the multi-fidelity method achieves above two order of magnitude speed-ups compared to the high-fidelity model.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physics-Informed Generative Adversarial Networks for Uncertainty Quantification in Fatigue and Fracture Applications

Author(s): *Patrick Leser, *NASA Langley Research Center*; Geoffrey Bomarito, *NASA Langley Research Center*; James Warner, *NASA Langley Research Center*; William Leser, *NASA Langley Research Center*; Julian Cuevas, *University of Puerto Rico Mayaguez*; Theodore Lewitt, *University of Southern California*; Sean Lai, *Portland State University*;

While standard generative adversarial networks (GANs) rely solely on data for training, physics-informed GANs (PIGANs) incorporate physical constraints in the form of partial differential equations using autodifferentiation. As a result, PIGANs can produce probabilistic and physically admissible solutions to PDEs without relying on traditional methods such as finite element analysis. Additionally, by relating observed data to unobserved quantities of interest through the differential equations, PIGANs can also be used to solve non-deterministic inverse problems. In this work, a numerical experiment is conducted in which PIGANs are used to learn the probability distribution of a spatially-varying elastic modulus given deformation data measured on the surface of a 2D plate in tension. The learned probability distribution can then be used to generate realizations of the material, or what are effectively virtual test specimens. The potential of this capability for uncertainty quantification in fatigue and fracture applications is discussed.

16th U.S. National Congress on Computational Mechanics
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Title: Non-Intrusive Coupling of a 3D Multi-Scale Generalized Finite Element Method with a Commercial FE Solver

Author(s): Haoyang Li, *University of Illinois at Urbana-Champaign*; *Patrick O'Hara, *Air Force Research Laboratory*; C. Armando Duarte, *University of Illinois at Urbana-Champaign*;

In many engineering applications, it is necessary to account for interactions among multiple spatial scales through numerical simulations. Resolving fine-scale features such as cracks and localized nonlinearities with high fidelity is critical for the accurate prediction of service life or failure of structures. Three-dimensional models with detailed meshes and advanced modelling techniques are often required to accurately resolve fine-scale behaviour. However, adopting such models on the structural/global scale is often computationally intractable, particularly for problems involving multiple local features. A coarse mesh is often sufficient for predicting the component-level response of a structure, and thus highly-adapted discretizations are only required on sub-sets of the component-scale model. In this talk, we present a multi-scale computational framework which couples Abaqus models and 3-D multi-scale Generalized FEM discretizations based on numerically-defined enrichment functions – the GFEMgl. The structural-scale problem is modelled in Abaqus using a coarse mesh of 3D elements suitable for capturing the macro/component-scale response of the structure. Fine-scale problems defined in regions of interest, and solved in parallel provide enrichment functions for the GFEMgl. These functions enable the GFEMgl to accurately approximate localized phenomena such as crack propagation without direct refinement of initially-coarse meshes. The interactions between structural (Abaqus) and GFEMgl models are captured using the Iterative Global-Local method (IGL). In this method, global-scale displacements are passed to GFEMgl models as boundary conditions while residual forces along the interface between the two models are applied to the structural model. The proposed multiscale framework is non-intrusive in the sense that only standard output quantities from the finite element simulations are exchanged during the coupling process. The interaction between Abaqus and the GFEMgl solver requires no knowledge of the discretization technique adopted in the other solver, and no access to source the source code of the commercial FE tool. Numerical examples of a T-joint structure exhibiting fatigue crack propagation are presented to demonstrate the accuracy and potential applicability of the proposed framework.

16th U.S. National Congress on Computational Mechanics
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Title: Regression Based Approach for Robust Finite Element Analysis on Arbitrary Grids (REBAR)

Author(s): *Paul Kuberry, *Sandia National Laboratories*; Pavel Bochev, *Sandia National Laboratories*; Jacob Koester, *Sandia National Laboratories*; Nathaniel Trask, *Sandia National Laboratories*;

REBAR is an approach for accurate and robust numerical simulation of partial differential equations for meshes that are of poor quality. Traditional finite element methods use the mesh to both discretize the geometric domain and to define the finite element shape functions. The latter creates a dependence between the quality of the mesh and the properties of the finite element basis that may adversely affect the accuracy of the discretized problem. Our approach breaks this dependence and separates mesh quality from the discretization quality. At the core of the approach is a meshless definition of the shape functions, which limits the purpose of the mesh to representing the geometric domain and integrating the basis functions without having any role in their approximation quality. A collection of numerical experiments will be presented: strongly coercive elliptic problems, linear elasticity in the compressible regime, and the stationary Stokes problem. Comparison of timestep and accuracy will be made with the continuous Galerkin finite element method.

16th U.S. National Congress on Computational Mechanics
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Title: Meso-Scale Finite Element Simulation on Impact Failure Behavior of Two-Dimensional Triaxially Braided Composites

Author(s): *Peng Liu, *Northwestern Polytechnical University, China*; Chao Zhang, *Northwestern Polytechnical University, China*;

Textile composites are widely used to manufacture large structural components of aircraft or aero-engine, because of its convenient forming, excellent mechanical properties, and better impact resistance than traditional laminate composites [1]. However, aircraft and aero-engine structures will inevitably suffer high-speed impact load during their service life. It is an urgent technical problem to evaluate the applicability of large-scale textile composite structures against impact loads, which is known to be a multi-scale problem from specimen level to the component level, and finally to the full-scale structure level. Experimental validation and certification processes are time and economy costly due to the large number of specimens and tests. Therefore, it is necessary to introduce computational methods to improve the design efficiency for impact resistance of composite structures. In this study, a high-fidelity meso-scale FE model is developed to study the progressive failure behavior of two-dimensional triaxially braided composites (2DTBC) under high-speed impact loads. The geometry features of the unit cell model were explicitly modeled based on the realistic geometry information. The model consisted of three components: fiber tow, matrix and interface. An orthotropic 3D continuous damage model was established to predict the damage initiation and propagation process in fiber tows [2]. The Johnson-Cook model was applied to describe the elastoplastic mechanical behavior of resin matrix and the interfaces between fiber tow and matrix were simulated using cohesive element model. The FE model was verified based on experimental results. Then the meso-scale FE model of the impact experiment of the material was established. The proposed model shows excellent correlation with the experimental results, not only capturing the global strain responses, but also capturing the Main mechanical response, failure mode and velocity threshold of 2DTBC under out-of-plane impact. [1] Marsh G. Aero engines lose weight thanks to composites. Reinforced Plastics, 2012, 56(6): 32-35. [2] Zhang C, Li N, Wang W Z, et al. Progressive damage simulation of triaxially braided composite using a 3D meso-scale finite element model[J]. Composite Structures, 2015, 125:104-116.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Fiber-Reinforced Constitutive Model for Earthen Structural Materials

Author(s): *Persid Koci, *University of Illinois at Chicago*; Craig Foster, *University of Illinois at Chicago*;

Earthen structures have seen renewed engineering interest in recent decades. With improved compaction techniques, the addition of cement or other stabilizers, and stronger mortars, the engineering properties of these materials have greatly improved. They can still be largely locally sourced, and are economical in areas with relatively cheap labor. They are also highly sustainable, often recyclable, and have excellent thermal mass. There are still some areas in which the materials can be improved. They are relatively weak in tension and not highly ductile. Fiber reinforcement may be one way to economically improve these properties in earthen materials. Though several reinforcement methods have been attempted, we focus here on polypropylene fibers. To understand the behavior of these materials and to optimize their performance, a new constitutive model is proposed. The model considers the effect of the fibers embedded in a matrix. A uniform distribution of the fiber orientations is assumed initially. A numerical technique is used to integrate the effect of the fibers over possible orientations, and the performance of that method is analyzed here. Under a given loading, the fibers may exhibit: elasto-plastic behavior approximated with linear hardening model with fracture; fiber slippage depending on the cohesive bond between the fiber and the matrix, and with frictional resistance; both behaviors; or neither of those. These possibilities result in a plasticity model employing multiple yield surfaces that are frequently met in plasticity theory. We do not account for fiber pull-out in this model, as this requires a crack of finite opening. The fiber model is coupled with Drucker-Prager model with linear hardening used for representing the soil (matrix), as a first approximation. The model is analyzed for uniaxial tensile loading and shear loading. Fiber parameters are calibrated to predict the model behavior in accordance with experimental data.

16th U.S. National Congress on Computational Mechanics
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Title: A Bond-Based Peridynamic Model for Coupled Heat Transfer and Water Flow with Phase Change Effects

Author(s): *Petr Nikolaev, *University of Manchester*; Majid Sedighi, *University of Manchester*; Andrey Jivkov, *University of Manchester*; Lee Margetts, *University of Manchester*;

A wide range of heat and mass transfer problems in natural and synthetic materials involve phase changes between solid and liquid states. Examples of such problems include seasonal and artificial freezing of soil/rock; solidification in metals, polymers and ceramics; thermal energy storage systems based on latent heat. Predicting the interphase boundary evolution in such systems is challenging for classical continuum approaches, as the boundary marks a discontinuous change of material properties and processes. For example, the water-ice boundary in freezing soil separates regions with different soil physical and mechanical properties and terminates water flow. An effective approach to such situations is offered by peridynamics. We present a bond-based peridynamic formulation for coupled heat and water transport in saturated porous media, which includes the effect of phase change on the transport processes. In our model, the domain is conceptually divided into three regions - liquid, mushy and solid - for which the boundaries depend on temperature. The thermo-physical properties are defined by the volume-averaged technique. Three types of bonds are defined: solid-solid; interfacial, which provide interconnection between different regions; and liquid-liquid. Heat transfer by conduction and convection is considered. The velocity of water calculated by the mass conservation of liquid is used to calculate the heat convection. The bonds emanating from the solid region transfer only heat, while all other bonds transfer both heat and water. The model is verified for 1D and 2D problems, using available analytical as well as alternative numerical solutions (FEA). The results from the verification exercise demonstrate that the proposed approach provides accurate prediction of the interphase boundary position and the temperature distribution for a wide range of initial and boundary conditions. Furthermore, we present a case study on thermal behavior of saturated soils under artificial ground freezing, by which we demonstrate the capability of the model to capture the effects of randomly distributed permeable and impermeable inclusions representing the heterogeneity of real soils.

16th U.S. National Congress on Computational Mechanics
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Title: Large-Scale Ab-Initio Polarizability Calculations using Real-Space Finite-Element Based Methods

Author(s): *Phani Motamarri, *Indian Institute of Science*; Krishnendu Ghosh, *Intel Corporation*; Vikram Gavini, *University of Michigan*;

Ab-initio calculations have played a significant role in determining a wide variety of material properties. In particular, large-scale ab-initio polarizability calculations are of paramount importance to understand the physics of di-electric screening behaviour and quasi-particle properties of layered materials, in surface plasmonics, strain engineering, optical properties of materials and so on. The state-of-the-art ab-initio computational technique to compute polarizabilities involve a combination of density functional theory calculation (mean-field) and random-phase approximated (RPA) density response calculation (post-mean-field). These post-mean-field calculations are computationally expensive with quartic computational complexity with number of electrons. Furthermore, one of the major challenges in these calculations lies in converging the polarizability tensor with respect to number of reciprocal G-vectors, Brillouin zone sampling and the number of empty states. This becomes even more challenging in semi-periodic or fully non-periodic material systems which require large vacuum in the non-periodic direction. To this end, we demonstrate a scalable real-space approach to conduct computationally efficient polarizability calculations within the framework of finite-element discretization which can accommodate unstructured coarse-graining and arbitrary conditions in a straightforward manner. Here, the underlying mean-field calculations employ a finite-element based DFT solver and the post mean-field calculation involving the computation of polarizability tensor is accomplished by efficiently evaluating the plane-wave matrix element in real-space on parallel computing architectures with the underlying wavefunction fields represented in finite-element basis. The accuracy and performance of the proposed implementation are demonstrated on a variety of benchmark examples including large-scale material systems involving few thousands of electrons.

16th U.S. National Congress on Computational Mechanics
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Title: Space-Time Continuous Galerkin hp-Finite Elements for Nonlinear Heat Problems

Author(s): *Philipp Kopp, *Technical University of Munich*; Stefan Kollmannsberger, *Technical University of Munich*; Ernst Rank, *Technical University of Munich*; Victor Calo, *Western Australian School of Mines*;

Many transient problems exhibit local features that need to be resolved in both, space and time. An important class of problems arises in the simulation of selective laser melting (SLM) processes. Here, a high energy laser is used to melt metal powder and ”print” three-dimensional objects layer by layer. The laser diameter is usually many orders of magnitude smaller than the printed object, and the distance traveled by the laser in the entire process can be as long as multiple kilometers. Thus, even partially simulating the evolution of the temperature poses an immense challenge for the discretization method. Clearly, local refinement in space-time is necessary for these kinds of problems. A natural choice is to use the finite element method for spatial and temporal discretization and apply existing refinement technology. To this end, we extend the multi-level hp-method introduced in [1] to four dimensions. The method allows arbitrary hanging nodes and provides the necessary flexibility to increase the polynomial degree in regions where the solution is smooth. We apply this methodology to discretize a transient heat equation with non-linear coefficients. To reduce the computational cost we split the problem into time slabs that are conforming to the base mesh. We first apply this to a standard Bubnov Galerkin discretization and then compare the results to a Galerkin-Petrov approach. [1] Zander, N. and Bog, T. and Elhaddad, M. and Frischmann, F. and Kollmannsberger, S. and Rank, E. The multi-level hp-method for three-dimensional problems: Dynamically changing high-order mesh refinement with arbitrary hanging nodes. Computer Methods in Applied Mechanics and Engineering (2017) 310:252–277. [2] Aziz, A.K. and Monk, P. Continuous finite elements in space and time for the heat equation. Mathematics of computation (1989) 52:255–274.

16th U.S. National Congress on Computational Mechanics
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Title: AMR for Unstructured T-Splines with Linear Complexity

Author(s): *Philipp Morgenstern, *Leibniz University Hannover*; Roland Maier, *Chalmers University of Technology and University of Gothenburg*; Thomas Takacs, *Johannes Kepler University Linz*;

We present an adaptive refinement algorithm for T-splines on unstructured 2D meshes. We consider unstructured spline spaces on manifolds as in [1], which yield C^{p-1}-continuous splines except in the vicinity of extraordinary nodes, where the continuity is reduced to C^0-continuity. Inspired by theory on higher-dimensional structured T-splines [2], we introduce the concept of direction indices, i.e., integers associated to each edge. These are a crucial ingredient refinement algorithm, in addition to the refinement levels of edges. We combine these ideas with an edge subdivision routine that allows for I-junctions, yielding a very flexible refinement scheme that nicely distributes the T-junctions, preserving sparsity of the system matrix and shape regularity of the mesh elements, and having linear complexity in the sense of a guaranteed upper bounds on a) the ratio of generated and marked mesh elements, and on b) the distance between marked and additionally refined elements. If used with conservative parameters, we also preserve analysis-suitability (local linear independence) except in the vicinity of extraordinary nodes. However, we also suggest the use of smaller edge neighborhoods in the refinement scheme for more localized refinement, sacrificing local linear independence for the sake of more localized refinement. In this case, we can still guarantee for the other properties mentioned above, such as sparsity of the system matrix, shape regularity, and linear complexity. [1] G. Sangalli, T. Takacs, and R. Vazquez, Unstructured spline spaces for isogeometric analysis based on spline manifolds, Computer Aided Geometric Design 47 (2016), 61–82. [2] P.Morgenstern, Mesh refinement strategies for the adaptive isogeometric method, Ph.D. thesis, Institut für Numerische Simulation, Rheinische Friedrich-Wilhelms-Universität Bonn, 2017.

16th U.S. National Congress on Computational Mechanics
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Title: A Unified Phase Field Approach to Elastic-Plastic Fracture

Author(s): *Pietro Pascale, *University of Cincinnati*; Kumar Vemaganti, *University of Cincinnati*;

A critical challenge associated with cohesive models of fracture resides in their phenomenological nature. The dependence on postulated surface energy laws results in a disconnect between the model and the underlying physical phenomena, which limits further developments of the model in multiscale settings. To overcome this issue, we propose an extension of the classical variational model of fracture that is capable of representing a wide range of behaviors, from brittle to ductile, without resorting to phenomenological assumptions. The approach we use is to separately model the two phenomena of plasticity (slip/gliding) and separation (crack) by identifying and tracking those phenomena with two distinct phase fields, called slip and damage, respectively. The proposed model embeds a mesoscale phase-field model of elastic-plastic behavior recently investigated by the authors that extends to the general load case the model of plastic slip presented by Ambrosio et al [1]. The second field, the damage, interacts with the slip field by the known phenomenon of pre-localization that is characteristic of some free-discontinuity formulations. Numerical results show that the proposed mesoscopic two phase field model is capable of reproducing a wide range of fracture behaviors, and can be easily correlated to ASTM standard testing results. We also show how the two-field approach can be harnessed to model a fatigue damage process. KEYWORDS: Phase-field model, Plasticity, Fracture, Damage [1] Ambrosio, L., A. Lemenant, and G. Royer-Carfagni (2013). A variational model for plastic slip and its regularization via gamma-convergence. J Elast 110, 201–235.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Personalized Virtual Cardiac Resynchronization Therapy to Predict and Optimize Long-Term Remodeling Outcome – A Case Study

Author(s): *Pim Oomen, *University of Virginia*; Èric Lluch, *Siemens Healthineers*; Tiziano Passerini, *Siemens Healthineers*; Tommaso Mansi, *Siemens Healthineers*; Kenneth Bilchick, *University of Virginia Health System*; Jeffrey Holmes, *The University of Alabama at Birmingham*;

Introduction: Cardiac resynchronization therapy (CRT) can restore coordinated contraction of the heart through biventricular pacing, which can stop and even reverse the progression of heart failure-induced remodeling. Yet 30-50% of patients do not have the desired response to CRT [1]. A major strength of CRT is the ability to tailor the therapy to individual patients; however, there are too many possible options to test during the implantation procedure. Therefore, there is a critical need for computational models that can predict long-term outcomes (left ventricle (LV) remodeling) for various possible pacing sites preoperatively. In this study, we test the feasibility of our novel virtual CRT simulation framework to predict and optimize long-term remodeling outcome for one individual patient. Methods: The virtual CRT framework consisted of a fast electrophysiology [2] and mechanical [3] model. Both models were personalized for a female non-ischemic LBBB patient (86-years-old female with non-ischemic LBBB, NYHA 3, QRS duration 155 ms). The electrophysiology model was used to simulate pre- and post-CRT regional electrical activation and QRS duration. The mechanical model, using the activation timing from the electrical model as input, was used to simulate strain-driven post-CRT cardiac remodeling. The models were customized for the patient using pre-CRT clinical MRI images, 12-lead ECG, and systolic and diastolic blood pressures, as well as pre- and post-CRT heart rates. Results: 6 Months of personalized post-CRT electrophysiology and remodeling were simulated in under 100s. When pacing from the clinical LV pacing site (apical lateral), simulated QRS duration shortening and reduction in LV end-systolic volume (LVESV, -43%) matched with 6-months post-CRT clinical data. Interestingly, when pacing from alternative LV free wall segments, we found a pacing site (mid anterior) that would have resulted in a greater reduction in LVESV (-52%). Discussion: We demonstrated that our virtual CRT framework can be used to predict and optimize long-term CRT outcome for one individual patient. The models are computationally efficient enough for routine clinical use and allow for personalized simulations at the bedside or in the electrophysiology lab. We will continue to test our model retrospectively on additional non-ischemic and ischemic LBBB patients treated in our center. References: [1] Brignole et al., Eur. Heart J., 34:2281–2329, 2013; [2] Neumann et al., Med. Image Anal., 34:52–64, 2016; [3] Witzenburg et al., J. Cardiovasc. Transl. Res., 11:109–122, 2018. Dislaimer: The concepts and information presented in this section are based on research results that are not commercially available

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Title: Mechano-Chemical Modeling of Microstructure Evolution and Grain Size Stabilization in Nano-Crystalline Metallic Alloys

Author(s): *Prakarsh Pandey, *University of Wisconsin-Madison*; Shiva Rudraraju, *University of Wisconsin-Madison*;

Nano-crystalline (NC) metallic alloys are fast evolving as a structural alloy of choice due to their superior mechanical properties (ductility and wear resistance) over the traditional coarse-grained micro-crystalline alloys. Key to the design and production of NC alloys is the challenge in ensuring the stability of their underlying microstructure. The classical understanding of metallic alloy microstructure evolution relies on grain boundary energy minimization through grain coarsening.However, NC alloys circumvent these grain growth mechanisms through kinetic and thermodynamic stabilization of the grain boundaries, resulting in many length-scale effects. Several mechanisms like grain boundary segregation, solute precipitation, and external loading have been known to affect the grain growth in NC alloys. In this work, we develop a novel phase-field representation of these mechanisms, and present a phase-field based finite-strain mechanics model of grain growth in NC alloys. Various parametric studies of NC microstructure evolution and its coupling to mechanical deformation will be discussed. Further, extensions of this framework to include length-scale effects through the incorporation of strain-gradient mechanics will be presented.

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Title: Kinetics of Self-Assembly due to Lipid Mebrane Thickness Interactions

Author(s): *Prashant Purohit, *University of Pennsylvania*; Xinyu Liao, *University of Pennsylvania*;

Self-assembly of proteins on lipid membranes underlies many important processes in cell biology, such as, exo- and endo-cytosis, assembly of viruses, etc. An attractive force that can cause self-assembly is mediated by membrane thickness interactions between proteins. The free energy profile associated with this attractive force is a result of the overlap of thickness deformation fields around the proteins which can be calculated from the solution of a boundary value problem. Yet, the time scales over which two inclusions coalesce has not been explored, even though the evolution of particle concentrations on membranes has been modeled using phase-field approaches. In this paper we compute this time scale as a function of the initial distance between two inclusions by viewing their coalescence as a first passage time problem [1]. The first passage time is computed using Langevin dynamics and a partial differential equation, and both methods are found to be in excellent agreement. Inclusions of three different shapes are studied and it is found that for two inclusions separated by about hundred nanometers the time to coalescence is hundreds of milliseconds irrespective of shape. An efficient computation of the interaction energy of inclusions is central to our work. We compute it using a finite difference technique and show that our results are in excellent agreement with those from a previously proposed semi-analytical method based on Fourier-Bessel series. The computational strategies described in this paper could potentially lead to efficient methods to explore the kinetics of self-assembly of proteins on lipid membranes. References: [1] Liao, X and Purohit, PK. Kinetics of self-assembly due to lipid membrane thickness interactions, to appear in Soft Matter, 2021.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analysis and Application of Peridynamics to Fracture in Solids and Granular Media

Author(s): *Prashant K Jha, *The University of Texas at Austin*; Robert Lipton, *Louisiana State University*;

In this talk, we will present our recent work on peridynamics and its application. We consider a bond-based peridynamics with a nonlinear constitutive law relating the bond-strain to the pairwise force. For the model considered, we can show well-posedness and existence in the Hölder and Hilbert H2 space under appropriate conditions and obtain apriori bounds on the finite-difference and finite-element discretization. We will present the application of the model to mode-I and mixed-mode fracture problems. One particular topic of interest is the kinetic relation for the crack tip velocity in the peridynamics and its link to the local kinetic relation (LEFM theory). We recover the classical kinetic relation from the peridynamics formulation. We will present numerical results that support the theory. Another application of peridynamics recently gaining much attention is in the granular media. DEM based methods can describe the interaction in particulate media very well but cannot model the intra-particle fracture. Prior works have shown the possibility of using peridynamics for the deformation of individual particles and DEM-like laws for the inter-particle interaction. We will present our work on the development of a high-fidelity model that we refer to as PeriDEM for granular media that promises to handle the arbitrarily shaped particles and their breakage. We will present some numerical results that demonstrate the effectiveness of the PeriDEM model. Work in the first part of the talk is joint work with Dr. R. Lipton and the second part of the work is collaborative work with Dr. R. Lipton and Dr. P. Desai.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Grain-Scale Modeling of Thermal and Mechanical Cycling of Coarse-Grain SAC305 Solder Joints

Author(s): *Qian Jiang, *University of Maryland, College Park*; Abhishek Deshpande, *University of Maryland, College Park*; Abhijit Dasgupta, *University of Maryland, College Park*;

Functional SAC solder joints in microelectronic assemblies commonly consist of a few highly anisotropic grains. The stochastic variations of the crystalline orientation and arrangement contribute to differences in stress conditions, even for different joints in a single component. This piece-to-piece variability in solder joints leads to significant uncertainty in their thermo-mechanical performance, thus necessitating a large number of repeated tests, to determine the statistical variability. In addition, numerical simulations based on simplified homogeneous isotropic material properties prove to be inadequate for realistic stress modeling and prediction of the variability of damage. An alternative grain-scale modeling approach is proposed in the current work, where the discrete grain morphology of coarse-grain solder joints is explicitly modeled with anisotropic viscoplastic and plastic properties of SAC single crystals. The viscoplastic behavior is modeled based on dislocation mechanics and typical microstructural features of multiple length scales. Rate-independent plastic behavior is determined by the orientation-dependent stress-strain data. Both models are calibrated by combining the results of in-house testing and those provided in the literature. Hill's anisotropic potential is then used to extract continuum-scale compact models of viscoplasticity and plasticity, respectively. This methodology enables computationally-efficient finite element simulations of multi-grain solder joints and facilitates parametric sensitivity studies of the nonlinear anisotropic response of different grain configurations. This capability will enable numerical exploration for the best-case and worst-case microstructural configurations and corresponding design margins of solder joints performance. Selected examples of SAC solder joints with triple crystals are presented, for modeling creep deformation under slow temperature cycling and plastic deformation under rapid mechanical cycling.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Scale-Free Phase-Field Modeling of Phase Transformation in Zirconium

Author(s): *Raghunandan Pratoori, *Iowa State University*; Hamed Babaei, *Iowa State University*; Valery Levitas, *Iowa State University*;

Zirconium is a widely used material in the nuclear and other industries owing to its superior mechanical properties. Hcp ? – phase at low pressure transforms to a simple hexagonal ? – phase under pressure. A scale-free phase field model for phase transformations at large strains [1] is advanced and used to study the ? - ? phase transformations in Zr. This phase field model is implemented using finite element algorithms in deal.II. Model is calibrated using available experimental data, including our [2]. It is applied to study forward and reverse phase transformations in Zr crystal under different hydrostatic and non-hydrostatic conditions and varying strain rates. The mesh size is also varied to study the microstructure evolution in detail. 1. Babaei H. and Levitas V.I. Finite-strain scale-free phase-field approach to multivariant martensitic phase transformations with stress-dependent effective thresholds. Journal of the Mechanics and Physics of Solids, 2020, 144, 104114. 2. Pandey K. K. and Levitas V. I. In situ quantitative study of plastic strain-induced phase transformations under high pressure: Example for ultra-pure Zr. Acta Materialia, 2020, 196, 338-346.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Low-Rank Registration Based Manifolds for Convection-Dominated PDEs

Author(s): *Rambod Mojgani, *Rice University*; Maciej Balajewicz, *Siemens Corporate Technology*;

We develop an auto-encoder type nonlinear dimensionality reduction algorithm tailored to convection-dominated nonlinear partial differential equations (PDEs) featuring traveling waves, shocks, and interfaces. Identifying an optimal manifold is a crucial step in the construction of efficient predictive machine learning (ML) models. Meanwhile, the slow decay of singular values, i.e. large Kolmogorov n-width, of such snapshots remains the fundamental challenge in these problems. Although the existing nonlinear methods in the ML community can break the so-called Kolmogorov n-width barrier, (i) they, except auto-encoders, lack a straightforward mapping from the identified manifold to the high-dimensional physical space, and (ii) they often lack interpretability. The proposed manifold is defined on a low-rank diffeomorphic spatio-temporal grid such that the Kolmogorov n-width of the mapped snapshots on the identified grid is minimized. The identified manifold can be incorporated similar to an auto-encoder layer into machine learning architectures, such as the neural-network models of PDEs, to increase accuracy and reduce the training costs of such models. Moreover, the identified grid approximates the path of convection/travelling features in the snapshots and is leveraged to predict beyond the training regime, i.e. forecasting. We demonstrate the efficacy and interpretability of the proposed approach on several manufactured and canonical systems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Stochastic Isogeometric Analysis by Spline Dimensional Decomposition for Arbitrary Multi-Patch Domains

Author(s): *Ramin Jahanbin, *The University of Iowa*; Sharif Rahman, *The University of Iowa*;

Stochastic Isogeometric Analysis by Spline Dimensional Decomposition for Arbitrary Multi-Patch Domains Ramin Jahanbin 1, Sharif Rahman 2 University of Iowa Abstract In many engineering problems, uncertainty needs to be propagated from the input to the output through a complex system. This process is referred to as uncertainty quantification and often involves solving a stochastic partial differential equation by numerical methods. Isogeometric analysis (IGA) was proposed to bridge the gap between design and numerical computations by avoiding the mesh generation step. Moreover, smooth basis functions, such as B-splines, non-uniform rational B-splines (NURBS), and T-splines are employed to form the approximation space in IGA and many common geometries are modeled precisely as well [1]. A new stochastic method, integrating spline dimensional decomposition (SDD) of a high-dimensional function and isogeometric analysis (IGA) on an arbitrary multi-patch domain is proposed for solving stochastic boundary-value problems from linear elasticity. The method, referred to as SDD-mIGA, involves (1) analysis-suitable T-splines for geometrical modeling, random field discretization, and stress analysis; (2) Bezier extraction operator for isogeometric mesh refinement; and (3) a novel Fourier-like orthogonal spline expansion of a high-dimensional output function. Compared with the past work [2], the method developed can handle arbitrary multi-patch domains in the context of IGA. For the stochastic part of the SDD-mIGA method, a standard least-squares regression is presented for efficiently calculating the expansion coefficients. Analytical formulae have been derived to calculate the second-moment properties of an SDD-mIGA approximation for a general output random variable of interest. Numerical results, including those obtained for a 54-dimensional, industrial-scale problem, demonstrate that a low-order SDD-mIGA is capable of efficiently delivering accurate probabilistic solutions when compared with the benchmark results from crude Monte Carlo simulation. Keywords: Uncertainty quantification, isogeometric analysis, T-splines, Bezier extraction operator, random field discretization. References [1] T. Hughes, J. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite element, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering 194 (2005) 4135-4195. [2] R. Jahanbin, S. Rahman, Stochastic isogeometric analysis in linear elasticity, Computer Methods in Applied Mechanics and Engineering 364 (2020) 112928. 1 Graduate Student and Presenting Author; e-mail: ramin-jahanbin@uiowa.edu. 2 Professor; e-mail: sharif-rahman@uiowa.edu.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Development of a Novel Hybrid Algorithm for Applications in Fluid-Structure Interaction (FSI)

Author(s): *Ramy Nemer, *Mines ParisTech - CFL - CEMEF*; Aurelien Larcher, *Mines ParisTech - CFL - CEMEF*; Thierry Coupez, *Mines ParisTech - CFL - CEMEF*; Elie Hachem, *Mines ParisTech - CFL - CEMEF*;

Key Words: Variational Multi-Scale Method, Solid Modeling, Fluid Modelling, Finite Elements, elastodynamcis, Hybrid Approach. Fluid--Structure Interaction (FSI) have been getting a lot of attention lately, due to its vast interval of applications. Ranging from everyday life applications, to complex engineering systems such as airplanes, pressure regulators, and biomechanical systems. While surrounded by the fluid, the solid experiences forces that dictates its behavior. The interaction is conversely felt by the fluid, when the solid is in motion. The detailed behavior of the aforementioned applications can help in the development, and sustainability of engineering tools. Embedded/Immersed methods for FSI have seen their fair share of development in the literature; one of which consists of adding a mesh adaptation algorithm. Existing methods are restricted in a couple of points: the convoluted interface coupling of both mediums, and the ability to handle arbitrary structures. For the above stated reasons, a novel Adaptive Immersed Mesh (AIM) method is introduced. The method couples the dynamics of the solid, with that of the fluid. The Navier-Stokes equations are solved for the fluid, and the hyperelastic elastodynamics equations are solved for the solid. The Variational Multi Scale (VMS) method is used for the stabilization of both methods. By modeling the sub-scales of the problem, we can solve the advection dominated regime of the Navier-Stokes equations using finite elements[1], and damp out spurious pressure oscillations for the incompressible regime of the solid[2]. The high accuracy of the method is achieved through anisotropic remeshing of the fluid-solid mesh, and the parallel framework for the solid mesh immersion using the level-set method[3]. 2D and 3D simulations are conducted to assess the precision, accuracy, and robustness of the hybrid method. REFERENCES [1] E. Hachem, B. Rivaux, T. Kloczko, H. Digonnet, and T. Coupez, Stabilized finite element method for incompressible flows with high Reynolds number. Journal of Computational Physics, Vol. 229, pp. 8643-8665, 2010. [2] R. Nemer, A. Larcher, T. Coupez, E. Hachem. (2021). Stabilized finite element method for incompressible solid dynamics using an updated Lagrangian formulation. arXiv: 2101.07057 [math.NA] (2021) (available at http://arxiv.org/abs/2101.07057). [3] P. DesJardin, B. Bojko, and M. McGurn, Initialization of high-order accuracy immersed interface CFDsolvers using complex CAD geometry. Int. J. Numer. Meth. Engng, Vol.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modal Operator Regression for Extracting Nonlocal Continuum Models

Author(s): *Ravi Patel, *Sandia National Laboratories*; Nathaniel Trask, *Sandia National Laboratories*; Mitchell Wood, *Sandia National Laboratories*; Eric Cyr, *Sandia National Laboratories*;

In this talk, we discuss a machine learning framework, MOR-Physics [1], capable of extracting coarse-grained, nonlocal models from data. This framework parameterizes spatial operators as compositions of local, point-wise applied operators and Fourier integral operators where both the point-wise operators and the symbols of the integral operators are parameterized by neural networks. We modify this parameterization to enforce a set of desirable inductive biases: translational and rotational invariance, global conservation, and reflective symmetry. We verify MOR-Physics by recovering the Laplacian and Burgers operators from their actions on a set of functions. We further demonstrate that MOR-Physics can recover the fractional Laplacian from coarse grained densities generated by Levy flights and show that the inductive biases improve model fit, particularly in the sparse, biased data regime. We conclude by extracting PDE's for colloidal suspensions from coarse grained molecular dynamics simulations. [1] Patel et al., "A physics-informed operator regression framework for extracting data-driven continuum models" CMAME 2021

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Machine Learning Constitutive Models

Author(s): *Reese Jones, *Sandia National Laboratories*; Ari Frankel, *Sandia National Laboratories*;

Traditional simulations of complex mechanical deformation are technologically crucial and computa- tionally expensive. Developing comparably accurate models with lower computational cost can enable more robust design and uncertainty quantification, as well as exhaustive structure-property exploration. Currently, high-throughput experimental techniques and microscale simulators can produce quantities of data that overwhelm traditional constitutive modeling methods and can provide sufficient data to train neural networks. As a modeling technique, neural networks are flexible in that their graph-like structure can be rearranged and functions of their nodes can be adapted to suit particular applications, such as image processing. On the other hand, Gaussian process models can outperform neural networks in the data limited regime. In this talk, I will discuss: how we construct input spaces and architectures to capture how microstructure affects mechanical outcomes given observations of the initial microstructure; how we draw upon classical constitutive theory to make predictions of the individual stress response that satisfy fundamental physical constraints, and, how we represent the time evolution of inelastic materials. References [1] Reese Jones, Jeremy A Templeton, Clay M Sanders, and Jakob T Ostien. Machine learning models of plastic flow based on representation theory. Computer Modeling in Engineering & Sciences, pages 309–342, 2018. [2] Ari L Frankel, Reese E Jones, Coleman Alleman, and Jeremy A Templeton. Predicting the mechanical response of oligocrystals with deep learning. Computational Materials Science, 169:109099, 2019. [3] Ari Frankel, Kousuke Tachida, and Reese Jones. Prediction of the evolution of the stress field of polycrystals undergoing elastic-plastic deformation with a hybrid neural network model. Machine Learning: Science and Technology, 2020. [4] Ari L Frankel, Reese E Jones, and Laura P Swiler. Tensor basis gaussian process models of hyperelastic materials. Journal of Machine Learning for Modeling and Computing, 1(01), 2020. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA- 0003525

16th U.S. National Congress on Computational Mechanics
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Title: On the Development of Fluid Flow Topology Optimization with High Reynolds Numbers and Turbulence Models

Author(s): *Renato Picelli, *University of Sao Paulo*; Eduardo Moscatelli, *University of Sao Paulo*; Shahin Ranjbarzadeh, *University of Sao Paulo*; Rafael dos Santos Gioria, *University of Sao Paulo*; Emílio Carlos Nelli Silva, *University of Sao Paulo*;

One of the current limitations in fluid flow topology optimization is its extension to high Reynolds flow, specially considering turbulence models. This is because three main issues exist in classic density-based methods with continuous variables when applied to fluid flow. First, the fluid boundaries are unclear during optimization. Fluid boundaries discretization are important when dealing with high Reynolds flow and wall functions are required in turbulence models. Second, the convergence to binary {0,1} designs might be highly dependent on the tuning of the optimization parameters, often requiring continuation schemes. Third, it is difficult to specify the maximum value of the inverse permeability in order to avoid the presence of fluid flowing inside the modeled solid medium. In this context, this work proposes a methodology to attack these three main issues and to solve fluid flow topology optimization including turbulence models. The method is based on the combination of a geometry trimming procedure and the recently developed TOBS (Topology Optimization of Binary Structures) algorithm. The TOBS is a gradient-based topology optimization method that employs binary design variables and formal mathematical programming. In this way, the fluid walls are explicitly defined and convergence to binary {0,1} designs is guaranteed. In the proposed geometry trimming procedure, the solid regions are removed out of the fluid flow domain, eliminating the use of the inverse permeability value. Herein, the Reynolds-averaged Navier–Stokes equations are solved together with the k-epsilon or k-omega turbulence equations. The analysis is done via the finite element package COMSOL Multiphysics. The total fluid energy dissipation (considering the viscous and turbulent effects) is minimized considering a fluid volume constraint. Numerical results show that the proposed method is suitable for turbulent fluid flow problems.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Nature-Inspired Vascular Materials

Author(s): *Reza Pejman, *Drexel University*; Ahmad Raeisi Najafi, *Drexel University*;

This study presents a systematic approach for the topology optimization of actively cooled microvascular composites using a geometrical reduced-order thermal/hydraulic model. Bio-inspired microvascular networks show a significant potential to offer a wide range of multi-functionality to fiber-reinforced polymer composites by enabling internal fluid/mass transport. Indeed, based on the choice of fluid flowing through the microchannels, microvascular material is capable of providing multifunctional applications such as thermal management, modifying the electromagnetic signature, self-healing, and tuning the electrical properties. The focus of this study is placed on the thermal regulation capability of multifunctional microvascular fiber-composites which has a broad range of applications including electric vehicle battery packaging, space re-entry, hypersonic aircraft, and heat exchangers for microelectronics. The considered objective function in this study is the p-norm temperature of the domain and there are constraints on the maximum allowable network pressure drop and the void volume fraction due to the presence of microchannels in the composite. Inspired by the Solid Isotropic Material with Penalization (SIMP) method, we define a set of design variables, which act analogously as the design variables in the SIMP method. Using this set of design variables, we can penalize the diameters of the microchannels by defining an effective diameter. In this approach, we collapse the microchannels embedded in the microvascular composite into line source/sinks and we project the microchannels on the edges of the elements to have a conforming mesh. The analysis module of this study is verified with FLUENT and the accuracy of the optimization scheme is examined through the so-called “cross-check” approach. We solve several numerical examples to compare the results of the proposed scheme with the Hybrid Topology/Shape (HyTopS) optimization and Shape optimization approaches in terms of several metrics such as (i) maximum temperature and p-norm temperature, (ii) network redundancy, (iii) manufacturability, and (iv) temperature uniformity. Our results reveal that the optimized design obtained by the presented TO scheme outperforms the designs of HyTopS and SO methods in terms of having lower maximum and average temperatures, higher temperature uniformity, and having a more redundant network.

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Title: An Image-Based Finite Element Model for Vascular Remodeling in Pediatric Pulmonary Arterial Hypertension

Author(s): *Reza Pourmodheji, *Michigan State University*; Zhenxiang Jiang, *Michigan State University*; Christopher Tossas-Betancourt, *University of Michigan*; C. Alberto Figueroa, *University of Michigan*; Seungik Baek, *Michigan State University*; Lik Chuan Lee, *Michigan State University*;

Pulmonary arterial hypertension (PAH) is a complex cardiovascular disease associated with elevation in pulmonary arterial (PA) pressure, typically with the mean pulmonary arterial pressure (mPAP) over 25 mmHg at rest. PAH is characterized by a progressive remodeling of the pulmonary arteries. Vascular remodeling in PAH, typically through a mechano-regulatory process is the direct cause of elevation in pulmonary vascular stiffness (PVS), a well-known marker of the disease progression [1]. Smooth muscle cells (SMC) hypertrophy and proliferation as well as extracellular matrix (ECM) accumulation such as collagen and elastin have been recognized as common features of PAH remodeling [2]. Due to an increase in the mass of these tissue constituents, the PA wall becomes thicker and stiffer. Computational modeling can help provide physical insights on the microstructural changes due to PAH, thus the impact on the global measures such as PVS in clinical settings. In this work, we develop a patient-specific computational platform based on the theory of constrained mixture [3] to study the vascular remodeling in large proximal PA due to mPAP elevation. Finite element (FE) model was reconstructed from magnetic resonance images (MRI) of the PA in a patient (16 y/o female) with idiopathic PAH with mPAP=46.7 mmHg. The fibrous structure of the PA wall was modeled as a mixture of vascular load-carrying micro-constituents. These constituents are, namely, collagen fibers and SMC whose passive behavior is described by a Holzapfel-type model, as well as elastin that is modeled as a Neo-Hookean solid. The constituents are continuously produced and removed over time (large time scale: months and years) to maintain the vascular homeostasis. They are produced under stress-regulated rates, i.e., the constituents with the stress near the homeostatic values will be produced under a sustained rate. A Heaviside function of a 30% pressure elevation is used as an input variable to study micro-structural changes. Our model predicts that as the response to the pressure elevation, the mass production of the constituents is accelerated, resulting in an immediate accumulation of collagen and SMC, and thus thicker PA. Our image-based computational model shows a potential to enhance prognosis and diagnosis and could serve as a useful tool for hypothesis generation. [1] Hunter, Kendall S., et al. J. Appl. Physiol. 108.4 (2010): 968-975. [2] Rabinovitch, Marlene. J. clin. Invest 122.12 (2012): 4306-4313. [3] Baek, S. et al. J. Biomedical Engineering (2006): 142-149.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The Kinetic Relations of Linear Elastic Fracture Mechanics from Nonlocal Dynamics

Author(s): Prashant Jha, *The University of Texas at Austin*; *Robert Lipton, *Louisiana State University*;

The hallmark and utility of peridynamic models is that fracture naturally emerges from the numerical simulation. Thus one should expect that the classic kinetic relations of LEFM be recovered directly from the equations of motion without any hypotheses. We recover the celebrated kinetic relations of Linear Elastic Fracture Mechanics directly from the nonlocal equations of motion in the limit of vanishing nonlocality. This is done analytically and numerically. We illustrate through numerical simulations when the nonlocal length scale is small.

16th U.S. National Congress on Computational Mechanics
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Title: Autonomous Microstructural Feature Characterization of Additively Manufactured Metals Using an Optimized Machine Learning Framework

Author(s): *Roberto Perera, *Auburn University*; Vinamra Agrawal, *Auburn University*; Davide Guzzetti, *Auburn University*;

Over the past decade, additive manufacturing of metallic materials has found applications towards aerospace rocket components, automotive parts, biomedical equipment, and infrastructural components. However, additively manufactured metals exhibit heterogeneous microstructure which dictates their material and failure properties. A vast number of imaging techniques have been developed to characterize these microstructural features. While these techniques have proved to be extremely useful, they generate a large amount of data that requires expensive computationally resources. Image segmentation is another valuable computational technique utilized for the characterization of pores, particles, grains, and grain boundaries (GBs). Well known algorithms such as city-block distance function + watershed segmentation, and the point-sampled intercept length method employ image segmentation to identify pores, particles, grains, and GBs. Although conventional segmentation tools have proved their use in these applications, they are restricted to time consuming pre-processing image operations such as gamma corrections, edge detection, threshold value selection, interpolation functions, morphological operators, and others. Additionally, prior to each analysis the user must know the specific microstructural features to be extracted, to then apply the corresponding conventional method. In this work, an optimized machine learning (ML) framework is proposed, to characterize pores, particles, grains, and GBs autonomously and efficiently from a given microstructure image. First, using a classifier Convolutional Neural Network (CNN), defects such as pores, powder particles, or GBs are recognized. Depending on the type of defect, two different processes are used. For powder particles or pores, binary segmentations are generated using an optimized Convolutional Encoder-Decoder Network (CEDN). These binary segmentations are then used to obtain particles', and pores' size and location using an object detection ML network (YOLOv5). For GBs, another optimized CEDN was developed to generate RGB segmentation images. These RGB segmentation images are then used to obtain grain size distribution using two regression CNNS. While conventional ML segmentation networks show advantages over conventional image segmentation methods, some of their main challenges are their high GPU usage, prolonged training time, and architecture's complexity. Therefore, to optimize the RGB CEDN, the Deep Emulator Network SEarch (DENSE) method which employs the Covariance Matrix Adaptation - Evolution Strategy (CMA-ES) was implemented. The optimized RGB segmentation network showed a substantial reduction in training time and GPU usage compared to the unoptimized network, while maintaining high accuracy. Lastly, the proposed framework showed a significant improvement in analysis time when compared to conventional methods.

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Title: Finite Element Tools for Performance Portability of Implicit and IMEX Simulations on Next Generation Architectures

Author(s): *Roger Pawlowski, *Sandia National Laboratories*; Matthew Bettencourt, *Sandia National Laboratories*; Eric Cyr, *Sandia National Laboratories*; Edward Phillips, *Sandia National Laboratories*; Eric Phipps, *Sandia National Laboratories*; John Shadid, *Sandia National Laboratories*; Christian Trott, *Sandia National Laboratories*; Sean Miller, *Sandia National Laboratories*;

Supporting scalable and performant finite element simulations across next generation heterogeneous architectures can add significant code complexity. This presentation will discuss the design of general finite element assembly tools applied to CFD, magnetohydrodynamics, and multi-fluid plasma simulations. Performance portability is achieved via the Kokkos programming model [1]. The assembly library uses a directed acyclic graph for composable physics kernels in a multiphysics setting. Mixed basis finite element formulations are used to enforce physics constraints for Maxwell's equations [2]. Embedded automatic differentiation, applied via templates and operator overloading, is used for generating machine precision sensitivities for implicit and IMEX solvers [3]. Performance results will be shown for NVIDIA GPU and Intel Haswell architectures. REFERENCES [1] H.C. Edwards, C.R. Trott and D. Sunderland, Kokkos: Enabling manycore performance portability through polymorphic memory access patterns. J. Parallel and Distrib. Comput., Vol. 74, pp. 3203?3216, 2014. [2] S.T. Miller, E.C. Cyr, J.N. Shadid, R.M.J. Kramer, E.G. Phillips, S. Conde, and R.P. Pawlowski, IMEX and exact sequence discretization of the multi-fluid plasma model, J. Comput. Phys., Vol. 397, 2019. [3] E.T. Phipps and R.P. Pawlowski, Efficient expression templates for operator overloading-based automatic differentiation, in Recent Advances in Algorithmic Differentiation, S. Forth, P. Hovland, E. Phipps, J. Utke, Lecture Notes in Computational Science, Vol 87, pp. 351-362, 2012.

16th U.S. National Congress on Computational Mechanics
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Title: Enhanced Data Efficiency Using Deep Neural Networks and Gaussian Processes for Aerodynamic Design Optimization

Author(s): Ashwin Renganathan, *Argonne National Laboratory*; *Romit Maulik, *Argonne National Laboratory*; Jai Ahuja, *Georgia Institute of Technology*;

Adjoint-based optimization methods are attractive for aerodynamic shape design primarily due to their computational costs being independent of the dimensionality of the input space and their ability to generate high-fidelity gradients that can then be used in a gradient-based optimizer. This makes them very well suited for high-fidelity simulation-based aerodynamic shape optimization of highly parametrized geometries such as aircraft wings. However, the development of adjoint-based solvers involves careful mathematical treatment and their implementation requires detailed software development. Furthermore, they can become prohibitively expensive when multiple optimization problems are being solved, each requiring multiple restarts to circumvent local optima. In this work, we propose a machine learning-enabled, surrogate-based framework that replaces the expensive adjoint solver, without compromising on predicting predictive accuracy. Specifically, we first train a deep neural network (DNN) from training data generated from evaluating the high-fidelity simulation model on a model-agnostic, design of experiments on the geometry shape parameters. The optimum shape may then be computed by using a gradient-based optimizer coupled with the trained DNN. Subsequently, we also perform a gradient-free Bayesian optimization, where the trained DNN is used as the prior mean. We observe that the latter framework (DNN-BO) improves upon the DNN-only based optimization strategy for the same computational cost. Overall, this framework predicts the true optimum with very high accuracy, while requiring far fewer high-fidelity function calls compared to the adjoint-based method. Furthermore, we show that multiple optimization problems can be solved with the same machine learning model with high accuracy, to amortize the offline costs associated with constructing our models. Our methodology finds applications in the early stages of aerospace design.

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Title: Metal 3D Printing: Controlling Interdependent Meso-Nanosecond Dynamics and Defect Generation Using a Digital Twin

Author(s): *Saad Khairallah, *Lawrence Livermore National Laboratory*;

State-of-the-art metal 3D printers based on laser powder bed fusion process (L-PBF) promise to revolutionize manufacturing, yet they still have not solved the variability problem. L-PBF technology uses a laser beam to scan 2D patterns over a flat bed of microscopic (~15-45 ?m) metal powder. This forms melt pool tracks that fuse with the lower layers. Repeating the layer-wise process thousands of times results in the build of a 3D object. However, a poor understanding of the interdependency between laser process parameters and complex powder and melt pool dynamics results in quality variability when building parts. The variability results from the accumulation of defects (~3-100?m) that are randomly generated at the powder bed layer and in the melt pool during each layer scan. These issues can lead to parts failing certification. We used a high-fidelity multi-physics model that we verified with in-situ X-ray and other diagnostics experiments to study laser-powder and laser-melt pool interactions. We captured different modes of laser powder interactions that involve laser expulsion of spatter (ejected molten and/or fused particles) and laser shadowing (spatter blocking the laser rays). We found that high laser power is necessary to prevent lack of fusion pores, distorted tracks, as low power is not able to expel spatter and negate their negative effects. We report on self-replicating spatter, that once formed, become hard to get rid of due to a self-replication mechanism that involves loose particles in the powder layer. We explain how pre-sintering the powder could be a strategy to mitigate this effect. We also report on first evidence on how spatter beyond a size threshold can cause pores due to laser shadowing. We identified the laser scan strategy as one source of these large spatter sizes and derived a stability criterion based on critical melt flow velocity and flow breakup to prevent them. The stability criterion is general and not specific to the problem at hand. We use it to devise new scan strategies that couple the laser power with scan speed and prevent end of track defects as well as keyholes (deep and narrow depressions). Diminishing the variability problem involves controlling random events generated by transient physical states. High-fidelity modeling coupled with in-situ diagnostics will be indispensable to introduce stability criteria to advance manufacturing and help usher in Industry 4.0 revolution. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE- AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-ABS-799067.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Space-Time Discretization of a Nonlinear Peridynamic Model on a 2D Lamina

Author(s): Luciano Lopez, *University of Bari*; *Sabrina Francesca Pellegrino, *Libera Università Mediterranea*;

Peridynamics is a nonlocal theory for dynamic fracture analysis consisting in a second order in time partial integro-differential equation. We consider a nonlinear model of peridynamics in a two-dimensional spatial domain. We implement a spectral method for the space discretization based on the Fourier expansion of the solution while we consider the Newmark-beta method for the time marching. This computational approach takes advantages from the convolutional form of the peridynamic operator and from the use of the discrete Fourier transform. We show a convergence result for the fully discrete approximation and study the stability of the method applied to the linear peridynamic model. Finally, we perform several numerical tests and comparisons to validate our results and provide simulations implementing a volume penalization technique to avoid the limitation of periodic boundary conditions due to the spectral approach.

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Title: Modeling the Plasticity and Fracture of the Reissener-Mindlin Shell in Peridynamics

Author(s): *Sai Li, *Wuhan University of Technology*; Xin Lai, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*;

In current work, plasticity and fracture are modelled and implemented in Reissener-Mindlin Shell by Peridynamics. Peridynamic Reissener-Mindlin shell theory is adopted here to provide the discretization of the shell, in which the shell is described and represented by the material points that stands in mean-plane of the shell structure with its drilling rotation ignored in the kinematic assumption. The plasticity of the material is realized by introducing the elastoplastic constitutive equation of the classical continuum mechanics which provides the nonlinear mechanical response of shell structure. Without losing generality, the Johnson-Cook constitutive and damage model is adopted here to characterize the elasto-plastic behavior of the material that including the plastic hardening and strain-rate effects. To improve the numerical accuracy, the stress-point integration method is utilized to eliminate the numerical instability induced by the zero-energy mode and rank-deficiency. Several numerical examples are presented to validate the modeling and implementation of the plastic shell, and also demonstrate the capability of proposed model on predicting the plastic fracture in finite deformation.

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Title: Transcatheter Heart Valve Accelerated Fatigue Modeling Parameters

Author(s): *Sailahari Ponnaluri, *The Pennsylvania State University*; Michael Sacks, *The University of Texas at Austin*; Keefe Manning, *The Pennsylvania State University*;

As of 2017, an estimated 138,400 patients died annually from heart valve disease (HVD) worldwide [1]. The primary treatment option is either a mechanical or bioprosthetic heart valve replacement. However, 30% of HVD patients are unable to receive surgical valves due to comorbidities and/or age [2]. Transcatheter aortic valve replacements (TAVRs) are a novel, minimally invasive HVD treatment whose long-term durability is unknown. Experimentally, durability testing is performed by an accelerated wear tester (AWT) in accordance with ISO:5840. This standard specifies a TAVR be tested for 200 million cycles while maintaining a delta pressure (~100 mmHg) across a closed valve for 5% of the cycle [3]. While AWT cycling replicates a “reasonable lifespan” in a timely manner, the accelerated environment may not be representative of in vivo fatigue. Variability in AWT designs, pressure loading conditions, and frequency can vary the life span. Therefore, to develop TAVR and future valve designs effectively, an accelerated fatigue model must be developed to simulate a valve life span. To do so, the parameters influencing TAVR durability must be determined. This study aims to identify parameters within the AWT by experimentally quantifying the fluid dynamics and TAVR motion under variable conditions. A TAVR was cycled in an Electroforce® DurapulseTM AWT. Four conditions were tested while adhering to ISO:5840: a standard intact TAVR and a trimmed TAVR at three frequencies (10, 15, and 20 Hz). The TAVR stent was trimmed to create windows to quantify the near valve fluid mechanics. Using enface imaging, the geometric orifice area (GOA), flow rate, and coaptation were quantified every 9% of the cycle. High speed particle image velocimetry (HSPIV) quantified the flow downstream of the TAVR. Two HSPIV data sets were captured: an averaged set every 9% of the cycle and an instantaneous set to visualize eddy formation. Reynolds normal and shear stresses were calculated. The TAVR motion and fluid dynamics demonstrated a clear dependence on the accelerated environment and testing frequency. While the fluid mechanics for the intact TAVR were similar to physiological beat rate studies, the valve motion demonstrated a reduced loading period of 21.6% and average transvalvular pressure of 72.55 mmHg. With increasing AWT frequency, the TAVR GOA, flow rate, loading period, maximum jet velocity, and turbulent stresses decreased, all factors influencing TAVR fatigue. 1. Yagdir, S., et al., Circulation, 141:1670-1680, 2020. 2. Leon M.B., et al., N Engl J Med, 363:1597-1607. 3. International Standards Organization:5840:3, 2013.

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Title: A Space-Time Gauge Theory Based on Translational Symmetry for Modelling Viscoplasticity in Polycrystalline Solids

Author(s): *Sanjeev Kumar, *Indian Institute of Science*;

A space-time gauge theoretic approach is used to describe viscoplasticity in polycrystalline solids, exploiting the invariance of an appropriate energy density under the action of local/inhomogeneous translations in both space and time. The invariance of the energy density is preserved through minimally replaced non-trivial space-time gauge covariant operators defined via the space-time minimal replacement construct. Translation in time leads to a new definition of gauge covariant temporal derivative; hence the classical notion of velocity gets modified and coupled with the compensating field variables. Using a space-time pseudo-Riemannian metric in a finite-deformation setup, we derive the evolution equation of the equivalent plastic strain rate. Dissipative terms and some higher order temporal and spatial derivative terms appear naturally in our space-time viscoplasticity model. We also establish a correspondence of the compensating fields appearing in our formulation due to spatial translation with Kr?ner's multiplicative decomposition of the deformation gradient, even though an introduction of the so called intermediate configuration is not required explicitly in this model. In order to explicate the efficacy of our theory, we carry out numerical simulation of homogeneous viscoplasticity and validate the simulated results against experimental data. Some interesting future studies include the effects of non-trivial higher order derivative terms on indentation and strain localization problems, e.g. the stability and width of the shear band. Key Words: Gauge theory, Translational symmetry, Gradient plasticity, Viscoplasticity, Large deformation, Shear banding

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Title: Intelligent Crack Growth Monitoring Using an Internet of Things Approach

Author(s): *Sarah Malik, *Drexel University*; Emine Tekerek, *Drexel University*; Abrar Zawad, *Drexel University*; Antonios Kontsos, *Drexel University*;

Real-time crack detection is a key area of Structural Health Monitoring (SHM) both for material performance and nondestructive evaluation (NDE), as well as for overall intelligent design purposes. For smart structural applications, while several monitoring and evaluation methods related to cracking have been proposed, recent needs for real-time assessment through advances in the Internet of Things (IoT) technology have created the need to connect data acquisition with analytics, machine learning and modeling for data-driven and adaptive decision making¬¬. In this context, this talk presents a novel approach to leverage multi-physics Nondestructive Evaluation (NDE) datasets in an IoT framework capable of providing near real-time diagnostics and prognostics for cracking. Specifically, compact-tension specimens of an aerospace-grade aluminum alloy were used in experiments conducted in accordance with ASTM standards. Acoustic Emission and Digital Image Correlation datasets were acquired and used to produce cross-validated information that was processed using an in-house built IoT system capable of Edge, Fog, and Cloud computing. The main innovation of this approach is the fact that a combination of hardware (Edge, Fog, and Cloud) and software proves to be advantageous in implementing machine learning through the testing and sensing process to successfully categorize the initiation and subsequent crack growth. The computation is distributed through the system to allow efficient real-time implementation and reduce latency. The optimal machine learning model is trained offline using feature engineering, information theory, and hyperparameter tuning. Signals are then sent through the three layers of hardware with smart filtering, dynamic data parsing and classification to the end user who can view the classified signals through a dashboard. The final output is then used to form inputs to both probabilistic and physics-based modeling to further illustrate the value of adopting this framework in fracture and fatigue investigations. A discussion is also provided on how this approach can further be implemented in digital twin applications.

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Title: Linking the Process-Structure-Property Relationship for Additively Manufactured Materials using Mechanistic Data Science Framework

Author(s): *Satyajit Mojumder, *Northwestern University*; Zhengtao Gan, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

Relating the process-structure-property (PSP) for a materials system is of particular importance to guide the manufacturing process for desired materials properties. For additive manufacturing systems, these linkages are essential to ensure the build quality of the materials through an optimized process; however, it requires enormous experimental and simulation efforts. In this study, we used Mechanistic Data Science (MDS) approach to relate the linkages between the process to structure (PS) and structure to property (SP) for an additively manufactured Ti64 alloy [1]. The process parameters include laser power and speed, scan spacing and orientations, and layer thickness, and for structure level, we considered the porosity and grain size which is a direct effect of these processing conditions. We applied a mechanistic active learning technique to learn from a small experimental dataset [1] and guide our simulation tool [2] to generate more data through an optimal design of experiment. The next step of MDS was applied by extracting the mechanistic features such as porosity from these simulations and experimental data. Dimensional analysis has been carried out on these extracted features and further a neural network-based symbolic regression has been applied to learn their relationship. This closed-form relation of PS provides a reduced-order model for structure prediction from given processing conditions. To establish SP relation, nanoindentation data has been collected for the same materials system and processing conditions [3]. Several features such as load curvature, unloading slope, plastic to total work ratio have been extracted from the nanoindentation data, and properties such as hardness and reduce modulus were calculated. We further applied dimensional analysis and symbolic regression to find the SP relationship. Our results indicate that MDS can effectively capture the PSP relationship through mechanistic active learning and reduce the experiment and simulation effort significantly. References: [1] Kumar, P., Prakash, O., & Ramamurty, U. (2018). Micro-and meso-structures and their influence on mechanical properties of selectively laser melted Ti-6Al-4V. Acta Materialia, 154, 246-260. [2] Gan, Z., Lian, Y., Lin, S. E., Jones, K. K., Liu, W. K., & Wagner, G. J. (2019). Benchmark study of thermal behavior, surface topography, and dendritic microstructure in selective laser melting of Inconel 625. Integrating Materials and Manufacturing Innovation, 8(2), 178-193. [3] Lu, L., Dao, M., Kumar, P., Ramamurty, U., Karniadakis, G. E., & Suresh, S. (2020). Extraction of mechanical properties of materials through deep learning from instrumented indentation. Proceedings of the National Academy of Sciences, 117(13), 7052-7062.

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Title: A Hierarchical Bayesian Approach to Regularization with Application to the Inference of Relaxation Spectra

Author(s): *Sayali Kedari, *University of Cincinnati*; Gowtham Atluri, *University of Cincinnati*; Kumar Vemaganti, *University of Cincinnati*;

The inference of the spectral function representing the relaxation process of a material is an ill-posed inverse problem and is usually solved by regularization. Obtaining a bias-variance trade-off is an important criterion in solving ill-posed problems and predicting reliable estimates of quantities of interest. Most current methods in this domain use ad hoc regularization procedures to solve this inverse problem. Various deterministic data-driven methods including L-curve and generalized cross-validation in Tikhonov (L2) regularization have been employed in the literature to find optimal levels of regularization. In this work, we formulate the inverse problem in a hierarchical Bayesian framework and consider the degree of regularization as a stochastic quantity and the relaxation spectra as the high-dimensional model parameters. We assume variable noise precision parameters so as to handle heteroscedastic data. Using real data (frequency-dependent storage and loss moduli), this novel approach is employed to characterize the linear viscoelastic response of materials and obtain sparse probabilistic solutions to linear regression. We consider two experimental datasets for polybutadiene and porcine brain tissue. The computations are carried out using a Metropolis-Hastings-within-Gibbs sampling algorithm. Numerical results demonstrating the performance of the hierarchical Bayesian approach and comparisons with the deterministic L-curve approach are presented. The novelty of the approach is that a hierarchical Bayesian approach is used to infer the spectra, with the experimental data informing not just the constitutive model but also the degree of regularization. Thus the approach eliminates any subjectivity about the choice of regularization parameter.

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Title: Blast-on-Structure Simulations Using Zapotec

Author(s): *Scott Miller, *Sandia National Laboratories*; Guy Bergel, *Sandia National Laboratories*; Gabriel de Frias, *Sandia National Laboratories*; Kevin Manktelow, *Sandia National Laboratories*; Matthew Mosby, *Sandia National Laboratories*; Julia Plews, *Sandia National Laboratories*; Jesse Thomas, *Sandia National Laboratories*; Ellen Wagman, *Sandia National Laboratories*;

Zapotec is a fluid-solid coupling software from Sandia National Laboratories that couples the shock physics code CTH to the Sierra/Solid Mechanics finite element code. One of the most common uses of Zapotec is blast-on structure calculations, wherein a shock wave is generated in CTH and impinges upon a (Lagrangian) solid mechanics model. The fluid-solid coupling is accomplished by immersing the solid into the fluid domain. This talk will provide details of the coupling methodology as well as showcase several production-level analyses completed with Zapotec. Sandia National Laboratories, P.O. Box 5800, MS 0380, Albuquerque, NM 87185-9999, USA. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

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Title: Not So HOT Triangulations

Author(s): *Scott Mitchell, *Sandia National Laboratories*; Patrick Knupp, *Dihedral, LLC*; Michael Deakin, *University of British Columbia*; Sarah Mousley, *Lawrence Livermore National Laboratory*;

Our title is a double entendre. We both show that optimizing the HOT (Hodge Optimized Triangulations[1]) energy has shortcomings, and propose new optimization objectives that are related to HOT, but are not the same. "Primal-dual meshes" are distinguished by the significance of the geometric relationship between primal elements and their dual Voronoi cells. Well-centered Delaunay-Voronoi pairs are a related ideal, but robust algorithms to construct them are elusive, especially for bounded domains. Weighting points extends (Delaunay mesh)---(Voronoi diagram) duality to (regular triangulation)---(power diagram) duality, and dramatically extends the types of constructions that are possible. The diagonalized Delaunay Hodge operator enables simulations involving primal and dual quantities. For fluid flow, divergence is stored on the primal edge, and curl on the dual perpendicular edge. If their midpoints are far apart the simulation has error. Good HOT energy improves many geometric processing algorithms in computer graphics, some of which cross-over to engineering, such as building self-supporting structures. The HOT energy[1] is a primal-dual mesh mesh metric, a bound on the diagonalized Hodge discretization error. Mullen et al. demonstrated using the HOT energy as the objective function in mesh position and weight optimization. The Delaunay Hodge operator is not even defined for non regular meshes, but their HOT energy is a continuous extrapolation of the error bound. They state the necessity of preconditioning the mesh, optimizing the position before the weight, and treating the boundary exceptionally, but did not describe fully describe why these are needed. Our contribution is a mathematical and algorithmic demonstration (in 2D) of * Why optimizing HOT is not robust; * Using the HOT energy to select discrete changes to the mesh; * New metrics that are simple, well-behaved under optimization, and require no preconditioning; * Algorithms that combine these concepts. Our new objectives are based on normalizations of the discretization error, with barriers to triangle inversion and edge collapse. When HOT would nearly-collapse an edge, we explictly collapse the edge by removing a node. Our new objectives drive the actual position and weight updates. By coupling discrete connectivity improvement and continuous position-weight optimization, we more fully explore the space of possible meshes and produce higher quality solutions. References [1] Mullen P., Memari P., de Goes F., Desbrun M. “HOT: Hodge-Optimized Triangulations.” ACM Transactions on Graphics (TOG), vol. 30, no. 4, 103, 2011

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Title: Physics-Aware, Probabilistic Learning of Reduced-Order Systems in the Small Data Regime

Author(s): *Sebastian Kaltenbach, *Technical University of Munich*; Phaedon-Stelios Koutsourelakis, *Technical University of Munich*;

Despite recent successes from applications of data-driven methods and Deep Learning in the field of computational physics [1], significant challenges remain especially in the context of multiscale systems and in Small-Data regimes. Given high-dimensional time-series' data from a multiscale dynamical system, we present a probabilistic framework that simultaneously addresses the tasks of dimensionality reduction and model compression by identifying interpretable representations [2], which capture slow-varying features and whose dynamics are guaranteed to be stable. These representations enable fully probabilistic reconstructions of the high-dimensional system into the future with the help of a suitable coarse-to-fine map. This map is parametrized by deep neural networks and incorporates an intermediate layer of physically motivated latent variables into our model that reflect domain knowledge and infuse inductive bias. Such physical knowledge or physical constraints can be shown to be useful when training in the Small Data regime [3]. In contrast to existing schemes, the proposed model does not require the a priori definition of projection operators from the fine-grained description and is completely probabilistic and therefore capable of capturing the predictive uncertainty due to the information loss because of dimension and model-order reduction. We apply our method to small amounts of simulation data of high-dimensional physical systems such as Fluid mechanics and demonstrate its efficacy and accuracy by generating extrapolative, long-term predictions with quantified uncertainty. Moreover, we extend the learned data-driven latent space by physically motivated dimensionless quantities, which are commonly used to characterize the system such as the Reynolds number in Fluid mechanics, and show that this approach facilitates knowledge transfer to unseen settings not contained in the training data. [1] Maziar Raissi, Paris Perdikaris, George Karniadakis: Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, 2019 [2] Sebastian Kaltenbach, Phaedon-Stelios Koutsourelakis: Physics-aware, probabilistic model order reduction with guaranteed stability, International Conference on Learning Representations (ICLR), 2021 [3] Sebastian Kaltenbach, Phaedon-Stelios Koutsourelakis: Incorporating physical constraints in a deep probabilistic machine learning framework for coarse-graining dynamical systems, Journal of Computational Physics, 2020

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Title: The Virtual Element Method for Magneto-Hydrodynamics in Polygonal Meshes.

Author(s): *Sebastian Naranjo, *Oregon State University*; Vrushali Bokil, *Oregon State University*; Vitaliy Gyrya, *Los Alamos National Laboratory*; Gianmarco Manzini, *Los Alamos National Laboratory*;

Abstract: The virtual element method (VEM) is a generalization of the classic finite element method (FEM). In the VEM framework the shape functions used to approximate the solution to PDE systems can be proven to exist but no explicit formula can be attained, thus they are said to be virtual. The "name of the game" in this method is to define a series of projectors onto polynomial spaces where an explicit basis is known and can be used to come up with approximations to mass and stiffness matrices. In this presentation we will discuss the design of a VEM for a model in magneto-hydrodynamics (MHD), a coupling between electromagnetics and fluid flow describing the behaviour of magnetized fluids. Implementations of VEM for MHD present two major advantages, the first is the possibility of its implementation in a very general class of meshes making VEM well-suited for problems posed in oddly shaped domains or with irregularly shaped material interfaces. The second involves the divergence of the magnetic field, it should remain close to zero at the discrete level in order to prevent the appearance of fictitious forces that render simulations unfaithful to the true physics involved, VEM captures this feature exactly.

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Title: Dual Horizon Peridynamic Formulation for Thermal Diffusion Analysis

Author(s): *Selda Oterkus, *University of Strathclyde*; Bingquan Wang, *University of Strathclyde*; Erkan Oterkus, *University of Strathclyde*;

Dual Horizon Peridynamic Formulation for Thermal Diffusion Analysis Bingquan Wang1, Erkan Oterkus2 and Selda Oterkus3 1University of Strathclyde, Glasgow, UK, e-mail: bingquan.wang@strath.ac.uk 2University of Strathclyde, Glasgow, UK, e-mail: erkan.oterkus@strath.ac.uk 3University of Strathclyde, Glasgow, UK, e-mail: selda.oterkus@strath.ac.uk Peridynamics is a new continuum mechanics formulation developed to overcome the limitations of classical continuum mechanics. Peridynamic formulation is based on integro-differential equations and does not contain any spatial derivatives. Therefore, the formulation is always valid regardless of discontinuities such as cracks. Original peridynamic formulation has been extended to other physical fields including thermal diffusion [1]. Peridynamic equations are usually solved by using numerical techniques especially meshless approach. Although uniform discretization and constant horizon are usually utilized in numerical calculations, non-uniform discretization and variable horizon can be required due to computational or physical reasons. To achieve this dual horizon peridynamic formulation has been introduced [2]. In this presentation, dual horizon peridynamic formulation for thermal diffusion analysis [3] will be presented and several numerical examples will be demonstrated. Funding This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-18-1-7004. References [1] Oterkus, S., Madenci, E. and Agwai, A. (2014). Peridynamic thermal diffusion. Journal of Computational Physics, 265, pp.71-96. [2] Ren, H., Zhuang, X., Cai, Y. and Rabczuk, T., 2016. Dual?horizon peridynamics. International Journal for Numerical Methods in Engineering, 108(12), pp.1451-1476. [3] Wang, B., Oterkus, S. and Oterkus, E., 2020. Thermal diffusion analysis by using dual horizon peridynamics. Journal of Thermal Stresses, 44(1), pp.51-74.

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Title: On the Coupling of Classical and Non-Local Models for Applications in Computational Mechanics

Author(s): *Serge Prudhomme, *Polytechnique Montréal*; Patrick Diehl, *Louisiana State University*;

It is often necessary to couple different models when dealing with multi-scale or multi-physics phenomena in order to ensure efficient simulations. For instance, non-local modeling theories, such as peridynamics, have recently been considered for fracture mechanics applications. Peridynamics models can be viewed as generalizations of classical continuum mechanics theories. However, they are computationally more expensive to solve than classical models. One objective is thus to design approaches that couple the two classes of models in the regions of the computational domain where they are compatible. We will describe in this talk a novel coupling method involving the classical linear elasticity and peridynamics models. The interface operators are mathematically justified and approximation errors due to the coupling are carefully analyzed. The approach will be compared to existing methods, and in particular, to those described in earlier works [1,2]. It will also be shown to provide an alternative way to those proposed in [3] for the application of boundary conditions in peridynamics. The efficiency of the coupling method will be illustrated on several numerical examples. References [1] P.T. Bauman, H. Ben Dhia, N. Elkhodja, J.T. Oden, and S. Prudhomme, On the application of the Arlequin method to the coupling of particle and continuum models, Computational Mechanics, Vol. 42, 511-530 (2008). [2] P. Seleson, S. Beneddine, and S. Prudhomme, A force-based coupling scheme for peridynamics and classical elasticity, Computational Materials Science, Vol. 66, 34-49 (2013). [3] S. Prudhomme and P. Diehl, On the treatment of boundary conditions for bond-based peridynamics models, Computer Methods in Applied Mechanics and Engineering, Vol. 372, 113391 (2020).

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Title: A Homogenized Continuum Model for Anisotropic Oxidation in Fiber-Reinforced Composites

Author(s): *Shabnam Konica, *Michigan Technological University*; Trisha Sain, *Michigan Technological University*;

High-temperature oxidation in polymer matrix composites (PMC) is a complex degradation process that starts with oxygen diffusion from the composite free surface within the bulk followed by a series of irreversible chemical reactions between oxygen and the matrix, producing volatile compounds. Concurrently, because of oxide product formation, the matrix becomes denser. This diffusion-reaction event results in a volume reduction at the macroscale, which eventually causes irreversible chemical shrinkage, leading to degradation and micro-crack and void formation in the PMC. Eventually, these cracks create a further diffusion path for oxygen toward the core, making the material susceptible to additional oxidation. In the case of a PMC, the process becomes more exigent because of fibers' presence and the anisotropy arising from it. Though fibers are mostly inert to oxide reactions, their presence introduces factors such as the fibers' orientation, fiber volume fraction, stacking sequence and sizing, etc., that play a significant role in the oxidation process. In PMC, the preferential diffusion of oxygen along the fiber direction visibly creates higher shrinkage strain along the fiber direction than the transverse direction, causing the debonding in the fiber-matrix interface and damage, which significantly reduces the material's lifetime expectancy. Modeling oxidative behavior of PMC poses additional complexity due to different constituent materials, presence interfaces, and fiber anisotropies. The model can be costly when all these different factors are considered separately. Hence, the problem is often resolved by using homogenized models. This work presents a continuum-level theory to model the anisotropic diffusion, chemical reactions, and a preferential oxide layer growth in a fiber-reinforced polymer composite. The present theory considers a homogenized approach to model the effect of thermo-oxidation in fiber-reinforced PMCs. In the homogenized scheme, the composite RVE is modeled as a mixture of fibers and isotropic matrix, where the fibers are characterized by their orientations and respective volume fractions. The oxygen diffusion and the resulting shrinkage strain developed due to the chemical reactions are considered as anisotropic, being dominant along the fiber direction. We have numerically implemented the model by writing user-element subroutines (UEL) in Abaqus/Standard and perform pertinent numerical simulations to demonstrate the model's capability. The homogenized model would help to predict the effect of oxidation in structural scale (component level) such as composite's lamina, panel, etc. in a computationally efficient manner.

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Title: Non-Intrusive Parametric Reduced-Order Modeling via Operator Inference

Author(s): *Shane McQuarrie, *The University of Texas at Austin*; Parisa Khodabakhshi, *The University of Texas at Austin*; Karen Willcox, *The University of Texas at Austin*;

This work extends Operator Inference, a scientific machine learning framework combining data-driven learning and physics-based modeling, to the setting of systems of parametrized partial differential equations (PDEs). The approach embeds the parametric structure of the governing equations directly into the reduced-order model and learns appropriate reduced-order model operators via a data-driven linear regression problem. The result is a reduced-order model that can be solved rapidly to map parameter values to approximate PDE solutions. Such parametrized reduced-order models may be used as physics-based surrogates for uncertainty quantification and inverse problems that require many forward solves of parametric PDEs. Numerical issues such as problem conditioning and the need for appropriate regularization in the learning problem are considered, and an algorithm for hyperparameter selection is presented. The method is demonstrated for several systems of PDEs arising in engineering applications.

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Title: A Stabilized Interface Method for Fluid-Structure Interaction Across Non-Matching Meshes: Non-Newtonian Blood and Finitely Deforming Arteries

Author(s): *Sharbel Nashar, *University of Illinois at Urbana-Champaign*; Soonpil Kang, *University of Illinois at Urbana-Champaign*; Arif Masud, *University of Illinois at Urbana-Champaign*;

This talk presents a stabilized interface method for fluid-structure interaction with application to blood-artery coupled response across non-matching interfacial meshes in cardiovascular flows. The proposed method is free of the restriction of employing nodally matched meshes at the fluid-structure interfaces, and this feature is very convenient for the discretization of complex patient-specific geometries. This method employs a stabilized formulation for incompressible fluids that implements a shear-rate dependent model for blood and couples it with a hyper-elastic solid model for the large deformation of arterial walls. The interface terms are derived via the Variational Multiscale (VMS) approach wherein we solve for the fine-scale variational problem locally to derive the analytical expressions for fine-scale models and the Lagrange multiplier field. These are subsequently embedded in the coarse-scale formulation and they result in variationally consistent and parameter-free formulation for weakly enforcing the interfacial constraints at the fluid-solid interface. We present a set of benchmark problems to investigate the mathematical attributes of the method and study its higher stability and accuracy properties. Test cases with patient-specific arterial models are presented to show the computational efficiency of the method for large scale meshes and to highlight its relevance in clinically relevant applications. References 1. A. Masud, J. Kwack, A stabilized mixed finite element method for the incompressible shear-rate dependent non-Newtonian fluids: Variational Multiscale framework and consistent linearization, Comput. Methods Appl. Mech. Engrg. 200 (2011) 577-596. 2. A Masud, TJ Truster, LA Bergman, A unified formulation for interface coupling and frictional contact modeling with embedded error estimation, Int. J. Numer. Meth. Engng. 92 (2012) 141-177. 3. T.J. Truster, P. Chen, A. Masud, Finite strain primal interface formulation with consistently evolving stabilization, Int. J. Numer. Meth. Engng. 102 (2015) 278-315.

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Title: Radiation Damage study of Ni/Inconel Multimetallic Layered Composite for Fluoride-Salt Reactor - A Molecular Dynamics study.

Author(s): *Shiddartha Paul, *The University of Alabama*; Daniel Schwen, *Idaho National Laboratory*; Michael Short Short, *Massachusetts Institute of Technology*; Kasra Momeni, *University of Alabama*;

Developing new radiation-resistant structural cladding materials for high temperatures and corrosive environments is one of the crucial obstacles for building Generation IV nuclear reactors. Recently, a new Ni-based Multi-metallic Layered Composite (MMLC) concept as a fuel cladding material has been proposed because of their low oxidation tendency. Our study has used the molecular dynamics (MD) approach to study the radiation-induced mixing through the heterostructure interface in five different Inconel/Ni MMLCs. We have investigated the irradiation effect on this particular MMLC by using successive collision cascades simulations up to the radiation dose of 0.5dpa. Our findings show that the thickness of the heterostructure interface and the number of defects have a linear relation with the radiation dose. Moreover, radiation-induced mixing profiles depict the higher tendency of Cr to get mixed through the diffusion. The lower migration barrier of Cr has assisted the vacancy and interstitial formation process. According to the result obtained from our study, the Ni/800H (Ni32Cr21Fe47) MMLC structure demonstrated a high radiation resistance among all five Inconel compositions that we have studied.

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Title: Numerical Study on Active Control of Limit Cycle Oscillation with Energy Harvesting

Author(s): *Shigeki Kaneko, *The University of Tokyo*; Shinobu Yoshimura, *The University of Tokyo*;

For mission of environmental survey and telecommunication service, an unmanned aerial vehicle (UAV) with high-altitude and long-endurance (HALE) flight has been developed recently. Because the HALE flight requires very efficient aerodynamics, high-aspect-ratio wings (HARW) with low weight have been widely investigated to realize high lift-drag ratio. Since the HARW may undergo large deformation, geometrical nonlinearity appears. Nonlinear flow may also happen due to the large deformation. As a result, the HARW is often exposed to limit cycle oscillation (LCO). Destructive vibration must be suppressed for safety. On the other hand, if a certain magnitude of vibration is allowed under the assumption that it does not harm the wing/aircraft performance, such vibration could serve as a source of energy harvesting. An experimental study on UAVs with piezoelectric energy harvesting was reported [1]. A numerical study on concurrent active control with piezoelectric energy harvesting was studied a few years ago [2], in which fluid force was calculated by a simple mathematical model. Since LCO is caused due to very complicated nonlinear behavior, a detailed fluid-structure interaction (FSI) model with large-scale degrees of freedom is appropriate to well capture LCO. In our previous work, we have been developing FEM-based fluid-structure-piezoelectricity coupled analysis considering active control systems to simulate the active control of FSI-induced vibration by piezoelectric sensors and actuators [3]. In the present study, we integrate an electric circuit into the coupled analysis to consider piezoelectric energy harvester and to calculate consumed energy by piezoelectric actuators. We show a two-dimensional numerical simulation on active control of LCO with piezoelectric energy harvesting. References [1] Anton, S. and Inman, D.: Vibration energy harvesting for unmanned aerial vehicles. In: Active and Passive Smart Structures and Integrated Systems (2008) [2] Tsushima, N. and Su, W.: Flutter suppression for highly flexible wings using passive and active piezoelectric effects. Aerosp. Sci. Technol. 65, 78-89 (2017) [3] Kaneko, S., Hong, G.-W., Mitsume, N., Yamada, T., Yoshimura, S.: Numerical study of active control by piezoelectric materials for fluid-structure interaction problems. J. Sound Vib. 435, 23-35 (2018)

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Mass Conserving Implicit-Explicit (IMEX) Methods for a Coupled Compressible Navier-Stokes Equations

Author(s): *Shinhoo Kang, *Argonne National Laboratory*; Emil Constantinescu, *Argonne National Laboratory*; Hong Zhang, *Argonne National Laboratory*; Robert Jacob, *Argonne National Laboratory*;

Earth system models require various components including atmosphere, ocean, and land. For decades, each component has been well-developed and continuously improved. When it comes to coupling, we need to address several challenges such as matching different grids at the interface and treating different time scales arising from each model. In this study, we focus on the coupling strategy in the sense of stable time integration methods. In particular, implicit-explicit (IMEX) tight and loose coupling strategies are explored to handle different time scales. For a simplified model for the air-sea interaction problem, we consider a coupled compressible Navier-Stokes equations with an interface condition. Under the rigid-lid assumption, horizontal momentum and heat flux are exchanged through the interface. Several numerical experiments are conducted to demonstrate the stability of the couplings schemes. We have numerically and theoretically shown that our IMEX coupling methods are mass conservative for a coupled compressible Navier-Stokes system with the rigid-lid condition.

16th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantified Parametrically Homogenized Constitutive Model for Polycrystalline Titanium Alloys

Author(s): *Shravan Kotha, *Johns Hopkins University*; Deniz Ozturk, *Johns Hopkins University*; Somnath Ghosh, *Johns Hopkins University*;

In this talk, an uncertainty quantified, parametrically homogenized constitutive model (UQ-PHCM) is developed for microstructure-sensitive modeling and simulation at the structural scale [1,2]. The PHCMs are thermodynamically consistent, macroscopic constitutive models, whose parameters are expressed as explicit functions of Representative Aggregated Microstructural Parameters (RAMPs) that represent statistical distributions of morphological and crystallographic descriptors of the microstructure. The forms of the PHCM equations are chosen to reflect the fundamental deformation characteristics of aggregated response of crystal plasticity finite element model (CPFEM) simulations of microstructural statistically equivalent RVEs [1]. Machine learning is used on datasets generated by CPFEM to obtain the functional forms of parameters in PHCM. Significantly reduced number of solution variables in the physics-based PHCM simulations, compared to direct numerical simulations of micromechanical models, make them several orders of magnitude more efficient with comparable accuracy. The UQ-PHCM framework is built from computational homogenization of CPFE simulations performed on a large set of microstructures and load paths, followed by Bayesian inference from these results to derive probabilistic, microstructure-dependent constitutive laws of the macroscopic material response [2]. The framework addresses three sources of uncertainty that accrue at the model development and response prediction stages, viz: (i) model reduction error (MRE), (ii) data sparsity (DS), and (iii) microstructural variability (MSV) of the material. A series expansion-based uncertainty propagation (UP) method, which is much more efficient than Monte Carlo sampling, is developed to propagate uncertainties to the material response variables. The UQ-PHCM framework is validated by comparing the stochastic predictions with a collection of CPFEM-based results and limited experimental data on the alpha-phase Ti alloy, Ti-7Al. Finally, UQ-PHCM is used to simulate structural components to test its viability in real applications. UQ-PHCMs have built-in microstructural dependencies and uncertainty propagation capabilities and thus facilitate computationally efficient, microstructure-sensitive structural simulations. These capabilities of UQ-PHCM represent a significant step in the multi-scale structure-material modeling. References: 1. Kotha, S., D. Ozturk, and S. Ghosh (2019). Parametrically homogenized constitutive models (PHCMs) from micromechanical crystal plasticity FE simulations, part I and II. Int. J. Plast.. 2. Ozturk, D., S. Kotha and S. Ghosh (2021). An uncertainty quantification framework for multiscale parametrically homogenized constitutive models (PHCMs) of polycrystalline Ti alloys. J. of Mech. Phys. of Solids., 148, pp. 1-31.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Isogeometric Finite Element-Based Simulation of the Aortic Heart Valve: Integration of Neural Network Structural Material Model and Structural Tensor ?ber Architecture Representations

Author(s): Wenbo Zhang, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*; Tan Bui, *The University of Texas at Austin*; *Shruti Motiwale, *The University of Texas at Austin*;

The functional complexity of native and replacement aortic heart valves are well known, incorporating such physical phenomenons as time-varying non-linear anisotropic soft tissue mechanical behavior, geometric non-linearity, complex multi-surface time varying contact, and fluid-structure interactions to name a few. It is thus clear that computational simulations are critical in understanding AV function and for the rational basis for design of their replacements. However, such approaches continued to be limited by ad-hoc approaches for incorporating tissue fibrous structure, high-fidelity material models, and valve geometry. To this end, we developed an integrated tri-lea?et valve pipeline built upon an isogeometric analysis (IGA) framework. A high-order structural tensor (HOST) based method was developed for ef?cient storage and mapping the two-dimensional ?ber structural data onto the valvular 3D geometry. We then developed a neural network (NN) material model that learned the responses of a detailed meso-structural model for both native and exogenously cross-linked planar soft tissues. The NN material model not only reproduced the full anisotropic mechanical responses but also demonstrated a considerable ef?ciency improvement, as it was trained over a range of realizable ?brous structures. Results of parametric simulations were then performed, as well as population based bicuspid aortic heart valve fiber structure, that demonstrated the ef?ciency and robustness of the present approach. In summary, the present approach that integrates HOST and NN material model provides an efficient computational analysis framework with increased physical and functional realism for the simulation of native and replacement tri-lea?et heart valves. while retaining the benefits of a high fidelity of the structural model, the present NN material models drastically reduced the computational cost. In comparison to the phenomenological models, regardless of speci?c form, the NN material model does not increase the computational cost for AV simulations. NN material models, as universal approximators, can be extended to represent more complex soft tissue mechanical behaviors, such as plasticity, fatigue, and related time-dependent behaviors. Finally, with the advance of the in-vivo imaging techniques, the present AV model can be easily adapted to patient specific geometry and fiber structures when such data is available. In such circumstances, the predictability of the AV simulation will be signi?cantly improved from a patient speci?c point of view.

16th U.S. National Congress on Computational Mechanics
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Title: A Fast Convolution-Based Method for Peridynamic Models of Elasticity and Fracture

Author(s): *Siavash Jafarzadeh, *University of Nebraska-Lincoln*; Farzaneh Mousavi, *University of Nebraska-Lincoln*; Longzhen Wang, *University of Nebraska-Lincoln*; Adam Larios, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

Computational cost of peridynamic (PD) simulations (and nonlocal models in general) is relatively higher compared to that of corresponding local models, due to the higher “connectivity” between nodes. Existing discretization methods for PD, such as the meshfree discretization or the finite element method, have the computational complexity of O(N2), with N being the total number of degrees of freedom. In this study, we introduce a fast convolution-based method (FCBM) for peridynamic problems in elasticity and brittle fracture on bounded domains with arbitrary shapes and arbitrary boundary conditions. We first express the bond-based and state-based PD models of elasticity in convolutional form, and then compute the convolutions by the fast Fourier transform (FFT), which converts these convolution integrals into multiplication operations. For fracture problems, we introduce a new energy-based bond failure criterion that leads to a nonlinear fracture model with convolutional structure, which is then exploited by the FFT. The complexity of this new method is O(Nlog2N). Unlike conventional Fourier methods which are limited to problems on periodic domains, the FCBM is applicable to general problems with arbitrary domains and boundary conditions. With a novel “Embedded Constraint” (EC) approach, we replace the boundary value problem on the bounded domain with an equivalent problem constructed on an extended periodic domain with volume constraints embedded in the domain. We verify our method by solving 3D elastic deformations in a complex geometry using a state-based model. The simulation results are compared with Abaqus finite element results. We also solve a dynamic brittle fracture problem with multiple crack branching events and compare the results with those obtained by the PD meshfree method based on the critical bond-strain criterion. We show that PD simulations with billions of nodes become possible on a single CPU, as FCBM cuts the run-time for PD simulations from years to days and from hours to seconds. Acknowledgements: This work has been supported by NSF grant No. 1953346, and by a Nebraska System Science award from the Nebraska Research Initiative. This work was completed utilizing the Holland Computing Center of the University of Nebraska, which receives support from the Nebraska Research Initiative. References [1] Jafarzadeh, S., Wang, L., Larios, A., & Bobaru, F. (2021). Computer Methods in Applied Mechanics and Engineering 375, 113633. [2] Jafarzadeh, S., Larios, A., & Bobaru, F. (2020). Journal of Peridynamics and Nonlocal Modeling 2, 185-110.

16th U.S. National Congress on Computational Mechanics
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Title: Unsupervised Discovery of Interpretable Hyperelastic Constitutive Laws

Author(s): *Siddhant Kumar, *Delft University of Technology*; Moritz Flaschel, *ETH Zurich*; Laura De Lorenzis, *ETH Zurich*;

We propose a new approach for data-driven automated discovery of hyperelastic constitutive laws. The approach is unsupervised, i.e., it requires no stress data but only displacement and global force data, which are realistically available through mechanical testing and digital image correlation techniques; it delivers interpretable models, i.e., models that are embodied by parsimonious mathematical expressions discovered through sparse regression of a large catalogue of candidate functions; it is one-shot, i.e., discovery only needs one experiment - but can use more if available. The problem of unsupervised discovery is solved by enforcing equilibrium constraints in the bulk and at the loaded boundary of the domain. Sparsity of the solution is achieved by lp regularization combined with thresholding, which calls for a non-linear optimization scheme. The ensuing fully automated algorithm leverages physics-based constraints for the automatic determination of the penalty parameter in the regularization term. Using numerically generated data including artificial noise, we demonstrate the ability of the approach to accurately discover five hyperelastic models of different complexity. We also show that, if a true feature is missing in the function library, the proposed approach is able to surrogate it in such a way that the actual response is still accurately predicted.

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Title: Accurate NDT Characterization of Hidden Flaws with Mechanics and Machine Learning

Author(s): *Sijun Niu, *Brown University*; Vikas Srivastava, *Brown University*;

Over 2.5 million miles of pipelines carrying hazardous hydrocarbons run across United States. Detailed non-destructive quantitative characterization of embedded and hidden flaws and accurate risk based failure models are critical to assess fitness for service and for avoiding catastrophic failures. Ultrasonic non-destructive test method is an important method for detecting and evaluating non-visible and embedded flaws. Even though there has been significant progress in developing advanced ultrasonic sensors and data accumulation and presentation methods, the final flaw detection and prediction relies on human expertise to evaluate the ultrasound signal, leading to very high variations, uncertainties, and errors in the prediction. With remarkable recent progress in the machine learning algorithms, we show that the ultrasound signal could be analyzed by machine learning algorithms to provide accurate predictions of critical crack characteristics. We have applied finite element simulations using software Abaqus to create large training datasets that contain A-scan ultrasonic signals of elliptical cracks with various geometries embedded in a steel plate. We have identified wavelet packet transform as our feature extraction technique to reduce the dimensionality of the raw ultrasonic signals for its capability to preserve information and to analyze signals in both time and frequency domains. Then a feedforward neural network model has been trained with the simulation datasets and used to predict multiple crack characteristic, including crack size, crack location and crack orientation, simultaneously with very high accuracy. We have also conducted ultrasound experiments with commercial ultrasonic units and 3D printed metal samples to validate our finite element simulations and predictive capabilities of our neural network on real signals.

16th U.S. National Congress on Computational Mechanics
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Title: The Source Transfer Domain Decomposition Preconditioner for High-Frequency Time-Harmonic Maxwell Equations

Author(s): *Socratis Petrides, *Lawrence Livermore National Laboratory*; Dylan Copeland, *Lawrence Livermore National Laboratory*; Tzanio Kolev, *Lawrence Livermore National Laboratory*;

We present a domain decomposition method with source transfer for the solution of high-frequency time-harmonic Maxwell equations. The method is built upon the work of Leng and Ju on the Diagonal Source Transfer method for the Helmholtz equation [1], and the work of Tsuji, Engquist, and Ying on the sweeping preconditioner for Maxwell equations [2]. In this work, we consider standard Finite Element discretizations with high order Nédélec elements for electromagnetic simulations posed in unbounded domains. The computational domain is partitioned into overlapping subdomains and a local Maxwell problem with a Perfectly Match Layer (PML) is defined on each subdomain. A special ordering of local subdomain solves and sweeping strategies that enable parallelization [1] lead to an effective preconditioner for the GMRES solver. For the case of a constant wavenumber, k, we observe iteration count of the preconditioned GMRES which grows logarithmically with the wavenumber. The efficacy of the preconditioner is showcased with several large scale simulations in two and three space dimensions, including problems with reflecting boundary conditions and variable wavenumber. [1] Wei Leng and Lili Ju. A Diagonal Sweeping Domain Decomposition Method with Source Transfer for the Helmholtz Equation. Communications in Computational Physics, 29(2):357–398, 2020. [2] Paul Tsuji, Bjorn Engquist, and Lexing Ying. A sweeping preconditioner for time-harmonic Maxwell’s equations with finite elements. Journal of Computational Physics, 231(9):3770–3783, 2012. Prepared by LLNL under Contract DE-AC52-07NA27344, LLNL-ABS-819303.

16th U.S. National Congress on Computational Mechanics
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Title: Bacterial Swimmers with a Polar Flagellar Bundle: Push, Pull, and Coil

Author(s): *Sookkyung Lim, *University of Cincinnati*; Yongsam Kim, *Chung-Ang University*; Jeungeun Park, *University of Cincinnati*; Wanho Lee, *National Institute for Mathematical Sciences*;

Flagellated bacteria swim in a fluid environment by rotating motors embedded in the cell membrane and consequently rotating helical flagella. Swimming strategies of such bacteria vary depending on the number of flagella and their arrangement across the cell body. In this talk, we present a mathematical model of lophotrichous bacteria such as Pseudomonas putida that have multiple flagella at one polar end. P. putida undergo a classical event of push-pull-push cycle. Alternatively, they reorient themselves by wrapping the cell body with their flagellar bundle. To investigate the fluid-cell interaction, we explicitly model the cell as a neutrally buoyant rigid body, treat the flagella as helical elastic rods modeled by a nonstandard Kirchhoff rod theory, and couple the bacterium to a viscous fluid with the regularized Stokes formulation. The simulation results may provide the insight into the underlying swimming mechanism of lophotrichous bacteria.

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Title: An Immersed Boundary Formulation for Thermally Coupled Incompressible Turbulent Flows

Author(s): *Soonpil Kang, *University of Illinois at Urbana-Champaign*; Arif Masud, *University of Illinois at Urbana-Champaign*;

This talk presents new developments in thermally coupled turbulent flows around immersed objects. The proposed method weakly imposes the Dirichlet boundary conditions for the momentum and the energy equations along the immersed boundaries. The boundary terms are derived via the Variational Multiscale (VMS) approach wherein we solve for the fine-scale variational problems locally to derive the analytical expressions for fine-scale velocity and temperature fields. In addition, locally resolving for the continuity conditions at the interface leads to analytical expression for the Lagrange multiplier field. These fine-scale models are then embedded in the coarse-scale formulation and they result in optimal enforcement of the Dirichlet boundary conditions at the non-boundary fitted discretization. These developments are done in the context of a residual-based multiscale turbulence method that is employed to model turbulent flows around the immersed objects. The surface geometry of the immersed object is represented via triangulated surface mesh that can readily be obtained from CAD models in the STL format. This helps drastically reduce the time-consuming pre-processing step of developing body conforming meshes around complex geometric shapes. Benchmark problems are presented to show the mathematical attributes of accuracy and stability of the method. Some sample industrial-strength problems are also presented to highlight the applicability of the method for large-scale computing. References 1. S. Kang, A. Masud, A Variational Multiscale method with immersed boundary conditions for incompressible flows, Meccanica (2020). https://doi.org/10.1007/s11012-020-01227-w 2. R Calderer, A Masud, Residual-based variational multiscale turbulence models for unstructured tetrahedral meshes, Computer Methods in Applied Mechanics and Engineering. 254 (2013) 238-253. 3. A. Masud, P. Chen, Thermoelasticity at finite strains with weak and strong discontinuities, Computer Methods in Applied Mechanics and Engineering. 347 (2019) 1050-1084.

16th U.S. National Congress on Computational Mechanics
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Title: Mechanics and Microstructurally Based Modeling of the Passive Right Ventricular Myocardium

Author(s): *Sotirios Kakaletsis, *The University of Texas at Austin*; Gabriella P. Sugerman, *The University of Texas at Austin*; Tomasz Jazwiec, *Spectrum Health*; Marcin Malinowski, *Spectrum Health*; Tomasz Timek, *Spectrum Health*; Manuel Rausch, *The University of Texas at Austin*;

The microstructure and mechanics of the right ventricle have been historically understudied compared to the left ventricle. Yet, right ventricular dysfunction -which can be described in terms of both mechanics and microstructural (mal)adaptations- is a major factor in severe cardiovascular diseases. For example, it contributes to the left ventricular dysfunction [1] and efforts to ameliorate it is the main treatment goal in pulmonary hypertension [2]. Thus, studying independently the right ventricle will enable us to describe the underlying mechanisms between histo-mechanics and healthy ventricle function. As a first step, we examine the passive mechanical properties of the right ventricular myocardium of 12 healthy sheep. First, in order to characterize the highly anisotropic response of the myocardium, we perform triaxial shear testing. Specifically, we excise cubic specimens of 10mm edge from the right ventricle and test them in six shear and three uniaxial testing modes. We then proceed by quantifying the fibrous microstructure of the tissue. We acquire histology sections at ten different levels throughout each specimen, over two normal anatomical directions. Next, we obtain continuous probability density functions of the fiber dispersion at each section level by using directional image analysis of the histology slides. Moreover, we model the right ventricular myocardium as a nearly incompressible hyperelastic material. To this end, we implement and modify an established material model of myocardium using FEBio, an opensource finite element software. Finally, we develop a custom inverse analysis pipeline in order to estimate material parameters. By gradually increasing the complexity of microstructural data as our pipeline’s input, we predict the response of unseen tested specimens. In this way, we investigate the extent of microstructural information that is necessary to capture and predict reliably the mechanical behavior of the right ventricular myocardium.References: [1] Zornoff, Leonardo AM, et al. "Right ventricular dysfunction and risk of heart failure and mortality after myocardial infarction." Journal of the American College of Cardiology 39.9 (2002): 1450-1455. [2] van de Veerdonk, M.C., Bogaard, H.J. & Voelkel, N.F. The right ventricle and pulmonary hypertension. Heart Fail Rev 21, 259–271 (2016).

16th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Analysis of Earthquake Load Mitigation on Two-Storey Building Using EPS Geofoam

Author(s): Panagiotis Karakitsios, *National Technical University of Athens*; *Spyridon Papoudos, *University of Patras*; George Mylonakis, *University of Bristol*;

The use of expanded polystyrene (EPS) geofoam fills for foundation in areas with intense seismic activity, such as Greece, has seen growing use worldwide in urban environments and presents technical challenges. Geofoam, which is manufactured into large lightweight blocks, is a geosynthetic product that can be used as a fill material in strap beam footing systems for seismic isolation of buildings against combined static and seismic activity. This paper introduces a novel seismic isolation technique implemented on a real-world project, where geofoam was used for a two-storey apartment building in Greece. The geofoam blocks, which exhibit nonlinear stress–strain behavior, were modeled with finite element analysis using Plaxis 2D (plane-strain) and isogeometric analysis using the Geomiso software. Parametric investigations were carried out to study the effect of EPS compressible inclusions density and thickness on the horizontal deformation, strain and stress fields. The numerical results indicate that geofoam reduces the total applied pressure on the ground and drastically increases the bearing capacity of the structure in static and seismic condition. The same results are obtained with NURBS-based isogeometric analysis with Geomiso. Geomiso (www.geomiso.com) achieves significantly increased accuracy and drastically reduced computational cost as far as the calculation of load carrying capacity and deformation/stress fields inside the layered soil body are concerned. This numerical simulation with both finite element analysis and isogeometric analysis shows that geofoam improves the building damage from severe to slight damage with lesser deformation. Geofoam is proved to be a new, more efficient, alternative seismic isolation technique for buildings. This is a novel practical technique for improving the earthquake resistance of the building, which combines speed, cost saving and safety, and leads to more efficient seismic isolation. This research and specifically the first author has been supported by the Alexander S. Onassis Foundation (G ZG 017/ 2010-2011). Keywords: Isogeometric analysis, finite element analysis, NURBS, geofoam, expanded polystyrene, seismic isolation, building, foundation, strap footing, earthquake REFERENCES [1] X. Karatzia, G. Mylonakis, G. Bouckovalas, Seismic isolation of surface foundations exploiting the properties of natural liquefiable soil, Soil Dynamics and Earthquake Engineering, 121 (2019) 233–251. [2] P. Karakitsios, G. Karaiskos, A. Leontaris, P. Kolios, Geomiso TNL: A software for non-linear static T-spline-based isogeometric analysis of complex multi-patch structures, 14th World Congress in Computational Mechanics (WCCM), ECCOMAS Congress (2020). [3] A. Karatarakis, P. Karakitsios, M. Papadrakakis, GPU accelerated computation of the isogeometric analysis stiffness matrix, Comput. Methods Appl. Mech. Engrg., 269 (2014) 334-355.

16th U.S. National Congress on Computational Mechanics
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Title: An Immersed-Interface Finite Element Method for Linear Elasticity using Four-Noded Rectangular Elements

Author(s): *Srivatsa Bhat Kaudur, *Virginia Polytechnic Institute and State University*; Mayuresh Patil, *Georgia Institute of Technology*;

We develop an immersed-interface finite element method (IIFEM) using four-noded rectangular elements. The IIFEM is based on a non-conformal, Petrov-Galerkin (ncPG) formulation similar to the one presented in [1] for triangular elements to solve linear elasticity problems. As the interface lies within the element, trial functions that satisfy the Hadamard conditions (displacement and traction continuity across the interface) are generated. We present trial functions which satisfy these conditions approximately in an integral sense. These functions are non-conformal on the element edges. We use a multimaterial patch test to confirm the consistency of the FE formulation. Standard finite element basis functions are used as test functions in the Petrov-Galerkin formulation. The developed ncPG-IIFEM is then used to solve a bi-material problem with uniform rectangular mesh. We expect that the convergence and error of the displacements and stresses to be equivalent to interface fitted mesh. Thus, the above method is expected to reduce the cost of meshing, especially during adaptive mesh refinement, without compromising on the accuracy of the solutions obtained. The developed immersed element also provides flexibility and accuracy while performing Topology optimization. References: [1] Mayuresh J Patil. Immersed-Interface Finite Element Method based on a Non-Conformal Petrov-Galerkin Formulation, International Journal of Numerical Methods in Engineering (accepted). [2] Lin T, Zhang X. Linear and bilinear immersed finite elements for planar elasticity interface problems. Journal of Computational and Applied Mathematics 2012; 236(18): 4681–4699.

16th U.S. National Congress on Computational Mechanics
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Title: Machine Learning Applications for Defeaturing and Model Preparation

Author(s): *Steven Owen, *Sandia National Laboratories*; Armida Carbajal, *Sandia National Laboratories*; Matthew Peterson, *Sandia National Laboratories*; Corey Ernst, *Sandia National Laboratories*;

We describe two new machine learning-based methods for model preparation. In the first, we demonstrate supervised machine learning to defeature CAD models for tetrahedral meshing. We show how ML-based predictions of mesh quality at localized topology in a CAD model prior to meshing can identify potential problem areas. Meshing outcomes can then be improved by predicting specific CAD modification operations that can best improve local mesh quality. In the second application, we use machine learning classification methods to identify common mechanical components such as fasteners, springs and bearings to speed model preparation of complex systems. Once classified, targeted operations can be rapidly applied to simplify or build reduced order representations of the mechanisms ready for analysis. We demonstrate how these applications can dramatically reduce time for CAD-to-simulation as well as improve reproducibility and credibility of analyst models. An interactive user environment using Sandia's Cubit Geometry and Meshing Toolkit demonstrates ML-based predictions and solutions to the user for validation and rapid execution.

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Title: A Robust and Accurate Variational Finite Element Formulation for Cavitating Hydrofoils with Fluid-Structure Interaction

Author(s): *Suraj Kashyap, *University of British Columbia*; Rajeev Jaiman, *University of British Columbia*;

Cavitation is ubiquitous in marine propeller operation and is known for deleterious effects such as flow-induced vibration and noise. Traditional approaches to fluid-structure interaction (FSI) studies in cavitating flows have often focused on a one-way coupling between a flow solver for the cavitation hydrodynamics and a separate finite element solver for structural deformation. In the current work, we develop a unified framework for the cavitating flow and the structural motion via a stabilized variational finite element formulation. To model the finite mass transfer in cavitation phenomena, we employ the phenomenological homogenous mixture-based approach via scalar transport differential equations, given by Merkle et al and Schnerr-Sauer models. The linearizations of the finite mass transfer terms for the mass continuity equation and the reaction term of the scalar transport equations are derived. The numerical solution of the cavitation equation is imparted by a positivity-preserving property to address the numerical oscillations arising from high-density gradients typical of two-phase cavitating flows. The proposed formulation is strongly coupled in a partitioned manner with a 3D Navier-Stokes finite element solver, and the unsteady problem is advanced in time using a fully-implicit generalized-\alpha time integration scheme. We first verify the implementation on the benchmark case of Rayleigh bubble collapse. We demonstrate the accuracy of the cavitation solver by comparing the numerical solutions with the analytical solutions of the Rayleigh-Plesset equation for bubble dynamics. We find our solver to be robust for large time steps and the absence of spurious oscillations/spikes in the pressure field. The cavitating flow solver is coupled with a hybrid URANS-LES turbulence model with a turbulence viscosity corrected for the presence of vapor. We validate the coupled solver on high Reynolds number turbulent cavitating flow over a NACA0012 hydrofoil section. Finally, the proposed method is solved in an Arbitrary Lagrangian-Eulerian framework to study turbulent cavitating flow over a pitching hydrofoil section and the coupled FSI results are explored for the characteristic features of cavitating flows such as re-entrant jet and periodic cavity shedding. References: 1. Joshi V, Jaiman R K. (2017). A variationally bounded scheme for delayed detached eddy simulation: Application to vortex-induced vibration of flexible riser. Computers and Fluids. 157, 84-111. https://doi.org/10.1016/j.compfluid.2017.08.013 2. Joshi V, Jaiman R K. (2018). A positivity preserving and conservative variational scheme for phase-field modeling of two-phase flows. Journal of Computational Physics. 360:137-166. https://doi.org/10.1016/j.jcp.2018.01.028.

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Title: Physics Guided Machine Learning in Fluid Dynamics

Author(s): *Suraj Pawar, *Oklahoma State University*; Omer San, *Oklahoma State University*; Adil Rasheed, *Norwegian University of Science and Technology*;

There is a growing interest in applying machine learning, particularly deep learning for scientific applications due to the abundance of data generated either from high-fidelity numerical simulations or sparse measurements. Despite the success of data-driven models for many problems in scientific computing, they lack the interpretability of the physics-based models. This motivates the need to address the generalizability and data efficiency of the data-driven approaches for physical systems. We present a novel physics guided machine learning (PGML) framework that improves the generalizability of nonintrusive models by fusing the domain knowledge directly into the machine learning model. The central idea in the PGML framework is to embed the knowledge from simplified theories directly into an intermediate layer of the neural network. The knowledge from the simplified theories aids in constraining the output of the neural network on a physical manifold. We demonstrate our framework for a variety of tasks, ranging from real-time airfoil aerodynamic prediction task [1] to reduced order modeling of fluid flows. We employ the potential flow solver and Galerkin projection as simplified models for the real-time airfoil forces prediction task and reduced order modeling of fluid flows, respectively. The PGML framework is successful in significantly reducing the model uncertainty (captured using the prediction from multiple models initialized with different parameters) of the neural network. The PGML framework can be applied in different branches of science and engineering, such as wind farm layout optimization, boundary layer flows, where simplistic models are very common. The simplified models are cheap to run and therefore the PGML framework can be attractive for applications such as model predictive control, data assimilation, and uncertainty quantification. The hybrid model built using the PGML framework can act as an enabler for predictive simulations paving the way for the digital twin of physical systems.
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16th U.S. National Congress on Computational Mechanics
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Title: Parallelization of a Stabilized Peridynamics Code Coupled with Finite Element Method Using OpenMP

Author(s): *Suyeong Jin, *Korea Advanced Institute of Science and Technology*; Young Kwang Hwang, *Korea Advanced Institute of Science and Technology*; Jung-Wuk Hong, *Korea Advanced Institute of Science and Technology*;

Peridynamics, based on a non-local theory, offers an effective feature for simulating the crack propagation as the integro-differential equation of motion in the peridynamics avoids the additional artificial criteria to describe the response at discontinuities such as cracks and voids [1]. However, such computation is expensive compared to the finite element method because each material point interacts with all material points within a non-local length scale, called horizon, and an appropriate stabilization scheme is required to suppress the zero-energy mode in the peridynamics [2]. In this paper, we extend the coupling scheme, originally developed to couple the bond-based peridynamics with finite elements [3], for the non-ordinary state-based peridynamics, implement the stabilization scheme for the peridynamics regime, and parallelize the code using the open multi-processing (OpenMP) library. The accuracy of the parallelized code is verified by comparing the numerical results of the serial and parallelized calculations, and then the performance of the parallelized code is investigated by increasing the number of threads. The parallelization significantly reduces the computation time by increasing the number of threads up to a certain value. The optimal number of threads is determined to efficiently conduct the numerical analyses using the proposed parallelized coupling code. References [1] S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, “Peridynamic states and constitutive modeling,” J. Elast., vol. 88, no. 2, pp. 151–184, 2007. [2] S. A. Silling, “Stability of peridynamic correspondence material models and their particle discretizations,” Comput. Methods Appl. Mech. Eng., vol. 322, pp. 42–57, 2017. [3] W. Liu and J.-W. Hong, “A coupling approach of discretized peridynamics with finite element method,” Comput. Methods Appl. Mech. Eng., vol. 245–246, pp. 163–175, 2012.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Probing Sea Ice Mechanics with a Lagrangian Discrete Element Model for Sea Ice

Author(s): *Svetoslav Nikolov, *Sandia National Laboratories*; Kara Peterson, *Sandia National Laboratories*; Adrian Turner, *Los Alamos National Laboratory*; Dan Bolintineanu, *Sandia National Laboratories*; Joel Clemmer, *Sandia National Laboratories*;

The representation of sea ice in Earth System Models (ESMs) has traditionally been carried out using a variety of continuum methods, like the visco-plastic model of Hibler and the elastic-viscous-plastic model by Hunke et al. [1]. The successful integration of such models into different ESMs has helped enhance the predictive capabilities of large-scale climate studies, which has had an important impact not only on climatology but also on marine biogeochemistry [2]. As computational resources have continued to grow and expand over the years however the resolution of some ESMs has begun to approach the 1–2-kilometer range. At these length scales the highly irregular structure and nonlinear response of sea ice causes the continuum assumption to breakdown. For these smaller length scales, the behavior of sea ice can be better represented with discontinuous Lagrangian schemes like the discrete element method (DEM), which can treat ice floes as individual particles interacting through a series of contact forces. In that regard, in the current work we develop a DEM model for sea ice (DEMSI) based on the Hopkins contact model, which includes both bonded and unbonded interactions [3]. The DEMSI code relies on the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to run the Hopkins contact model which enables the utilization of the Kokkos performance portability programming ecosystem. As a result, DEMSI is highly scalable and easily portable across different high performance computing architectures. For sensitivity analysis and parametrization of our model we rely on the Dakota software. We validate our model by examining compressive, tensile, shear modes of failure and comparing against previous studies in literature. 1. Hunke, E. C., and J. K. Dukowicz. "An elastic–viscous–plastic model for sea ice dynamics." Journal of Physical Oceanography 27.9 (1997): 1849-1867. 2. Notz, Dirk, et al. "The CMIP6 Sea-Ice Model Intercomparison Project (SIMIP): understanding sea ice through climate-model simulations." Geoscientific Model Development 9.9 (2016): 3427-3446. 3. Hopkins, Mark A., Susan Frankenstein, and Alan S. Thorndike. "Formation of an aggregate scale in Arctic sea ice." Journal of Geophysical Research: Oceans 109.C1 (2004). Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Non-Intrusive Reduced Order Modeling of Poroelasticity of Heterogeneous Media Based on a Discontinuous Galerkin Approximation

Author(s): *T. Kadeethum, *Cornell University*; F. Ballarin, *Scuola Internazionale Superiore di Studi Avanzati*; N. Bouklas, *Cornell University*;

A simulation tool capable of speeding up the calculation for linear poroelasticity problems in heterogeneous porous media is of large practical interest for engineers, in particular, to effectively perform sensitivity analyses, uncertainty quantification, optimization, or control operations on the fluid pressure and bulk deformation fields. Towards this goal, we present here a non-intrusive model reduction framework using proper orthogonal decomposition (POD) and neural networks, based on the usual offline-online paradigm. As the conductivity of porous media can be highly heterogeneous and span several orders of magnitude, we utilize the interior penalty discontinuous Galerkin (DG) method as a full order solver to handle discontinuity and ensure local mass conservation during the offline stage. We then use POD as a data compression tool and compare the nested POD technique, in which time and uncertain parameter domains are compressed consecutively, to the classical POD method in which all domains are compressed simultaneously. The neural networks are finally trained to map the set of uncertain parameters, which could correspond to material properties, boundary conditions, or geometric characteristics, to the collection of coefficients calculated from an L^2 projection over the reduced basis. We then perform a non-intrusive evaluation of the neural networks to obtain coefficients corresponding to new values of the uncertain parameters during the online stage. We show that our framework provides reasonable approximations of the DG solution, but it is significantly faster. Moreover, the reduced order framework can capture sharp discontinuities of both displacement and pressure fields resulting from the heterogeneity in the media conductivity, which is generally challenging for intrusive reduced order methods. The sources of error are presented, showing that the nested POD technique is computationally advantageous and still provides comparable accuracy to the classical POD method. We also explore the effect of different choices of the hyperparameters of the neural network on the framework performance.

16th U.S. National Congress on Computational Mechanics
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Title: Temporal Convergence and Stability Assessment of the Generalized Finite Element Method for Localized 1-D Heat Transfer

Author(s): *TJ Miller, *The Ohio State University*; Patrick O'hara, *Air Force Research Laboratory*; Jack McNamara, *The Ohio State University*;

The Generalized Finite Element Method (GFEM) is applied to the model heat transfer problem outlined previously by Merle and Dolbow. This equation has features of practical interest to structures in extreme environments, namely a sharp-transient thermal gradient that moves in space. As such, numerical solutions to this model problem using standard finite element methods requires fine meshing over a broad domain to accurately resolve the response. Previous work by O'Hara, Duarte and Eason demonstrated global-local GFEM enables efficient handling of this problem. However, that work did not formally investigate temporal convergence or stability of the time marching procedure. This presentation will overview a detailed study on this for the model problem; specifically, an analysis of the temporal stability and convergence of GFEM using both solution-tailored and analytical enrichments for multiple time stepping methods (Forward Euler, Crank-Nicholson, etc.). We hypothesize that solution-tailored enrichments will allow for stable, high-order GFEM solutions with less stringent stability requirements and better temporal convergence compared to GFEM without solution-tailored enrichments. Improved convergence in the L2 norm is also expected with a significant reduction in error levels in the GFEM with exponential enrichments when compared to GFEM with polynomial enrichments at similar element sizes.

16th U.S. National Congress on Computational Mechanics
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Title: Asymptotic Analysis of a Coupled System of Nonlocal Equations with Oscillatory Coefficients

Author(s): *Tadele Mengesha, *University of Tennessee*; James Scott, *University of Pittsburgh*;

In this talk I will discuss on the asymptotic behavior of solutions to systems of strongly coupled integral equations with oscillatory coefficients. The system of equations is motivated by a peridynamic model of the deformation of heterogeneous media that additionally accounts for short-range forces. We consider the vanishing nonlocality limit on the same length scale as the heterogeneity and show that the system's effective behavior is characterized by a coupled system of partial differential equations that are elliptic in the sense of Legendre-Hadamard. This effective system is characterized by a fourth-order tensor that shares properties with Cauchy elasticity tensors that appear in the classical equilibrium equations for linearized elasticity. This is a joint work with James M. Scott.

16th U.S. National Congress on Computational Mechanics
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Title: Error-Curve Analysis of Neural Network and Linear Stochastic Estimation for Fluid Flow Problems

Author(s): *Taichi Nakamura, *Keio University*; Kai Fukami, *University of California, Los Angeles*; Koji Fukagata, *Keio University*;

Neural networks (NNs) have recently acquired citizenship in fluid mechanics as a surrogate modeling tool for conventional linear methods thanks to their capability to handle fluid big data efficiently [1]. However, the conventional linear methods are still indispensable from the perspective on interpretability in results provided by models. Therefore, it can easily be expected that a clarification of the difference between linear methods and NNs enables us to develop more advanced NN-based techniques. For reduced order modeling efforts, the understanding of the relationship between them has already been progressing. For example, Milano \& Koumoutsakos [2] reported that an autoencoder-shaped NN with linear activation function is equivalent to proper orthogonal decomposition (POD). Otherwise, Murata et al. [3] also exhibited the analogy between a linear convolutional neural network based autoencoder and POD, and indicated the superiority of utilizing the nonlinear activation function. Motivated above, of particular interest here is to investigate the relationship between linear methods and NNs for regression tasks in fluid mechanics. For our investigation, we consider the estimation of high-order POD coefficients from low-order counterparts for a flow around a two-dimensional cylinder. A linear stochastic estimation (LSE) and a multi-layer perceptron (MLP) are utilized for the estimation. We perform the visualization of error surfaces in the optimization process of both LSE and MLP, which enables us to reveal the cause of their difference in various characteristics including noise robustness. At last, we also consider a state estimation of turbulent channel flow as a more practical regression problem. [1] Brunton, S. L., Noack, B. R., and Koumoutsakos, P., "Machine learning for fluid mechanics," Annu. Rev. Fluid Mech. 52, 477–508 (2020). [2] Milano, M. and Koumoutsakos, P., "Neural network modeling for near wall turbulent flow," J. Comput. Phys. 182, 1–26 (2002). [3] Murata, T., Fukami, K., and Fukagata, K., "Nonlinear mode decomposition with convolutional neural networks for fluid dynamics," J. Fluid Mech. 882, A13 (2020).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Computational Assessment of Stenoses Severity and Aortic Wall Mechanics in Patients with Supravalvular Aortic Stenosis

Author(s): *Talha Lone, *Duquesne University*; Angelica Alday, *Duquesne University*; Rana Zakerzadeh, *Duquesne University*;

Supravalvular aortic stenosis (SVAS) is a condition characterized by a narrowing in the aorta directly above the level of the aortic valve. SVAS is a challenging condition to assess as routine Doppler ultrasound exams provide inaccurate blood flow and pressure information surrounding this lesion. In clinical practice, it is often observed that pressure gradients measured from ultrasound imaging tend to be higher than those obtained from invasive cardiac catheterization due to the conversion of velocity to pressure drop by means of the Bernoulli equation. These overestimated pressure measurements may suggest premature surgical treatment for patients. Thus, the need for a reproducible, comprehensive, non-invasive, method to obtain an accurate estimation of the pressure drop across the stenosed region is pressing. In this work, we develop the first SVAS computational model that embraces different constitutive models for the arterial wall. We apply the model to different stenosis severities to investigate the effect of viscous loss and discrepancies between pressure gradient calculations in catheterization and ultrasound techniques. The goal is to develop an algorithm that evaluates diagnostic parameters using a fluid-structure interaction (FSI) computational model. To this aim, we created finite element geometric models using FreeFem++, an open-source software package, for the FSI simulations. Blood is modeled as an incompressible, viscous fluid and the arterial wall consists of a thick material that accounts for its multilayer structure. Our solver used Navier-Stokes equations to model blood flow and a hyperelastic material was employed to model deformable arterial wall. An Arbitrary Lagrangian-Eulerian mesh was generated to perform the FSI simulations. To simulate the response to stenosis, we modified the geometry to exhibit a defined degree of narrowing. Wall mechanical properties in the geometrical models were tuned to account for the wide range of stenotic wall features reported in the literature. Using this model, Fractional Flow Reserve (FFR), Pressure Drop Coefficient (CDP), and fluid pressure gradient across the stenosed region are measured. Computational results quantify the effects of stenosis severity and arterial wall stiffening on local hemodynamics, artery compression, and viscous energy loss. The results suggest that the range of clinically observed stenosis levels has little influence on pressure drop at different wall stiffness values. We found that, with an increase in stenosis severity, FFR decreased whereas CDP increased. Moreover, our findings indicate that differences in diagnostic parameters could lead to misinterpretation of stenosis severity.

16th U.S. National Congress on Computational Mechanics
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Title: Solving Interface Inverse Problems by an Immersed Finite Element Method with a Fixed Mesh

Author(s): *Tao Lin, *Virginia Polytechnic Institute and State University*;

This talk is about a shape optimization algorithm based on immersed finite elements for solving some interface inverse problems with a fixed mesh. We consider an underlying interface forward problem modeling a certain physics in a domain formed with multiple materials; hence, the coefficients in the involved partial differential equation are discontinuous across the interface separating the materials. An interface inverse problem associated with this forward problem is to use measurements about the solution to the underlying forward problem, either on the boundary and/or in the interior of the domain, to determine the material interface. We formulate the interface inverse problem as a shape optimization problem whose objective functional depends on the interface. Both the governing partial differential equation and objective functional are discretized accurately by an immersed finite element (IFE) method on a fixed mesh independent of the interface varying in the shape optimization. Formulas for the shape sensitivities of the discretized objective function are derived within the IFE framework that can be computed accurately and efficiently through the discretized adjoint method. We demonstrate features of this IFE-based shape optimization algorithm by a group of representative interface inverse/design problems.

16th U.S. National Congress on Computational Mechanics
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Title: Learning Missing Mechanisms in a Dynamical System from a Subset of State Variable Observations

Author(s): *Teresa Portone, *Sandia National Laboratories*; Erin Acquesta, *Sandia National Laboratories*; Raj Dandekar, *Massachusetts Institute of Technology*; Chris Rackauckas, *Massachusetts Institute of Technology*; Ahmad Rushdi, *Sandia National Laboratories*;

Universal differential equations (UDEs) are an approach to scientific machine learning in which one or more universal approximators (UAs), such as neural networks (NNs) or Chebyshev expansions, is embedded within a differential equation model. The UAs are embedded such that they respect physical constraints, both through the structure of the differential equation model and possibly through additional constraints in the loss function. UDEs were shown to have success in a range of applications in Rackauckas, et al. 2020. This talk extends the work by asking the following question: “just how much data is required to accurately and automatically discover a model?” To approach this problem, we focus on a generalized compartment-based model of disease spread using UDEs. Given that in the context of disease spread it is common for only a subset of state variables to be observed, we investigate under which conditions it is possible to successfully learn the dynamics of this generalized model when observations of only a subset of the state is available. The study is carried out by generating synthetic data from an existing compartment-based model and training the generalized UDE model using combinatorial subsets of the state variables as data. The success of the training is judged in terms of the recovery of the original terms in the model used to generate the data. Depending on success of the initial study, the case in which the model used to generate the synthetic data carries more states than the UDE-based model will also be examined. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: Bridging the Gap between Atomistic Simulations and Microscale Experiments in Understanding the Dislocation-Mediated Plastic Flow and its Interactions with the Interfaces in Amorphous/Crystalline Composites

Author(s): *Thanh Phan, *Iowa State University*; Ashraf Bastawros, *Iowa State University*; Liming Xiong, *Iowa State University*;

A fundamental characterization of the interactions between dislocations and the amorphous/crystalline interfaces (ACI) is essential to understand the mechanical behavior of amorphous/crystalline composites systems. Due to the length-scale limitation, traditional atomistic simulation is inadequate to accommodate a large number of dislocations, which may suppress the large-scale features of dislocation/ACI interaction. A recently developed concurrent atomistic-continuum (CAC) approach, which unifies the atomistic and continuum description of materials, has been shown to have the capability of simulating a series of a large number of dislocations at a fractional cost of traditional atomistic simulation. However, our previous CAC approach may introduce artificial obstacle to the dislocation migration due to its coarse-grain nature. In this work, we expand our previous CAC capability by employing an adaptive meshing scheme that eliminate the artificial obstacle and assure a smooth passage for dislocation migration. With this newly developed adaptive CAC, we have: (i) simulated the effect of long-range stress or strain gradient associated with a large number of dislocations approaching the ACI on shear transformation zones (STZs) formation and percolation; and (ii) setup a tri-layer Cu/CuZr/Cu model to assess the collective behavior of dislocations and STZs in the crystalline and amorphous layers respectively. There are two major findings in this work: (a) the number of dislocations accumulated near an ACI greatly affect the critical stress at which the amorphous phases become instable; and (b) the long-ranged stress from piled up dislocations promotes the formation of STZs and the transmission of dislocations in the other crystalline layer. The knowledge to be gained from this work may provide researchers with opportunities to connect the atomistic deformation physics of an A/C-MC with its overall mechanical performance, which is currently difficult to achieve in laboratory experiments.

16th U.S. National Congress on Computational Mechanics
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Title: Bayesian Calibration of Continuum Crystal Plasticity Models

Author(s): *Thao Nguyen, *Los Alamos National Laboratory*; Devin C. Francom, *Los Alamos National Laboratory*; Saryu J. Fensin, *Los Alamos National Laboratory*; Justin W. Wilkerson, *Texas A&M University*; D.J. Luscher, *Los Alamos National Laboratory*;

Bayesian calibration is a powerful statistics-based approach to identify the optimal sets of model parameters given experimental observations and physical constraints. In this work, we extend and apply a two-stage Bayesian approach to calibrate continuum crystal plasticity models to a diverse range of experimental data. The two-stage approach is particularly suited for computationally intensive models combined with a large number of free parameters, especially when separate subsets of experimental observations are known to be independently sensitive to two possibly overlapping subsets of the free parameters. We demonstrate two variations of this Bayesian approach via application to single crystal tantalum and copper. Application to the dynamic thermomechanical behavior of single crystal body-centered cubic (BCC) tantalum uses a diverse set of experimental measurements including uniaxial stress-strain curves obtained from quasi-static and split Hopkinson pressure bar (SHPB) compression tests and velocity-time histories from single crystal flyer plate impact experiments. Multiple combinations of slip systems for tantalum are compared to identify the optimal choice of slip systems, given the targeted experimental measurements. Application to the dynamic ductile failure behavior of single crystal face-centered cubic (FCC) copper uses experimental measurements including uniaxial stress-strain curves obtained from SHPB compression tests and pullback velocities from spallation signal of plate impact tests on single crystal copper. The talk will present the calibration approach, highlights of the constitutive models, results of the calibration, and subsequent simulations of validation experiments used to assess the performance of the parameterized models.

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Title: Mixed Data Driven Fracture Mechanics

Author(s): *Trenton Kirchdoerfer, *Lawrence Livermore National Laboratory*; William Schill, *Lawrence Livermore National Laboratory*;

The paradigm of Data Driven computational mechanics aims to provide simulation methodologies capable of performing analysis without constitutive models. Such methods are highly amenable to a variety of data sources including data sources with stochastic data sources. Here we will show how these methods can mix with traditional deterministic models to provide coupled domain solutions. Demonstrations will involve include an example problem of crack propagation in bulk material. Document Number: LLNL-ABS-819156

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The CGL2 A Posteriori Error Estimator for Isogeometric Analysis

Author(s): *Trond Kvamsdal, *Norwegian University of Science and Technology*; Mukesh Kumar, *College of Charleston*; Abdullah Abdulhaque, *Norwegian University of Science and Technology*; Kjetil A. Johannessen, *SINTEF Digital*; Arne Kvarving, *SINTEF Digital*; Knut M. Okstad, *SINTEF Digital*;

The new paradigm of Isogeometric analysis, which was introduced by Thomas J. R. Hughes et al. [1], demonstrates that much is to be gained with respect to efficiency, quality and accuracy in analysis by replacing traditional Finite Elements by volumetric B-splines or NURBS elements. However, B-splines and NURBS are not flexible as they lack the possibilities of local refinement. However, the LR B-splines proposed by [2] facilitate adaptive mesh refinement [3]. Kumar, Kvamsdal and Johannessen [4] developed Superconvergent Patch Recovery (SPR) and Continuous Global L2 (CGL2) error estimation methods for Poisson problems applicable for LR B-splines. We will herein focus on the CGL2-estimator and present numerical examples illustrating that for certain problems we get a significant improved accuracy obtained for IGA-elements based on splines basis function compared to classical finite elements based on Lagrange basis functions. We will end the talk by showing the use of CGL2 for mixed IGA-elements on fluid problems. T. J. R. Hughes, J. A. Cottrell and Y. Bazilevs: Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering, 194:4135-4195, 2005. T. Dokken, T. Lyche and K. F. Pettersen: Polynomial Splines over Locally Refined Box-Partitions. Computer Aided Geometric Design, 30:331-356, 2013 K. A. Johannessen, T. Kvamsdal, and T. Dokken. Isogeometric analysis using LR B-splines. Computer Methods in Applied Mechanics and Engineering, 269:471–514, 2014. Kumar, M., Kvamsdal, T. and Johannessen, K. A. Superconvergent patch recovery and a posteriori error estimation technique in adaptive isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 316:1086-1156, 2017.

16th U.S. National Congress on Computational Mechanics
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Title: Parametric Topology Optimization and Design Space Exploration with Deep Learning and Scientific Visualization

Author(s): *Vahid Keshavarzzadeh, *The University of Utah*; Robert Kirby, *The University of Utah*; Akil Narayan, *The University of Utah*;

We present deep learning approaches for topology optimization of parametrized linear structures. In this talk we consider two scenarios for parametric topology optimization. First, we consider the problem of robust topology optimization and present an approach which approximates the high fidelity structural analysis solutions, design sensitivities and subsequently the robust design with a neural network which is trained by the data associated with the map between low resolution images and the low rank approximation coefficients in a bi- fidelity approximation setting. We verify these parametric topology optimization computations with computable error estimates and demonstrate them via illustrative numerical examples [1]. Second, we consider the problem of design space exploration and present an approach which approximates near-optimal high resolution designs with respect to varying simulation parameters, namely in the loading and boundary conditions, via a deep neural network machinery which learns building blocks of the images (or segments of the images) mainly using low resolution designs. We show this approach on benchmark topology optimization problems on 2D and 3D linear elastic and heat sink problems [2]. We also present systematic numerical studies on computational time which demonstrate the superior performance of our scientific visualization approach (while considering the training time) compared to standard SIMP approach for high-dimensional design space exploration. References [1] Keshavarzzadeh V., Kirby R.M., Narayan A. Parametric Topology Optimization with Multiresolution Finite Element Models, International Journal for Numerical Methods in Engineering, 119 (7) (2019), pp. 567-589. [2] Keshavarzzadeh V., Alirezaei M., Tasdizen T., Kirby R.M. Image-Based Multiresolution Topology Optimization Using Deep Disjunctive Normal Shape Model, Computer-Aided Design, (2021), 102947.

16th U.S. National Congress on Computational Mechanics
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Title: Phase-Field Nano- and Scale-Free Approaches to Interaction between Martensitic Phase Transformations and Plasticity

Author(s): *Valery I. Levitas, *Iowa State University*;

The following basic problems of the phase-field approach (PFA) and simulations will be presented: 1. Multivariant martensitic phase transformations (PTs): formulation of explicit requirements for phase-field potentials, nano- and microscale PFAs, large strain formu-lation, and crystal lattice instability conditions. Lattice instability conditions under the action of all six components of the stress tensor are derived and calibrated for phase transformations between Si I and Si II iteratively by combining phase-field analytic the-ory with atomistic (molecular dynamics and first principle) simulations. 2. PFA to dislocations at the nanoscale and modeling of the localized shear bands at the microscale at large strains. The nanoscale PFA satisfies similar requirements for phase-field potentials like for martensitic PTs. Localized shear bands are modeled using contact problem formulation, which is scale-free. 3. Interaction between PTs and dislocations at the nanoscale and scale-free mod-eling of coupled PTs and localized shear bands at large strains. Inheritance of disloca-tions during direct and reverse PTs is included. For similar problem formulations, a much simpler scale-free approach reproduces reasonably well results of the nanoscale approach. 4. Application to plastic strain-induced PTs at high pressure and large plastic shear strains. Our experiments on compression and torsion of various materials in rota-tional diamond anvil cell show drastic reduction (by a factor of 2 to 10, and even 100 for transformation from graphite to diamond) of transformation pressure in comparison with hydrostatic loading, as well as the appearance of new phases. These results are ex-plained and quantitatively interpreted by solving problems on nucleation of a high-pressure phase at evolving dislocation pileups followed by growth, in bicrystal and pol-ycrystal. A very strong concentrator of all components of the stress tensor at the tip of the dislocation pileup (roughly proportional to the number of dislocations) is responsi-ble for the observed phenomena. 1. Javanbakht M. and Levitas V.I. Nanoscale mechanisms for high-pressure mechano-chemistry: a phase field study. Journal of Materials Science, 2018, 53, 13343-13363. 2. Levitas V.I., Esfahani S.E., and Ghamarian I. Scale-free modeling of coupled evo-lution of discrete dislocation bands and multivariant martensitic microstructure. Physi-cal Review Letters, 2018, 121, 205701. 3. Levitas V.I. High-Pressure Phase Transformations under Severe Plastic Defor-mation by Torsion in Rotational Anvils. Material Transactions, 2019, 60, 1294-1301, invited review.

16th U.S. National Congress on Computational Mechanics
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Title: Metal Additive Manufacturing Process-Informed Topology Optimization

Author(s): *Vignesh Perumal, *Drexel University*; Alex Riensche, *University of Nebraska-Lincoln*; Reza Yavari, *University of Nebraska-Lincoln*; Lars Jacquemetton, *Sigma Labs Inc.*; Darren Beckett, *Sigma Labs Inc.*; Harold Scott Halliday, *Navajo Technical University*; Kevin Cole, *University of Nebraska-Lincoln*; Prahalada Rao, *University of Nebraska-Lincoln*; Ahmad Najafi, *Drexel University*; Antonios Kontsos, *Drexel University*;

Adapting topology optimization formulation for use in the design for metal additive manufacturing (AM) has recently raised significant research. The main reason is that heat accumulation during metal AM is a process and geometry-induced condition that is typically not taken into account in the design phase. Specifically, low heat accumulation can lead to lack of fusion whereas over accumulation to local material evaporation creating gas porosity. Furthermore, an uneven thermal accumulation profile in the printed part can lead to residual stresses and nonuniform microstructure, which deteriorate the overall AM part quality and reduce its technology readiness level. In this context, design considerations for AM rely on thermomechanical process simulations, which although they provide valuable insights on the role of manufacturing parameters and overall geometry on the print quality do not offer direct ways to adapt the target part geometry into the specific AM process used, creating in this way a disconnect between the model and the produced part. To address this critical issue, this talk presents an approach to directly couple process simulation results or in situ monitoring data of the AM process with a gradient-based topology optimization approach. To accomplish this goal, a database of thermal data is generated in the results presented by using a graph theory approach. The database is used thereafter in creating a temperature constraint which is fed into the topology optimization using a surrogate model approach. The surrogate model is used to infer the temperature and its gradient as a function of the target geometry. The upper and lower temperature bounds are set with respect to the lack of fusion and local thermal accumulation of the material. The method has been formulated and implemented for 2D Topology optimization and is currently being reformulated for handling complex 3-D geometries. The optimization results are compared with metal AM parts while preliminary efforts to also use in situ monitoring thermal data in this approach are presented.

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Title: Space-Time Meshes in Droplet Formation and Detachment During GMA Welding

Author(s): *Violeta Karyofylli, *RWTH Aachen University*; Marek Behr, *RWTH Aachen University*;

Key Words: space-time FEM, simplex, GMA welding, level-set field, enthalpy-porosity method, multi-phase flows. Gas Metal Arc Welding (GMAW) is a welding process with a plasma arc forming between the wire and the workpiece. The plasma arc temperature is high, resulting in the electrode melting and a droplet formation at the electrode tip. The droplet is afterwards detached and advected through the arc plasma to the workpiece. Gravity, surface tension, arc pressure, and non-isothermal phenomena influence the droplet formation and detachment by regulating the shape, volume, frequency, and acceleration of the detached droplet [1], although the main driving forces for the droplet detachment in GMAW are electromagnetic. Since the gradients on the droplet's boundary are very high due to the thermal and electromagnetic arc-droplet attachment processes, a fast and robust method is desired that allows for local refinement in both time and space. This application can be characterized as a multi-phase problem. The droplet formation and detachment during GMA welding is described by an incompressible non-isothermal two-phase flow, with phase-transition effects, while not considering the electromagnetic processes, in a first approach. The transient incompressible Navier-Stokes equations govern this flow since we assume that the fluids of our interest are incompressible and Newtonian, which are coupled with the heat equation. For the description of the moving droplet front, the level-set method is used. To reduce the dimensionality and, consequently, the complexity of our problem, we use an axisymmetric description of the governing equations. Regarding the phase-change phenomena, we account for them using a source-based method. A stabilized finite element method is also adapted for unstructured space-time meshes, allowing us for a space-time refinement in the vicinity of the evolving interface. The space-time method has the inherent ability to admit completely unstructured meshes with varying levels of refinement in spatial dimensions and in the time dimension, giving us the flexibility to use a type of local time-stepping for our simulations [2]. REFERENCES [1] Semenov, O. and Demchenko, V. and Krivtsun, I. and Reisgen, U. and Mokrov, O. and Zabirov, A. A dynamic model of droplet formation in GMA welding. Model. Simul. Mater. Sci. Eng. (2012) 20(4): 045003. [2] Karyofylli, V.and Wendling, L. and Make, M. and Hosters, N. and Behr, M. Simplex space-time meshes in thermally coupled two-phase flow simulations of mold filling. Comput. Fluids (2019) 192: 104261.

16th U.S. National Congress on Computational Mechanics
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Title: Output-Based Mesh Adaptation for Fluid-Structure Interaction Simulations

Author(s): *Vivek Ojha, *University of Michigan*; Krzysztof Fidkowski, *University of Michigan*; Carlos Cesnik, *University of Michigan*;

This work extends output-based mesh adaptation to the multi-physics problem of Fluid-Structure Interaction (FSI). A high-order FSI solver based on the partitioned approach is developed to tightly couple the fluid and the structural subsystems. The fluid subsystem governed by the Navier-Stokes equations is solved by an arbitrary Lagrangian–Eulerian (ALE) approach, using a discontinuous Galerkin finite-element method in space, while the structural subsystem uses a continuous Galerkin discretization [1]. Output-based methods [2] are used to estimate the errors in the output of interest due to the spatial discretization in the fluid and structural meshes. These error estimates require the coupled adjoint which is evaluated by solving the coupled unsteady adjoint equations. Adaptive indicators based on the error estimates inform the mesh adaptation procedure. The adaptive meshing procedure adapts in the spatial order of the fluid mesh, i.e., p-refinement, and in the element size in the structural mesh, i.e., h-refinement. A planar cantilevered beam and a finite plate subjected to a uniform flow are the two aeroelastic cases chosen for this study. Varied outputs of interest are chosen for this study and the effectiveness of adaptive mesh refinement is shown by comparing the convergence of coupled outputs against a uniform refinement strategy. References 1. Ojha, V., Fidkowski, K., and Cesnik, C. E. S., “High-Fidelity Coupled Fluid-Structure Interaction Simulations with Adaptive Meshing,” AIAA Aviation 2019 Forum, 2019, p. 3056. 2. Fidkowski, K. J. and Darmofal, D. L., “Review of Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics,” American Institute of Aeronautics and Astronautics Journal, Vol. 49, No. 4, 2011, pp. 673–694.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Momentum-Based Accelerated Mirror Descent Stochastic Approximation for Robust Topology Optimization under Stochastic Loads

Author(s): *Weichen Li, *University of Illinois at Urbana-Champaign*; Shelly Zhang, *University of Illinois at Urbana-Champaign*;

Robust topology optimization (RTO) improves the robustness of designs with respect to random sources in real-world structures, yet an accurate sensitivity analysis requires the solution of many systems of equations at each optimization step, leading to a high computational cost. To open up the full potential of RTO under a variety of random sources, we present a momentum-based accelerated mirror descent stochastic approximation (AC-MDSA) approach to efficiently solve RTO problems involving various types of load uncertainties. The proposed framework can perform high-quality design updates with highly noisy and biased stochastic gradients. The sample size is reduced to two (minimum for unbiased variance estimation) and shows only two samples are sufficient for evaluating stochastic gradients to obtain robust designs, thus drastically reducing the computational cost. The AC-MDSA update formula based on l1-norm with entropy function is derived, which is tailored to the geometry of the feasible domain. A momentum-based acceleration scheme is integrated to accelerate the convergence, stabilize the design evolution, and alleviate the step size sensitivity. Several 2D and 3D examples with various sizes demonstrate the effectiveness and efficiency of the proposed AC-MDSA framework to handle RTO involving various types of loading uncertainties. Comparison with other methods such as Monte Carlo method with Method of Moving Asymptotes (MMA) updates and MDSA algorithm shows that the proposed AC-MDSA is superior in stability, computational cost, and convergence speed. Although using a biased gradient estimate, the AC-MDSA algorithm successfully solves the stochastic RTO problem and produces robust designs with various levels of robustness.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Numerical Methods for Tracking Topological Changes in Multiphase Fluid-Structure Interaction Simulations

Author(s): *Wentao Ma, *Virginia Polytechnic Institute and State University*; Xuning Zhao, *Virginia Polytechnic Institute and State University*; Shafquat Islam, *Virginia Polytechnic Institute and State University*; Kevin Wang, *Virginia Polytechnic Institute and State University*;

Simulation of multiphase fluid-structure interaction problems requires accurate prediction of the motion and deformation of fluid-fluid and fluid-solid material interfaces. The occurrence of topological changes — such as the contact, merging and separation of bubbles in a liquid, the contact of a bubble or droplet with a solid structure, and the fracture in a structure — adds another level of complexity to the simulation. In this talk, we present and compare several numerical methods for interface tracking and load transferring in the context of the FIVER (FInite Volume method with Exact multi-material Riemann solvers) framework, with an emphasis on the proper handling of topological changes. The FIVER framework couples a three-dimensional multiphase finite volume compressible fluid dynamics solver and a nonlinear finite element structural dynamics solver through the construction and solution of local fluid-fluid and fluid-structure Riemann problems. Fluid-fluid interfaces are tracked by solving level set equations, while fluid-structure interfaces are tracked in an unstructured, non-interface-conforming fluid grid using an embedded boundary method. The talk will first briefly review the key model equations and algorithms implemented in the computational framework. Recent efforts on verification and validation will also be discussed. Then, the design and implementation of algorithms for detecting and tracking topological changes will be discussed. Finally, several model problems will be presented to demonstrate and assess the numerical methods, including problems related to underwater explosion and implosion, cavitation erosion, and hypervelocity impact.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Polyurethane Foam Manufacturing Models Using a FEM-Level Set-Population Balance Approach

Author(s): *Weston Ortiz, *University of New Mexico*; Rekha Rao, *Sandia National Laboratories*;

Polyurethane foams are often used in manufacturing as they offer many benefits such as low thermal conductivity, adjustable density, and manufacturability. We are developing computational models to predict useful material properties of injected polyurethane foam to improve overall design of manufactured parts. Our main focus is PMDI foam parts which are used for electronic encapsulation and lightweight structural parts. Evolution of the foam is predicted using a kinetic based model [1] modified to include a population balance equation which is solved using the quadrature method of moments (QMOM) [2]. We solve our system of equations using a stabilized finite element method. The foam-air interface is modeled using the level set method. Mesh adaptivity is employed to reduce computational costs while effectively capturing the level set interface. Results are compared against experimental data such as X-ray CT density measurements and bubble size distributions for our target polyurethane foam. [1] Rao, Rekha, Lisa Mondy, David Noble, Victor Brunini, Kevin Long, Christine Roberts, Nick Wyatt, Mathew Celina, Kyle Thompson, and James Tinsley. “Density Predictions Using a Finite Element/Level Set Model of Polyurethane Foam Expansion and Polymerization.” Computers & Fluids 175 (October 2018): 20–35. https://doi.org/10.1016/j.compfluid.2018.08.010. [2] Karimi, Mohsen, Hermes Droghetti, and Daniele L. Marchisio. “Multiscale Modeling of Expanding Polyurethane Foams via Computational Fluid Dynamics and Population Balance Equation.” Macromolecular Symposia 360, no. 1 (February 2016): 108–22. https://doi.org/10.1002/masy.201500108.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: HiDeNN: An AI Platform for Scientific and Materials Systems Innovation

Author(s): *Wing Kam Liu, *Northwestern University*;

Hierarchical Deep Learning Neural Networks-Artificial Intelligence (HiDeNN-AI) is a mechanistic artificial intelligence framework that uses machine learning methods such as active deep learning and hierarchical neural network(s) to process the input data, extract mechanistic features from it, reduce dimensions, learn hidden relationships through regression and classification, and provide a knowledge database in reduced order form that can be further exploited for design and optimization of new scientific and engineering systems. HiDeNN-AI is a multi-objective, multi-tasking, end-to-end integrated machine learning tool which serves as a platform for discovering new scientific knowledge from various sources of data through mechanistic and mathematical principles. Using this AI platform, a systematic analysis of a given system can be performed through active and transfer learning and the extracted knowledge can be transferred for a new or revised system for design and optimizations. The major innovations can be identified as: (a) a systematic approach to analyze system data and derive the scientific knowledge from it, (b) faster and accurate solution method for large scale problems, (c) design and optimization of engineering material systems, and (d) multiresolution analysis of material systems and manufacturing method. The outcome of the platform is a HiDeNN-AI tool that can be used to design the engineering process or materials system. This proposed AI platform can be applied to address the pressing global issues such as STEM education, manufacturing, health, energy, materials and can further be extended to include the education of a new generation of scientist, engineers, and STEM educators. References • L. Zhang, L. Cheng, H. Li, J. Gao, C. Yu, R. Domel, Y. Yang, S. Tang, and W. K. Liu, "Hierarchical Deep Learning Neural Networks: Finite Elements and Beyond," Comput Mech 67, 207–230 (2021). • S. Saha, Z. Gan, L. Cheng, J. Gao, O. L. Kafka, X. Xie, H. Li, M. Tajdari, A. H. Kim, and W. K. Liu, "Hierarchical Deep Neural Network (HiDeNN): An artificial intelligence (AI) framework for Computational Science and Engineering," Comput. Methods Appl. Mech. Engrg. 373 (2021) 113452. • M. Tajdari, A. Pawar, H. Li, F. Tajdari, A. Maqsood, E. Cleary, S. Saha. Y.J. Zhang, J. F. Sarwark, W. K. Liu, "Image-based Modeling for Adolescent Idiopathic Scoliosis: Mechanistic Machine Learning Analysis and Prediction" Comput. Methods Appl. Mech. Engrg. 374 (2021) 113590

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Hybridizing Superconvergent Spectral Elements and Generalized Weighted Residuals on Irregular Domains via Schwarz Alternation

Author(s): Rebecca Conley, *Saint Peters University*; *Xiangmin Jiao, *Stony Brook University*; Jacob Jones, *Stony Brook University*;

Spectral element methods, such as those using tensor-product Gauss-Lobatto points, are well known to superconverge over regular domains [3]. However, it is difficult to generalize such superconvergence properties to irregular domains due to significant challenges in mesh generation and the potential loss of accuracy due to distorted tensor-product elements. We introduce a novel hybrid method, which leverages a Schwarz alternating process to combine superconvergent spectral elements in the interior with a method of generalized weighted residuals (GWR) [2] near the boundary. Specifically, we use a GWR formulation called the extended adaptive stencil finite element method (AES-FEM) [1], which overcame element-quality dependence of Lagrange finite elements by replacing the trial functions with discontinuous generalized Lagrange basis functions while preserving the C0 continuity of the test functions. Our resulting hybrid method, called SPEAF, preserves the global superconvergence and overall efficiency of tensor-product spectral elements with Gauss-Lobatto points while being much more flexible to accommodate irregular domains by using hybrid meshes with simplicial (such as triangular and tetrahedral) and transitional (such as pyramidal) elements near irregular boundaries. We present numerical results in solving parabolic partial differential equations in 2-D and 3-D and demonstrate the O(h^{p+2}) convergence rate in l^2 norm and O(h^{p+1}) in H^1 norm with degree-p spectral elements in the interior for even-degree-p, matching the superconvergence of spectral elements and exceeding the convergence rates of equidistant finite elements by one order, while approximately preserving their efficiencies. We describe the simplified mesh-generation process of SPEAF with sublinear time complexity and compare the accuracy and efficiency of SPEAF with standard Lagrange finite elements and spectral elements. References [1] R. Conley, T. J. Delaney, and X. Jiao. Overcoming element quality dependence of finite elements with adaptive extended stencil FEM (AES-FEM). Int. J. Numer. Meth. Eng., 108(9):1054–1085, 2016. [2] R. Conley, T. J. Delaney, and X. Jiao. A hybrid method and unified analysis of generalized finite differences and Lagrange finite elements.J. Comput. Appl. Math., 376:112862, 2020. [3] M. Křižek and P. Neittaanmäki. Bibliography on superconvergence. In Finite Element Methods: Superconvergence, Post-processing, and A Posteriori Estimates, pages 315–348. CRC Press, 1998

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Variational Interface-Preserving and Conservative Phase-Field Method for the Surface Tension Effect in Two-Phase Flows

Author(s): *Xiaoyu Mao, *University of British Columbia*; Vaibhav Joshi, *University of British Columbia*; Rajeev Jaiman, *University of British Columbia*;

We present a finite element based variational interface-preserving and conservative phase-field formulation for the modeling of incompressible two-phase flows with surface tension dynamics. The preservation of the hyperbolic tangent interface profile of the convective Allen-Cahn phase-field formulation relies on a novel time-dependent mobility model. The mobility coefficient is adjusted adaptively as a function of gradients of the velocity and the order parameter in the diffuse interface region in such a way that the free energy minimization properly opposes the convective distortion. The ratio of the convective distortion to the free energy minimization is termed as the convective distortion parameter, which characterizes the deviation of the diffuse interface profile from the hyperbolic tangent shape due to the convection effect. In the phase-field formulation, the mass conservation is achieved by enforcing a Lagrange multiplier with both temporal and spatial dependence on the phase-field function. We integrate the interface-preserving and conservative phase field formulation with the incompressible Navier-Stokes equations and the continuum surface tension force model for the simulation of incompressible two-phase flows. A positivity preserving scheme designed for the boundedness and stability of the solution is employed for the variational discretization using unstructured finite elements. We examine the convergence and accuracy of the Allen-Cahn phase-field solver through a generic one-dimensional bistable diffusion-reaction system in a stretching flow. We quantify and systematically assess the relative interface thickness error and the relative surface tension force error with respect to the convective distortion parameter. Two- and three-dimensional rising bubble cases are further simulated to examine the effectiveness of the proposed model on the volume-preserving mean curvature flow and the interface-preserving capability. Finally, we demonstrate the applicability of the proposed model for a complex case of two bubbles rising and merging with a free surface, which includes complex topological changes and the surface tension dynamics using unstructured finite elements.

16th U.S. National Congress on Computational Mechanics
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Title: A Study of Wave Propagation of Coupling Nonlocal and Local Elasticities

Author(s): *Xingjie Li, *University of North Carolina at Charlotte*; Hayden Pecoraro, *University of North Carolina at Charlotte*; Pablo Seleson, *Oak Ridge National Laboratory*; Kelsey Wells, *University of Nebraska-Lincoln*;

We study the dispersion relations of two consistent nonlocal-to-local coupling methods in 1D: (1) the quasi-nonlocal coupling and (2) the blending-based coupling. We analyze the dispersion relations and the reflection coefficients on the transitional regions for both methods, respectively. Both coupling methods are rigorously proved that the imaginary artifacts of their dispersion relations due to the coupling will disappear with first order speed as the horizon size goes to zero. In addition, we employ a finite difference numerical discretizations and find that the artificial imaginary parts of the dispersion relation and the reflection coefficients of the blending-based coupling are all cases smaller than those of the quasi-nonlocal coupling on the transitional region, hence, the waves are preserved better by the blending-based method. Several numerical tests are performed to confirm these theoretical findings. This is a joint work with Hayden Pecoraro, Kelsey Wells and Pablo Seleson.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physics-informed Model-Based Deep Reinforcement Learning for Dynamic Control

Author(s): *Xinyang Liu, *University of Notre Dame*; Jian-xun Wang, *University of Notre Dame*;

Model-based reinforcement learning (MBRL) is believed to have much higher sample efficiency compared to traditional model-free reinforcement learning by learning a world model of the environment. However, the performance of MBRL highly relies on the quality of the learned model, which is usually built in a black-box manner and may have poor predictive accuracy outside of the data distribution. The deficiencies of the learned model may prevent the learned policy from being fully optimized. Although some uncertainty analysis-based remedies have been proposed to alleviate this issue, model-bias still poses a great challenge for MBRL, particularly when interactions with the environment are costly and limited. In this work, we propose to leverage the prior knowledge of underlying physics of the environment, where the governing laws are known or partially known. In particular, we developed a physics-informed MBRL in Dyna-style formulation, where governing equations and physical constraints are utilized to inform the model learning and policy search. By incorporating the prior information of the environment, the quality of the learned model can be notably improved, while the required interactions with the environment are significantly reduced, leading to better sample efficiency and learning performance. The effectiveness and merit have been demonstrated over a handful of classic control problems, where the environments are governed by canonical ordinary/partial differential equations.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of 2D Heat Exchangers for Additive Manufacturing Based on Isogeometric Analysis and Machine Learning

Author(s): *Xuan Liang, *Carnegie Mellon University*; Angran Li, *Carnegie Mellon University*; Anthony Rollett, *Carnegie Mellon University*; Yongjie Zhang, *Carnegie Mellon University*;

Heat exchangers (HXs) have gained increasing attention due to the intensive demand of performance improving and energy saving for various equipment and machines. As a natural application, topology optimization has been involved in the structural design of HXs aiming at improving heat exchange performance. In this work, a topology optimization framework is developed to maximize the heat exchange between two fluids with different temperatures in 2D cross-flow HXs. Isogeometric analysis (IGA) is employed to solve the steady-state Navier-Stokes and heat convection-diffusion equations to evaluate the heat exchange amount in the entire domain of the HXs. Computing parallelization is also incorporated to ensure fast solution of the governing equations. Control points involved in IGA are defined as the design variables for the topology optimization. In order to implement the optimization process, genetic programming is selected to drive evolution of the 2D design domain. In addition, to facilitate additive manufacturing (AM) of the HXs, machine learning is employed to minimize unwanted geometrical features such as overhang regions for the HXs so that layer-wise AM fabrication process is more likely to succeed. Numerical examples show that the heat exchange performance in terms of kW per unit weight can be greatly increased (potentially by ~50 %) between the flow inlet and outlet of the 2D cross-flow HXs based on the proposed topology optimization framework. Moreover, good printability of the designed HXs can be ensured with respect to the AM processing.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multi-Fidelity Bayesian Neural Networks for Inverse PDE Problems with Noisy Data

Author(s): *Xuhui Meng, *Brown University*; George Karniadakis, *Brown University*;

We propose a new class of Bayesian neural networks (BNNs) that can be trained using noisy data of variable fidelity, and we apply them to learn function approximations as well as to solve inverse problems based on partial differential equations (PDEs). These multi-fidelity BNNs consist of three neural networks: The first is a fully connected neural network, which is trained following the maximum a posteriori probability (MAP) method to fit the low-fidelity data; the second is a Bayesian neural network employed to capture the cross-correlation with uncertainty quantification between the low- and high-fidelity data; and the last one is the physics-informed neural network, which encodes the physical laws described by PDEs. For the training of the last two neural networks, we first employ the mean-field variational inference (VI) to maximize the evidence lower bound (ELBO) to obtain informative prior distributions for the hyperparameters in the BNNs, and subsequently we use the Hamiltonian Monte Carlo method to estimate accurately the posterior distributions for the corresponding hyperparameters. We demonstrate the accuracy of the present method using synthetic data as well as real measurements. Specifically, we first approximate a one- and four-dimensional function, and then infer the reaction rates in one- and two-dimensional diffusion-reaction systems. Moreover, we infer the sea surface temperature (SST) in the Massachusetts and Cape Cod Bays using satellite images and in-situ measurements. Taken together, our results demonstrate that the present method can capture both linear and nonlinear correlation between the low- and high-fidelity data adaptively, identify unknown parameters in PDEs, and quantify uncertainties in predictions, given a few scattered noisy high-fidelity data. Finally, we demonstrate that we can effectively and efficiently reduce the uncertainties and hence enhance the prediction accuracy with an active learning approach, using as examples a specific one-dimensional function approximation and an inverse PDE problem.

16th U.S. National Congress on Computational Mechanics
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Title: A Rate-Dependent Peridynamic Optimization Model for Dynamic Mechanical Behavior of Ceramic Materials

Author(s): *Yaxun Liu, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*; Qiwen Liu, *Wuhan University of Technology*; Hai Mei, *Wuhan University of Technology*;

As a mathematical expression describing the dynamic mechanical behavior of ceramics, the constitutive model plays an indispensable role in the numerical simulation of ceramic materials. The existing constitutive model can describe the dynamic mechanical behavior of ceramic materials under impact load, but the Poisson’s ratio predicted by the constitutive model is 0.25 under three-dimensional condition, and most of the known ceramics are not 0.25. This difference makes the original constitutive model unable to study many different types of ceramics. Based on the existing constitutive model, this study uses the description method of tangential bond force and considers the effect of the bond on rotation, so that the model breaks the limit of Poisson's ratio and can accurately predict different types of ceramic materials (SiC, B4C, etc.). The basic mechanical properties include Poisson’s ratio, and a new damage judgment criterion is added, that is the comprehensive damage judgment of tensile-shear and compressive-shear failures, and the rate-dependent bond-based peridynamics constitutive model is improved, so as to realize the optimization of the original model. The improved constitutive model was used to conduct several numerical experiments, including frontal impact, side impact, and uniaxial compression experiments. The simulation results were compared with the classical finite element results and experimental results, and it was found that the optimized model can accurately simulate different kinds of ceramics. The damage behavior of materials verifies the effectiveness of the optimized model in describing the damage behavior of ceramic materials.

16th U.S. National Congress on Computational Mechanics
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Title: Efficient Hyper-Reduced Order Model for Additive Manufacturing Thermal Fluid Analysis

Author(s): *Ye Lu, *Northwestern University*; Kevontrez Jones, *Northwestern University*; Zhengtao Gan, *Northwestern University*; Wing Liu, *Northwestern University*;

The thermal fluid coupled analysis is essential to enable an accurate temperature prediction in additive manufacturing. However, numerical simulations of this type are time-consuming, due to the high non-linearity, the underlying large mesh size, and the small time step constraints. In this work, we will present a possibility for accelerating these simulations via model order reduction techniques. The method of focus is the hyper-reduction method [1] which was initially proposed to tackle the nonlinearity difficulties associated with standard model reduction methods. We try to extend this method to additive manufacturing related problems and discuss the underlying challenges with standard snapshot-based reduced order modeling. In particular, we propose a novel adaptation strategy for the reduced basis and reduced domain for the hyper-reduced order model. Some representative 3D examples of additive manufacturing models, including single-track and multi-track cases, will be presented [2]. This talk will be closed by some potential applications and the coupling with other data-driven methods [3]. References: [1] D. Ryckelynck, Hyper-reduction of mechanical models involving internal variables, Internat. J. Numer. Methods Engrg. 77 (1) (2009) [2] Lu, Y., Jones, K. K., Gan, Z., Liu, W. K. Adaptive hyper reduction for additive manufacturing thermal fluid analysis. Computer Methods in Applied Mechanics and Engineering, (2020). [3] Lu, Y., Blal, N., Gravouil, A. Adaptive sparse grid based HOPGD: Toward a nonintrusive strategy for constructing space-time welding computational vademecum. International Journal for Numerical Methods in Engineering, (2018).

16th U.S. National Congress on Computational Mechanics
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Title: Precise and Efficient Time Integration Method for Linear Dynamics Systems

Author(s): *Yi Ji, *Beihang University*; Yufeng Xing, *Beihang University*;

Time-dependent hyperbolic equations are widely encountered in engineering. Accurate and fast simulation for such equations has attracted continuous attention. Time integration methods are a powerful numerical tool in solving transient responses of dynamics systems, and can be classified into explicit methods and implicit methods. Although the implicit methods can be designed to be unconditionally stable, indicating the arbitrary selection of time step size, achieving high accuracy by conventional time integration methods requires small time steps, calling for expensive computations. To address this issue, the present authors constructed, in 2018, a highly precise time integration method (HPTIM) [1] where a precise integrated amplification matrix was created, and a 2m algorithm and a method of storing incremental matrix were used to improve efficiency and avoid rounding error. Numerical experiments showed that HPTIM can get higher precision than existing methods. But HPTIM is only suitable for solving linear time-invariant homogenous equations. For using HPTIM, nonhomogeneous equations need to be transformed into homogeneous ones, expanding the sizes of structural matrices. The expanded stiffness matrices are always unsymmetrical, so the consistent stability needs to be examined. For improving HPTIM, this paper proposes a new strategy of developing precise and efficient time integration methods for linear structural dynamics systems. In this work, an unconditionally stable single-step method with controllable dissipation is proposed first, then its precise integrated amplification matrix is created. Like in HPTIM, to reduce computations and rounding error, the 2m algorithm and the method of storing incremental matrix are also considered. Different from HPTIM, the new method can directly solve nonhomogeneous equations, since the external load terms are precisely computed by the Gaussian-Legendre quadrature. The new method is unconditionally stable, and its degree of dissipation is exactly controlled by ??, the spectral radius ranging from 0 to 1 at high-frequency limit. For the case ??=1, the new method is symplectic, so it is suggested for conservative systems. For the case 0???<1, the new one precisely preserve essential low-frequency modes and completely damp out unexpected high-frequency information. Compared to some advanced methods, the new method enjoys advantages both in precision and efficiency. Keywords: high precision and efficiency; integrated amplification matrix; Gaussian-Legendre quadrature; structural dynamics; unconditional stability; controllable dissipation [1] Xing YF., Zhang HM., Wang ZK. Highly precise time integration method for linear structural dynamics analysis. Int. J. Numer. Methods Eng. 2018; DOI: 10.1002/nme.5934

16th U.S. National Congress on Computational Mechanics
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Title: Entropy Stable Modal Discontinuous Galerkin Schemes and Wall Boundary Conditions for the Compressible Navier-Stokes Equations

Author(s): *Yimin Lin, *Rice University*; Jesse Chan, *Rice University*; Timothy Warburton, *Virginia Polytechnic Institute and State University*;

Entropy stable schemes ensure that physically meaningful numerical solutions also satisfy a semi-discrete entropy inequality under appropriate boundary conditions. In this work, we describe a discretization of viscous terms in the compressible Navier-Stokes equations which enables simpler methods for imposing entropy stable no-slip wall boundary conditions for discontinuous Galerkin (DG) discretizations. Numerical results confirm the robustness and accuracy of the proposed approaches.

16th U.S. National Congress on Computational Mechanics
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Title: Understanding Nanoparticle Transport in Human Vasculature Through Large-Scale Fluid-Structure Interaction Simulations

Author(s): *Ying Li, *University of Connecticut*; Huilin Ye, *University of Connecticut*; Zhiqiang Shen, *University of Connecticut*;

A large number of nanoparticles (NPs) have been raised for diverse biomedical applications and some of them have shown great potential in treatment and imaging of diseases. Design of NPs is essential for delivery efficacy due to a number of biophysical barriers, which prevents the circulation of NPs in vascular flow and their accumulation at tumor sites. The physiochemical properties of NPs, so-called ‘4S’ parameters, such as size, shape, stiffness and surface functionalization, play crucial roles in their life journey to be delivered to tumor sites. NPs can be modified in various ways to extend their blood circulation time and avoid their clearance by phagocytosis, and efficiently diffuse into tumor cells. Nevertheless, there are limited understandings on the blood circulation, near-wall adhesion and tumor transmigration behaviors of NPs under the influence of realistic physiological condition. In this talk, I will highlight a recently in-house developed fluid-structure interaction simulation package based on Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). We have implemented a parallelized lattice Boltzmann simulator within LAMMPS to handle the fluid flow simulation. The deformation and motion of red blood cells (RBCs) and NPs have been resolved by the spring-network models embedded within LAMMPS framework. These two components are seamlessly integrated within LAMMPS through immersed boundary method. The scaling performance and speedup test further confirm the high efficiency and robustness of proposed computational method. With this method, we have computationally explored the following phenomena: 1) anomalous vascular dynamics of nanoworms within blood flow; 2) adhesion effect on margination of elastic micro-particles; and 3) motion of magnetic particles under external magnetic field. In the end, I will discuss the future opportunity to extend the current simulation package for multiple different HPC platforms, such as Intel Xeon Phi, Knights Landing (KNL) and GPU (Pascal).

16th U.S. National Congress on Computational Mechanics
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Title: Coarse-Grained Atomistic Simulation of Phase Transformation in Materials Under General Stresses: Methodology, Algorithm, and Applications

Author(s): *Yipeng Peng, *Iowa State University*; Rigelesaiyin Ji, *Iowa State University*; Thanh Phan, *Iowa State University*; Wei Gao, *The University of Texas at San Antonio*; Valery I. Levitas, *Iowa State University*; Liming Xiong, *Iowa State University*;

The phase transformations (PT) process in multiphase materials under deformation by general stress is multiscale in nature. It nucleates at the atomic scale and grows up to the micrometer level and even above. Such a wide range of length scale is obviously within the reach of neither a fully atomistic model nor a traditional continuum approach. A multiscale computational approach that can capture not only the atomic-level phase nucleation but also the micrometer-level phase growth is thus in need. Here we argue that our previous coarse-grained (CG) atomistic model is one such approach, if not the best because it: (1) unifies the atomistic and continuum descriptions of PTs in one single framework; and (2) enables a smooth assage of PTs from the atomistic to the continuum domain. Through equipping it with a phonon density states-guided finite temperature algorithm, in this work, we perform a set of CG simulations of PTs in a prototype multiphase materials under deformation. Results show that our CG models successfully capture the PT processes when the material is subjected to a combined compression (σ) and shear (τ). The critical σ and τ for the onset of the PT fit into a straight line, for which an instability criterion based on the concept of transformation work is then formulated. This criterion can be used for predicting the PTs in multiphase materials under a general stress loading at the continuum level. The effects of the sample size, image stress, temperature, and also the mesh size on the PTs are systematically studied. The CG-simulation-predicted PT processes are found to be in good agreement with that from fully atomistic simulations. This work will significantly expand the applicability of our previous concurrent atomistic-continuum (CAC) method for predicting the inelastic behavior in multiphase materials subjected to complex mechanical loadings.

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Title: In Silico Experiments of Bone Remodeling Towards Predicting Drug Treatment of Bone Diseases

Author(s): *Yoshitaka Kameo, *Kyoto University*; Yuki Miya, *Kyoto University*; Taiji Adachi, *Kyoto University*;

Bone structure and function are maintained by well-regulated bone remodeling depending on the surrounding mechanical and biochemical environment. An imbalance between bone resorption and formation due to disuse or sex hormone aberrations causes metabolic bone diseases, such as osteoporosis. Even though the underlying molecular and cellular mechanisms of bone metabolism system are now being clarified, the complexity of intercellular signaling makes it difficult to predict the changes in bone morphology during metabolic bone diseases and their drug treatment. In this study, we have developed a novel in silico experimental platform based on image-based finite element analysis to synthetically understand the mechanism of bone remodeling by linking microscopic molecular/cellular interactions to macroscopic tissue/organ adaptations [1]. In order to show the validity of the proposed platform, we conducted in silico experiments to investigate the morphological changes of cancellous bone in a mouse distal femur subjected to compressive loading, using an image-based model reconstructed from micro-computed tomography. First, we reproduced osteoporosis due to unloading, which is characterized by acute bone erosion. Then, we reproduced osteoporosis due to overexpression of RANKL, a key protein that can induce osteoclastogenesis, which is characterized by chronic bone loss. These results were qualitatively in good agreement with previous experimental data. As a clinical application of the proposed platform, we conducted in silico medication experiments to predict the therapeutic effects of four drugs (bisphosphonate, anti-RANKL, anti-sclerostin, and Sema3A) against osteoporosis due to RANKL overexpression. Bisphosphonate and anti-RANKL only inhibit bone resorption, while anti-sclerostin and Sema3A have dual effects of inhibiting bone resorption and promoting bone formation. Quantitative comparison of the therapeutic effects of four drugs showed that drugs that promote bone formation but inhibit bone resorption, such as anti-sclerostin and Sema3A, are more effective in improving both bone quantity and quality. The data suggest that in silico medication experiments may potentially provide a powerful way for comprehensive drug assessment and formulation of effective treatment regimens. Taken together, the developed in silico experimental platform enables to investigate spatial and temporal behavior of bone remodeling regulated by complex mechano-biochemical couplings. We anticipate that these in silico experiments will significantly accelerate research into bone metabolism and remodeling. This work was supported by AMED-CREST (Mechanobiology), Japan. [1] Y. Kameo, Y. Miya, M. Hayashi, T. Nakashima, T. Adachi, In silico experiments of bone remodeling explore metabolic diseases and their drug treatment. Sci. Adv. 6, eaax0938, (2020).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Mesh Generator for Storm Surge-Rainfall Events

Author(s): *Younghun Kang, *The Ohio State University*; Ethan Kubatko, *The Ohio State University*;

Many operational storm surge models, such as ADCIRC (ADvanced CIRculation) and DG-SWEM (Discontinuous Galerkin Shallow Water Equation Model), have been developed to account for a number of factors (e.g., wind, atmospheric pressure, and tides) that influence flooding associated with the storm. However, the impact of rainfall has not yet been included in these models, which can, in many cases, have a large impact on the resulting flooding. To address this deficiency, an efficient multidimensional model of overland/open-channel flows, DG-SAKE, is coupled to DG-SWEM. In this study, as a preliminary step for this coupling, a mesh generator is developed that focuses on accurate and efficient representation of coastal floodplains. One of the main features of the mesh generator is the ability to approximate narrow channels by 1D finite elements in order to preserve channel networks with relatively low computational overhead. Numerical studies are performed on the Lower Niches River in Texas, where results from the coupled approach are compared to results obtained from ADCIRC and DG-SWEM.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Analysis of Semi- and Quarter-Elliptical Fatigue Crack Propagation

Author(s): *Yozo Mikata, *Fluor Corporation*;

Introduction The fatigue crack propagation of a 3D crack is investigated under a uniform loading. As for crack geometry, a semi-elliptical crack and a quarter-elliptical crack are considered. The focus of this paper is to solve a pair of coupled differential equations derived from Paris law [1]. Stress intensity factors are approximate. The approximate stress intensity factors used for semi- and quarter-elliptical cracks are based on empirical equations given by Newman and Raju [2,3]. Mathematical formulations The governing equations for fatigue crack propagation of semi- and quarter-elliptical cracks are derived from Paris law. By introducing an intermediate special function, it is shown that the governing equation for both cases can be exactly solved. As an application of the mathematical result, numerical examples will be shown. Conclusion Exact solutions are obtained for fatigue crack propagation of semi- and quarter-elliptical cracks based on the assumption that the crack shape stays self-similar (semi-elliptical or quarter-elliptical). References 1. Paris, P.C., Erdogan, F. (1963). “Critical Analysis of Crack Propagation Laws,” Journal of Basic Engineering, Vol. 85, pp. 528-534. 2. Newman, J.C., Raju, I.C. (1981). “An Empirical Stress-Intensity Factor Equation for the Surface Crack,” Engineering Fracture Mechanics, Vol. 15, pp. 185-192. 3. Anderson, T.L. (1995). Fracture Mechanics, Second Edition, CRC Press.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Using Poro-Elasticity to Model the Large Deformation of Tissue During Subcutaneous Injection

Author(s): *Yu Leng, *Purdue University*; Mario de Lucio, *Purdue University*; Hector Gomez, *Purdue University*;

Subcutaneous injection of therapeutic monoclonal antibodies (mAbs) has recently attracted unprecedented interests in the pharmaceutical industry. The drug transport in the tissue and mechanical response of the tissue after injection are not yet well-understood. We are motivated to study the subcutaneous injection using poro-elasticity. We first investigate the model assumption of linear poro-elasticity using numerical solutions. In the case of small permeability, linear model is not adequate to account for the large deformation of the tissue due to injection. We then adopt a nonlinear poro-elastic model combined with the Ogden hyperelastic constitutive relation. For large deformation, numerical solutions of the nonlinear model differ significantly from that of the linear model, especially near the injection site. The calculation is enabled using the fixed-stress iterative scheme for nonlinear poro-elastic models by splitting the strain-energy function into isochoric and volumetric contributions.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Adaptive Isogeometric Analysis Collocation Method with Higher Order PHT-Splines

Author(s): *Yue Jia, *Northwestern Polytechnical University, China*; Cosmin Anitescu, *Bauhaus University Weimar*; Yongjie Zhang, *Carnegie Mellon University*; Timon Rabczuk, *Bauhaus University Weimar*;

We extend the Gaussian isogeometric analysis (IGA) collocation method [1] to arbitrary higher order polynomial degrees. The current IGA collocation method applies a new hierarchical basis over T-meshes (PHT-splines), which take the advantage of the tensor product structure avoiding the decay phenomenon appears in the original PHT basis [2]. The improved method collocates at Gaussian points [3] which are the superconvergent points for the new PHT elements. Based on the new PHT basis, the current collocation method can be extended to arbitrary higher order approximation. The local refinement strategy is driven by a recovery-based error estimator which invokes computing an improved approximation without knowledge of the exact solution. The proposed collocation method can obtain the optimal convergent rates which are also compared with the IGA Galerkin method and the Greville-abscissae collocation method. Key Words: Isogeometric analysis, collocation, PHT-splines, Gaussian collocation points. REFERENCES [1] Y. Jia, C. Anitescu, Y. Zhang and T. Rabczuk, An adaptive isogeometric analysis collocation method with a recovery-based error estimator. Computer Methods in Applied Mechanics and Engineering, Vol. 345, pp. 52-74, 2019. [2] J. Deng, C. Fa, X. Li, C. Hu, W. Tong, Z. Yang and Y. Feng, Polynomial splines over hierarchical T-meshes. Graphical Models, Vol. 70, pp. 76-86, 2008. [3] C. De Boor and B. Swartz, Collocation at Gaussian Points. SIAM Journal on Numerical Analysis, Vol. 10, pp. 582-606, 1973.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multiscale Modeling of Fibrin Through Neural Network Homogenization of Discrete Fiber Networks

Author(s): *Yue Leng, *Purdue University*; Sarah Calve, *University of Colorado Boulder*; Adrian Tepole, *Purdue University*;

Fibrin is an important biopolymer with crucial roles in wound healing and thrombus formation. Due to its fibrous structure, fibrin's mechanical behavior at the macroscale depends on the microscale fiber network mechanics. Accordingly, accurate modeling of fibrin can be achieved by multiscale models, with discrete fibrin network models coupled to a nonlinear continuum mechanics framework [1]. Current multiscale strategies are computationally inefficient. Machine learning has emerged as an alternative approach to replace detailed physics-based models by inexpensive yet accurate metamodels [2]. Here we use fully connected neural networks (FCNN) trained on discrete fiber network data to predict the macroscale behavior of fibrin gels [3]. The significant speed up from the FCNN enables an efficient multiscale coupling. We showcase this by programming the FCNN into a user subroutine UMAT for the finite element software Abaqus and running representative examples of gels deforming at the macroscale. To train the FCNN, 1100 representative volume elements (RVEs) were generated and subjected to a combination of biaxial deformations. Each RVE modeled the behavior of a discrete fiber network. The energy and stresses on the RVE were obtained for every simulation. Based on the assumption that the macroscale response of fibrin is hyperelastic, we posed the existence of an unknown strain energy for the macroscale response. By using the FCNN, we were able to capture the macroscale based on the RVE data without ever having an analytical function for the strain energy. During FCNN training, the loss function was modified in order to impose meaningful constraints on the strain energy: symmetry and positive definiteness of its Hessian. Lastly, the inputs to the FCNN were the strain invariants from the deformations imposed on the RVEs. The invariant formulation allowed us to implement the FCNN as a material model in a UMAT subroutine. The FCNN was able to capture the nonlinear response of the RVEs. The FCNN offered significant speedup compared to the RVE problem, and thus enabled an efficient multiscale coupling by coding the FCNN into the finite element software Abaqus. Our work is an important step towards integration of machine learning and computational mechanics to improve modeling and understanding of biological materials. Acknowledgements: NSF grant 1911346-CMMI to PIs Tepole and Calve and Bilsland Dissertation Fellowship to Dr. Leng. [1] Aghvami, et al. J Biomech Eng. 2013,135(7). [2] Vlassis, et al. Comput Methods Appl Mech Eng. 2020, 371. [3] Leng, Calve, Tepole, 2021. arXiv preprint arXiv:2101.11712.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling the Fracture Behavior of Fiber Networks Using Discrete Element Method

Author(s): *Yujun Li, *Northwestern Polytechnical University*; Jiao Huang, *Northwestern Polytechnical University*; Xing Chen, *Northwestern Polytechnical University*;

Fiber network materials have been used in a large variety of applications due to their unique properties, such as high porosity, flexibility, and toughness. Few studies have investigated the influence of fiber networks' microstructure on the fracture behavior in any systematic way. This study aims to develop an efficient approach toward addressing this issue by simulating the 3D structure of fiber networks. The first step for assessing fiber networks' mechanical response is the generation of virtual fibrous architectures. In this work, a physics-based deposition technique was used to deposit fibers from the top of the cell in an iterative manner until they entered contact with other fibers or the plate surface. Instead of fiber architectures consisting of straight fibers considered in most of the literature, a random polygonal tracks representation for describing single fibers was employed in multivariate time series to achieve virtual networks with curved fibers configuration. It could mimic the typical in-plane course of fibers that have been extracted from SEM images. To obtain a configuration where fibers cannot overlap other fibers, the discrete element method (DEM) was used for contact computation, with external forces applied on fibers to achieve a controllable bending level. The model considered fibers' practical mechanical properties by discretizing each fiber as an array of identical spheres connected via springs and dampers. The elastic deformation of a single fiber was simulated and validated against elastic beam theories. Consequently, the fibers could experience bending and axial extension/compression during the deposition process. In the second step, uniaxial tension simulations were conducted on generated fiber networks with DEM models. The above spring-damper algorithm was further extended to incorporate the single fiber's fracture properties by applying a crack criterion for coupled tension and bending cases. Additionally, the fiber-fiber bond broken when its traction load exceeded a critical value. In this way, fracturing fiber networks of different void volume fractions, fiber diameters, and fiber orientations were statistically analyzed and analyzed in detail. The simulation results fitted well with the measured data from polyvinylidene difluoride (PVDF) fiber networks. It was mainly found that both strength and toughness significantly increase simultaneously as the mean diameter of fiber decreases.

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Title: Time Multi-Scale Implicit/Explicit Co-Simulation Method for Extreme Loadings on Safety Elements

Author(s): *Yvan Le Nôtre, *Université Lyon - INSA Lyon*; Michael Brun, *Université de Lorraine, Arts et Métiers Paris Tech, CNRS, LEM3, Metz F-57000, France*; Clément Grenat, *Framatome*; Anthony Gravouil, *Université Lyon - INSA Lyon*;

Due to the increasing difficulty in components justification, Framatome is developing more realistic dynamical models with 3D finite element methods. These models allow more complex studies to be performed and a better representation of local phenomena such as friction and impacts. They are well suited for nonlinear resolution of vibration problems with implicit solvers, but are less effective regarding stiff dynamical problems such as impact, friction or wave propagation. In the dynamical response of such problems, several time scales are coexisting. Especially, the time scales associated with the stiff phenomena are very small. To well simulate such dynamical response using explicit time integration scheme, a reduction of the time step to fit the smaller time scale is necessary, increasing significantly the compution time. In this work, a new adapted method to deal with localized stiff dynamical phenomenon called “time multi-scale implicit/explicit co-simulation” will be presented. The new method (based on [GCB15]) consists in dividing a structure into several sub-domains solved with their own time integration scheme and time step. Indeed, subdomains experiencing stiff dynamical phenomena can be finely meshed and solved using the appropriate time integration scheme and time step, while the rest of the structure can have a coarser mesh dealt with a larger time step [Cha14], [Fek17]. Such development strategy for 3D modelling results in the reduction of computation time as well as in the improvement of physical representativeness. A proof of concept of the new co-simulation method will be presented on relevant examples to demonstrate its industrial usefulness References [Cha14] Teddy Chantrait. Approche multi-échelle en espace et en temps pour la prévision des endommagements dans les structures composites soumises à un impact de faible énergie. page 170, 2014. [Fek17] Fatima-Ezzahra Fekak. Etude de la réponse dynamique des ponts roulants soumis à des chocs multiples pendant un séisme: Co-simulation implicite / explicite multi-échelle en temps pour la dynamique du contact. page 169, 2017. [GCB15] A. Gravouil, A. Combescure, and M. Brun. Heterogeneous asynchronous time integrators for computational structural dynamics: Heterogeneous asynchronous time integrators. International Journal for Numerical Methods in Engineering, 102(3-4):202–232, April 2015.

16th U.S. National Congress on Computational Mechanics
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Title: Constitutive Model of Erythrocyte Membranes with Distributions of Spectrin Orientations and Lengths

Author(s): *Zhangli Peng, *University of Illinois at Chicago*; Zhe Feng, *University of Illinois at Chicago*; Richard Waugh, *University of Rochester*;

We present an analytical hyperelastic constitutive model of the red blood cell (erythrocyte) membrane based on recently improved characterizations of density and microscopic structure of its spectrin network from proteomics and cryo-electron tomography. The model includes distributions of both orientations and natural lengths of spectrin and updated copy numbers of proteins. By applying finite deformation to the spectrin network, we obtain the total free energy and stresses in terms of invariants of shear and area deformation. We generalize an expression of the initial shear modulus, which is independent of the number of molecular orientations within the network and also derive a simplified version of the model.We apply the model and its simplified version to analyze micropipette aspiration computationally and analytically and explore the effect of local cytoskeletal density change. We also explore the discrepancies among shear modulus values measured using different experimental techniques reported in the literature. We find that the model exhibits hardening behavior and can explain many of these discrepancies. Moreover, we find that the distribution of natural lengths plays a crucial role in the hardening behavior when the correct copy numbers of proteins are used. The initial shear modulus values we obtain using our current model (5.9–15.6 pN/um) are close to the early estimates (6–9 pN/um). This new, to our knowledge, constitutive model establishes a direct connection between the molecular structure of spectrin networks and constitutive laws and also defines a new picture of a much denser spectrin network than assumed in prior studies.

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Title: Parareal Physics-Informed Neural Network for Solving Time-Dependent PDEs

Author(s): *Zhen Li, *Clemson University*; Xuhui Meng, *Brown University*; George Karniadakis, *Brown University*;

Physics-informed neural networks (PINNs) encode physical conservation laws and prior physical knowledge into the neural networks, ensuring the correct physics is represented accurately while alleviating the need for supervised learning to a great degree. While effective for relatively short-term time integration, when long time integration of the time-dependent PDEs is sought, the time–space domain may become arbitrarily large and hence training of the neural network may become prohibitively expensive. To this end, we develop a parareal physics-informed neural network (PPINN), hence decomposing a long-time problem into many independent short-time problems supervised by an inexpensive/fast coarse-grained (CG) solver. In particular, the serial CG solver is designed to provide approximate predictions of the solution at discrete times, while initiate many fine PINNs simultaneously to correct the solution iteratively. There is a two-fold benefit from training PINNs with small-data sets rather than working on a large-data set directly, i.e., training of individual PINNs with small-data is much faster, while training the fine PINNs can be readily parallelized. Consequently, compared to the original PINN approach, the proposed PPINN approach may achieve a significant speed-up for long-time integration of PDEs, assuming that the CG solver is fast and can provide reasonable predictions of the solution, hence aiding the PPINN solution to converge in just a few iterations. To investigate the PPINN performance on solving time-dependent PDEs, we first apply the PPINN to solve the Burgers equation, and subsequently we apply the PPINN to solve a two-dimensional nonlinear diffusion–reaction equation. Our results demonstrate that PPINNs converge in a few iterations with significant speed-ups proportional to the number of time-subdomains employed.

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Title: Crash Safety Evaluation of Three-Bar Metal Bridge Rail Using Finite Element Analysis

Author(s): *Zheng Li, *University of North Carolina at Charlotte*; Howie Fang, *University of North Carolina at Charlotte*; Qian Wang, *Manhattan College*;

Crash safety involving bridge rails is one of the major concerns in highway safety due to the severe consequence of a failed system under vehicular impacts. With the adoption of the new highway safety standard, Manual for Assessing Safety Hardware (MASH), it is necessary to evaluate existing bridge rails to ensure they meet the MASH safety requirements. The objective of this study was to evaluate the impact performance of an NCDOT three-bar metal bridge rail under MASH Test Level 2 (TL-2) conditions, i.e., under impacts by a small passenger car and a pickup truck at 70 km/h and a 25-degree angle. Finite element modeling and simulations were employed as the major tool of investigation in this study. The effectiveness of the three-bar metal bridge rail was evaluated using the MASH exit box criterion, vehicle row and pitch angles, dynamic barrier deflections, and occupant safety in terms of occupant impact velocity (OIV), occupant ridedown acceleration (ORA). Following a successful evaluation at Test Level 2, the bridge rail was further evaluated under Test Level 3 conditions along with a parametric study on the effect of the stiffness of reinforcement bars on occupant risk factors (i.e., OIV and ORA). This research provided insights on the performance of the three-bar metal bridge rail as well as guidance on improving the current bridge rail design for safety enhancement.

16th U.S. National Congress on Computational Mechanics
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Title: Machine Learning-Enabled Discrete Element Method for Contact Detection and Resolution of Irregular-Shaped Particles

Author(s): *Zhengshou Lai, *Sun Yat-sen University*; Qiushi Chen, *Clemson University*; Linchong Huang, *Sun Yat-sen University*;

This paper presents a machine learning (ML)-enabled discrete element method (DEM) for the computational mechanics of irregular-shaped particles. ML-enabled DEM, as with most conventional DEMs, encompasses four main steps in one typical calculation cycle, namely, (1) the detection and resolution of contacts, (2) the evaluation of contact behavior, (3) the calculation of particle motion, and (4) the updating of particle geometric descriptions. Unlike conventional DEMs, the proposed method constructs and employs neural networks to detect particle contacts and resolve contact geometric features. Neural networks take particle geometric descriptors as inputs and output the contact status and contact geometric features. Using two-dimensional elliptical particles as an example, the performance of the ML-enabled DEM is investigated through five numerical experiments and compared with analytical solutions or conventional DEM methods. A sixth numerical experiment involving irregular-shaped particles is also presented to showcase the potential and applicability of the proposed method for other particle shapes. ML-enabled DEM can accurately capture the trajectory and energy evolution of individual particles, the fabric characteristics of dense packing, and the mechanical behavior of packing under large loads, while demonstrating computational efficiency over conventional methods. A remaining challenge, as an intrinsic limitation of ML-based prediction tools, resides in the errors in the predicted contact geometric features. The spurious particle oscillation and surface roughness effects as a result of the errors in the predicted contact geometric features are identified and discussed.

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Title: Development of Time-Discontinuous Peridynamic Method for Transient Crack Propagation Problems

Author(s): *Zhenhai Liu, *Dalian University of Technology*; Hongfei Ye, *Dalian University of Technology*; Dong Qian, *The University of Texas at Dallas*; Hongwu Zhang, *Dalian University of Technology*; Yonggang Zheng, *Dalian University of Technology*;

To accurately simulate the sharp gradient features of the stress wave propagation and reduce spurious numerical oscillations in transient problems, a time-discontinuous peridynamic method (TDPD) is developed. In this method, the displacement and velocity fields are interpolated by cubic and linear functions respectively and the field functions are constructed considering the potential discontinuities in the temporal domain. The discrete equations of TDPD are derived based on the bond-based peridynamics and the time-discontinuous Galerkin method. It is found that the method can be regarded as a new step-by-step integration method, and the displacement field between each time step is continuous, while the velocity field is discontinuous. Due to these features, the TDPD can effectively characterize discontinuous characteristics of stress and eliminate spurious numerical oscillations that usually appear in the transient solutions obtained by the PD with conventional time integration method for transient problems. Numerical results of many representative problems demonstrate that the TDPD can effectively suppress the spurious numerical oscillations and predict reasonably the crack propagation. Furthermore, since the numerical formulas in the temporal and spatial domains are constructed separately, the TDPD can be easily extended to incorporate more sophisticated ordinary and nonordinary state-based PD theories. This method is expected to have wide applications in various engineering problems involving cracking. This work is supported by the NSFC (Nos. 12072061 and 12072062), the LiaoNing Revitalization Talents Program (XLYC1807193), Key Research and Development Project of Liaoning Province (2020JH2/10500003) and Fundamental Research Funds for the Central Universities (DUT20LAB203). References: [1] Liu Z, Ye H, Qian D, Zhang H, Zheng Y. A time-discontinuous peridynamic method for transient problems involving crack propagation, Int J Numer Meth Eng. https://doi.org/10.1002/nme.6602, 2020. [2] Lu M, Zhang J, Zhang H, Zheng Y, Chen Z. Time-discontinuous material point method for transient problems. Comput Methods Appl Mech Eng. 2018;328:663-685. [3] Nicely C, Tang S, Qian D. Nonlocal matching boundary conditions for non-ordinary peridynamics with correspondence material model. Comput Methods Appl Mech Eng. 2018;338:463-490.

16th U.S. National Congress on Computational Mechanics
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Title: Using Multiphysics and Multiscale Modeling Methods to Explore the Cross-Functional Application of Composites in Sustainable and Resilient Civil Infrastructure

Author(s): *Zhiye Li, *Stanford University*; Michael Lepech, *Stanford University*;

The adoption of fossil-based hydrocarbon polymer composites has been successful in both automotive and aircraft industries. However, few extension has been achieved in civil infrastructure and building construction industry. This gap is partly due to (i) the lack of multiphysics and multiscale models unifying degradation?deformation damage phenomena to assess the safety and durability of newly adopted or proposed material and structural systems, and (ii) no available computational models that are succinctly fundamental and directly interactable with other digital files from architecture designer or manufacturer. To begin addressing this gap, this study presents a multi-physics and multiphysics model that uses the UV and moisture deterioration variables homogenized from a micromechanics model to integrate a nonlocal continuum damage model (CDM) into a curvilinear coordinate system. The macro-level model links the application of analysis to the architecture or manufacturing digital model by enabling more accurate predictions of mechanical performance. An example of the model is presented for analysis of a group of glass fiber?reinforced polymer (GFRP) composite plates in SFMOMA Façade System, the first and largest architectural application of fiber reinforced polymer (FRP) in the United States. The benefits of utilizing the GFRP in buildings and civil infrastructures include higher material usage efficiency, more economical construction and life-cycle costs. This model also offers the potential for structural engineers and architects to create novel solutions in sustainable design and construction.

16th U.S. National Congress on Computational Mechanics
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Title: Neural Operator for Parametric Partial Differential Equations

Author(s): *Zongyi Li, *California Institute of Technology*;

In this talk, I will introduce our recent works Neural Operator. The classical development of neural networks has primarily focused on learning mappings between finite-dimensional Euclidean spaces. Recently, this has been generalized to neural operators that learn mappings between function spaces. For partial differential equations (PDEs), neural operators directly learn the mapping from any functional parametric dependence to the solution. Thus, they learn an entire family of PDEs, in contrast to classical methods which solve one instance of the equation. We formulate a new neural operator by parameterizing the integral kernel directly in Fourier space, allowing for an expressive and efficient architecture. We will demonstrate the experiments on Burgers' equation, Darcy flow, and the Navier-Stokes equation (including the turbulent regime).

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Title: Real-Space Density Functional Theory Adapted to Cyclic and Helical Symmetry

Author(s): *Abhiraj Sharma, *Georgia Institute of Technology*; Phanish Suryanarayana, *Georgia Institute of Technology*;

One-dimensional nanostructures such as nanotubes, nanowires, and nanocoils have received increased attention over the past three decades due to their fascinating mechanical, electronic, optical, and thermal properties. In this work, we present a cyclic and helical symmetry-adapted formulation and large-scale parallel implementation of real-space Kohn-Sham DFT for 1D nanostructures, with application to the mechanical and electronic response of carbon nanotubes subject to torsional deformations. Specifically, we derive symmetry-adapted variants for the energy functional, electronic ground state's variational problem, Kohn-Sham equations, atomic forces, and axial stress, all posed on the fundamental domain, while employing a semilocal exchange-correlation functional and a local electrostatic formulation. Within this framework, we develop a representation for nanotubes of arbitrary chirality subject to external twists. We develop a high-order finite-difference parallel implementation capable of performing cyclic and helical symmetry-adapted Kohn-Sham calculations in both the static and dynamic settings. Using this implementation, we study the mechanical and electronic response of carbon nanotubes to twist-controlled deformations, at both small and large deformations. In the linear regime, we find the torsional moduli to be proportional to the cube of the diameter; metallic nanotubes undergo metal-insulator transitions; and the band gap as well as effective mass of charge carriers to be proportional to the shear strain and the sine of three times the chiral angle. In the nonlinear regime, we find that there is significant Poynting effect, particularly at the chiral angle-dependent ultimate strain; torsional deformations provide a possible mechanism for the irreversible phase transformation from armchair to zigzag nanotubes; and the band gap as well as effective mass have an oscillatory behavior, with the period for metal-insulator transitions being inversely proportional to the square of the diameter and sine of three times the chiral angle.

16th U.S. National Congress on Computational Mechanics
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Title: Multi-Physics Models of Soft Tissue Mechanobiology, from Wounds to Organoids

Author(s): *Adrian Tepole, *Purdue University*; Yifan Guo, *Purdue University*; David Sohutskay, *Purdue University*; Bumsoo Han, *Purdue University*; Sherry Voytik-Harbin, *Purdue University*; Sarah Calve, *University of Colorado Boulder*;

A hallmark of soft tissue function is its ability to regulate its mechanical form and function by morphogenesis, growth, and remodeling. These processes are ultimately controlled by cellular activity at the microscale. Cell adhesion and contractility, as well as extra cellular protein (ECM) deposition and turnover, are the main mechanisms that couple microscale changes to the macroscale mechanical adaptation of tissues. However, there is a lack of coupled models that can account for these interactions across scales. We present first a theoretical framework that describes soft tissue as a mixture of cell populations and soluble chemical signals modeled as continuous fields (biochemical variables), as well as a solid ECM component (biomechanical variables). The deformation of the solid obeys mechanical equilibrium, and the cells and chemical species follow reaction diffusion partial differential equations (PDE) for mass balance. At the macroscale, the key coupling points between the biochemical and biomechanical components are three: i) the stress in the tissue is a combination of passive and active parts, the active part generated by the cell density field; ii) growth is captured through the multiplicative split of the deformation gradient; iii) the mechanical properties of the solid change based on tissue composition. At the microscale, the key coupling points between the biochemical and biomechanical components are two: i) cell adhesion and contractility are modeled with the well-established model proposed by Bell, which explicitly depends on ECM stiffness and deformation, and determines the active stress field; ii) production of ECM proteins by cells is modeled with rate equations, which drive the changes in growth and composition of the tissue. We solve the coupled equations with a custom finite element implementation in 2D and 3D. To showcase the wide applicability of this model, we apply it to a range of different scenarios: fibrin gel compaction by fibroblasts, wound healing in rats, and organoid formation. The model is able to capture the extreme changes in shape and mechanical properties characteristic of these scenarios, setting up the stage for further advances in theories and computational methods that can help us improve the treatment of diseases in which the mechanical form and function of tissues is at the center.

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Title: Extension of the Spectral Difference method using Raviart-Thomas elements to the sixth-order of accuracy on triangles and formulation on tetrahedra

Author(s): *Adèle Veilleux, *ONERA*; Guillaume Puigt, *ONERA*; Hugues Deniau, *ONERA*; Guillaume Daviller, *Cerfacs*;

The Spectral Difference (SD) method is an efficient and accurate high-order discontinuous spectral method dealing with the strong form of equations. The standard SD scheme introduced in 1996 by Kopriva and Kolias as the staggered-grid Chebyshev multidomain method is today well defined in the one-dimensional case and for tensor product cells. In particular, the stability was demonstrated for all accuracy orders by Jameson. When considering the standard SD method on simplex cells (triangles in 2D, tetrahedral in 3D), stability analysis leads to different conclusions. In 2008, Van den Abeele showed that for an order of accuracy strictly greater than two, the scheme stability is not ensured for triangular cells. To overcome this limitation, Balan et al. proposed in 2012 an alternative SD formulation using Raviart-Thomas elements on triangles, leading to the naming SDRT. The SDRT scheme is proven to be linearly stable up to the fourth-order under a Fourier stability analysis originally initiated by May and Schöberl and validated on Euler test cases. The SDRT method was recently extended to simulate 2D viscous flows on unstructured hybrid grids up to the fourth-order by Li et al. and used for the simulation of vortex-induced vibrations using a sliding-mesh method on hybrid grids by Qiu et al. The present study first extends the SDRT method on triangular and 2D hybrid grids to accuracy orders higher than four. To determine stable SDRT formulations, an optimization process of the interior flux points location is used. The SDRT scheme based on interior flux points determined by the optimization algorithm is shown as linearly stable under a Fourier analysis up to the sixth-order of accuracy. The high accuracy of the proposed SDRT scheme is verified using a nonlinear Euler test case for both triangular and 2D hybrid grids. Then, the SDRT implementation is used to simulate a steady flow over a NACA0012 airfoil on a quadratic triangular mesh for three different flow conditions. Secondly, the SDRT method is established for tetrahedral elements and the linear stability is studied using Fourier analysis. A 3D Euler test case is used to retrieve the expected orders of accuracy. Finally, the simulation of a Taylor-Green vortex is run using tetrahedral grids.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multi-Phase MPM Approaches for Unsaturated Soils

Author(s): *Alba Yerro, *Virginia Polytechnic Institute and State University*; Veronica Girardi, *University of Padua*; Francesca Ceccato, *University of Padua*;

Many geotechnical hazards involve large deformations of soils. Some examples are landslides, embankment collapses, tailings dam failures, seepage-induced instabilities of levees, etc. These phenomena are usually studied in the framework of porous media in soil mechanics. This requires to account for the multi-phase interactions between solid skeleton (i.e., solid grains) and pore fluids (i.e., liquid and gas). Climate events such as heavy rainfall or changes in the river water table are complicated boundary conditions that also need to be accounted for to predict failure and post-failure scenarios. In particular, the prediction of large deformations and post-failure behavior poses significant computational challenges. Several multi-phase hydromechanically formulations in the framework of the Material Point Method (MPM) were recently developed to model saturated and unsaturated soils. The purpose of this presentation is to offer an overview of the available MPM approaches to model unsaturated soils, including those proposed by the authors, and to highlight the differences and similarities of the formulations and their impact on the results in the application field of slope stability. These include the work by Yerro et al (2015), which proposed a three-phase approach in which the governing equations are derived from the momentum balance and the mass balance of solid, liquid, and gas-phase assuming non-zero gas pressure. In contrast, Bandara et al (2016) and Ceccato et al (2021) among others, use simplified approaches that neglect the momentum and the mass balance equations of the gas, thus reducing the computational cost. These approaches are slightly different in terms of governing equations, integration schemes, and benefit from various computational features. All use an explicit time integration scheme, and stability issues limit the time step increment size, introducing numerical artifacts to simulate real-time scale processes. The critical time step of the formulation presented by Ceccato et al (2021) is investigated. Preliminary results show that the stability criterion for unsaturated conditions is generally less restrictive than for saturated conditions; however, a larger variability of hydraulic properties can lead to smaller critical time steps. Yerro, A., E.E. Alonso, N.M. Pinyol, 2015. The material point method for unsaturated soils, Geotechnique. 65:201–217. Bandara, S.S., A. Ferrari, L. Laloui, 2016. Modelling landslides in unsaturated slopes subjected to rainfall infiltration using material point method, Int. J. Numer. Anal. Methods Geomech. 40(9):1358-1380. Ceccato, F., A. Yerro, V. Girardi, P. Simonini, 2021. Two-phase dynamic MPM formulation for unsaturated soil, Comput. Geotech. 129:103876.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Topology Optimization Considering Uncertainties via Stochastic Reduced Order Models

Author(s): *Alberto Torres, *Johns Hopkins University*; James Warner, *NASA Langley Research Center*; James Guest, *Johns Hopkins University*; Miguel Aguilo, *Sandia National Laboratories*;

A non-intrusive, computationally efficient approach for propagating uncertainties within a robust topology optimization framework is presented. Advancements in the field of topology optimization have addressed a wide assortment of mechanics and applications, but most work has assumed deterministic input parameters. Interest is growing, however, in approaches that incorporate uncertainties within the optimization formulation, such that optimized structures contain redundant features capable of efficiently withstanding variations in input parameters. Towards this goal, a computationally efficient method for the propagation of uncertainties at each iteration of the optimization must be implemented. We herein propose an efficient simulation-based approach capable of achieving Monte Carlo level accuracy in the propagation of uncertainties without a significant increase in the computational cost of sensitivities. The approach utilizes stochastic reduced order models (SROMs) in which a small subset of optimal samples and their corresponding probabilities are found by performing an inexpensive optimization problem that aims to reduce the error that the SROM exhibits when approximating statistical quantities of interest (CDF, moments, correlation). These samples are analogous to a classical Monte Carlo simulation, in which each realization is used to evaluate the state equation to obtain a sample of the random output. The framework allows for accurate propagation of uncertainties in an inexpensive, non-intrusive manner that is capable of modeling both analytic and/or empirical distributions with arbitrary correlation structure. The algorithm is simple to implement due to its similarities to other Monte Carlo methods. We demonstrate the approach with several continuum examples under uncertain loading conditions, and verify results using Monte Carlo-based optimization results.

16th U.S. National Congress on Computational Mechanics
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Title: Computational Fluid Dynamics of Blood Flow in the Human Heart

Author(s): *Alberto Zingaro, *Politecnico di Milano*; Luca Dede', *Politecnico di Milano*; Alfio Quarteroni, *Politecnico di Milano / École polytechnique fédérale de Lausanne*;

We develop a mathematical and numerical pipeline for the numerical simulation of blood flows in the human heart. In our CFD model, we use the Navier-Stokes (NS) equations in Arbitrary Lagrangian Eulerian (ALE) framework with prescribed motion, in order to account for the endocardium displacement. We use a Variational Multiscale - Large Eddy Simulation (VMS-LES) model [1] to get a stable formulation of the NS equations discretized by means of FEM and, then, to account for turbulence modeling within the framework of LES to consider typical transitional effects of blood flows. We mimic the presence of valves by means of the Resistive Immersed Implicit Surface (RIIS) method [2]. We propose a computational model on the haemodynamics of a left atrium (LA) to improve the general understanding of blood flow in the LA in normal conditions. We then investigate the use of the VMS-LES model in a situation of transitional blood flow: we show that VMS-LES model is more accurate to predict transitional blood flow indicators than the standard SUPG stabilization technique, especially when relatively coarse meshes are adopted [3]. We apply our model for the simulation of the left heart (LH) in physiological conditions, i.e. a multiple chambers study made of LA, left ventricle (LV) and ascending aorta, using a realistic geometry and a realistic displacement (simulated by electromechanical simulation of the LV). To prescribe realistic boundary conditions to our problem and to get physiological results, we present a coupling strategy between the 3D CFD model of the LH and a 0D closed-loop circulation model of the whole cardiovascular system. Finally, advances regarding the fluid-dynamics simulation of the whole human heart will be presented and discussed. This project has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme: grant agreement No 740132, iHEART – “An integrated Heart Model for the Simulation of the Cardiac Function”, 2017–2022. [1] Forti D., Dede' L., Semi-implicit BDF time discretization of the Navier-Stokes equations with VMS-LES modeling in a High Performance Computing framework, Computers & Fluids, 117, pp. 168-182, 2015. [2] Fedele M., Faggiano E., Dede’ L., Quarteroni A. A patient-specific aortic valve model based on moving resistive immersed implicit surfaces. Biomech Model Mechanobiol, 16(5), pp. 1779-1803, 2017. [3] Zingaro A., Dede' L., Menghini F., Quarteroni A. Hemodynamics of the heart's left atrium based on a Variational Multiscale-LES numerical model. MOX-Report, Politecnico di Milano, 80, 2020

16th U.S. National Congress on Computational Mechanics
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Title: Experimental-Numerical Analysis of Microstructure-Property Linkages for Additively Manufactured Materials

Author(s): *Alexander Raßloff, *Dresden University of Technology*; Paul Schulz, *Dresden University of Technology*; Robert Kühne, *Fraunhofer Institute for Material and Beam Technology*; André Till Zeuner, *Dresden University of Technology*; Marreddy Ambati, *Dresden University of Technology*; Ilja Koch, *Dresden University of Technology*; Maik Gude, *Dresden University of Technology*; Martina Zimmermann, *Fraunhofer Institute for Material and Beam Technology*; Markus Kästner, *Dresden University of Technology*;

The innovation of new or improved products fabricated from additive manufacturing processes with desired properties and its reliable utilization depends on a multitude of trials [National Science and Technology Council (2011): Materials genome initiative for global competitiveness]. Therefore, a systematic approach is essential to accelerate materials development. This can be realized by developing systematic materials knowledge in the form of process-structure-property (PSP) linkages. In this envisioned framework, the present work aims to derive the SP linkages of additively manufactured Ti-6Al-4V alloy. The main focus is to investigate the influence of potential defects (pores) inherited from the fabrication process on the fatigue properties. The complicated polycrystalline structure geometry, including the porosity at a microscale, is obtained by processing the Light Microscopy (LM), Electron Back-Scatter Diffraction (EBSD) and Computed Tomography (CT) measurements. A detailed statistical analysis is performed to obtain a low-dimensional representation of the structure (inputs). Based on these statistical measurements, a suitable reconstruction algorithm is developed to create pore distributions that are incorporated into synthetic Statistically Similar Volume Elements (SSVEs) generated from DREAM.3D [http://dream3d.bluequartz.net/]. Using these SSVEs, microscale crystal plasticity finite element simulations in DAMASK [F. Roters et al. DAMASK - The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale. Computational Materials Science 158: 420-478, 2019] are performed to obtain the material properties (outputs) such as yield strength and Fatigue Indicator Parameters (FIPs). The linkages of inputs and outputs are established through classical regression techniques using datasets generated by simulations on selected microstructure exemplars. A detailed numerical analysis is carried out to study the influence of pore statistics such as spatial distribution, size distribution or porosity fraction. Data analysis is carried out to rank-order the SSVEs based on FIPs. Furthermore, a comparison with the empirical Murakami's square root area concept is made.

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Title: A High-Order Generalized Finite Element Method for Multiscale Structural Dynamics and Wave Propagation

Author(s): *Alfredo Sanchez-Rivadeneira, *University of Illinois at Urbana-Champaign*; Carlos Armando Duarte, *University of Illinois at Urbana-Champaign*;

This work introduces a high-order multiscale Generalized/eXtended Finite Element Method tailored for the solution of structural dynamics and wave propagation problems exhibiting fine-scale and/or localized solution features. This type of special attributes encompasses singularities and discontinuities usually associated with fracture problems, moving/evolving interfaces, localized material nonlinearities, among others, occurring in different engineering applications. The proposed method uses an explicit time-marching scheme together with a block-diagonal lumped mass matrix applicable to arbitrary patch approximation spaces, and adopts shape functions computed numerically on-the-fly through the solution of local initial/boundary value problems. The usage of numerically-calculated shape functions to capture multi-scale phenomena has proven viable, effective and efficient in other applications. In addition, the block-diagonal structure of the lumped mass matrix allows the solution of each block independently. Thus, amenable to an efficient parallel implementation that can provide fully-explicit performance levels. Numerical studies in one-, two-, and three-dimensions show that the proposed framework is able to capture relevant features of the response using structural-scale meshes that are much coarser than those required by Direct Generalized Finite Element Analyses (DGFEAs) of comparable accuracy. In addition, a detailed study of the critical time step size of the method, as a consequence of the conditional stability of the explicit time-marching scheme, is presented and compared against the one for DGFEA discretizations that provide similar levels of accuracy, showing that the proposed method attains considerably looser time step size restrictions than available DGFEAs.

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Title: Using Multi-phase Cahn-Hilliard-Navier-Stokes Models to Extract Interfacial Properties of Molten Metal Mixtures

Author(s): *Ali Rabeh, *Iowa State University*; Makrand Khanwale, *Iowa State University*; Jonghyun Lee, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

We deploy an optimization based approach to extract surface tension properties of molten core-shell metal droplets. This has significant implications in continuous casting of alloys. The forward model is well represented by a multi-phase Cahn Hilliard Navier Stokes (air-metal1-metal2). However, numerical simulations are complicated by the very large density ratios ~ 120,000 that such systems exhibit. We use a thermodynamically consistent coupled Cahn Hilliard Navier-Stokes equations with a residual based variational multi-scale method to model this system. We present several cases to validate our framework and to illustrate the mass conservation and energy stability of our scheme under very high density ratios. Next, we integrate this ‘forward model’ with a Bayesian optimization routine to identify various system properties. We showcase this framework by identifying the surface tension of the core-shell system, given micro-gravity experiments of an oscillating core-shell droplet.

16th U.S. National Congress on Computational Mechanics
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Title: Probabilistic Modeling of Tau Propagation in Alzheimer's Disease

Author(s): *Amelie Schaefer, *Stanford University*; Mathias Peirlinck, *Stanford University*; Kevin Linka, *Hamburg University of Technology*; Ellen Kuhl, *Stanford University*;

In the United States, one out of ten people over the age of 65 is suffering from Alzheimer's disease and the case numbers are projected to grow rapidly over the next 30 years as the number of older adults in our society increases [1]. It has become widely accepted that the cerebral accumulation of hyperphosphorylated tau is one of the disease initiators and closely related to neurodegeneration and cognitive impairment [2]. However, until recently, our understanding of how this pathological protein aggregates and propagates across the brain has relied almost exclusively on postmortem histopathology. Now, the emerging imaging technology of positron emission tomography allows to visualize the distribution of tau protein in the brain in vivo, offering the opportunity to track disease progression in a patient over time. Using the extracted quantitative characteristics of the evolution of tau, data-driven computational models can provide crucial insights into critical factors and time points for early diagnosis and intervention and allow for personalized predictions of disease progression. We use a network diffusion model on a weighted Laplacian graph to compute the propagation of hyperphosphorylated tau protein across the brain's connectome [3]. We compare our model to longitudinal positron emission tomography images from the Alzheimer's Disease Neuroimaging Initiative, following 76 subjects over three to four annual scans. Using Bayesian hierarchical modeling, we infer model parameters that best reproduce the neuropathological patterns of the image data on subject- and group-levels. This probabilistic approach allows us to quantify the uncertainty associated with the inferred parameters, making optimal use of individual and population evolution data. Propagation of the quantified uncertainty allows us to estimate the confidence on our personalized model predictions. As such, our Bayesian framework provides clinically relevant information on the progression of the disease and may serve as an important tool to optimize the subject-specific scheduling of follow-up imaging with the goal of improving the accuracy of predictions while minimizing cost. [1] Alzheimer's Association, 2019 Alzheimer's disease facts and figures. Alzheimer's & Dementia, 15(3), pp.321-387. [2] Bejanin, A., et al., 2017. Tau pathology and neurodegeneration contribute to cognitive impairment in Alzheimer's disease. Brain, 140(12), pp.3286-3300. [3] Schäfer, A., Mormino, E.C. and Kuhl, E., 2020. Network Diffusion Modeling Explains Longitudinal Tau PET Data. Frontiers in Neuroscience, 14, p.1370.

16th U.S. National Congress on Computational Mechanics
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Title: ParaMonte: A Parallel High-Performance Cross-Language Cross-Platform Toolbox for Monte Carlo Sampling, Uncertainty Quantification, and Visualization

Author(s): *Amir Shahmoradi, *The University of Texas at Austin*; Fatemeh Bagheri, *The University of Texas at Arlington*; Shashank Kumnhare, *The University of Texas at Arlington*; Joshua Alexander Osborne, *The University of Texas at Arlington*;

Monte Carlo simulation techniques, in particular, the Markov Chain Monte Carlo (MCMC) are among the most popular methods of quantifying uncertainty in scientific inference. Together with Bayesian probability theory, these techniques lie at the heart of machine learning and predictive computing. A major challenge in developing and deploying Bayesian models is often the mathematical and computational complexity of the final objective function of the Bayesian models which is intractable to explore using traditional Monte Carlo techniques. Here we present our efforts in developing an open-source library named ParaMonte, comprised of a set of parallel scalable adaptive Monte Carlo algorithms for sampling and integrating the mathematical objective functions of arbitrary shapes and dimensions. The principal design goals of ParaMonte are: 1. full automation of all Monte Carlo simulations, 2. interoperability of the core library with multiple programming languages, including C, C++, Fortran, Julia, MATLAB, Python, and R, 3. high-performance 4. parallelizability and scalability of simulations, 5. zero-dependence of the kernel routines on external libraries, 6. fully-deterministic reproducibility of all simulations, 7. automatic comprehensive-reporting, post-processing, and visualization of the simulation results. We discuss how these design goals can help ParaMonte users readily and efficiently solve a variety of machine learning and scientific inference problems on a wide range of platforms, from Jupyter notebooks on personal laptops to supercomputers. ParaMone is MIT-licensed and permanently maintained at https://github.com/cdslaborg/paramonte

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Title: Implicit Shock Tracking and the Method of Lines for Shock-Dominated, Unsteady Flows

Author(s): *Andrew Shi, *University of California, Berkeley*; Matthew Zahr, *University of Notre Dame*; Per-Olof Persson, *University of California, Berkeley*;

In [Zahr, Shi, Persson; 2020], we introduce a novel framework for resolving discontinuous solutions of conservation laws using high-order implicit shock tracking (HOIST) with a high-order discontinuous Galerkin (DG) discretization. Central to the framework is an optimization problem whose solution is a discontinuity-aligned mesh and the corresponding high-order approximation to the flow that does not require explicit meshing of the unknown discontinuity surface. We formulate an optimization problem featuring an error-based objective function which penalizes violation of the DG residual in an enriched test space which is shown to have excellent tracking properties. We develop an associated sequential quadratic programming (SQP) solver which simultaneously converges the nodal coordinates of the mesh and DG solution to their optimal values and is equipped with a number of features to ensure robust, fast convergence: Levenberg-Marquardt approximation of the Hessian with weighted elliptic regularization, backtracking line search based on the l1 merit function, and rigorous convergence criteria. We use the proposed method to solve a range of inviscid, steady conservation laws and unsteady problems via a space-time approach. We show the method is able to deliver accurate solutions on coarse, high-order meshes and the SQP solver is robust and usually able to drive the first-order optimality system to tight tolerances. In [Shi, Persson, Zahr; 2021], we extend the shock tracking framework to the case of unsteady conservation laws using a method of lines discretization by “solving a steady problem at each timestep”. The key ingredients of the method-of-lines approach are: 1) an Arbitrary Lagrangian-Eulerian formulation of the conservation law to handle the deforming mesh (which deforms to track the shock through the domain), 2) semi-discretization with DG to obtain a system of ordinary differential equations, 3) high-order temporal discretization with a diagonally implicit Runge-Kutta (DIRK) method, and 4) implicit shock tracking at each time step following the previously developed approach. A Rankine-Hugoniot based prediction of the shock location together with a high-order, untangling mesh smoothing procedure provides a high-quality initial guess for the optimization problem at each time, which results in Newton-like convergence of the SQP optimization solver. We demonstrate this framework on a series of inviscid, unsteady conservation laws in both one- and two- dimensions. We also verify that our method is able to recover the design order of accuracy of our time integrator in the presence of a strong discontinuity.

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Title: Calibration and Validation of Regularized Failure Models Applied to Dynamic Puncture

Author(s): *Andrew Stershic, *Sandia National Laboratories*; Kyle Karlson, *Sandia National Laboratories*; Sharlotte Kramer, *Sandia National Laboratories*; Brandon Talamini, *Sandia National Laboratories*;

The ability to accurately predict the response of structures to mechanical insults has motivated significant investment in computational modeling and simulation tools. However, in order to realize the benefits of simulation, an analyst must be able wield feature-rich material constitutive and failure models in combination with adequate foundational experimental data. Deter-mining the model parameters to reflect this data poses a particular challenge, as the potential parameter space grows rapidly as material and failure models include more physics, and there-fore model parameters. In this presentation, we present our strategy of material constitutive and failure model calibration using Sandia's MatCal, an optimization tool extending the DAKOTA optimization frame-work. Particular attention is given reviewing and analyzing the experimental data from a suite of characterization tests in order to choose the proper constitutive model form and the approach for characterizing regularized failure models. We include consideration of regularized failure models – phase field and nonlocal regularization – as their nonlocal features are advantageous for establishing mesh-convergent predictions. The calibration strategy is demonstrated through application, with the problem of interest being dynamic puncture of an aluminum plate. We conclude with comparisons between simulation results and experimental data. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honey-well International, Inc., for the U.S. Department of Energy's National Nuclear Security Ad-ministration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: Reynolds-Averaged and Large-Eddy Simulation Strategies for Langmuir Turbulence in the Coastal Ocean

Author(s): *Andrés Tejada-Martínez, *University of South Florida*; Juan Penaloza-Gutierrez, *University of South Florida*; Qiming Zhu, *University of Illinois at Urbana-Champaign*; Anthony Perez, *University of South Florida*; Jinhui Yan, *University of Illinois at Urbana-Champaign*; Yuri Bazilevs, *Brown University*;

Langmuir turbulence in the coastal ocean is driven by winds and waves and is characterized by Langmuir cells (LCs) that can span the full depth of unstratified water columns. A solution strategy based on Reynolds averaging is introduced, relying on the coherency and persistence of full-depth LCs. Here these cells are treated as a secondary component to the wind and/or pressure gradient-driven primary flow. The strategy is used to investigate LCs engulfing unstratified shallow water regions representative of a shallow shelf zone and a surf-shelf transition zone. The resolved LCs and associated statistics will be compared with their counterparts in large-eddy simulation (LES). The comparison shows that the Reynolds-averaged approach can successfully reproduce cell meandering and merging (i.e. the so-called Y-junctions), a requisite for capturing the proper crosswind width of the LCs. The merging occurs less frequently over time as the cells grow after being spun from rest. Additional studies via the Reynolds-averaged approach will be presented investigating the impact of variable water column depth, the coastal shore and wave direction on the width of the LCs and their intensity. Traditionally LES of Langmuir turbulence has been performed with pseudo-spectral methods on domains of constant depth with periodicity in the horizontal directions, representative of locations where lateral boundaries do not affect the turbulence. To handle variable water column depths and non-periodic directions, LES will be performed using a residual-based variational multiscale (RBVMS) method with non-uniform rational basis splines. The Craik-Leibovich vortex force appearing in the momentum equations accounting for the surface wave-current interaction that generates Langmuir turbulence is treated as a generalized advective term in the RBVMS method leading to modifications of the method’s stabilization parameters.

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Title: An Entropy-Stable Discontinuous Galerkin Scheme for Compressible Magnetohydrodynamics with Subcell Finite Volume Shock Capturing

Author(s): *Andrés M Rueda-Ramírez, *University of Cologne*; Sebastian Hennemann, *German Aerospace Center (DLR)*; Florian J Hindenlang, *Max Planck Institute for Plasma Physics*; Andrew R Winters, *Linköping University*; Gregor J Gassner, *University of Cologne*;

We present robust entropy stable shock-capturing methods for discontinuous Galerkin spectral element (DGSEM) discretizations of the compressible magneto-hydrodynamics (MHD) equations. Specifically, we use the resistive GLM-MHD equations, which include a divergence cleaning mechanism that is based on a generalized Lagrange multiplier (GLM). For the continuous entropy analysis to hold, and due to the divergence-free constraint on the magnetic field, the GLM-MHD system requires the use of non-conservative terms, which need special treatment. Hennemann et al. [1] recently developed entropy stable shock-capturing strategy for DGSEM discretizations of the Euler equations that blends the DGSEM scheme with a subcell first-order finite volume (FV) method. Our first contribution is the extension of the method of Hennemann et al. to systems with non-conservative terms, such as the GLM-MHD equations. As the baseline scheme, we use the entropy stable DGSEM scheme for the GLM-MHD equations proposed by Bohm et al. [2]. In our approach, the advective and non-conservative terms of the equations are discretized with a hybrid FV/DGSEM scheme, whereas the visco-resistive terms are discretized only with the high-order DGSEM method. We prove that the extended method is entropy stable on three-dimensional unstructured curvilinear meshes. Our second contribution is the derivation and analysis of an additional entropy stable shock-capturing method that provides enhanced resolution by using a subcell reconstruction procedure that is carefully built to ensure entropy stability. We provide a numerical verification of the properties of the hybrid FV/DGSEM schemes on curvilinear meshes and show their robustness and accuracy with common benchmark cases, such as the Orszag-Tang vortex and the GEM (Geospace Environmental Modeling) reconnection challenge. Finally, we simulate a space physics application: the interaction of Jupiter's magnetic field with the plasma torus generated by the moon Io. References [1] S Hennemann, AM Rueda-Ramírez, FJ Hindenlang, GJ Gassner. “A provably entropy stable subcell shock capturing approach for high order split form DG for the compressible Euler equations". JCP, 2020. [2] M Bohm, AR Winters, GJ Gassner, D Derigs, F Hindenlang, J Saur. “An entropy stable nodal discontinuous Galerkin method for the resistive MHD equations. Part I: Theory and numerical verification”. JCP, 2018.

16th U.S. National Congress on Computational Mechanics
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Title: High-Spatial Resolution Ice-Sheet Modeling: Leveraging Parallelized Techniques to Accelerate Time to Solution

Author(s): *Anjali Sandip, *University of North Dakota*; Mathieu Morlighem, *University of California, Irvine*;

Since the Fifth Assessment Report (AR5) of the Intergovernmental Panel on Climate Change, there have been several advances in models developed to project glacier and ice-sheet evolution in a warming climate. Despite the progress made, the existing ice-sheet flow models do not accurately describe polar ice-sheet discharge. One of the primary limitations is the low spatial resolution (> 5 km in the interior of the ice sheet and >1 km at the coast). High-spatial resolution models do not achieve reasonable time to solution [1-3]. The objective of this study was to utilize massively parallelized techniques to accelerate the time to solution for high-spatial resolution numerical ice-sheet flow models. The models tested in this study were two-dimensional (2-D) based on shallow-shelf approximation of non-linear Stokes equations. Utilization of the parallelized techniques accelerated the time to solution by 45%, for the real glaciers included in this study. Future work would include extending this study to higher-order models followed by Full-Stokes. References: [1]. Church, J.A., Clark, P.U., Cazenave, A., Gregory, J.M., Jevrejeva, S., Levermann, A., Merrifield, M.A., Milne, G.A., Nerem, R.S., Nunn, P.D. and Payne, A.J., 2013. Sea level change. PM Cambridge University Press. [2]. Pattyn, F., 2018. The paradigm shift in Antarctic ice sheet modelling. Nature communications, 9(1), pp.1-3. [3]. Tezaur, I.K., 2019. An Overview of the State-of-the-Art in Computational Modeling of Ice Sheets.

16th U.S. National Congress on Computational Mechanics
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Title: Towards the Computational Design of Smart Nanocarriers

Author(s): *Annalisa Quaini, *University of Houston*; Maxim Olshanskii, *University of Houston*; Alexander Zhiliakov, *University of Houston*; Shereen Majd, *University of Houston*; Yifei Wang, *University of Houston*;

Membrane fusion is a potentially efficient strategy for the delivery of macromolecular therapeutics into the cell cytoplasm. However, existing nano-carriers formulated to induce membrane fusion suffer from a key limitation: the high concentrations of fusogenic lipids needed to cross cellular membrane barriers lead to toxicity in vivo. To overcome this limitation, we are developing complimentary in silico and in vitro models that will explore the use of membrane phase separation to achieve efficient membrane fusion with minimal concentrations of fusion-inducing lipids and therefore reduced toxicity. The in silico research is based on a novel multiphysics model formulated in terms of partial differential equations posed on evolving surfaces.

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Title: Refactorization of Cauchy's Method: a Second-Order Partitioned Method for Fluid-Thick Structure Interaction Problems

Author(s): Martina Bukac, *University of Notre Dame*; *Anyastassia Seboldt, *University of Notre Dame*; Catalin Trenchea, *University of Pittsburgh*;

This work focuses on the derivation and the analysis of a novel, strongly-coupled partitioned method for fluid-structure interaction problems. The flow is assumed to be viscous and incompressible, and the structure is modeled using linear elastodynamics equations. We assume that the structure is thick, i.e., modeled using the same number of spatial dimensions as fluid. Our newly developed numerical method is based on generalized Robin boundary conditions, as well as on the refactorization of the Cauchy's one-legged 'theta-like' method, written as a sequence of Backward Euler–Forward Euler steps used to discretize the problem in time. This family of methods, parametrized by theta, is B-stable for any theta contained in [0.5,1] and second-order accurate for theta = 0.5 +O(tau), where tau is the time step. In the proposed algorithm, the fluid and structure sub-problems, discretized using the Backward Euler scheme, are first solved iteratively until convergence. Then, the variables are linearly extrapolated, equivalent to solving Forward Euler problems. We prove that the iterative procedure is convergent, and that the proposed method is stable provided theta is contained in [0.5,1]. Numerical examples, based on the finite element discretization in space, explore convergence rates using different values of parameters in the problem, and compare our method to other strongly-coupled partitioned schemes from the literature. We also compare our method to both a monolithic and a non-iterative partitioned solver on a benchmark problem with parameters within the physiological range of blood flow, obtaining an excellent agreement with the monolithic scheme.

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Chicago, IL, July 25-29. 2021

Title: Uncertainty Quantification for Microstructure Reconstruction of Additively Manufactured Microstructures

Author(s): *Arulmurugan Senthilnathan, *Virginia Polytechnic Institute and State University*; Pinar Acar, *Virginia Polytechnic Institute and State University*;

Microstructure data is experimentally measured over small spatial domains as obtaining large-scale data through experiments is usually not preferable or even feasible due to cost and time constraints. Such large-scale data required to compute the mechanical response of materials can be generated by mathematical reconstruction methods using small-scale experimental inputs. Popular techniques capture the global features of the image by matching the features and point probability functions with the experimental microstructures. Nevertheless, most reconstruction techniques cause local per-pixel data loss in computations. Markov Random Field (MRF) overcomes this issue by computing the local probability distributions of pixels [1]. With the inclusion of the local information, the evolution of 2D experimental microstructure maps is predicted using the data that is routinely obtained over small spatial domains with diffraction and optical techniques. However, this prediction is influenced by the effects of the uncertainties in computations and experiments [2]. These uncertainties can propagate onto the synthesized microstructures and thus affect the material properties. While the uncertainty quantification (UQ) of crystallographic texture and grain size is addressed with state-of-the-art methods, the UQ of grain shapes is still an unexplored research challenge. We address this challenge in our present work by proposing a new methodology for the UQ of grain topology and texture of metallic microstructures. We utilize the concept of shape moment invariants in physics to quantify the grain shapes and the effects of microstructural uncertainties on material properties. According to this concept, the shape of a physical object can be mathematically quantified with a set of invariant parameters. To generate sufficient statistical information, synthetic microstructures are reconstructed from the experimental data of Titanium-7wt%- Aluminum (Ti-7Al) microstructures using the MRF method. The texturing of the synthetic microstructures is described with the Orientation Distribution Function (ODF), while the shape moment invariants are used to represent the grain shapes. The propagation of the microstructural uncertainty on the stress-strain response is investigated by performing crystal plasticity simulations. References: [1] Acar, Pinar, and Veera Sundararaghavan. "A Markov random field approach for modeling spatio-temporal evolution of microstructures." Modelling and Simulation in Materials Science and Engineering 24.7 (2016): 075005. [2] Acar, P?nar. "Recent progress of uncertainty quantification in small-scale materials science." Progress in Materials Science (2020): 100723.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Predicting Microstructure-Dependent Mechanical Properties in Additively Manufactured Metals using Machine- and Deep-Learning Methods

Author(s): Carl Herriott, *The University of Utah*; *Ashley Spear, *The University of Utah*;

The microstructure of additively manufactured (AM) metals has been shown to be heterogeneous and spatially non-uniform when compared to conventionally manufactured metals. Consequently, the effective mechanical properties of AM-metal parts are expected to vary both within and among builds. In this work, the efficacy of machine-learning (ML) and deep-learning (DL) models to predict microstructure-sensitive mechanical properties in AM metals is assessed using results from high-fidelity, multi-physics simulations from prior work as training data. In the prior work [1], physics-driven models were developed to predict grain nucleation and competitive growth as a function of thermal history for a multi-pass, multi-layer direct laser deposition process. The resulting 3D microstructures were then automatically sub-sampled to perform virtual mechanical testing throughout multiple build domains using a parallelized elasto-viscoplastic fast Fourier transform code, accounting for grain-boundary strengthening. The microstructural subvolumes and corresponding homogenized yield-strength values (~7700 data points) are used in the current work [2] to train two types of ML models (Ridge regression and XGBoost) and one type of DL model (a custom 3D convolutional neural network (CNN) based on VGGNet). Morphological and crystallographic features describing each microstructure serve as the inputs for the Ridge regression and XGBoost models. The CNN is trained with a 3D image of the microstructure represented by progressively informative input data (ranging from grain ID to crystal orientation, and supplemented with auxiliary features describing the mechanical loading) to determine the relative improvement among different feature types. Comparisons are drawn between the predictive performance of each data-driven model in terms of different scoring metrics and spatial-property maps. The computational efficiency of each data-driven model and the physics-driven modeling framework is also reported. Among all of the data-driven models tested, the CNN models that use crystal orientation as input (with or without auxiliary input features) provide the best predictions, require little pre-processing, and predict spatial-property maps in a matter of seconds. [1] Herriott, C., et al. (2019). A multi-scale, multi-physics modeling framework to predict spatial variation of properties in additive-manufactured metals. Modelling and Simulation in Materials Science and Engineering, 27(2), 025009. [2] Herriott, C. & Spear, A. D. (2020). Predicting microstructure-dependent mechanical properties in additively manufactured metals with machine-and deep-learning methods. Computational Materials Science, 175, 109599. https://doi.org/10.1016/j.commatsci.2020.109599

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Computational Modeling of Two-Phase Flow in Deformable Porous Media

Author(s): *Beatrice Riviere, *Rice University*; Boqian Shen, *Rice University*;

The poroelasticity model for two-phase flow in porous media is discretized by an interior penalty discontinuous Galerkin methods. These models are important in the prediction of subsidence, which can be significant and can result in costly remediation. The proposed scheme solves for the phase pressures, and the displacement sequentially and each equation is treated implicitely in time. With the sequential approach, the resulting scheme is computationally cheaper than the fully implicit method. Optimal convergence of the numerical method is obtained as the mesh size and time-step decrease.

16th U.S. National Congress on Computational Mechanics
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Title: Time-Lapse In Vivo Imaging of Bone Formation and Resorption in Mouse Models and Humans using Microcomputed Tomography and High-Resolution Peripheral Quantitative Computed Tomography

Author(s): Seyedmahdi Hosseinitabatabaei, *McGill University / Shriners Hospital for Children-Canada*; Isabela Vitienes, *McGill University / Shriners Hospital for Children-Canada*; Maximillian Rummler, *McGill University / Shriners Hospital for Children-Canada*; Annette Birkhold, *Siemens Healthcare GmbH*; *Bettina Willie, *McGill University / Shriners Hospital for Children-Canada*;

Bone undergoes structural changes through bone modeling and remodeling. Modeling (spatially independent resorption and formation) and remodeling (spatially and temporally dependent resorption and formation) processes construct and reconstruct the skeleton by removal and formation of bone packets that modulate size, architecture, mass, and consequently the bone's strength. Bone (re)modeling is measured using biochemical markers or histomorphometry, both of which have limitations. Advances in microcomputed tomography have enabled non-invasive in vivo monitoring of structural changes in cortical and trabecular bone of mice in 3D-space over time. We developed a computational imaging method to monitor bone (re)modeling over time in living mice using registered longitudinal microcomputed tomography data (1, 2). Attempts to translate time-lapse imaging to humans have been made using first generation high-resolution peripheral-quantitative computed tomography (HR-pQCT) datasets (3). HR-pQCT is a non-invasive imaging tool for measuring volumetric bone mineral density and microstructure at peripheral sites such as the radius and tibia. Second generation HR-pQCT scanners now provide an isotropic voxel size of approximately 60?m. We recently adapted and extended our preclinical time-lapse method to quantify bone formation and resorption using a two-year longitudinal HR-pQCT dataset from a phase 2b, multi-centre, multinational, double-blind, dose-finding study in 120 adult patients with Type I, III or IV osteogenesis imperfecta (OI) treated with Setrusumab™ (Mereo BioPharma), a bone formation inducing drug. OI is a devastating genetic disorder resulting in bone fragility and deformity with no approved medication. In this method, grayscale images of follow-ups and baseline were aligned using rigid 3D-registration. Next, voxel-based intensity values of the two images were subtracted, resulting in a grayscale image representing local changes. To reduce the effects of noise and interpolation errors, a two-step filter was applied. First, only voxels with changes larger than a threshold are defined as formation or resorption. Secondly, clusters of formation and resorption smaller than a certain size were removed. Finally, formed and resorbed bone volumes and surface areas were determined relative to the baseline image. We demonstrate the potential of this emerging in-vivo imaging techniques to identify local changes in bone turnover in patients and potentially avoid the need for histomorphometric assessment of invasive bone biopsies. This noninvasive imaging biomarker for bone formation and resorption will allow clinicians to longitudinally examine disease progression and treatment efficacy on bone (re)modeling processes in patients. References: 1-2. Birkhold et al., Bone-2014, Biomaterials-2015; 3. Christen et al., Nat.Commun-2014 Acknowledgement: This study was supported by Mereo BioPharma.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Adaptive Interface-Preserving Variational Formulation for Fully-Eulerian Fluid-Structure Interaction

Author(s): *Biswajeet Rath, *University of British Columbia*; Xiaoyu Mao, *University of British Columbia*; Rajeev Jaiman, *University of British Columbia*;

Body-fitted finite element techniques such as Arbitrary Lagrangian Eulerian (ALE) have long dominated the realm of numerical solutions for fluid-structure interaction (FSI) problems. They have been very successful for accurate interface tracking of several complicated multiphase and multi-physics engineering applications. However, difficulties arise when we attempt to employ these methods to solve problems dealing with flexible multibody contact dynamics or those involving large topological changes such as the bursting of a pipeline or rupture of an aortic aneurysm. In this study, we present a novel interface-driven adaptive model using the fully-Eulerian method for FSI problems. The fully-Eulerian approach involves a fixed background mesh on which the interface is treated implicitly. The two domains are modeled by the phase-field finite element formulation [1], involving the convective Allen-Cahn equation coupled with the unified momentum equation for both solid and fluid. A bounded and stable solution of the Allen-Cahn equation is ensured through the use of the positivity preserving variational formulation [2]. The finger tensor is convected at each time step to trace the material coordinates in the Eulerian reference frame based on its initial position to evaluate the stresses correctly. The adaptive refinement/coarsening for the unstructured grid is determined by appropriate indicators and carried out by the newest vertex bisection algorithm. The proposed nonlinear adaptive partitioned procedure carries out the refining/coarsening steps at the first or last non-linear iterations, hence ensuring the convergence of the non-linear governing differential equations [3]. The convergence and accuracy analysis are first carried out systematically for the fully-Eulerian formulation using two simple benchmark problems namely, the pure solid system and a coupled fluid-solid system with an interface in a rectangle domain. We then demonstrate our fully-Eulerian interface-driven adaptive FSI model to simulate a popular bouncing elastic ball problem i.e. free-fall of an elastic ball under gravity and its subsequent bounce back from the rigid floor. References: [1] Mao, X., Joshi, V., and Jaiman, R. K. A variational interface-preserving and conservative phase-field method for the surface tension effect in two-phase flows. (2020) arXiv preprint arXiv:2007.15887. [2] Joshi, V. and Jaiman, R. K. A positivity preserving and conservative variational scheme for phase-field modeling of two-phase flows. Journal of Computational Physics 360 (2018), pp. 137-166. [3] Joshi, V. and Jaiman, R. K. An adaptive variational procedure for the conservative and positivity preserving Allen-Cahn phase-field model. Journal of Computational Physics 366 (2018), pp. 478-504.

16th U.S. National Congress on Computational Mechanics
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Title: On Entropy Conservation and Kinetic Energy Preservation Methods

Author(s): H. C. Yee, *NASA Ames Research Center*; *Bjorn Sjogreen, *MultiD Analyses AB*;

The Tadmor-type entropy conservative method using the mathematical logarithmic entropy function and two forms of the Sjogreen & Yee entropy conservative methods using the Harten entropy function are examined for their nonlinear stability and accuracy in very long time integration of the Euler equations of compressible gas dynamics. Following the same procedure as Ranocha (2019) these entropy conservative methods can be made kinetic energy preserving with minimum added computational effort. The focus of this work is to examine the nonlinear stability and accuracy of these newly introduced high order entropy conserving and kinetic energy preserving methods for very long time integration of selected test cases when compared with their original methods. Computed entropy, and kinetic energy errors for these methods are compared with the Ducros et al. and the Kennedy-Gruber-Pirozzoli skew-symmetric splittings.

16th U.S. National Congress on Computational Mechanics
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Title: A Higher-Order Thermo-Mechanical Homogenization Method For Heterogeneous Porous Material

Author(s): *Bozo Vazic, *The University of Utah*; Pania Newell, *The University of Utah*;

Porous materials, such as geomaterials, porous metals, and ceramics are used in many engineering and scientific applications. Most natural and man-made porous materials are highly heterogeneous in nature, and they contain large variations in their pore structures (e.g., pore sizes, pore distribution, pore shapes, and pore strut/wall size). For instance, the variation of pore structures at microscopic level presents considerable challenges when accounting for thermo-mechanical mechanisms occurring in the porous material. However, such variation in the underlying pore structure is usually ignored in continuous modeling. This is mainly due to the difficulty of capturing complex relationship between macroscopic material properties and stochastic microscopic pore structure. For example, accurate definition of thermo-mechanical properties of porous ceramics used in active cooling for spaceflight technology is extremely important because the components are exposed to severe environments with ultrahigh temperature, high pressure, and usually supersonic velocity. This in turn requires porous ceramics to have high temperature melting point, high mechanical strength, low thermal conductivity, open pore structure, and special pore distribution. In this presentation, the effect of a complex micropore morphology on effective thermo-mechanical properties of a porous material will be numerically investigated. A coupled thermo-mechanical problem is governed by the balance equations of linear momentum and energy, in which linear momentum equation is a function of Cauchy stress tensor and the body force per unit of deformed volume, while energy equation is defined by using the Fourier equation for heat transfer. To account for the variability in the pore shapes and sizes, we adopt higher-order homogenization method. The second-order scheme used in this study is an extension of the first-order computational homogenization framework as it incorporates third-order macroscopic second gradient deformation tensor into the kinematical macro–micro scale transition and accounts for a microscopic length scale. The developed formulation is fully coupled and encapsulates the two physics of the problem, through firstly determining the thermal parameters and then considering thermal effects onto the mechanical behavior. By employing this model we are able to solve a nonlinear and temperature dependency of porous materials' deformation response at the microscopic level and then transmit this information to the macroscopic level. The new formulation is benchmarked against various tests to showcase its capability.

16th U.S. National Congress on Computational Mechanics
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Title: Phase Field Disconnections: Exploring Complex Grain Boundary Migration from the Mesoscale Perspective

Author(s): *Brandon Runnels, *University of Colorado Colorado Springs*;

Grain boundary (GB) migration is a key mechanism underlying such phenomena as deformation twinning, recrystallization, solidification, and many others. While GB migration has received a great deal of attention at the atomistic level (both experimentally and computationally), the mesoscale picture of GBs has remained relatively unexplored. Consequently, mesoscale models of GBs have tended to be overly simplistic, failing to capture some of the key mechanisms of interest in microstructure evolution. The overarching goal of this work is to develop a comprehensive and predictive mesoscale treatment of GB migration. The contributions of this presentation are threefold: The first contribution of this work is the development of a rigorous continuum thermodynamic framework for GB migration. GBs are known to exhibit a wide range of migration behavior that is highly dependent on GB character, temperature, and loading conditions. In this work we show that shear-coupled GB migration is analogous to crystal plasticity (CP), and admits a corresponding formulation using the principle of minimum dissipation potential. It is shown that this general principle, when specialized to a number of different boundaries, is able to accurately reproduce the observed shear coupling behavior. The second contribution of this work is the demonstration that the mechanism of disconnection-mediated GB migration is, in fact, a natural consequence of (i) GB energy anisotropy and (ii) the minimum dissipation potential governing GB migration. Disconnections may be thought of as “facets” resulting from strong orientation dependence. These facets then create stress concentrations, which in turn produce strong driving forces localized at the facet corners. A phase field implementation of this model is developed, and results for several boundaries undergoing shear coupling are presented. The third contribution of this work is the development of a novel nucleation model that is used to introduce thermal dependence into the phase field disconnection framework. Just as with real disconnections, phase field disconnections require nucleation in order to propagate. We present a general algorithm that is able to consistently generate disconnections at the GB in a temperature-dependent manner. This model makes it possible to explore the effects of temperature and GB size on GB mobility from a continuum perspective.

16th U.S. National Congress on Computational Mechanics
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Title: A Variational Phase-Field Model of Ductile Fracture

Author(s): *Brandon Talamini, *Sandia National Laboratories*; Andrew Stershic, *Sandia National Laboratories*; Michael Tupek, *Sandia National Laboratories*;

Phase field approaches have become well-established in the domain of brittle fracture due to their remarkable ability to represent arbitrary evolving crack geometries, including branching, bifurcation, and merging. Given the widespread use of ductile alloys in engineering applications, there has been increasing effort put towards extending the phase field methodology to ductile failure. In this talk, we exhibit a new family of phase-field models of elastic-plastic fracture that attains several important milestones. First, the model predictions of elastic-plastic crack growth resistance are insensitive to the phase field interface length parameter. Taking this further, we make an informal argument for convergence of solutions in the limit of a sharp cracks, a conjecture which is borne out by numerical calculations. Second, the model incorporates effects of stress triaxiality in a fashion consistent with theories of ductile rupture based on void growth and coalescence. Even when this is the dominant driver of crack propagation, the theory retains its regularized character and produces solutions that converge with mesh refinement. Third, both the continuous and discretized equations of the theory are derivable from the minimization of a scalar action principle, including the irreversible effects of plasticity and damage. The energy landscape (or the generalized potential in this case) of phase field models of fracture are known to be non-convex, and spurious unstable saddle-points solutions can be produced by naïve solution techniques. Difficulties and crude approximations are also common for imposition of inequality constraints such as damage irreversibility. We show that the variational approach is thus especially useful in this case, as it allows use of modern constrained optimization techniques that are efficient, robust, accurate, and guarantee physically meaningful stable solutions. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
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Title: Computational Modeling of Transcatheter Heart Valves in Bicuspid Aortic Valves for Clinical Planning

Author(s): *Breandan Yeats, *Georgia Institute of Technology / Emory University*; Sri Krishna Sivakumar, *Georgia Institute of Technology / Emory University*; Pradeep Yadav, *Piedmont Hospital*; Vekateshwar Polsani, *Piedmont Hospital*; Vinod Thourani, *Piedmont Hospital*; Lakshmi Dasi, *Georgia Institute of Technology / Emory University*;

Bicuspid aortic valve (BAV) disease is the most common congenital heart defect effecting 2-4% of the general population and has increased risk of developing calcific aortic valve disease [1, 2]. Transcatheter aortic valve replacement (TAVR) therapies are becoming increasingly popular to treat BAV diseased patients however, these cases present with increased adverse outcomes likely due to abnormal anatomies and irregular calcium distributions [3]. We aim to reduce adverse outcome occurrence for TAVR in BAV cases through pre-procedural computational modeling. Our computational analysis encompasses the major complications associated with balloon and self-expandable TAVR use in BAVs. This includes finite element analysis to simulate deployment followed by a stress analysis to predict aortic root injury (maximum stress) and permanent pacemaker implantation (stress on the membranous septum). This is followed by pressurization of the bioprosthetic leaflets to predict improper opening of the cusps which, along with pre-operative hemodynamic data, is used to estimate thrombosis risk. Finally, paravalvular regurgitation risk is evaluated through computational fluid dynamics after finite element deployment. Several of our finite element deployments have been validated through geometric comparison to 30-day post-operation CT scans which have shown reasonable agreement. Although limited in number, all cases avoided root rupture, moderate to severe paravalvular regurgitation, and thrombosis at 30 days post-operation. Computational modeling is a powerful TAVR clinical planning tool that can lead to excellent patient outcomes. Its accuracy is very promising when compared to post operation data and is rapidly expanding its use to encompass more clinical risks. TAVR use in BAV patients has proven to be very complex and increased risk compared to tricuspid diseased patients however, is rapidly increasing in popularity. Computational modeling can greatly assist in the transition of normal TAVR use for BAV patients by offering safe techniques and guidelines unique for each patient. 1. Siu, S.C. and C.K. Silversides, Bicuspid aortic valve disease. Journal of the American College of Cardiology, 2010. 55(25): p. 2789-2800. 2. Yutzey, K.E., et al., Calcific aortic valve disease: a consensus summary from the Alliance of Investigators on Calcific Aortic Valve Disease. Arteriosclerosis, thrombosis, and vascular biology, 2014. 34(11): p. 2387-2393. 3. Yoon, S.-H., et al., Bicuspid aortic valve morphology and outcomes after transcatheter aortic valve replacement. Journal of the American College of Cardiology, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Unraveling the Implications of Finite Specimen Size on the Interpretation of Dynamic Experiments for Polycrystalline Metals through Numerical Simulations

Author(s): *Bryan Zuanetti, *Los Alamos National Laboratory*; Darby Luscher, *Los Alamos National Laboratory*; Kyle Ramos, *Los Alamos National Laboratory*; Cynthia Bolme, *Los Alamos National Laboratory*;

Normal (NPI) and/or combined Pressure-shear (PSPI) plate impact experiments are often employed for studying the mean-field macroscopic response of polycrystalline metals under dynamic loading. However, even for high symmetry metals such as those with a Face-Centered Cubic (FCC) crystal structure, their single crystal or multi-crystal response is inherently anisotropic. The contribution to uncertainties in the macroscale response of polycrystalline metals resulting from the heterogeneity at smaller scales remains an open question in the literature. In the present study, we perform direct numerical simulations (DNS) of statistically representative microstructures composed of randomly distributed and orientated equiaxed grains within macroscale polycrystalline specimens subjected to dynamic compression and compression-shear loading. The results from DNS are reviewed for the two loading configurations to discuss the effects of grain size on the variability of the macroscale measurements (typically from free surface velocimetry) expected in NPI and PSPI experiments. The results from DNS show that in both cases, the grain size directly correlates with the coefficient of variation in the macroscale measurements, showing a decrease in the coefficient of variation with decreasing grain size. For NPI simulations, after propagating over one millimeter, the coefficient of variation of the elastic precursor amplitude is observed to decrease from approximately 5 – 9 % to 2 – 3 % (for upper and lower values of the HEL) when the grain size was reduced from 200 to 35 μm. Similarly, in PSPI simulations, the coefficient of variation (after the ring-up period) of the transverse free surface particle velocity history was shown to decrease from approximately 5 – 7 % to 1 – 2 % when the grain size (along the shearing direction) was reduced from about 400 to 50 μm. The results from DNS are used to generate a distribution of predicted outcomes, which are compared to the prediction from a dislocation kinetics-based isotropic plasticity model developed in our previous study, to ascertain the limits of agreement that can be reasonably expected between the isotropic model against experimental data on pure polycrystalline aluminum. This information is expected to provide a quantitative framework for guiding the parameterization of isotropic plasticity models when correlating with macroscale measurements in dynamic experiments on polycrystalline metals with a finite specimen size.

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Title: A Stable GFEM ersion Based on Nonconventional Partitions of Unity for Constructing Shape Functions

Author(s): *Caio Ramos, *University of Sao Paulo*; Sergio Proença, *University of Sao Paulo*; Murilo Bento, *University of Sao Paulo*;

The methodology adopted aims to achieve a version for the Generalized Finite Element Method (GFEM) that proves to be efficient and stable. Nonetheless, the main conceptual fundamentals of the method are preserved. In this sense, we seeked to preserve optimal order of convergence and conditioning comparable to the conventional Finite Element Method (FEM). Such aspects can be essentially contemplated by guaranteeing the linear independence of the shape functions, typically generated by enriching the Partition of Unity (PU). Basically the alternative herein adopted to achieve the above mentioned goals, consists in the use of appropriate bases for the generation of the enriched shape functions (for example, flat-top or nonconventional trigonometric PUs). Different aspects involved in the numerical implementation will be addressed, in addition to error convergence analyses to demonstrate the optimal convergence rates and computational efficiency gains. Applications to be presented include two and three-dimensional analysis. In this regard, we outline the extension of the shape function formulation based on the flat-top and trigonometric PU to the tetrahedral element.

16th U.S. National Congress on Computational Mechanics
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Title: Physics-Based Data-Driven Discovery of Continuum Equations

Author(s): *Celia Reina, *University of Pennsylvania*;

Can atomistic simulations tell us their corresponding evolution equations in the continuum limit? Can a non-equilibrium process be interpreted as an equilibrium one? In this talk, various coarse-graining strategies will be discussed to elucidate these questions, and provide important connections between atomistic and continuum models.

16th U.S. National Congress on Computational Mechanics
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Title: Risk-Averse Optimal Experiment Design Using R-Optimality for Vibration Control Inverse Problems

Author(s): *Chandler Smith, *Sandia National Laboratories*; Drew Kouri, *Sandia National Laboratories*; Timothy Walsh, *Sandia National Laboratories*;

Goal of ground-based vibration testing is to inexpensively emulate desired field responses, such as those measured during expensive flight tests, by controlling vibration sources. This problem can be formulated as a PDE-constrained inverse problem for the unknown boundary conditions. However, the predictive capabilities of the calibrated model are typically unreliable since the measured data is imperfect and represents a sparse subset of the full-field system response. In this talk, we formulate and solve an optimal experiment design (OED) problem to intelligently place sensors that minimize a conservative measure of prediction uncertainty. In particular, we investigate a new risk-adapted optimality criterion called R-optimality and compare its performance with that of the traditional I- and G-optimality criteria. R-optimality seeks a user weighted risk-averse design that balances the trade-off between minimizing worst-case prediction variance (G-optimality), which may be overly conservative, and average prediction variance (I-optimality), which does not penalize heavy tailed statistics. We apply the R-optimality criterion to the Box Assembly with Removable Component (BARC) model for ground-based vibration testing and leverage massively parallel computing capabilities to solve the resulting OED problem.

16th U.S. National Congress on Computational Mechanics
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Title: Computational Model For Biochemical Transport In Large Arterial Thrombus Neighborhood

Author(s): *Chayut Teeraratkul, *University of Colorado Boulder*; Debanjan Mukherjee, *University of Colorado Boulder*;

Pathological blood clotting or thrombosis is the primary cause of most major cardiovascular diseases worldwide. Blood flow and biochemical transport around a thrombus are central to thrombus growth, disease progression, and thrombolysis. A comprehensive understanding of such phenomena is central to evaluation of stroke scenarios and treatment planning efficacy. Specific examples include: (a) thrombolytic drug transport to thrombus site and subsequent permeation efficacy into the thrombus; (b) thromboxane and ADP released from thrombus aggregate which further activate platelets and promotes disease progression. Computational approaches offer a non-invasive method to study flow and transport around a thrombus. Realistic arterial thrombi are aggregates of platelets and fibrin strands which makes their micro-composition highly heterogeneous and variable among each individual thrombus. Thrombus microstructural features play a significant role in flow driven permeation and transport inside the thrombus [1]. Comprehensive investigation of thrombus-hemodynamics interactions requires resolving both the fast macro-scale transport around the thrombus and the slower micro-scale diffusion dominated transport inside the thrombus simultaneously. Resolving this inherent multiscale nature of the system is a key challenge. Previous attempts have been made to study transport process in thrombi using microscale particle-based approaches as well as a continuous media approach [2]. Comprehensive three-dimensional unsteady models which resolve the microstructural features of the thrombus are rare. In prior works, we proposed a hybrid particle-continuum approach which allow for variations in thrombus shape and microstructure independent of the computational domain discretization [3]. Using this approach, here we devised a microstructure aware model for unsteady multiscale biochemical species transport within and around a three-dimensional arterial thrombus. We present numerical investigations of transient flow and transport inside and around a large arterial thrombus. We demonstrate the formation of coherent flow structures which organizes advective transport of biochemical species around the thrombus. Finally, the role of permeation processes at the thrombus boundary and the transport to and from the thrombus is illustrated. [1] C. Teeraratkul, and D. Mukherjee. Microstructure Aware Modeling Of Biochemical Transport In Arterial Blood Clots. bioRxiv 2021.01.25.428179; 2021. [2] K. Leiderman and A. Fogelson. An overview of mathematical modeling of thrombus formation underflow.Thrombosis research, 133:S12–S14, 2014. [3] D. Mukherjee and S. Shadden. Modeling blood flow around a thrombus using a hybrid particle–continuum approach. Biomechanics and Modeling in Mechanobiology, 17(3):645–663, 2018

16th U.S. National Congress on Computational Mechanics
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Title: Mesh Convergence Study for Fluid-Structure Interaction Problems Using Non-Conforming Methods

Author(s): *Chen Shen, *Rensselaer Polytechnic Institute*; Scott Miller, *Sandia National Laboratories*; Lucy Zhang, *Rensselaer Polytechnic Institute*;

In this study, we present a mesh convergence study approach for fluid-structure interaction (FSI) problems modeled using non-conforming mesh techniques. Non-conforming meshing techniques such as the Immersed Boundary method (IB), the Immersed Interface method (IIM), the Immersed Finite Element Method (IFEM), and fictitious domains, etc. are emerging to be popular approaches to model multiphysics problems for their robustness in handling independent meshes and moving interfaces. However, as of now, only heuristic guidelines have been provided to ensure system solution convergence and stability. A rigorous approach in performing mesh convergence study for non-conforming meshing techniques is necessary. In this work, mesh convergence is defined as a combination of mesh compatibility and mesh sensitivity. Mesh compatibility refers to the compatibility between the mesh sizes of the overlapping domains; while given a compatible mesh size ratio, the mesh sensitivity determines the accuracy of the numerical solutions. Our study shows that the mesh compatibility test is vital to the FSI solution stability, a pre-requisite for accuracy. Specifically, we show that rather than the individual solid/fluid mesh that determines convergence of the solution, it is the solid/fluid mesh size ratio that dominates solution convergence. Once the mesh compatibility range is determined, then the mesh sensitivity study can further determine the accuracy of the solution by varying either the fluid or the solid mesh size. We systematically performed both the mesh compatibility and sensitivity tests for two FSI examples. The first example is a thin solid structure blocking the fluid flow where the numerical stability needs to be strictly satisfied to preserve the sharp jump occurring at the interface. We performed a mesh convergence test by first identifying the range of compatibility ratios for a very thin (one-layer) solid structure. The accuracy (convergence rate) of the numerical solution is then performed by changing either the solid or the fluid mesh. The second case is a 3-D flow past a cantilever beam to demonstrate that our definition can be extended to any general FSI problems. For the first time, this work creates a paradigm to systematically study the subtlety that lies within the mesh convergence studies when using the non-conforming mesh techniques.

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Title: Massively Parallel Implementation of the Finite Cell Method on Incomplete Octrees

Author(s): *Cheng-Hau Yang, *Iowa State University*; Kumar Saurabh, *Iowa State University*; Hari Sundar, *The University of Utah*; Adarsh Krishnamurthy, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

We present an open-source implementation of the Finite Cell method integrated with octree meshes for highly efficient and accurate structural simulations. A novel incomplete octree based adaptive discretization approach allows carving out arbitrarily shaped regions from a bounding hyper-cube. In conjunction with parallel incomplete octree-based top-down and bottom-up traversal methods, the computational framework enables us to perform efficient finite element (FE) computations on arbitrary carved out regions. Such a strategy allows high-order finite elements, adaptive quadrature, and Nitsche's method to weakly enforce Dirichlet boundary conditions on the immersed geometries. We demonstrate the scalability of the proposed method up to 30,000 processors. We illustrate this approach for small and large deformation linear elasticity problems.

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Title: Fault-Tolerant Meshing Workflow in ANSYS Fluent

Author(s): *Chenglong Wang, *Ansys Inc.*; Nagendra Gannamanedi, *Ansys Inc.*; Hamid Ghazialam, *Ansys Inc.*; Elijah Gravenhorst, *Ansys Inc.*;

Commercial computational fluid dynamics (CFD) software has come a long way in the last few decades. It has become a standard tool for all levels of engineering expertise, assisting prototype design and model optimization for product development. Different commercial software offers different capabilities and ease-of-use. However, there are still technical challenges to utilizing computer-aided design (CAD) models for CFD analysis. Challenges include automatic de-featuring of inconsequential details and automatic repairing of leakages, overlaps, intersections, and other geometry defects that are commonly found in CAD models. According to~\citet{Hughes05a}, analysts spend 80\% of their design time generating the CFD mesh for their CAD, using an inefficient process that lacks reliability. Meanwhile, the interface for CFD software is less than user-friendly, requiring a lot of time for the user to understand the interface well enough to generate meshes from complex models. In this work, we present a new fault-tolerant meshing workflow for CFD analysis that can directly use the CAD models from complex assemblies to automatically generate a high quality mesh using the Cartesian shrink-wrapping technique. We have implemented a workflow in ANSYS Fluent and have performed multiple simulations of exterior aerodynamics cases to verify the accuracy and efficiency of our new workflow which can reduce the design time from days to hours. The proposed fault-tolerant meshing workflow will significantly shorten and streamline the geometric preprocessing and provide a high fidelity mesh for CFD analysis.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physics Informed Neural Networks for Extracting Phenomenological Models from Molecular Dynamics Simulations.

Author(s): *Chih-Hsuan Yang, *Iowa state University*; Balaji Pokuri, *Iowa state University*; Shi Li, *University of Kentucky*; Martin Bazant, *Massachusetts Institute of Technology*; Chad Risko, *University of Kentucky*; Baskar Ganapathysubramanian, *Iowa State University*;

Continuum approaches that model morphology evolution of organic thin films can account for macro scale effects like evaporation rates and fluid shear stresses. However, the phenomenological model (here, the free energy) is generally incorrectly calibrated, making it insensitive to the underlying molecular architecture and interactions. Recent efforts have focused on constructing this free energy from molecular simulations. Here, we use a physics informed neural network as a mechanism to extract the free energy landscape from a finite set of molecular simulations. The physics informed neural network acts as an inverse mapping between continuum models (here, the Cahn-Hilliard and Alan-Cahn equations) and corresponding molecular simulations exhibiting phase change (Allen-Cahn) or phase separation (Cahn-Hilliard). We illustrate the approach using canonical problems, including binary phase separation and solidification. This opens up the way for systematic MD-continuum simulations while ensuring that a minimal number of compute-intensive MD simulations are required.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Nonlocal-to-Nonlocal Coupling via Subdomain-Dependent Kernels

Author(s): *Christian Vollmann, *Trier University*; Volker Schulz, *Trier University*;

We discuss a nonlocal convection-diffusion model on a bounded domain with a subdomain-dependent kernel. More precisely, we assume that the domain is divided into several disjoint subdomains. The governing kernel is assumed to have bounded support and to vary on the possible combinations of subdomains. The resulting model can be interpreted as nonlocal-to-nonlocal coupling. The diffusion case has been studied for a two-domain setting in [1] and is also related to the nonlocal domain decomposition framework presented in [2]. Here, we discuss the case of a possibly nonsymmetric kernel and also provide a two-domain example where we are able to identify the two subdomains from a given solution via shape optimization [3]. REFERENCES [1] G. Capodaglio, M. D'Elia, P. Bochev, M. Gunzburger, An energy-based coupling approach to nonlocal interface problems, Computers and Fluids, 2020, arXiv:2001.03696. [2] G. Capodaglio, M. D'Elia, M. Gunzburger, P. Bochev, M. Klar, C. Vollmann, A general framework for substructuring-based domain decomposition methods for models having nonlocal interactions, submitted, 2020, arXiv:2008.11780. [3] V. Schulz and C. Vollmann: Shape Optimization for Interface Identification in Nonlocal Models, 2019, arXiv:1909.08884

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Accelerating the Simulation of Highly Stiff HVAC Systems with Continuous-Time Echo State Networks

Author(s): *Christopher Rackauckas, *Massachusetts Institute of Technology*;

Acausal mechanical systems which arise from component-based modeling, such as HVAC systems, are differential algebraic equations with a highly stiff irregular construction which can be difficult to capture with many model order reduction techniques. However, efficient and high fidelity simulation of these systems is required in order to design energy efficient buildings. Thus we investigated the development of data-driven surrogates for accelerating the simulation of these systems. In this talk we will highlight a new data-driven surrogate technique, the continuous-time echo state network (CTESN), and show it it utilizes a global training via SVD-factorization in order to model highly ill-conditioned systems. We will demonstrate how the continuous nature of the surrogate exploits the information of adaptive differential-algebraic equation solvers to highlight essential training points for the surrogate in order to reduce the time cost and increase the accuracy. Specifically, we will show how typical data-driven surrogates, such as echo state networks, recurrent neural networks, and physics-informed neural networks, fail to train on these highly stiff systems due to gradient pathologies which are present in the training, while the CTESN's architecture completely avoids this difficulty. We showcase how on these HVAC systems the Julia SciML differential equation solvers accelerate the simulation of the HVAC system 6x over the Dymola Modelica compiler, while the CTESN surrogate then brings the acceleration to 60x-560x. We will end by highlighting the upcoming work on a new acasual modeling language with automated data-driven surrogatization via CTESNs.

16th U.S. National Congress on Computational Mechanics
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Title: Coupled Mechanical-Electrochemical Phase-Field Model for Crack Propagation and Li Dendrite Growth in Solid-State Battery

Author(s): *Chunhao Yuan, *University of North Carolina at Charlotte*; Jun Xu, *University of North Carolina at Charlotte*;

All solid-state batteries (ASSBs) are considered as the promising candidates to replace conventional lithium-ion batteries due to the safety performance of nonflammable inorganic solid electrolyte and significant improved energy density based on the pure lithium metal electrode. However, dendrite growth and interface defects are two fatal issues hindering the commercialization of ASSBs. Although solid electrolyte is much harder than liquid electrolyte, lithium dendrite is still able to grow within the interface defects and grain boundaries. To further understand the inner mechanism of dendrite growth, especially under mechanical pressure, a coupled electrochemical-mechanical phase-field model for crack propagation and dendrite growth is proposed in this study. The effects of pre-defect patterns and stacking pressure are comprehensively investigated. Results show that longer defect with sharp edge and angle causes more severe crack propagation thus larger dendrite growth area, due to larger Von Mises stress and strain energy density. The pre-defect within grain plays an irrelevant role in the dendrite growth within the grain boundary. Stacking pressure greater than 10 MPa significantly speeds up crack propagation as well as dendrite growth due to large mechanical driving force. On the other hand, pressure below 10 MPa has little influence on dendrite growth and crack propagation, which may be applied to improve the interface properties without sacrificing safety performance. The developed multiphysics phase-field modeling framework in this study is generally applicable for ASSBs and provides insight for further improvement.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Data Driven Modeling of Interfacial Traction Separation Relations Using a Thermodynamically Consistent Neural Network

Author(s): *Congjie Wei, *Missouri University of Science and Technology*; Jiaxin Zhang, *Oak Ridge National Laboratory*; Kenneth Liechti, *The University of Texas at Austin*; Chenglin Wu, *Missouri University of Science and Technology*;

For multilayer structures, interfacial failure is one of the most important elements related to device reliability. For cohesive zone modelling, traction-separation relations represent the adhesive interactions across interfaces. However, existing theoretical models do not currently capture traction-separation relations that have been extracted using direct methods, particularly under mixed-mode conditions. Given the complexity of the problem, models derived from the neural network approach are attractive. Although they can be trained to fit data along the loading paths taken in a particular set of mixed-mode fracture experiments, they may fail to obey physical laws for paths not covered by the training data sets. In this paper, a thermodynamically consistent neural network (TCNN) approach is established to model the constitutive behavior of interfaces when faced with sparse training data sets. Accordingly, three conditions are examined and implemented here: (i) thermodynamic consistency, (ii) maximum energy dissipation path control and (iii) J-integral conservation. These conditions are treated as constraints and are implemented as such in the loss function. The feasibility of this approach is demonstrated by comparing the modeling results with a range of physical constraints. Moreover, a Bayesian optimization algorithm is then adopted to optimize the weight factors associated with each of the constraints in order to overcome convergence issues that can arise when multiple constraints are present. The resultant numerical implementation of the ideas presented here produced well-behaved, mixed-mode traction separation surfaces that maintained the fidelity of the experimental data that was provided as input. The proposed approach heralds a new autonomous, point-to-point constitutive modeling concept for interface mechanics.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Functional Tensor Network Approximations for Earth System Models

Author(s): *Cosmin Safta, *Sandia National Laboratories*; Alex Gorodetsky, *University of Michigan*; John Jakeman, *Sandia National Laboratories*; Khachik Sargsyan, *Sandia National Laboratories*;

Sensitivity analysis and model calibration studies for large scale models are challenged by both the large computational cost and large number of parameters typically associated with these models. These challenges are exacerbated by the non-linear input-output dependencies that limit the number of reduced-order techniques that could be leveraged in these studies. In this work we focus on the E3SM land component, and we exploit its internal structure to construct low-rank functional tensor network surrogates that model the spatio-temporal dependencies for select quantities of interest. We present a set of functional representations and model construction techniques to create parsimonious approximations commensurate with the flow of information between various model components. We investigate the efficiency of this approach for uncertainty quantification studies at both regional and global scales.

16th U.S. National Congress on Computational Mechanics
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Title: Stress-Based Multi-Material Topology Optimization to Prevent Interface Fracture

Author(s): *Daiki Watanabe, *Nagoya University*; Hiroya Hoshiba, *Nagoya University*; Junji Kato, *Nagoya University*;

Multi-materialization attracts attention in advanced structure designs and is promoted to satisfy various mechanical properties such as strength, stiffness and weight in industries. For this reason, many multi-material topology optimization techniques have been proposed so far. However, some fundamental and important problems have yet to be solved from a viewpoint of the structural design. One of the difficulties is that it is complicated to formulate the stress-based multi-material topology optimization when mechanical behaviour on the interface between materials is considered while ensuring material interface strength is particularly vital for their integrity and durability because bonding of materials with adhesives can lead to brittle behaviour of the adhesive over time, which can lead to dangerous fracture. To the best of theauthors? knowledge, a method which considers the strength of both materials and the interface has yet to be established. Under this circumstance, we propose a multi-material topology optimization method which satisfies the allowable strengths of each material and the interface. In this study, we use DMO approach because it is suitable when considering multiple material properties such as Young?s modulus, strength, and weight. Furthermore, we adopt the gradient-based interface representation to evaluate the strength of the interface on density-based methods which cannot describe the boundary explicitly.

16th U.S. National Congress on Computational Mechanics
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Title: Reduced Order Homogenization of Polycrystalline Materials Undergoing Large Deformation

Author(s): *Damin Xia, *Vanderbilt University*; Caglar Oskay, *Vanderbilt University*;

In this study, we present a novel finite-strain reduced order computational homogenization formulation for analysis of structures made of polycrystalline materials. The proposed formulation leverages and generalizes the principles of the Eigenstrain-based reduced order homogenization (EHM) approach [1]. At the microstructural scale, the deformation behavior characteristic volume (e.g., representative or statistical volume element) of the material is modeled using crystal plasticity constitutive laws. In particular, rigid-crystal plasticity is considered in the present formulation. Asymptotic analysis with multiple scales is employed to decompose the original governing equations into a microscopic problem defined over the characteristic volume and a macroscopic problem defined over the structure. The model order reduction is applied on the microstructure problem by employing the idea of representing the inelastic rate of deformation using microstructure scale influence functions and a coarse basis approximation of the microstructure kinematics. The constitutive equation at the microscale is approximated in terms of a two-term Taylor Series expansion. An efficient implementation scheme is proposed to evaluate the multiscale system without the need to recompute the reduced basis as a function of evolving deformation. The accuracy and efficiency characteristics of the reduced order model in capturing homogenized and localized behavior as well as texture evolution is demonstrated by comparing with crystal plasticity finite element simulations in the context of single crystal and polycrystal microstructures. References [1] Zhang X, Oskay C. Eigenstrain based reduced order homogenization for polycrystalline materials. Computer Methods in Applied Mechanics and Engineering, 2015, 297: 408-436.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Hypercomplex-Variable Finite Element Method-Based Inverse Methodology to Extract Constitutive Parameters Using Experimental Data

Author(s): *Daniel Ramirez Tamayo, *The University of Texas at San Antonio*; Ayoub Soulami, *Pacific Northwest National Laboratory*; Varun Gupta, *ExxonMobil Upstream Research Company*; Arturo Montoya, *The University of Texas at San Antonio*; Harry Millwater, *The University of Texas at San Antonio*;

The structural performance prediction of a joint requires mechanical characterization of the interface resulting from the joining process. Cohesive zone modeling (CZM) is a popular approach to investigate fracture, seams, and joints in structures. The CZM requires a cohesive constitutive law, which in the context of a welded joint, relates the tractions at the interface to the separation displacement of the two surfaces. The existing mechanical test techniques to obtain the parameters for a cohesive law place restriction on the test geometries and require the existence of analytical solutions, making those techniques unsuitable for dissimilar joints produced using, for example, friction stir technique. In order to address this challenge, we developed a novel approach that utilizes the full-field kinematic measurements from a suitable test geometry obtained using the Digital Image Correlation (DIC) procedure and inversely identifies the cohesive parameters by solving an optimization problem. The desired interfacial parameters will be estimated as the solution of a nonlinear optimization problem where the objective function will quantify the discrepancy between the experimental data obtained from DIC procedure and the analogous quantities computed from the finite element simulation of the corresponding test geometry. A key ingredient in this proposed approach is the sensitivity analysis with respect to the unknown parameters. These sensitivities are useful to solve the optimization problem using an accurate and efficient gradient-based method. The hypercomplex-variable finite element method, ZFEM a specialized computational method developed by the research group at UTSA, was enhanced to carry out the sensitivity analysis within the Abaqus commercial finite element program. The use of ZFEM's accurate derivatives to inversely determine material parameters was demonstrated for several examples. First, the cohesive material parameters of the adhesive were be determined using a double cantilever beam test using both, synthetic and experimental data. Then, the cohesive material properties that govern the interfacial behavior of a joint resulting from a friction stir weld were obtained using DIC data from a T-peel test. Last, the mechanical properties of steel DP-590 were obtained using a tensile test specimen. The results showed the value of using highly accurate and truncation error free first order derivatives: the parameters determined using ZFEM were superior to those obtained using finite difference and a non-gradient optimization method, and were obtained in less computational time.

16th U.S. National Congress on Computational Mechanics
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Title: Calibration of Elastoplastic Constitutive Model Parameters from Full-Field Data with Automatic Differentiation-Based Sensitivities

Author(s): *Daniel Seidl, *Sandia National Laboratories*; Brian Granzow, *Sandia National Laboratories*;

Two of the most widely used inverse methods in experimental mechanics are finite element updating (FEMU) and integrated digital image correlation (IDIC). Both approaches take full-field displacement or strain measurements provided by digital image or volume correlation techniques as input and produce estimates of constitutive model parameters. In these methods the finite element model is typically treated as a black box and is used to produce finite difference (FD) approximations of the objective function gradient or forward sensitivity matrices required for Gauss-Newton optimization. The cost of computing these approximations scales with the dimension of the parameter space, as a full nonlinear finite element solve is required for each component of the parameter vector. Techniques from local sensitivity analysis have been applied in various fields to produce numerically-exact sensitivities though the formulation and solution of auxiliary linear partial differential equations (PDEs). They require an invasive modification of standard finite element formulations, but they also reduce the computational cost of inversion relative to techniques that use FD approximations. There are two primary challenges with the application of such methods to plasticity models. The first is the proper treatment of the coupled nature of the internal variables evolution equations and the equilibrium PDE in the derivation of the sensitivity computations. The second is the history-dependence inherent in these models, which causes the sensitivity matrices or adjoint variables to vary in time. A key aspect of our approach is the reliance on automatic differentiation (AD) to compute derivatives of the constraints and objective function required for gradient-based optimization. We present results from our AD-based approach and compare its accuracy and computational cost to FD FEMU for parameter estimation in a finite deformation J2 plasticity model driven by synthetic DIC data.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling of Orthotropic Hygrothermal Behavior for Various Wood Species Based on Collected Isotherm Database

Author(s): *Danyang Tong, *Northwestern University*; Brown Susan Alexis, *Northwestern University*; David Corr, *Northwestern University*; Gianluca Cusatis, *Northwestern University*;

Wood and wood composites interest many researchers and engineers due to their great potential as a sustainable substitute for traditional concrete structures. However, the sensitivity of timber to changes in humidity and temperature creates challenges in the design process. Specifically, the mechano-sorptive effect, where the wood is subjected to cyclic moisture content under constant loading. This effect leads to increased viscosity and a corresponding increase in the creep phenomenon, regardless of the magnitude of loading. To accurately capture the long-term effects of environmental changes on wood, heat and moisture transfer is investigated for structural applications. A database is compiled of the nonlinear isotherm curves for various wood species, where the internal moisture content of timber was obtained according to external relative humidity cycling based on different wood species. A hygrothermal finite element model was developed based on the mass balance between water vapor in the environment and bound water in cell walls for moisture transport, and energy balance for heat conduction by using the classical form of Fourier's Laws. After analysis, the GAB isotherm model (Themelin 1998) was implemented in the hygrothermal model to obtain nonlinear behavior of moisture diffusion through wood. Consideration for the orthotropic behavior is reflected by a diffusion parameter matrix. To validate the model, several experimental tests were used, which including variations in dimensions, species, and material directions. Moisture permeability parameters for all directions were fit to the data. The comparison of numerical results with experimental tests gives satisfactory results for all data. The hygrothermal model can display a very non-linear adsorption or desorption process and in a large humidity range. It was also observed from the results that the parameter values for permeability largely depends on species, indicating a diffusion database according to wood species is critical for structural application. [1] Themelin, A., 1998. Comportement en sorption de produits ligno-cellulosiques. BoisFor. Trop. 256, 55–67.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: E-Optimum Sensor Selection for Estimating a Subset of Parameters

Author(s): *Dariusz Ucinski, *University of Zielona Gora*;

A fundamental problem towards parameter estimation of spatiotemporal systems described by partial differential equations is sensor location. Although engineering judgment and trial-and-error procedures are quite often used, some systematic means should still be developed in order to reduce the cost of instrumentation and the efficiency of the identifiers. The most common approach consists in quantifying the quality of sensor configurations through various measures defined on the Fisher information matrix (FIM) associated with the estimated parameters. One of these measures to be minimized is the E-optimality criterion, which is the maximum eigenvalue of the inverse of the FIM. Its use amounts to minimizing the largest asymptotic variance of the least-squares estimator. This criterion is more involved than others due to its nondifferentiability in case a multiple maximum eigenvalue is observed. In this contribution an even more difficult problem is considered, in which interest is in accurately estimating only a subset of unknown parameters while the accuracy of the other parameters is of no importance. An additional difficulty that arises here is that the FIM may tend to be be singular when approaching an optimal solution. This problem is investigated in the context of selecting gauged sites from among a given number of accessible sites. A convex relaxation of this highly combinatorial problem is proposed here. Then a simple computational algorithm is set forth for minimizing the largest eigenvalue of the inverse of the FIM associated with the parameters of interest over the set of all convex combinations of a finite number of nonnegative definite matrices subject to additional box constraints on the weights of those combinations. The potential singularity of the FIM is avoided through imposing the additional constraint that the D-efficiency of the optimal solution evaluated for all unknown parameters must be no less than an arbitrary positive threshold. The idea of the algorthm is to apply the method of outer approximations for solving the associated convex semi-infinite programming problem, which reduces to solving a sequence of finite min-max problems. A key novelty here is that solutions to the latter are found using generalized simplicial decomposition, which is a recent extension of the classical simplicial decomposition to nondifferentiable optimization. Thereby, the dimensionality of the design problem is drastically reduced. The use of the algorithm is illustrated by an example involving a large sensor network collecting measurements for parameter estimation of a spatiotemporal process.

16th U.S. National Congress on Computational Mechanics
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Title: Sensitivity and Uncertainty Quantification Analysis in Phononic Metamaterials through Complex-Variable Finite Element Method

Author(s): Juan David Navarro, *The University of Texas at San Antonio*; Matthew Balcer, *The University of Texas at San Antonio*; Harry Millwater, *The University of Texas at San Antonio*; *David Restrepo, *The University of Texas at San Antonio*;

The new kind of materials called metamaterials has captured the attention of researchers in recent years. Remarkable mechanical properties like negative stiffness, negative density, and negative bulk modulus have been achieved by designing the unit cell's geometry. Also, periodic phononic metamaterials lead to frequency band gaps in their dispersion diagrams. This exciting property is found to be useful in different applications, such as noise absorption and seismic wave abatement. However, the bandgap behavior is extremely sensitive to small variations in the unit cell. Current manufacturing techniques used to produce periodic metamaterials, such as additive manufacturing, does not ensure mechanical or geometric consistency to preserve theoretical predictions. Therefore, it is of primal importance to investigate and quantify the band gaps' sensibility to the different parameter variations to close the breach between the scientific predictions and the industrial applications. In this talk, we will present a new computational methodology to perform parameter sensibility and uncertainty quantification in the dispersion relation of phononic metamaterials. The method is based on the complex-variable finite element method (ZFEM) coupled with Bloch's periodic boundary. Preliminary results show that our proposed method can reproduce probability density functions with the same accuracy as Monte Carlo modeling and polynomial chaos but at a fraction of the computational cost.

16th U.S. National Congress on Computational Mechanics
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Title: Variational Multiscale Large Eddy Simulations for Very High Rayleigh Number Rayleigh-Benard Convection

Author(s): *David Sondak, *Harvard University*; Thomas Smith, *Sandia National Laboratories*; Roger Pawlowski, *Sandia National Laboratories*; Sidafa Conde, *Sandia National Laboratories*; John Shadid, *Sandia National Laboratories*;

High Rayleigh number (Ra) large eddy simulations (LES) are performed for Rayleigh-Benard convection in two and three dimensions for two different Prandlt (Pr) numbers. A new family of LES models is developed based off the residual-based variational multiscale (VMS) formulation. The resulting mixed model uses the VMS formulation to model cross-stress terms and the Wall-Adapting Local Eddy-viscosity (WALE) model to model Reynolds stresses. The models were incorporated into the finite element code Drekar and simulations were run for 10^6 < Ra < 10^15. The two-dimensional simulations were performed for Pr=1 in a domain with aspect ratio 2 whereas the three dimensional simulations were conducted in a cylinder of aspect ratio 1/4. The primary diagnostic parameter in Rayleigh-Benard convection is the non-dimensional heat transport, represented by the Nusselt number (Nu). The scaling of Nu with Ra of the mixed model LES is in excellent agreement with the existing direct numerical simulations. We also consider the effect of diffusive flux reconstruction in the VMS residuals, describe generalizations of the mixed model to rotating Rayleigh-Benard convection, and show early results of simulations for the rotating system.

16th U.S. National Congress on Computational Mechanics
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Title: Application of Mass Lumping and Nodal Quadrature to the Immersed Boundary Finite Element Method

Author(s): *David Wells, *University of North Carolina at Chapel Hill*; Ben Vadala-Roth, *US Army Engineer Research and Development Center*; Jae Ho Lee, *Johns Hopkins University*; Boyce Griffith, *University of North Carolina at Chapel Hill*;

The immersed-boundary finite-element (IBFE) method couples an immersed and neutrally buoyant structure to a fluid. In the IBFE method, the structure is discretized with the finite element method and typically uses an explicit time integration scheme, while the fluid is discretized with a finite difference method on an Eulerian grid. The structure's evolution and coupling equations are a good candidates for mass lumping, meaning that the consistent linear systems used at each time step are replaced by diagonal and inconsistent versions. This presentation examines the effects of this replacement both for evaluation of the structure's stress and for the IB coupling operators. We perform a theoretical investigation on a potential loss of accuracy and the benefits of replacing both the stress projection and coupling operators with the same lumped scheme. The theory is validated with numerical experiments, including standard solid mechanics tests and examination of a bioprosthetic heart valve.

16th U.S. National Congress on Computational Mechanics
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Title: SCA - Applications to Multiscale Modeling for Self-Piercing Riveting Process

Author(s): *Derick Suarez, *Northwestern University*; Sourav Saha, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

Self-piercing riveting (SPR), a cold-forming process where two similar or dissimilar sheet materials are joined through a rivet via plastic deformation, remains abundant in aerospace and automotive applications, particularly in scenarios where other joining methods such as welding are not satisfactory. Typically expensive and timely experiments are performed to assess SPR joint performance. Therefore, it is lucrative to have an efficient computational model for SPR joint performance prediction. The first step in such a model is accurate prediction of the piercing process itself. In this work we model SPR through a concurrent multiscale finite element simulation using a representative volume element (RVE) to capture the sheet material's underlying microstructure. Previous SPR simulation studies have restricted themselves to 2d macro-scale models to limit computational expense. To ameliorate this deficit, we have leveraged Self-consistent Clustering Analysis (SCA), a data-driven multiscale scheme in which RVE voxel elements are clustered a priori in an "offline" process and voxel elements within the same cluster share the same mechanical response for subsequent arbitrary loading in an "online" process, thereby reducing the computational complexity of the simulation allowing for a full 3D simulation. The multiscale framework presented here provides the basis for bottom-up design and joint prediction for SPR based on the sheet material's microstructure. The model is validated against literature data for a steel rivet and Al6060 T4 plates. In the future, the output of model will be used as the initial state for a fatigue simulation.

16th U.S. National Congress on Computational Mechanics
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Title: Microstructure-Based High Cycle Fatigue Life Prediction Based on A Data-Driven Computational Approach

Author(s): *Dong Qian, *The University of Texas at Dallas*; Rui Zhang, *The University of Texas at Dallas*; Yingjian Liu, *The University of Texas at Dallas*; Derick Suarez, *Northwestern University*; Sourav Saha, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

High cycle fatigue (HCF) is the dominant failure mechanism of many engineering applications. For fatigue life predictions safe-life and damage-tolerance approaches have been used extensively, however, they are limited due to the empirical nature. In this work, I will present a multiscale HCF simulation approach based on integrating the space-time finite element method with an enrichment scheme. The resulting approach is called extended space-time FEM (XTFEM). By augmenting the standard FEM interpolation with enrichment function that represents the problem physics, the XTFEM is capable of handling multiple temporal scales for simulations of the HCF problem [1]. To address the challenge in capturing nonlinear material behavior associated with material microstructures under the HCF loading condition, we established a microstructure-based HCF damage model based on machine learning [2-3] and the Continuum Damage Mechanics (CDM). This implementation enables the direct modeling of complex material microstructures with much reduced computational cost. Finally, Examples of HCF life prediction are presented to demonstrate the robustness of the proposed multiscale approach. References: [1] R. Zhang, S. Naboulsi, T. Eason, and D. Qian. A high-performance multiscale space-time approach to high cycle fatigue simulation based on hybrid CPU/GPU computing. Finite Elements in Analysis & Design, 2019, 166: 103320. [2] Z. Liu, M.A. Bessa, and W.K. Liu. Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials. Computer Methods in Applied Mechanics and Engineering, 2016, 306: 319-341. [3] C. Yu, O.L. Kafka, W.K. Liu. Self-consistent clustering analysis for multiscale modeling at finite strains. Computer Methods in Applied Mechanics and Engineering, 2019, 349: 339-359.

16th U.S. National Congress on Computational Mechanics
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Title: On the Significance of Integration Consistency for Galerkin Meshfree Accuracy

Author(s): *Dongdong Wang, *Xiamen University*; Junchao Wu, *Huaqiao University*;

Numerical integration plays a very important role on the accuracy of Galerkin meshfree methods due to the rational nature of meshfree shape functions and the misalignment of meshfree shape function supports with integration cells. Up to date, many versatile integration schemes have been designed to improve the efficiency and accuracy for Galerkin meshfree methods [1]. However, there still lacks a theoretical foundation which can explains that how numerical integration affects the Galerkin meshfree accuracy. In this work, an accuracy analysis of Galerkin meshfree methods is presented in order to reveal the reason behind the numerical integration [2]. Firstly, an error measure is proposed to evaluate the loss of Galerkin orthogonality condition, which is related to the order of integration consistency for Galerkin meshfree formulation. Subsequently, based upon the proposed orthogonality error measure, both H1 and L2 error estimates are developed for Galerkin meshfree methods. It is shown that the meshfree solution errors essentially contains two parts, one attributes to the standard interpolation error, and the other one is due to the numerical integration error. According to the proposed error estimates, it is evident that for the conventional Gauss integration schemes violating the integration consistency, the solution errors eventually are controlled by the integration error and optimal convergence cannot be achieved even with high order quadrature rules. On the other hand, when consistent integration approaches [3] are employed, the integration and interpolation errors have the same accuracy order which ensures an optimal convergence of Galerkin meshfree methods. Numerical results well conform the proposed theoretical error estimates for Galerkin meshfree methods. Acknowledgements: The support of this work by the National Natural Science Foundation of China (12072302, 11772280) is gratefully acknowledged. References 1. J.S. Chen, M. Hillman, S.W. Chi, Meshfree methods: progress made after 20 years, Journal of Engineering Mechanics-ASCE 143 (2017) 04017001. 2. J. Wu, D. Wang. An accuracy analysis of Galerkin meshfree methods accounting for numerical integration, Computer Methods in Applied Mechanics and Engineering, 375 (2021) 113631. 3. D. Wang, J. Wu, An inherently consistent reproducing kernel gradient smoothing framework toward efficient Galerkin meshfree formulation with explicit quadrature, Computer Methods in Applied Mechanics and Engineering 349 (2019) 628-672.

16th U.S. National Congress on Computational Mechanics
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Title: Investigating the Effect of Grain Structure on Compressive Response of Open-Cell Metal Foam Using High-Fidelity Crystal-Plasticity Modeling

Author(s): *Dongfang Zhao, *The University of Utah*; Kristoffer Matheson, *The University of Utah*; Quinton Johnson, *The University of Utah*; Brian Phung, *The University of Utah*; Steve Petruzza, *Utah State University*; Michael Czabaj, *The University of Utah*; Ashley Spear, *The University of Utah*;

Open-cell metallic foams are hierarchical structural-material systems that have applications as light-weight impact absorbers, noise insulators, and heat sinks, to name a few. The mechanical response of open-cell metallic foams depends strongly on their hierarchical structure, which ranges from the grain scale, to the scale of individual struts, to the scale of the bulk foam. The objective of this study is to investigate the effect of grain structure on the compressive mechanical response of open-cell metallic foam using a crystal-plasticity finite-element-based (CPFEM) framework. Multiple polycrystalline instantiations (overlaid on a foam volume derived from X-ray tomography) are simulated to quantify the grain-size effect on the global compressive response of investment-cast aluminum foam. The high-fidelity numerical framework captures the deformation mechanisms across multiple length scales and is able to predict the inhomogeneous grain-to-continuum compressive response in the foams. Also, by incorporating grain-boundary strengthening and free-surface softening mechanisms, the current framework accounts simultaneously for the Hall-Petch effect in polycrystalline alloys and the effect of unconstrained slip-based deformation at the strut free surfaces. The crystal-plasticity simulations explicitly account for the coupled effects of grain structure and surface conditions (oxidized or non-oxidized) and provide new insights into the mechanical behavior of open-cell metallic foams. Results show that the relationship between grain size and plateau stress in the foams follows a Hall-Petch-like trend provided there is at least approximately one complete grain along the strut length and approximately one grain through the strut thickness; below this threshold, the effective plateau stress of the foam tends to saturate. In the presence of an oxidation layer, when the dislocations are blocked at the strut boundaries, the effect of grain structure on plateau stress is less pronounced than when an oxidation layer is absent. It is also shown that by accounting for grain size and surface condition through the parameters ?_y and C_4, the accuracy and generalizability of the well-established Gibson-Ashby model for plastic collapse strength can be significantly enhanced. The high-fidelity numerical framework is subsequently leveraged to investigate micromechanical failure evolution (e.g., local plastic collapse and fracture initiation) in a real, grain-resolved foam sample characterized in-situ using high-energy X-ray diffraction microscopy (HEDM). Results from the CPFEM simulation are correlated with the 4D experimental observations to provide insight into the micromechanical failure mechanisms of open-cell metallic foam. Zhao, D., et al. (2021). Materials Science and Engineering A. https://doi.org/10.1016/j.msea.2021.140847

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Reduced Deep Networks: a Framework for Nonlinear Model Reduction

Author(s): *Donsub Rim, *New York University*; Luca Venturi, *New York University*; Joan Bruna, *New York University*; Benjamin Peherstorfer, *New York University*;

Nonlinear reduced models of various forms have been introduced recently to overcome the limitations of low-rank linear representations. Reduced deep networks (RDNs) are a sub-class of feedforward deep neural networks whose approximation power strictly supersedes that of their shallower analogues. In this talk, we will introduce RDNs and discuss how previous nonlinear reduced models can be expressed as special cases of RDNs, and how many important notions from classical model reduction such as empirical interpolation generalize to RDNs in a straightforward manner. The computational efficiency of RDNs will be illustrated through numerical examples.

16th U.S. National Congress on Computational Mechanics
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Title: Validating Sub-Grid Scale Approaches for Modeling of Cross-Barrier Flows in Flood Control Systems for Hydrodynamic Storm Hazard Models

Author(s): *Dylan Wood, *University of Notre Dame*; Collin Lester, *The Ohio State University*; Ethan Kubatko, *The Ohio State University*; Mehrzad Rahimi, *The Ohio State University*; Abdollah Shafieezadeh, *The Ohio State University*;

The effective performance of flood control systems is key to mitigating the negative impacts of natural flooding hazards, such as hurricane storm surge, in developed areas. Occasionally, flood barriers such as levees and dykes may permit flows to occur across the top of or through the body of the structure, either by design (e.g., culverts) or by consequence of local flow conditions in excess of design characteristics (e.g., water elevations above the structure crest). Current hydrodynamic models used for assessing impacts of storm flooding apply sub-grid scale approaches, which prescribe cross-barrier flow rates based on empirical or analytical relations. These models include as mechanisms for cross-barrier flow, overtopping by mean sea level rise, overtopping by waves, and piping. Despite the widespread use of these sub-grid scale approaches, they have yet to be thoroughly validated for applications towards storm-hazard modeling. In this study, we present these sub-grid scale methods as well as recent, ongoing and proposed near-future efforts to validate them and improve upon their applications within the context of a hydrodynamic shallow water equations model used for storm hazard modeling, by comparisons to physical measurements as well as to results from more detailed hydrodynamic modeling.

16th U.S. National Congress on Computational Mechanics
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Title: An Adaptive Space-Time FE Method for the Shallow Water Equations

Author(s): *Eirik Valseth, *The University of Texas at Austin*; Clint Dawson, *The University of Texas at Austin*;

We introduce a Petrov-Galerkin method, the automatic variationally stable finite element (AVS-FE) method [1] for the shallow water equations (SWE). This method uses a first order system integral formulation of the underlying partial differential equations (PDEs) and, in the spirit of the discontinuous Petrov-Galerkin (DPG) method by Demkowicz and Gopalakrishnan [2], employs the concept of optimal test functions to ensure discrete stability. The AVS-FE method distinguishes itself by using globally conforming FE trial spaces, e.g., H1and H(div) and their broken counterparts for the test spaces. The broken topology of the test spaces allows us to compute numerical approximations of the local restrictions of the optimal test functions in a completely decoupled fashion, i.e. element-by-element. The test functions are computed with sufficient numerical accuracy by using the same local p-level as applied for the trial space. The unconditional discrete stability of the method allows for straightforward implementation of transient problems into existing FE solvers without the need for additional stability constraints commonly encountered for commonly used time-stepping schemes. Furthermore, a built-in a posteriori error estimate as well as element-wise error indicators allows us to perform adaptive refinements in both space and time. The global trial spaces we consider leads to FE approximations using classical polynomial FE bases such as Lagrangian interpolants and Raviart-Thomas basis functions. Hence, from a user point-of-view the AVS-FE approximations are standard FE solutions. We present numerical veri cations including numerical convergence stud- ies as well as commonly applied benchmark problems for the shallow water equations. [1] Calo, V.M., Romkes, A., and Valseth, E., Variationally Stable Analysis for Finite Element Computations: An Introduction, in: Barrenechea G., Mackenzie J. (eds) Boundary and Interior Layers, Computational and Asymptotic Methods BAIL 2018, Springer, 2020, pp. 19-43. [2] L. Demkowicz and J. Gopalakrishnan. A Class of Discontinuous Petrov-Galerkin Methods. II. Optimal Test Functions. Numerical Methods for Partial Di erential Equations, 27(1):70-105, 2011.

16th U.S. National Congress on Computational Mechanics
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Title: Multiphase Lattice Discrete Particle Model for the Prediction of Early-Age Properties of Cement Paste

Author(s): *Elham Ramyar, *Northwestern University*; Gianluca Cusatis, *Northwestern University*;

Cement-based materials demonstrate heterogeneity at different length scales. The impact of nano-scale characteristics on the macro-scale response is undeniable. At the nano and microscale level, grid-nanoindentation experimental plots reveal the existence of at least five significant phases. These phases are listed as a low stiffness capillary pore, the low-density Calcium-Silicate-Hydrate (CSH), the high-density CSH, Portlandite, and unhydrated cement. Although properties of these phases can be classified as intrinsic characteristics, the formation and distribution of each phase depend on the degree of hydration, mix design, and drying treatments. The change in volume fractions of these phases fundamentally alters the long-term strength, creep, shrinkage, viscoelasticity, and permeability of mesoscale concrete over time. The primary purpose of this study is to develop a computational microscale multiphase model bridge between the micro and mini scale with consideration for the effect of nano and micro pores. To this end, an algorithm was developed for postprocessing the voxelated microstructure cement paste data at different hydration degrees from NIST's CEMHYD3D model [1] which is a three-dimensional cement hydration modeling package. Based on available nanoindentation test results and the significant influence of the above-mentioned cement unhydrated constituents and hydration products on the overall behavior of cement paste, CEMHYD3D's voxelated products are classified into five main phases. It must be pointed out that the current CEMHYD3D model does not differentiate between CSH phases. Therefore, a formulated CSH densification was integrated into the model to calculate variable volume fractions for the CSH phases over time. Finally, the processed data were used to formulate a multiphase Lattice Discrete Particle Model (LDPM) [2] at the sub-micron-scale to simulate the structural behavior of multiphase cement paste. Since the five constituents also vary in time, depending upon hydration, the microstructural model updates over time. The results show that the microscale multiphase LDPM model can accurately predict the linear and nonlinear cement paste behavior at different ages. Bulk properties resulting from the microscale cement-paste model are promising in terms of usability for developing a mini-scale high-resolution model that includes aggregate, interfacial transition zone (ITZ), and cement paste. [1] Bentz, Dale P. (2000). "CEMHYD3D: A three-dimensional cement hydration and microstructure development modeling package", US Department of Commerce, National Institute of Standards and Technology. [2] Cusatis, Gianluca, Daniele Pelessone, and Andrea Mencarelli. (2011) "Lattice discrete particle model (LDPM) for failure behavior of concrete. I: Theory." Cement and Concrete Composites 33(9), 881-890.

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Title: Multilevel Best Linear Unbiased Estimators for Uncertainty Quantification

Author(s): Daniel Schaden, *Technical University of Munich*; *Elisabeth Ullmann, *Technical University of Munich*;

We discuss novel multilevel best linear unbiased estimators (BLUEs) introduced in [1]. The goal is the estimation of the expectation of a scalar-valued quantity of interest associated with a family of multi-fidelity models. The key idea is to reformulate the estimation as a generalized linear regression problem where we treat the output of the computer simulations as observations of an unknown parameter. By construction, BLUEs have the smallest variance among all linear unbiased estimators. Hence the BLUEs use the information provided by the observations optimally and independently of the simulation cost. In a further optimization step, we then construct a specific BLUE which minimizes the estimator variance given a total cost budget. We compare our proposed estimator to alternative multilevel estimators in the literature such as multilevel Monte Carlo, multi-fidelity Monte Carlo, and Approximate Control Variates. In addition, we show that the variance of our estimator approaches a sharp lower bound that holds for any linear unbiased multilevel estimator in the infinite low-fidelity data limit. Finally, we specialize our results to PDE-based models [2] which are parameterized by a discretization quantity, e.g. the finite element mesh size. We prove that in this case the computational cost of the BLUE is not larger than the complexity of multilevel Monte Carlo. In addition, we discuss random elliptic PDE problems where the multilevel BLUE outperforms the state-of-the-art multilevel Monte Carlo estimator. REFERENCES [1] D. Schaden and E. Ullmann, “On multilevel best linear unbiased estimators”, SIAM/ASA J. Uncert. Quantif., 8, pp. 601 – 635 (2020). [2] D. Schaden and E. Ullmann, “Asymptotic analysis of multilevel best linear unbiased estimators”, available from arXiv:2012.03658.

16th U.S. National Congress on Computational Mechanics
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Title: Physics-Informed Neural Networks for Geometry Identification of Inhomogeneities

Author(s): *Enrui Zhang, *Brown University*; Guofei Pang, *Brown University*; Ming Dao, *Massachusetts Institute of Technology*; George Karniadakis, *Brown University*; Subra Suresh, *Nanyang Technological University*;

Identifying the geometry of inhomogeneities within solids is a difficult task, especially for materials governed by nonlinear constitutive relations such as hyperelasticity and plasticity. In this contribution, we propose a unique method based on Physics-Informed Neural Networks (PINNs) [1] for solving inverse problems in continuum solid mechanics involving both material and geometry identification. While the material identification with PINNs involves the parameterization of governing equations that has been extensively studied for problems in various fields [1] including solid mechanics [2], there has been no research regarding geometry identification with PINNs. For the first time, we propose to directly parameterize the computational domain by trainable parameters of the PINN and hence assign geometry-dependent training points accordingly. As a proof of concept, our method is applied to the identification problem of inhomogeneities encompassed in a matrix: with the matrix under static loading, the PINN seeks to identify the unknown geometric (and material) parameters of the void (inclusion) given data of displacement measurement. We test the performance of our method with various problem setups, including different shapes and topologies of the inhomogeneities and different constitutive models (linear elasticity, hyperelasticity, and deformation plasticity). The results show that our method can accurately predict the unknown material and geometric parameters given limited amount of data. By inheriting and extending the applicability and advantages of PINNs, our method provides a generic, unified, flexible framework for a wide range of inverse problems in practice. [1] Raissi, Maziar, Paris Perdikaris, and George E. Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations." Journal of Computational Physics 378 (2019): 686-707. [2] Zhang, Enrui, Minglang Yin, and George Em Karniadakis. "Physics-informed neural networks for nonhomogeneous material identification in elasticity imaging." arXiv preprint arXiv:2009.04525 (2020).

16th U.S. National Congress on Computational Mechanics
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Title: Numerical Modeling of Phase Transformation Induced Material Fracture and Crack Propagation

Author(s): *FNU Sindhusuta, *University of Illinois at Chicago*; Sheng-Wei Chi, *University of Illinois at Chicago*; Craig Foster, *University of Illinois at Chicago*;

Abstract The key mechanisms behind intermediate-depth earthquakes remains a puzzle for the scientific community. However, many studies discussed phase transformation being primary mechanism behind the generation of these damaging earthquakes. The objective of this study is to develop a numerical model for simulation of phase transformation-induced failure in geo-materials. The materials of interest include different groups of minerals found in the earth crust such as granulite, eclogite, and olivine. To model the phase transformation behavior, a thermo-mechanical phenomenological model approach has been taken. A thermodynamically consistent mesoscale model, based on Mahnken et al, 2015, has been developed to capture the evolution of phase transformation taking place in such materials under different pressure and temperature conditions. The model also considers visco-plasticity and heat conduction and uses an averaging scheme to link different length scales. In the numerical scheme, coupled non-linear equations for the evolution of visco-plasticity and phase transformation have been obtained by a staggered algorithm. The algorithm uses Newton's iteration with an active set strategy and a radial return method for obtaining the solution. For the simulation of microstructural failure in the material, the extended finite element method (XFEM) in ABAQUS has been used and the above-mentioned model with phase transformation has been implemented in a user-defined subroutine (UMAT). The model thus obtained will be validated with the data from the experimental study by Shi et al. (2018) showing eclogitization of dry granulite as a trigger for mechanical instability leading to large fault generation. For further study, the model will eventually be upscaled to simulate the fault generation at the macroscale (kilometer-scale) and investigate the role of phase transformation in the formation of large-scale cracks or faults. Keywords: Phase transformation, Fracture, Mesoscale model, Crack propagation References: Mahnken, R., Schneidt, A., Antretter, T., Ehlenbröker, U. and Wolff, M., 2015. Multi-scale modeling of bainitic phase transformation in multi-variant polycrystalline low alloy steels. International Journal of Solids and Structures, 54, pp.156-171. Shi, F., Wang, Y., Yu, T., Zhu, L., Zhang, J., Wen, J., Gasc, J., Incel, S., Schubnel, A., Li, Z. and Chen, T., 2018. Lower-crustal earthquakes in southern Tibet are linked to eclogitization of dry metastable granulite. Nature communications, 9(1), pp.1-13.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling Blasting Induced Rock Fractures with Non-Ordinary State-Based Peridynamics

Author(s): *Fan Zhu, *The Hong Kong University of Science and Technology*; Jidong Zhao, *The Hong Kong University of Science and Technology*;

Blasting has been a primary means for rock excavation in mining and geoengineering. Numerical simulation of blasting induced rock fractures remains a challenging task owning to the complex physical process involved. The material response under blasting load is highly nonlinear and is known to be pressure- and strain rate dependent. Blasting causes significant discontinuities to develop in the rock mass with crack branching, intervening, arresting, and jointing. Those processes remain difficult to simulate with traditional numerical approaches. Peridynamics has recently emerged as an alternative of classical continuum mechanics and has been applied for modelling geomaterials [1]. The method exhibits amiable features for handling discontinuities since it does not involve differentiation of displacement field. Among the various types of peridynamics, the non-ordinary state-based peridynamics (NOSB-PD) [2] is a versatile one that allows implementation of classical stress or strain based constitutive models. In this study we propose a novel computational approach based on the NOSB-PD to model blasting induced rock fractures. The approach is proposed in conjunction with a Johnson-Holmquist (JH2) constitutive model [3] to consider the pressure dependency, strain rate effect, and viscoplasticity of rocks under blasting loads. Fracture is assessed based on the JH2 damage model in conjunction with a tension failure model. The former is used to evaluate the material response pertaining to excessive plastic strain and the latter is employed to gauge failure based on tensile stress in consideration of strain rate effect. 3D simulations of single hole blasting in granite rock are presented and compared with experimental records. The proposed approach is shown to capture reasonably well the plastic material failure surrounding the borehole as well as the tensile cracks on both radial and circumferential directions. The simulated crack density and radial pressures are also comparable with experimental data. The presented computational approach offers a rigorous basis for future development of more versatile, multi-physics-integrated computational framework on rock blasting simulations. References: [1]. Zhu F, Zhao J. A peridynamic investigation on crushing of sand particles, Géotechnique 2019;69(6):526-540. [2]. Silling SA, Epton M, Weckner O, Xu J, Askari A. Peridynamics states and constitutive modeling, J Elasticity 2007;88(2):151–184. [3]. Johnson GR, Holmquist TJ. An improved computational constitutive model for brittle materials. AIP Conf Proc 1994;309(1):981–4.

16th U.S. National Congress on Computational Mechanics
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Title: Computing the Effective Elasticity of Anisotropic Porous Media from X-Ray Computed Micro-Tomography Images

Author(s): *Federico Semeraro, *NASA Ames Research Center*; Marcos Acin, *NASA Ames Research Center*; Francesco Panerai, *University of Illinois at Urbana-Champaign*; Arnaud Borner, *NASA Ames Research Center*; Nagi Mansour, *NASA Ames Research Center*; Jeremie Meurisse, *NASA Ames Research Center*;

Development and optimization of composite materials designed for thermal protection of NASA's spacecraft requires the understanding of their physical response to high-enthalpy environments. To predict their macro-scale properties and behavior, high-fidelity 3D simulations are performed at the micro-scale on realistic representations of these composites. The digital micro-structures are generated either synthetically or through X-ray micro-tomography reconstructions. One of the main challenges in the prediction of heatshield material structural response is the computation of the effective elasticity of the fibrous composite, as well as the understanding of the deformation and stresses generated at the micro-scale. These are driven by the fiber layout within the micro-structure and the distribution of the infused matrix. In this effort, the micro-mechanical linear elastic behavior of fibrous ablators is modeled through the use of a numerical method based on the Multi-Point Stress Approximation (MPSA) finite volume scheme [1]. The MPSA, a generalization of the more commonly used Multi-Point Flux Approximation (MPFA), was discussed in a previous presentation at the 15th USCCN and in reference [2]. To predict the behavior of fibrous and woven architectures, algorithms that compute the local fiber orientation are used [3]. The implementation of the MPSA was verified using analytical solutions, engineering test cases and compared against legacy Finite Element Analysis (FEA) software. The stress analysis models were then applied to real geometries used by NASA in thermal protection systems such as fibrous preforms and woven materials and the results were compared to experimental data. [1] Keilegavlen, Eirik, and Jan Martin Nordbotten. "Finite volume methods for elasticity with weak symmetry." International Journal for Numerical Methods in Engineering 112, no. 8 (2017): 939-962. [2] Semeraro, Federico, Joseph C. Ferguson, Marcos Acin, Francesco Panerai, and Nagi N. Mansour. "Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity." Computational Materials Science 186 (2021): 109956. [3] Semeraro, Federico, Joseph C. Ferguson, Francesco Panerai, Robert J. King, and Nagi N. Mansour. "Anisotropic analysis of fibrous and woven materials part 1: Estimation of local orientation." Computational Materials Science 178 (2020): 109631.

16th U.S. National Congress on Computational Mechanics
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Title: A Probabilistic Learning Approach for Uncertainty Quantification of Oil Reservoir Waterflooding

Author(s): *Fernando Rochinha, *Universidade Federal do Rio de Janeiro*; Jeferson Almeida, *Universidade Federal do Rio de Janeiro*;

Waterflooding is the most common oil secondary recovery strategy, in which water is injected through wells to maintain or increase reservoir pressure and displace oil from the pores of the reservoir rock towards the producing wells [1]. In that context, computational simulation is often applied during field development and management. However, the computational burden of large-scale reservoir simulation is very high, specially in the presence of uncertainties. To consider the uncertainties and study their effects on the quantities of interest (QoIs), several uncertainty propagation methods are available in the literature. Here, to reduce the computational cost with respect to the classical methods, the probabilistic learning methodology (PLoM) proposed in [2] can be used for risk analysis and oil recovery performance in reservoir development and management applications. In this work, risk analysis is carried out by applying the probabilistic learning methodology. The risk of optimal water injection strategies in a waterflooding process is addressed considering a set of geological and economic uncertainties. The reservoir computational model considers a two-phase (oil and water) immiscible flow with a heterogeneous permeability field adopted from Matlab reservoir simulation toolbox (MRST). The reservoir with one vertical producer (pressure-controlled by constant bottom-hole pressure (BHP) of 1 bar) and a vertical injector (rate-controlled with an injection rate) is considered, which has a size of $20x20x5m^3$. The production period is fixed to 2 years. In the numerical study, the input is the injection history characterized by 8 constant values for different timesteps (each one of a 90-day duration) and, also, the random permeability field. The quantities of interest (QoIs) are the bottom-hole pressure (BHP) of injection well, the cumulative water and oil production along the injection, and the water breakthrough time. The methodology is applied to generate risk curves of each quantities of interest for different production strategies.

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Title: Physics-Informed Neural Networks for Cardiac Activation Mapping

Author(s): *Francisco Sahli Costabal, *Pontificia Universidad Católica de Chile*; Yibo Yang, *University of Pennsylvania*; Paris Perdikaris, *University of Pennsylvania*; Daniel E. Hurtado, *Pontificia Universidad Católica de Chile*; Ellen Kuhl, *Stanford University*;

A critical procedure in diagnosing atrial fibrillation is the creation of electro-anatomic activation maps. Current methods generate these mappings from interpolation using a few sparse data points recorded inside the atria; they neither include prior knowledge of the underlying physics nor uncertainty of these recordings. Here we propose a physics-informed neural network for cardiac activation mapping that accounts for the underlying wave propagation dynamics and we quantify the epistemic uncertainty associated with these predictions. These uncertainty estimates not only allow us to quantify the predictive error of the neural network, but also help to reduce it by judiciously selecting new informative measurement locations via active learning. We illustrate the potential of our approach using a synthetic benchmark problem and a personalized electrophysiology model of the left atrium. We show that our new method outperforms linear interpolation and Gaussian process regression for the benchmark problem and linear interpolation at clinical densities for the left atrium. In both cases, the active learning algorithm achieves lower error levels than random allocation. Our findings open the door toward physics-based electro-anatomic mapping with the ultimate goals to reduce procedural time and improve diagnostic predictability for patients affected by atrial fibrillation. Open source code is available at https://github.com/fsahli/EikonalNet.

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Title: MATBOX, an Open-Source Microstructure Analysis Toolbox for Meshing, Generation, Segmentation, and Characterization of 3D Heterogenous Volumes

Author(s): *Francois Usseglio-Viretta, *National Renewable Energy Laboratory*; Prehit Patel, *University of Alabama*; Jeffery Allen, *National Renewable Energy Laboratory*; Aashutosh Mistry, *Argonne National Laboratory*; Partha Mukherjee, *Purdue University*; Kandler Smith, *National Renewable Energy Laboratory*;

Battery performance is strongly correlated with electrode microstructural properties. To account for its impact, lithium-ion battery (LIB) models either abstract the microstructural heterogeneity of composite electrodes using effective macroscopic properties (macro- or meso- scale models) or directly solve the system of equations on the microstructure geometry or mesh (microstructure-scale models). Therefore, to be adequate, both families of models require information from the microstructure geometry, which can be provided by the numerical tool presented in this work. MATBOX is a MATLAB open-source application [1] developed by NREL for performing various microstructure-related tasks including microstructure numerical generation, image filtering and microstructure segmentation, microstructure characterization and correlation, visualization, and microstructure meshing. MATBOX was originally developed for the analysis of LIB electrode microstructures; however, the algorithms provided by the toolbox are widely applicable to other heterogeneous materials. The toolbox provides a user-friendly experience thanks to a Graphical-User Interface, requires no coding by the user, and is well documented. This presentation will illustrate various MATBOX features for the characterization of a LIB electrode, including a fully automated Representative Volume Element (RVE) analysis, the numerical generation of complex ‘virtual’ microstructure, including dual-layer electrodes and carbon-binder additive phase, and the meshing of a complex NMC/graphite full cell microstructure suitable for 3D finite-element modeling. Other modules (segmentation, visualization, and correlation) will be briefly presented. Thanks to its modular, open-source approach, MATBOX can easily incorporate third-party algorithms to eventually build a standard in the field that will benefit the whole scientific community. Effective diffusion coefficient [2], additive phase numerical generation [3], and meshing [4] third-party algorithms have been already integrated in the toolbox with more to come. [1] F. Usseglio-Viretta et al., MATBOX: an open-source microstructure analysis toolbox for microstructure generation, segmentation, characterization, visualization, correlation, and meshing (2020) https://github.nrel.gov/fussegli/Microstructure_analysis_toolbox. [2] S. J. Cooper et al., TauFactor: An open-source application for calculating tortuosity factors from tomographic data. Softwarex 5, 203–210 (2016). [3] Mistry, A., Smith, K. & Mukherjee, P. P. Secondary Phase Stochastics in Lithium-ion Battery Electrodes. ACS Applied Materials & Interfaces (2018) doi:10.1021/acsami.7b17771. [4] Q. Fang et al., Tetrahedral mesh generation from volumetric binary and grayscale images. 2009 Ieee Int Symposium Biomed Imaging Nano Macro 1142–1145 (2009) doi:10.1109/isbi.2009.5193259.

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Title: Novel Coupling Approach to Topology and Shape Optimization

Author(s): *Gabriel Stankiewicz, *University of Erlangen-Nuremberg*; Chaitanya Dev, *University of Erlangen-Nuremberg*; Paul Steinmann, *University of Erlangen-Nuremberg*;

Density-based topology optimization and node-based shape optimization are often used sequentially to generate production-ready designs. In this presentation, we address the challenge to couple topology and shape optimization into a single optimization problem by using an embedding domain discretization technique. In this technique, the outline of the embedded body, defined by a d ? 1 dimensional mesh, segregates the elements of the embedding domain into inner, boundary and outer collection. The boundary elements require a special integration approach, which involves oversampling of the integration points to approximate the geometry of embedded body. In our approach, a variable shape is explicitly represented by the boundary of an embedded body. Large design changes of the shape are easy to handle, since no morphing of the interior of the embedded body is necessary. Hence, complex regularization and remeshing schemes which are used in standard node-based shape optimization methods are not required. Furthermore, the embedding domain in form of a structured mesh allows us to introduce a variable, pseudo density field. This provides a full flexibility in handling topological changes. In regions that reach zero pseudo density, the algorithm introduces additional shape variables. In this novel approach we couple topology and shape optimization by using an embedding domain discretization. This way, we bring the advantages of both methods together and provide an efficient way to design fine-tuned structures without predefined topological features.

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Title: Discrimination of Operating Regimes using Physics-Informed Neural Networks in Motorized Systems

Author(s): Jeremy Shen, *Stuyvesant High School*; Sourav Banerjee, *University of South Carolina*; *Gabriel Terejanu, *University of North Carolina at Charlotte*;

Identifying abnormal operating regimes of motorized systems is important for a large number of applications such as monitoring the condition of helicopter rotors, windmills, and CNC machines. In this work, we derive features to discriminate between various operating regimes by querying the predictive models that are constrained to conserve the energy of the system. The experimental data collected in this study is from a motor that drives a shaft where various defects are introduced. The data collected consists of vibrations, sound, and speed measurements. We observed that while the energy is conserved in all operating regimes, the behavior of the system is different and it is reflected in the shape of the learned energy function, which provides discriminatory information between various scenarios considered.

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Title: Isogeometric Singular Enrichments for Multi-Material Corners

Author(s): Chun-Pei Chen, *Purdue University*; *Ganesh Subbarayan, *Purdue University*;

Crack tips and multi-material corners are common concerns in engineering analysis. The singular stress arising at multi-material corners and its special case of crack tips require very refined meshes or special elements for analysis. In this talk we describe an isogeometric enrichment method for multi-material corners that enables accurate estimations of generalized stress intensity factors with relatively coarse and uniform discretizations. Specifically, explicitly modeled geometries of material junctions, crack tips and debonded interfaces are isoparametrically and hierarchically enriched to construct approximations with the known local behavior. The analysis procedure is termed enriched isogeometric analysis since the enrichments are constructed directly (explicitly) on the parametric spline geometry of the vertex or crack face unlike in procedures where the influence of the enriching entity is implicitly inferred on the underlying mesh. The developed method allows direct extraction of generalized stress intensity factors without needing a posteriori evaluation of path independent integrals for decisions on crack propagation. The numerical implementation is first validated through analysis of a bi-material corner and growth of an inclined crack in a homogeneous solid. Next, a detailed analysis of a representative back end of line structure of a semiconductor chip with multiple singular corners is carried out to identify critical corners susceptible to crack initiation. The developed procedure demonstrates rapid convergence to the solution stress intensity factors with relatively fewer degrees of freedom, even with uniformly refined coarse discretizations.

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Title: Multiresolution Spline Topology Optimization with Volumetric Subdivision Representation of Complex Geometry

Author(s): *Gang Xu, *Hangzhou Dianzi University*; Jin Xie, *Hangzhou Dianzi University*; Zhenyu Dong, *Hangzhou Dianzi University*; Jinlan Xu, *Hangzhou Dianzi University*; Jessica Zhang, *Carnegie Mellon University*; Bernard Mourrain, *Inria*; Charlie Wang, *University of Manchester*;

Topology optimization plays a key role in generative design. However, some post-processing operations are required to make the optimization results suitable for CAD systems, and it is also a challenging problem to achieve seamless data integration of design, simulation and optimization phases for complex shapes. In order to tackle these problems, in this paper, we propose a novel multi-resolution 3D isogeometric topology optimization framework with an unstructured trivariate spline model. Firstly, explicit limit point formula of Catmull-Clark subdivision solids is given with mathematical proof. Secondly, based on the proposed limit point formula, the approximation representation of Catmull-Clark subdivision solid with a minimal set of tricubic volumes is given. That is, for an input hex-mesh, we can construct an unstructured tricubic spline representation with C2/C0-continuity. Finally, a multi-resolution 3D isogeometric topology optimization framework is proposed with the proposed unstructured spline solid representation. In our framework, consistent spline language is used for geometry representation, isogeometric analysis and topology optimization, which leads to an optimal shape represented by smooth spline patches that can be imported for CAD applications directly. In particular, for generative design problem with shape constraints, the interface geometry between different components can be exactly preserved during topology optimization. Moreover, the proposed topology optimization framework naturally has a multi-resolution property, that is, a volume parameterization with fixed resolution is used to perform the simulation, and a volume parameterization with high-resolution is used for design optimization, which can achieve computationally efficient and high-resolution designs. Several topology optimization examples for linear elasticity and heat conduction problems are presented to show the effectiveness and efficiency of the proposed framework.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Data-Driven Bayesian Crack Nucleation Model for Fatigue in Ni-Based Superalloys

Author(s): *George Weber, *Johns Hopkins University*; Max Pinz, *Johns Hopkins University*; Somnath Ghosh, *Johns Hopkins University*;

A data-driven Bayesian approach is developed to identify the underlying mechanics that drive crack nucleation in Ni-based superalloy Rene88-DT. Over 20 experimental 2D micrographs containing crack nucleation sites after undergoing low cycle fatigue are virtually replicated and simulated within an automated crystal plasticity finite element framework, providing mechanical state variable values at each material point of the microstructures. The virtual representations of these microstructures are embedded within a homogenized constitutive model to alleviate inherent boundary condition errors and provide an accurate simulation of the microstructure. A Bayesian classification method is applied in order to optimally select the most informative state variable predictors of crack nucleation and construct a near-pareto frontier of models with varying complexity. Following the selection of optimal variables, an expectation maximization component is added, allowing the model to select the most likely location of a crack nucleation point. This adaptation is critical for this application as the micrographs do not pinpoint the precise location of initial crack nucleation, but rather the cracked region after some small amount of propagation. The paradigm of this Bayesian approach is to allow the micro-mechanical state variables responsible for causing crack nucleation events to arise naturally from existing data. This method allows the experimental data to inform a theory of crack nucleation, rather than generating a theory to test against data. The final Bayesian model highlights specific mechanistic features of crack initiation in superalloys, such as parallel slip and thermodynamic driving forces. The result is a model capable of predicting the probability of nucleating a crack at a microstructural position, given the mechanical state of the material.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Grain Size Dependence of Polycrystalline Plasticity Modeling in Cylindrical Indentation

Author(s): *George Z. Voyiadjis, *Louisiana State University*; Juyoung Jeong, *Louisiana State University*; Jeffrey W. Kysar, *Columbia University*;

The grain boundary strengthening effect for polycrystalline copper is studied numerically using crystal plasticity in conjunction with cylindrical indentation simulations under the plane strain condition. In order to compare with an isotropic, heterogeneous continuum model a new constitutive relation is developed. This new nonlocal continuum model that encompasses the heterogeneity in yield strength based on the exponentiated Weibull function can predict the plastic properties of materials in the micron length scale. Two physical material parameters which are a length scale of grains and degree of heterogeneity are introduced in the Weibull averaging method. The spatial description of the deformation gradient two-point tensor is utilized to capture the intrinsic size effect in line with the subsequent deformation measures. Moreover, the total geometrically necessary dislocation density is obtained from the non-zero components of the Nye dislocation density tensor. From the simulation, the relationship between the effective Green–Lagrange strain and effective stress measures is explained using the persistent long-range order and intermittent short-range order. The observation derived from the analogy between the cylindrical indentation and the progress in cylindrical voids describes how different average grain sizes of polycrystalline materials are compared with the behavior of isotropic materials. The trajectories of directions of both principal stretch and maximum shear strain explain that the internal stresses induced by cylindrical indentation either hinder or reinforce the dislocation flow, forming strain localization sporadically. The grain size dependence of polycrystalline modeling incorporates the Hall–Petch strengthening as well as the homogenization of anisotropic polycrystalline metal into the isotropic effective medium. This is a physically-based model that is used to model failure characterization in metals.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Reduced Order Methods for Computational Fluid Dynamics: State of the Art, Perspectives and Applications

Author(s): *Gianluigi Rozza, *Scuola Internazionale Superiore di Studi Avanzati*;

We provide the state of the art of Reduced Order Methods (ROM) and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Efficient parametrizations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: a better use of stable high fidelity methods, considering also spectral element method and finite volume discretisations, to enhance the quality of the reduced model too, and allowing to incorporate turbulent patterns and increasing the Reynolds number; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; as well as the guarantee of the stability of the approximation with proper space enrichments. For nonlinear systems, also the investigation on bifurcations of parametric solutions are crucial and they may be obtained thanks to a reduced eigenvalue analysis of the linearised operator. All the previous aspects are very important in CFD, especially when dealing with real time complex parametric industrial, environmental and biomedical flow problems, even in a control flow setting. We will show few benchmark cases, from simple fluid-structure interaction problems to shape optimisation applied to industrial problems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Uncertainty Quantification and Well-Posedness for Damage Mechanics

Author(s): Petr Plechac, *University of Delaware*; *Gideon Simpson, *Drexel University*; Jerome Troy, *University of Delaware*;

Many important materials, including glasses and ceramics, are of the linearly elastic/brittle variety, obeying a classical Hookean law until an applied load reaches a yield stress, at which point they break into some number of fragments. Predicting the behavior of such materials, through modelling and simulation, is of obvious value to a variety of applications. In this work, we add randomness in material properties into the problem, modelling them via random fields within a damage mechanics framework. We establish the well-posedness of our model, identifying key regularizations. We then apply tools from uncertainty quantification to investigate the robustness to deformation of materials in the presence of this randomness.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Combinatorial Optimal Control of PDEs with Deep Reinforcement Learning

Author(s): *Gradey Wang, *Stanford University*; Adrian Lew, *Stanford University*; Eric Darve, *Stanford University*;

Partial differential equations (PDEs) are used to model a broad range of phenomena (e.g., diffusion, electromagnetism, elasticity, options pricing) and are particularly pervasive in the physical sciences. Many current, long-standing challenges in engineering, such as wave, diffusion, and electromagnetic control problems, are approximately governed by partial differential equation are either combinatorial control problems or can be reduced to one. Combinatorial PDE-constrained optimal control problems are particularly difficult because 1) combinatorial optimization is generally computationally expensive and 2) optimizing over fields arising from PDEs can be difficult due to the lack of understanding of their behavior under nonlinear control. Reinforcement learning techniques have demonstrated state-of-the-art performance on board games, which can be represented as sequential combinatorial control problems. Motivated by applications in metal additive manufacturing and the objective of controlling the temperature history of their produced objects, we build on deep reinforcement learning techniques in order to identify high-quality control sequences for objective functions of time-dependent PDEs' field histories. More specifically, our method augments techniques a la DeepMind's AlphaZero with the Traveling Salesperson Problem-inspired k-opt heuristic to outperform other leading methods to identify high-quality solutions in cardinality up to O(10^{41}) in less than 24 hours. We further introduce advances in this algorithm that use multiscaling to optimize over larger search spaces. Our results demonstrate the efficacy of deep reinforcement learning as a method for combinatorial control of PDEs and illustrate its potential for understanding and optimizing PDE behavior.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Scale Bridging Materials Physics: Active Learning Workflows and Integrable Deep Neural Networks for Free Energy Function Representations in Alloys

Author(s): *Gregory Teichert, *University of Michigan*; Anirudh Natarajan, *University of California, Santa Barbara*; Sambit Das, *University of Michigan*; Murat Aykol, *Toyota Research Institute*; Chirranjeevi Gopal, *Toyota Research Institute*; Vikram Gavini, *University of Michigan*; Anton Van der Ven, *University of California, Santa Barbara*; Krishna Garikipati, *University of Michigan*;

The free energy plays a fundamental role in theories of phase transformations and microstructure evolution. It encodes the thermodynamic coupling between different fields, such as mechanics and chemistry, within continuum descriptions of non-equilibrium materials phenomena. In mechano-chemically interacting materials systems, even consideration of only compositions, order parameters and strains results in a free energy description that occupies a high-dimensional space. Scale bridging between the electronic structure of a solid and continuum descriptions of its non-equilibrium behavior can be realized with integrable deep neural networks (IDNN) that are trained to free energy derivative data generated by first-principles statistical mechanics simulations and then analytically integrating to recover a free energy density function. We also combine the IDNN with an active learning workflow to ensure well-distributed sampling of the free energy derivative data in high-dimensional input spaces, thereby enabling true scale bridging between first-principles statistical mechanics and continuum phase field models. As prototypical material systems, we focus on Ni-Al and the battery material LCO. This work advances the treatment of scale bridging, starting with electronic structure calculations and proceeding through statistical mechanics to continuum physics. Its coupling of Cahn-Hilliard and Allen-Cahn phase field descriptions with nonlinear elasticity through the free energy density ensures a rigorous treatment of phase transformation phenomena. Reference: G.H. Teichert, at al. Computer Methods in Applied Mechanics and Engineering, Vol. 371, 2020, 113281

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Coreform IGA: Enabling Commercial Application of IGA

Author(s): *Gregory Vernon, *Coreform*;

Coreform is developing a new isogeometric analysis solver, called Coreform IGA, based on our U-spline and Flex IGA technologies. We have been developing a full-stack suite of tools to bring the power of IGA to end-users, not just to IGA researchers. Our preprocessor Coreform Cubit and our isogeometric solver Coreform IGA are being integrated into a seamless workflow in order to bring the full power of IGA to users. To drive this effort, Coreform has partnered with industry-leading organizations via strategic projects. These projects are beginning to yield exciting results in private industry. Our partners provide some of their most challenging simulation analysis problems as well as insight into their workflow needs, and we develop IGA capabilities and workflows that enable the solution to those problems. In this presentation, we will demonstrate how Coreform Cubit and Coreform IGA, have been used to solve several of these problems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Smoothed Particle Hydrodynamics for Hybrid Robot Motion on Granular Terrain

Author(s): *Guanjin Wang, *University of Maryland, College Park*; Balakumar Balachandran, *University of Maryland, College Park*;

Navigating an unmapped environment is one of the ten biggest challenges facing the robotics community. Wheeled robots can move fast on flat surfaces but suffer from loss of traction and immobility on soft ground because of sinkage and slipping. However, legged machines have superior mobility over wheeled locomotion when they are in motion over flowable ground or a terrain with obstacles but can only move at relatively low speeds on flat surfaces. This is the case, since with legged machines one makes use of discrete footholds instead of a continuous support surface for adapting to surface irregularities. Also, the feet establish contact with the ground at selected points according to the terrain conditions. A plausible question is the following: If legged and wheeled locomotion are combined, can the resulting hybrid leg-wheel locomotion move fast in any terrain condition? Locomotive interactions are sensitive to the material properties of the underlying ground soil, which is a granular material. Continuum treatment is a good choice for dealing with dynamic interaction problems when the particle size of the ground is smaller than the intruder size. The authors have proposed a Smooth particle hydrodynamics framework for this problem. The mesh-free nature of SPH makes it easy to capture the large deformation and the post-failure state of the granular substrate. Good agreement is found amongst the obtained numerical results and theoretical and experimental results across a wide range of robot leg shapes. Parametric studies have been conducted to compare and evaluate the efficiency and robustness of different robot locomotion modes on complex terrains. The results are expected to form a good basis for robot navigation and exploration in unknown and complex terrains. 1. Wang, G., Riaz, A., and Balachandran, B. 2021. Continuum Modeling and Simulation of Robotic Appendage Interaction with Granular Material. Journal of Applied Mechanics. 88(2): 021013. 2. Wang, G., Riaz, A. and Balachandran, B., 2020. Smooth Particle Hydrodynamics Studies of Wet Granular Column Collapses. Acta Geotechnica, 15, pp.1205-1217.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The Shifted Fracture Method

Author(s): Kangan Li, *Duke University*; Nabil Atallah, *Duke University*; Antonio Rodriguez-Ferran, *Universitat Politecnica de Catalunya*; *Guglielmo Scovazzi, *Duke Univerisity*;

We propose a new framework for fracture mechanics, based on the idea of an approximate fracture geometry representation combined with approximate interface conditions. Our approach evolves from the shifted interface method, and introduces the concept of an approximate fracture surface composed of the full edges/faces of an underlying grid that are geometrically close to the true fracture geometry. The original interface conditions are then modified on the surrogate fracture, by way of Taylor expansions, to achieve a prescribed level of accuracy. The shifted fracture method does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with specific integrals on the approximate fracture. Furthermore, the energetics of the true fracture are represented within the prescribed level of accuracy and independently of the grid topology. The computational framework is presented here in its generality and then applied in the specific context of cohesive zone models, with an extensive set of numerical experiments. Reference: Kangan Li, Nabil Atallah, Antonio Rodriguez-Ferran, Guglielmo Scovazzi "The Shifted Fracture Method," Int. J. Num. Meth. Eng. (2021), Submitted.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: OnsagerNet: Learning Stable and Interpretable Dynamics Using a Generalized Onsager Principle

Author(s): *Haijun Yu, *Chinese Academy of Sciences*; Xinyuan Tian, *Chinese Academy of Sciences*; Weinan Ee, *Princeton University*; Qianxiao Li, *National University of Singapore*;

We propose a systematic method for learning stable and interpretable dynamical models using sampled trajectory data from physical processes based on a generalized Onsager principle. The learned dynamics are autonomous ordinary differential equations parameterized by neural networks that retain clear physical structure information, such as free energy, diffusion, conservative motion and external force. The neural network representations for the hidden dynamics are trained by minimizing the loss between sample data and predictions using multiple steps of Runge-Kutta methods. For high dimensional problems with a low dimensional slow manifold, an autoencoder with metric preserving regularization is introduced to find the low dimensional generalized coordinates on which we learn the generalized Onsager dynamics. Our method exhibits clear advantages in two benchmark problems for learning ordinary differential equations: nonlinear Langevin dynamics and the Lorenz system. We further apply this method to study Rayleigh-Bernard convection and learn Lorenz-like low dimensional autonomous reduced order models that capture both qualitative and quantitative properties of the underlying dynamics. Reference: 1. H. Yu, X. Tian, W. E and Q. Li, OnsagerNet: Learning Stable and Interpretable Dynamics Using a Generalized Onsager Principle, arXiv:2009.02327

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physical Stability Analysis and Domain Decomposition Preconditioner for Dynamic Fracture Problems

Author(s): Lampros Svolos, *Los Alamos National Laboratory*; Luc Berger-Vergiat, *Sandia National Laboratories*; *Haim Waisman, *Columbia University*;

Iterative methods used for analysis of multiphysics problems that result in localized solution features may be highly demanding from a computational standpoint and often require special treatment to be more efficient. Dynamic fracture of metals is one such example in which a nonlinear thermo-mechanical system leads to strain localization, resulting in shear bands and/or cracks, in which iterative solvers may have difficult time converging. In the current paper, we develop a novel updating domain decomposition preconditioner for parallel solution of dynamic fracture problems, in which shearbands are modeled using a temperature-dependent viscoplastic material model and fracture is modeled by the phase-field method. The domain decomposition method is based on the Additive Schwarz Method. The key idea is to decompose the computational domain into two subdomains, a localized subdomain that includes all localized features of the solution and a healthy subdomain for the remaining part of the domain. In this way, one can apply different solvers in each subdomain, i.e. focus more effort in the localized subdomain. In this work, an LU solver is applied in both subdomains, however, while the localized subdomain is solved exactly at every nonlinear iteration, the healthy subdomain LU operator is reused and only selectively updated. Hence, significant CPU time savings associated with the setup of the preconditioner can be achieved. To this end, we propose a strategy for updating the preconditioner in the healthy subdomain. The strategy is based on an idealized performance-based optimization procedure that takes into account machine on-the-fly execution time. Three dynamic fracture problems corresponding to different failure modes are investigated. Excellent performance of the proposed updating preconditioner is reported in serial and parallel computers. References: [1] L. Svolos, L. Berger-Vergiat and H. Waisman, Updating strategy of a domain decomposition preconditioner for parallel solution of dynamic fracture problems, Journal of Computational Physics, 422, 109746, 2020. [2] L. Berger-Vergiat and H. Waisman, An overlapping Domain Decomposition preconditioning method for monolithic solution of shear bands, Computer Methods in Applied Mechanics and Engineering, 318:33-60, 2017.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Recent Progress on Computational Methods for Seismic Analysis of Underground Structures

Author(s): *Haitao Yu, *Tongji University*; Yong Yuan, *Tongji University*;

Seismic analysis of tunnel structures is one of the most important topics on the disaster prevention of underground engineering. Nowadays, tunnels are widely constructed with the characteristics of long and large in dimensions and complex joints. Critical issues such as the longitudinal seismic design theory, large-scale seismic response analysis method, and non-uniform earthquake excitation effects, etc., are challenging for seismic analysis of large and long tunnels. Based on the literature reviews and urgent demands on seismic design of tunnel structures, this paper focuses on the seismic analysis theories and computational methods for long tunnels subjected to non-uniform seismic loadings. Firstly, several simplified models for seismic design of long tunnels are introduced and analytical solutions for longitudinal responses of long tunnels under arbitrary dynamic loads are derived, and degraded solutions are presented for the special load case of travelling waves. These solutions can be conveniently used to obtain the overall response of the tunnel structure subjected to seismic loading. Based on the proposed multi-mass-spring-beam model, a simplified method is also developed for the longitudinal seismic design of long tunnels. Secondly, a multiscale method is developed for the large-scale seismic analysis of long tunnels, with coarse and refined finite element meshes, or with the discrete element method and the finite difference method to compute the overall seismic response of the tunnel while including detailed dynamic response at positions of potential damage or of interest. This multiscale method does not have spurious wave reflections at the fine/coarse interface and does not need filtering procedures. Finally, hybrid simulation methods with numerical and physical sub-models for underground structures were also introduced. With application in major projects such as the immersed tunnel of Hongkong-Zhuhai-Macau Linkage, examples are presented to demonstrate the applicability of the proposed analytical, numerical and hybrid simulation methods.

16th U.S. National Congress on Computational Mechanics
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Title: Hybrid CT Imagine-FEA Modeling and its Application in Medical Device Fatigue Analysis

Author(s): *Haitao Zhang, *Medtronic Plc.*;

Neuromodulation is among one of the fastest-growing areas of the medical device industry. Neural stimulators are being used to provide therapies to patients with chronic pains, movement disorders, overactive bladders, and psychiatric disorder symptoms. In these therapies, well-controlled stimulation current is delivered to the target nerves through implantable leads. The implantable leads must have sufficient fatigue durability to last for many years of implantation. An implantable lead is composed of a lead body and conductor coils/cables. The lead body is commonly made from polymer materials and the conductor coils/cables are generally made from metal alloys. A recent emerging technology is to use braided metal wire-reinforced polymer composite to make the lead body to enable MRI conditional safe. The braided lead body makes it quite challenging to use the conventional FEA approaches to analyze the stress and strain of lead conductors. In this work, we approached the stress and strain of lead conductors with a hybrid CT image-FEA methodology. The method was illustrated with the example of lead fatigue analysis under bending load. Under a desired loading condition, the DICOMS files obtained with the CT scanner were analyzed using the Mimics Medical 19.0 and 3-Matic 11.0 software to obtain the curvatures of lead conductor coil centerline. The obtained centerline curvatures were then used as coil FEA analysis boundary conditions. FEA analysis was performed with Abaqus 6.14. The stress/strain from FEA analysis was then fed into a Bayesian Random Fatigue-Limit Model for lead fatigue prediction.

16th U.S. National Congress on Computational Mechanics
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Title: Optimal Finite-Rank Approximation of Koopman Operators: Theory, Methods and Challenges

Author(s): *Hao Wu, *Tongji University*;

Transfer operators such as Perron-Frobenius or Koopman operator play a key role in modeling and analysis of complex dynamical systems, which allow linear representations of nonlinear dynamics by transforming the original state variables to feature spaces. A lot of analysis and modeling methods of Markov processes, including TICA, DMD, EDMD and MSM, can be interpreted as finite-rank approximation method of transfer operators. However, it remains challenging to identify the optimal low-dimensional feature mappings from data. The variational approach for Markov processes (VAMP) provides a comprehensive framework for the evaluation and optimization of feature mappings based on the variational estimation of modeling errors. In this talk, I will review the related theory and methods (including deep learning based methods) of VAMP. Moreover, some open problems and challenges will be discussed.

16th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification of TMS Simulations Considering Spatially-Determined MRI Data Segmentation Errors

Author(s): *Hao Zhang, *Duke University*; Luis Gomez, *Purdue University*; Johann Guilleminot, *Duke University*;

TMS (transcranial magnetic stimulation) is a non-invasive brain stimulation method that is used to study brain function and conduct neuropsychiatric therapy. High fidelity numerical simulations have been widely used to study the electric field (E-field) dosimetry of TMS inside the brain. However, the simulation results are highly sensitive to the geometrical uncertainties introduced during the process of segmenting brain magnetic resonance image (MRI) data into various tissue types. This work presents a methodology that models the segmentation errors and studies their impacts on accuracy and precision of TMS computational E-field dosimetry. The segmentation errors of brain MRI data are modeled as random fields defined on the boundaries between different tissue types. In particular, the random fields are defined to capture the spatially-determined features of the geometric perturbations due to the segmentation algorithm and patient-specific brain geometry. An in-house solver is further employed to conduct the forward uncertainty propagation analysis and quantify the tissue boundary uncertainties on the computational E-field dosimetry. Two parameters of the geometric uncertainties are particularly studied, i.e., the perturbation height together with the correlation length of the random field. This work would provide support to ensure safe and effective use of TMS simulation results on patient-specific brain models.

16th U.S. National Congress on Computational Mechanics
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Title: Accelerated Computational Micromechanics and its Applications to Polydomain Liquid Crystal Elastomers

Author(s): *Hao Zhou, *California Institute of Technology*; Kaushik Bhattacharya, *California Institute of Technology*;

We present an approach to solving problems in micromechanics that is amenable to massively parallel calculations through the use of graphical processing units and other accelerators. We demonstrate the approach by studying liquid crystal elastomers (LCEs), an emerging class of responsive materials, that are obtained by incorporating nematic mesogens into the underlying polymer chains of the elastomer. Various problems of micromechanics, including those of LCEs, lead to nonlinear differential equations that are typically second order in space and first order in time. This combination of nonlinearity and nonlocality makes such problems difficult to solve in parallel. However, this combination is a result of collapsing nonlocal, but linear and universal physical laws (kinematic compatibility, balance laws), and nonlinear but local constitutive relations. We propose an operator-splitting scheme inspired by this structure. The governing equations are formulated as (incremental) variational problems, the differential constraints like compatibility are introduced using an augmented Lagrangian, and the resulting incremental variational principle is solved by the alternating direction method of multipliers. The resulting algorithm has a natural connection to physical principles, and also enables massively parallel implementation on structured grids. We apply the method to study polydomain LCEs where disorder disrupts natural nematic order. Our simulations reveal a new and unexpected liquid-like behavior in membranes, as well as the mechanism for this exotic behavior.

16th U.S. National Congress on Computational Mechanics
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Title: Mechanistic Machine Learning-Based Multiscale Simulation of Short-Fiber-Reinforced Composites

Author(s): C. T. Wu, *Livermore Software Technology LLC, Ansys, Inc*; *Haoyan Wei, *Livermore Software Technology LLC, Ansys, Inc*; Dandan Lyu, *Livermore Software Technology LLC, Ansys, Inc*; Wei Hu, *Livermore Software Technology LLC, Ansys, Inc*; Tung-Huan Su, *Livermore Software Technology LLC, Ansys, Inc*; Hitoshi Oura, *JSOL Corporation*; Masato Nishi, *JSOL Corporation*; Tadashi Naito, *Honda Motor Co., Ltd.*; Leo Shen, *CoreTech System Co., Ltd.*; Kevin Zhang, *Livermore Software Technology LLC, Ansys, Inc.*; Philip Ho, *Livermore Software Technology LLC, Ansys, Inc.NSYS*; Zeliang Liu, *Livermore Software Technology LLC, Ansys Inc.*; Tianyu Huang, *Livermore Software Technology LLC, Ansys Inc.*;

Short-fiber-reinforced composites (SFRC) have been widely used as high-performance engineering materials for structural applications in automotive and electronics industries. Typically, SFRC are manufactured by injection molding, which induces heterogeneous microstructures across different length scales, and predicting the resulting nonlinear anisotropic behaviors by conventional micromechanical methods are challenging. In this work, we present a data-driven multiscale modeling framework that integrates the injection molding simulation, material homogenization, and a mechanistic machine learning model referred to as Deep Material Network (DMN) [1]. The physics-embedded DMN learns the microscale material morphologies hidden in Representative Volume Elements (RVE) of composites through offline training, and the trained network is able to predict the nonlinear material behaviors at a computational speed orders-of-magnitude faster than the high-fidelity RVE simulation. Through transfer learning [2] of different material microstructures, a unified DMN database is created to cover a full range of SFRC geometric descriptors. Recently, we have coupled the trained DMN database with macroscale finite element models in the engineering simulation software LS-DYNA to perform concurrent multiscale structural simulations [3]. The proposed multiscale simulation framework achieves extraordinary computational performance, and it is quite promising for the design and analysis of composite structures. References: (1). Liu, Z., & Wu, C. T. (2019). Exploring the 3D architectures of deep material network in data-driven multiscale mechanics. Journal of the Mechanics and Physics of Solids, 127, 20-46. (2). Liu, Z., Wu, C. T., & Koishi, M. (2019). Transfer learning of deep material network for seamless structure–property predictions. Computational Mechanics, 64(2), 451-465. (3). Liu, Z., Wei, H., Huang, T., & Wu, C. T. (2020). Intelligent multiscale simulation based on process-guided composite database. arXiv preprint arXiv:2003.09491.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling and Isogeometric Analysis of Thin Layered Structures Using Volumetric NURBS

Author(s): *Harshil Shah, *Iowa State University*; Onur Rauf Bingol, *Iowa State University*; Emily Johnson, *Iowa State University*; Manoj Rajanna, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Laminated fiber-reinforced polymer (FRP) composites have been increasingly used in structural applications because of their combination of good mechanical properties and low weight along with their ability to conform to complex shapes. However, owing to their high manufacturing costs, computational modeling of composites can provide valuable insights into their design and repair decisions. Traditionally, composite laminates are modeled using Kirchhoff-Love thin shells for performing structural analysis. However, the thin shell method has limitations on computing the interlaminar stress and strains of the composite laminates and does not allow modeling of common interlaminar defects, such as delaminations. In this work, we have developed an integrated modeling and structural analysis framework for multi-layered composite laminates using volumetric NURBS elements using isogeometric analysis (IGA). We showcase the approach by generating multi-layered models from complicated shell structures with variable thickness. Our framework starts from the original shell model and generates an optimized surface offset considering the adjacent surfaces. This allows us to handle degenerate elements during the generation of multiple layers. Using NURBS volumes instead of thin shells provides higher fidelity for the structural analysis by generating the digital twin of the composite manufacturing processes and allowing for integration of interlaminar stresses in the structure. Moreover, isogeometric analysis with NURBS volumes allows a direct analysis without complicated meshing when compared to traditional finite element analysis methods. We demonstrate the utility of our framework by comparing the results of a well-studied benchmark problem using our method. We also use our framework to model the complex composite structure of a wind turbine blade and perform static structural analysis using IGA.

16th U.S. National Congress on Computational Mechanics
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Title: A Generalized Image Preprocessing Workflow for High Fidelity 3D Rendering of Natural Sands from X-Ray Computed Tomography Images

Author(s): Peng Tan, *University of California, Berkeley*; *Hasitha Sithadara Wijesuriya, *University of California, Berkeley*; Nicholas Sitar, *University of California, Berkeley*;

Abstract: Micromechanical analysis of granular media is contingent upon accurate identification of grain-to-grain contact regions. The challenge in dealing with naturally deposited sands is that they are usually polymineralic, contain a wide range of shapes and grain sizes. Herein we introduce three-step image preprocessing workflow that improves the grain segmentation for heterogeneous granular media. The first step in our approach is to denoise the CT images by applying a non-local means filter, which identifies and averages neighborhoods across an entire image, based on the degree of similarity with the source instead of the proximity. The resulting denoised images preserve edge sharpness and significantly remove noise. In the second step, we utilize a learning-based image super-resolution method (Yang et al., 2010) to enhance the resolution of the images based on sparse signal representation. This method produces a sparse representation for each patch of the low-resolution input and then uses the coefficients of this representation to generate high-resolution output. In the third step, we use the image segmentation method developed by Zhang et al. (2001) to differentiate individual objects from the background. This method clusters pixels via Hidden Markov Random Field (HMRF) with Weighted Expectation Maximization (WEM) algorithm, wherein each group of pixels (void, water, solid etc.) is modelled as a distinct Gaussian and the spatial connectivity is imposed via a stochastic Markov network. Conventional methods such as that developed by Otsu (1979), K-means, or histogram analysis serve as priors for the optimal label configuration of an image. Such configuration maximizes the maximum a posterior (MAP) estimation or minimizes the likelihood energy. We show that this 3-step workflow is robust and leads to more accurate binary segmentation of X-Ray CT images for heterogeneous granular materials. Keywords: Non-Local Mean Filter, Image Super-resolution, Hidden Markov Random Field, Weighted Expectation Maximization Algorithm Reference: Otsu, N. (1979). A Threshold Selection Method from Gray-Level Histograms. IEEE Transactions on Systems, Man, and Cybernetics, 9(1), 62-66. Yang, J., Wright, J., Huang, T. S., & Ma, Y. (2010). Image super-resolution via sparse representation. IEEE transactions on image processing, 19(11), 2861-2873. Zhang, Y., Brady, M., & Smith, S. (2001). Segmentation of brain MR images through a hidden Markov random field model and the expectation-maximization algorithm. IEEE transactions on medical imaging, 20(1), 45-57.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: On the Construction of Locally Refined B-Splines with Preservation of Local Linear Independence

Author(s): *Hendrik Speleers, *University of Rome Tor Vergata*; Carla Manni, *University of Rome Tor Vergata*; Francesco Patrizi, *Max Planck Institute for Plasma Physics*; Francesca Pelosi, *University of Rome Tor Vergata*;

Adaptive refinement is crucial in simulations for balancing accuracy and computational cost. Classical multivariate B-spline spaces are formulated as tensor products of univariate B-spline spaces and therefore cannot properly address local refinements. In order to break the tensor structure of the underlying mesh and achieve local refinements, new formulations of multivariate B-splines have been introduced during the last decades. One of these is Locally Refined B-splines, or in short, LR B-splines [1]. The definition of LR B-splines is roughly similar to classical B-splines, even though they allow for local refinements. Furthermore, LR B-splines satisfy the same properties as classical B-splines, such as nonnegativity, local support, and partition of unity (when using positive scaling weights). However, a particular structure of the mesh is required to guarantee local linear independence. Such a characterization in terms of meshing constraints has been provided in the literature [2], but no truly adaptive refinement strategy was available to produce LR-meshes with such a structure until recently. In this talk, we describe the first refinement of this kind [3]. Then we exploit this feature for the construction of efficient quasi-interpolation schemes and the numerical solution of elliptic problems. [1] T. Dokken, T. Lyche, and K. F. Pettersen. Polynomial splines over locally refined box-partitions. Computer Aided Geometric Design 30 (2013), pp. 331-356. [2] A. Bressan and B. Jüttler. A hierarchical construction of LR meshes in 2D. Computer Aided Geometric Design 37 (2015), pp. 9-24. [3] F. Patrizi, C. Manni, F. Pelosi, and H. Speleers. Adaptive refinement with locally linearly independent LR B-splines: Theory and applications. Computer Methods in Applied Mechanics and Engineering 369 (2020), art. 113230.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Estimating the Mechanical Property of Short Fiber Reinforced Plastic using Viscosity Model with Multiscale Simulation

Author(s): *Hirofumi Sugiyama, *University of Yamanashi*; Shigenobu Okazawa, *University of Yamanashi*;

This study evaluates the macroscopic mechanical properties of short fiber reinforced plastics under various conditions using multi-scale analysis. The composite material satisfies the desired mechanical properties by combining the base material and the fiber. Composite materials have a strain rate dependence and an environmental temperature dependence, and many types of composite have been proposed considering the characteristic of such dependency. Therefore, various combinations are used to obtain the desired characteristics, but it is very costly to evaluate them experimentally. Evaluation using a numerical simulation method such as the finite element method (FEM) plays an important role. In particular, various methods based on the multi-scale analysis for evaluating macroscopic characteristics considering the microscopic structure have been proposed. Although it is possible to use a complicated microscopic structure, an increase in calculation cost is unavoidable due to multi-scale analysis. We can expect to reduce the calculation cost if we can evaluate many cases that reflect the dependence using a more straightforward microscopic structure. Therefore, in this study, we use multi-scale analysis using a simple microscopic structure to examine microscopic structures that satisfy various conditions based on material tests. We will analyze composite materials with polyamide base material and glass fiber. Tensile test results are used with varying fiber orientation and tensile speed. First, FE model called unit cell considering a microscopic structure generate. In this context, the unit cell is assumed to be a single layer that completely contains fibers. We examine a material model for changing the base constitutive law and reflecting the nonlinear characteristics. On the other hand, since the fiber is glass, it remains in an elastic state. Next, a numerical material test is applied to the microscopic structure to calculate macroscopic characteristics. Then, macrostructure analysis is performed using the obtained material properties. In the macro-structural analysis, the material test conditions are applied, and the difference from the material test result is compared. Furthermore, it is examined whether the material test properties can be handled by changing the base metal's material properties. Besides, by considering each material's constants applied to the microstructure, the difference from the characteristic of material models will be clarified.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Topology Optimization of Anisotropic Plate Structures with Designable Reinforcement

Author(s): *Hollis Smith, *University of Connecticut*; Julián Norato, *University of Connecticut*;

Design with composite materials is largely motivated by weight reduction and enhanced performance compared to design with traditional isotropic materials. An important consideration for structures made of composite materials is their manufacturing. Composites reinforced with long, continuous-fibers typically exhibit superior mechanical properties when compared to those reinforced with discontinuous-fibers. However, the shapes of components that can be manufactured with continuous-fiber reinforcements is far more restrictive. Typically, components made with continuous-fiber reinforcements correspond to geometric primitives such as bars or plates. Plate-like components are generally made of multiple plies, with each ply having a different layout of fibers. In order to produce structural layouts composed of geometric primitives that are prevalent in the fabrication of structures with continuous-fiber reinforcements, the geometry projection method has been employed in [1] and [2] to generate designs exclusively composed of bars or plates respectively. In these existing approaches to topology optimization using geometric components made of anisotropic materials, the orientation of the reinforcement in each primitive is assumed a priori, and the layout of the primitives is optimized. In this work we introduce a topology optimization method for the design of structures composed of rectangular plates in which each plate is made of a designable anisotropic material. This work is a natural extension of the geometry projection method presented in [2] which introduced a topology optimization framework that renders designs made exclusively of plates made from a predetermined orthotropic material that is oriented with the geometric components. In the presented topology optimization framework, the designable anisotropic material is included as a part of the optimization. This designable anisotropic material may represent, e.g., a homogenized material corresponding to a composite laminate consisting of a layup of stacked orthotropic fiber-reinforced composite plies. We demonstrate the efficacy of the proposed method with a numerical example comparing optimized beam designs obtained using (a) predetermined and (b) designable-material plates. For this example, we maximize the stiffness of the structure for a fixed amount of material. The example demonstrates the advantage of simultaneously optimizing material properties and structural layout in the design of composite plate structures. References [1] Smith, H., & Norato, J. A. (2021). Topology optimization with discrete geometric components made of composite materials. Computer Methods in Applied Mechanics and Engineering. [2] Smith, H., & Norato, J. (2020). A Topology Optimization Method for the Design of Orthotropic Plate Structures. In IDETC-CIE ASME.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Real Space Density Functional Theory Method for Twisted Structures

Author(s): *Hsuan Ming Yu, *University of California, Los Angeles*; Amartya Banerjee, *University of California, Los Angeles*;

We present a real-space formulation and implementation of Kohn-Sham density functional theory suited to twisted geometries, and apply it to the study of torsional deformations of Group IV (i.e., C, Si, Ge, Sn) nanotubes. Our formulation is based on higher order finite difference discretization in helical coordinates, uses ab intio pseudopotentials, and naturally incorporates rotational (cyclic) and screw operation (i.e., helical) symmetries. We discuss several aspects of the computational method, including the form of the governing equations, details of the numerical implementation, as well as its convergence, accuracy and efficiency properties. The technique presented here is particularly well suited to the first principles simulation of quasi-one-dimensional structures and their deformations, and many systems of interest can be investigated using small simulation cells containing just a few atoms. We apply the method to systematically study the properties of zigzag and armchair group-IV nanotubes in the range of 1 to 3 nm radius, as they undergo twisting. We extract the mechanical response of these materials ab initio, and also elucidate different aspects of their variation in electronic properties as they undergo torsional deformation. Using our simulations, we are able to extend some well-known features of the electromechanical properties of carbon nanotubes to the broader class of Group IV nanotubes.

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Learning of Peridynamic Models for Graphene Sheets

Author(s): *Huaiqian You, *Lehigh Univerisity*;

Peridynamics, as a reformulation of the classic continuum mechanics, has been widely used because of its advantage in treating solution discontinuities such as cracks directly. Unlike the more classical PDE models, peridynamics require constitutive models (“kernels”) that define physical interactions across finite distances. These nonlocal interactions, while offering opportunities to make improvements in the fidelity of simulations, introduce ambiguity into the task of formulating a constitutive model. Moreover, works that provide rigorous well-posedness analysis of peridynamic models typically require mathematically complex and lengthy derivations, often relying on restrictive assumptions on the kernel. To overcome these challenges, We propose a machine learning approach to infer a well-posed peridynamic model description of 2D graphene sheets from coarse-grained molecular-dynamics (MD) simulations. This method is based on an optimization-based technique in which the nonlocal kernel function is approximated via Bernstein polynomials. The kernel, including both its functional form and parameters, is derived so that when used in a peridynamic solver, it generates solutions that closely match MD data. We demonstrate the capability of the learned peridynamic model by comparing its solution with new MD simulations in applications that are substantially different from the problems used as training data.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Peridynamic Modelling of Desiccation Induced Cracking of Cohesive Soils

Author(s): *Huaxiang Yan, *University of Manchester*; Majid Sedighi, *University of Manchester*; Andrey Jivkov, *University of Manchester*;

Desiccation of cohesive soils due to the loss of moisture is a geo-environmental challenge and it is increasingly becoming a wide spread problem due to climate changes. The understanding of desiccation in clay soils and how it leads to cracking has substantially been improved during the last 20 years through experimental investigations and theoretical developments. However, very limited predictive models for the initiation and propagation of cracks during clay desiccation have been presented in the literature. The slow progress in this field is essentially due to the limitations of the local (differential) formulations, solved by classical numerical methods. We will present a non-local (peridynamic) formulation of clay desiccation and fracture propagation, which couples weakly the moisture flow and the mechanical deformation and allows for the emergence and evolution of discontinuities. This model is incorporated into a multi-physics computational implementation of peridynamics (Pyramid). Two series of validation exercises by comparing the model predictions with experimental data with very different setups and consequently experimental outcomes will be presented. The validations presented will include the shrinkage and cracking of a soil sample in a ring test and desiccation-induced cracking of a long clay sample. It will be shown that the model captures accurately the experimentally observed behaviour for crack initiation to occur at a narrow water content range. The simulation results, including crack initiation and number of generated cracks, correlate well with the experimental observations, lending strong support for the predictive capabilities of the model and its computational implementation in the Pyramid code.

16th U.S. National Congress on Computational Mechanics
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Title: Goal-Adaptive Meshing for Structural Shell Analysis Problems

Author(s): *Hugo Verhelst, *Delft University of Technology*; Matthias Möller, *Delft University of Technology*; Henk Den Besten, *Delft University of Technology*;

Isogeometric Analysis enables seamless integration between Computer-Aided Design (CAD) and numerical analysis by employing the spline basis functions for geometric representation in CAD in the analysis. Applications of Isogeometric Analysis include structural shell analysis problems among other disciplines. In some structural analysis applications, for example fatigue analysis, accurate descriptions of stress fields are of importance to predict structural safety. Accurate description of these fields are enabled by the higher-order continuity of the basis functions in isogeometric shells. To balance computational costs with a desired level of accuracy – hence enabling accurate and reliable design-through analysis – adaptive meshing can be employed. Elements are typically refined based on their contribution to the total error measure (Buffa & Giannelli, 2016). In our work, we present an adaptive refinement and coarsening procedure based on goal functionals dedicated to different structural analysis problems, varying from linear bending-dominated response to non-linear membrane problems at large strains. We employ the Dual-Weighted Residual method (Rannacher, 2004) to compute element-wise error contributions with respect to a goal functional (e.g. a stress measure) and Truncated Hierarchical B-splines (THB splines) (Giannelli et al. 2012) to provide local mesh refinements. We will evaluate different goal functionals for both (non-)linear equilibrium analyses (i.e. static, dynamic and post-buckling) as well as eigenvalue analyses (i.e. modal and buckling) and assess their effectivity or different problems. The results of our study will both include global error analysis accuracy per degree-of-freedom as well as computational costs involved in the assembly and the solving of additional linear systems.

16th U.S. National Congress on Computational Mechanics
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Title: An Immersed Boundary Method for Concrete Printing Applications

Author(s): *Ignasius Wijaya, *University of Illinois at Urbana-Champaign*; Soonpil Kang, *University of Illinois at Urbana-Champaign*; Arif Masud, *University of Illinois at Urbana-Champaign*;

We present an immersed boundary method to simulate extrusion-based layered printing with cementitious material where the mechanical properties are continuously evolving due to chemical curing. The goal is to analyze the feasibility of print design which is significantly influenced by the geometry, printing speed, and material evolution as a function of curing. Immersed boundary method is used to bridge the gap between geometric design and numerical simulation by removing the need to create the Ghost-mesh that aligns with the geometry of the object to be printed. A new technique that is derived based on the Variational Multiscale (VMS) method is employed to weakly impose the Dirichlet boundary conditions in the interior of the elements. To model the mechanical behavior of the printed concrete, Drucker-Prager plasticity model is employed. Incorporating plasticity model allows for analysis of two main modes of failure, namely (i) elastoplastic buckling, and (ii) plastic collapse. The material parameters evolve as a function of time to model chemical curing of the layered cementitious material. The evolution of material parameters gives rise to the bounce-back phenomenon where the deformation under constant load decreases as a result of increasing stiffness in the material model. In extrusion based layered printing, this results in swelling of the lower layers as they cure, thereby pushing the subsequent layers upwards. This numerical manifestation of curing induced deformation contradicts the experimental observation of the behavior of printed cementitious materials that gain strength at an almost constant deformation. An algorithm is presented that prevents the non-physical bounce-back via enforcing a constraint on the Drucker-Prager model in the material space. The process of 3D layered printing is modeled via a finite deformation finite element method with embedded modified Drucker-Prager model in conjunction with immersed boundary method. All integration points in the background mesh are initially assigned a relatively small stiffness and zero density. Then, a moving point is defined to represent the kinematics of the printing nozzle. At each step, integration points around the nozzle are activated and assigned the actual stiffness and density of the material. As the nozzle moves around, more integration points are activated. This process simulates layered printing of the structure. The model and method are validated with experimental data, and several interesting test cases are presented.

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Title: A Thermo-Mechanical Model of Permafrost for the Simulation of Arctic Coastal Erosion

Author(s): Alejandro Mota, *Sandia National Laboratories*; Jennifer Frederick, *Sandia National Laboratories*; *Irina Tezaur, *Sandia National Laboratories*; Diana Bull, *Sandia National Laboratories*;

Accelerating Arctic coastal erosion rates have put critical infrastructure and native communities at risk due to a number of changes in the Arctic environment. Although the Arctic comprises one-third of the global coastline, current tools for quantifying permafrost erosion are unable to explain the episodic, storm-driven events. This presentation will describe the terrestrial component of a new thermo-mechanics-based model known as ACE (Arctic Coastal Erosion) for the simulation of the erosion of permafrost off the Arctic coast of Alaska. The ACE model is intended to inform our scientific understanding of coastal erosion processes, contribute to estimates of biogeochemical and sediment loading, and facilitate infrastructure susceptibility assessments. The terrestrial component of the ACE model [1] is comprised of two main ingredients: (1) a solid mechanics model that calculates the three-dimensional (3D) stress, strain and displacement fields of the underlying permafrost developing in response to a frozen water content dependent plasticity model, and (2) a novel thermal model governing the 3D heat conduction and solid-liquid phase change occurring within the permafrost. These two physics sets are coupled via a sequential thermo-mechanical coupling scheme developed within the Albany LCM open-source finite element code [2]. Elements are dynamically removed from the underlying finite element mesh so as to simulate transient permafrost erosion events. Oceanographic boundary conditions are provided by a numerical modeling suite comprised of a circum-Arctic Wave Watch III model forcing a two-way coupled SWAN-Delft3D-FM local model. Combined with atmospheric conditions, this suite produces time-dependent surge and run-up output to force the Albany terrestrial model. Unlike prior approaches, our modeling approach enables failure from any allowable deformation (block failure, thermo-denudation, thermo-abrasion); moreover, failure modes develop from constitutive (rather than empirical) relationships inherent in the underlying finite element model. Following a description of the key features of the ACE terrestrial model, we will present the results of a validation study of ACE devised from field surveys and data collected at the Drew Point site in Northern Alaska during a 2018-19 field campaign. [1] A. Mota, J. Frederick, I. Tezaur, D. Bull. “A thermo-mechanical terrestrial model of Arctic coastal erosion”, submitted to J. Comput. Appl. Math. [2] A. Salinger et al. “Albany: using agile components to develop a flexible, generic Multiphysics analysis code”. Int. J. Multiscale Comput. 14(4) (2016) 415-438.

16th U.S. National Congress on Computational Mechanics
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Title: Eigenanalysis and Non-Modal Analysis of Collocated Entropy Stable Discontinuous Galerkin Discretizations with the Summation-by-Parts Property

Author(s): *Irving Enrique Reyna Nolasco, *King Abdullah University of Science and Technology*; Lisandro Dalcin, *King Abdullah University of Science and Technology*; Matteo Parsani, *King Abdullah University of Science and Technology*;

In recent years, high-order methods based on summation-by-part (SBP) operators have shown a good maturity level in efficiency and accuracy for dealing with wave propagation problems on complex geometries. In general, high-order discretization schemes have demonstrated an ability to produce accurate solutions with smaller numerical dissipation and dispersion compared to lower order methods. Moreover, numerical diffusion plays a crucial role in the robustness and accuracy of under-resolved turbulent computations. Therefore, the analysis of the numerical errors arising in any scheme is essential to understand the accuracy of a numerical solution, and to design robust and accurate numerical discretizations. In the present work, the dispersion and diffusion properties are analyzed for the semi-discrete equation of the one-dimensional linear advection and linear advection-diffusion equation. The spatial derivatives of the equations are discretized through a differentiation matrix collocated at the Legendre-Gauss-Lobatto points, which satisfy the SBP property. The boundary data is weakly imposed through the simultaneous-approximation-term technique (SAT). The analysis performed here is based on the traditional Fourier analysis or eigenanalysis technique similar to the work presented in [1], and the non-modal analysis introduced by P. Fernández et. al. in [2]. The non-modal analysis aims to characterize the methods' numerical diffusion properties by taking into account all modes for each wavenumber. This is achieved through the study of the short-term dynamics of the semi-discretization equation of the linear advection-diffusion equation. The short-term diffusion behavior is investigated as a function of the spatial discretizations and speed regimes. In this work's eigenanalysis, the behavior of the so-called primary and secondary eigenmodes are analyzed. Additionally, the energy loss of the initial wave is computed in order to describe the diffusion for different spatial discretizations. The main goal of the analysis presented in this work is to characterize the numerical dispersion and diffusion properties arising in the SBP-SAT discretizations. At the same time, we get some insights into the discretization scheme's robustness and the effects of numerical dissipation on the unresolved-scales. The analysis observations are validated with numerical results. [1] F. Q. Hu, M. Y. Hussaini, and P. Rasetarinera, An analysis of the discontinuous Galerkin method for wave propagation problems, J. Comput. Phys., 151 (1999), pp. 921--946. [2] P. Fernandez, R. C. Moura, G. Mengaldo, and J. Peraire, Non-modal analysis of spectral element methods: Towards accurate and robust large-eddy simulations, Comput. Methods Appl. Mech. Engrg., 346 (2019), pp. 43--62.

16th U.S. National Congress on Computational Mechanics
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Title: Robust Modal Decomposition of Corrupt Fluid Flows

Author(s): *Isabel Scherl, *University of Washington*; Benjamin Strom, *University of Washington*; Jessica Shang, *University of Rochester*; Owen Williams, *University of Washington*; Brian Polagye, *University of Washington*; Steven Brunton, *University of Washington*;

Modal analysis techniques have been used to identify patterns and structures in a variety of fluid applications. However, experimentally acquired flow fields may be corrupted with incorrect and missing entries, which will degrade subsequent modal analyses. Here we explore how robust principal component analysis (RPCA) can be used to leverage global coherent structures to identify and replace spurious data points. RPCA decomposes a data matrix into a sparse component and low-rank matrix of coherent structure. We explore RPCA on a range of fluid simulations and experiments of varying complexity and assess how accurately the low rank structure in the data is recovered.In all cases, we find that RPCA extracts dominant fluid coherent structures and identifies and fills in incorrect or missing measurements. The performance is particularly striking when flow fields are analyzed using dynamic mode decomposition, which is sensitive to noise and outliers.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling the In-Plane and Out-Of-Plane Mechanical Response of Paper Using Fiber Networks

Author(s): Greta Kloppenburg, *RWTH Aachen University*; Hagen Holthusen, *RWTH Aachen University*; *Jaan-Willem Simon, *RWTH Aachen University*;

Many natural and synthetic materials possess fibrous microstructures, such as nonwoven fabrics, paper, and fiberboard. In most applications, it is difficult to evaluate the mechanical behavior of these fiber networks experimentally because of their small-scale nature. Particularly in the out-of-plane direction, performing experiments is challenging due to the small specimen thickness. Hence, to predict mechanical properties properly, network-scale models are required to obtain effective material properties by considering fiber-scale mechanisms. The current study demonstrates a three-dimensional representative volume element (RVE) for fiber networks using the finite element method. First, the classical deposition procedure has been adopted to generate fiber networks with preferential fiber orientations followed by an artificial compression step. The hollow fibers, described with elastic-plastic material behavior implemented into brick finite elements, have been joined by interface-based cohesive zone elements introduced in all fiber-fiber contact areas. Then, the fiber networks have been subjected to displacement boundary conditions, and their apparent mechanical responses have been evaluated by means of averaging the resulting stresses. Further, an RVE size convergence study has been conducted in order to determine the appropriate RVE dimension. Noteworthy, the responses in compression and in tension have been investigated for both, in-plane and out-of-plane loading scenarios. Since the thickness of the considered networks is much smaller than the in-plane dimensions, the principle of scale separation does not hold in the thickness direction. Thus, the RVE size is investigated by varying the specimen length while keeping the specimen thickness constant. From this investigation it can be concluded, that an RVE exists even in cases where debonding is taken into account. Further, the required RVE size for the sample to be representative can be reduced if multiple realizations of the same size are considered. The framework established in this work can be used to model numerous kinds of fiber networks at the individual fiber level and pass the information up to the macro scale for further analysis. This model is suitable to analyze both, the in-plane and the out-of-plane deformation.

16th U.S. National Congress on Computational Mechanics
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Title: Sparsity of the Tight Binding Potential Energy Surface

Author(s): *Jack Thomas, *University of Warwick*; Christoph Ortner, *University of British Columbia*; Huajie Chen, *Beijing Normal University*;

We survey some recent results on the sparsity of the potential energy surface (PES) aimed to justify and extend the theory of machine-learning for interatomic potentials. Firstly, we show that the PES in a wide range of tight binding models can be decomposed into site contributions which only depend on an exponentially small atomic neighbourhood. The asymptotic behaviour of the pre-factors and exponents in these estimates are characterised with respect to vanishing Fermi-temperature and, in the case of insulators, the band gap. Moreover, we show that the site contributions may be approximated by a body-order expansion of low body-order. Specifically, we prove that the resulting body-order expansion for analytic observables has an exponential rate of convergence both at finite Fermi-temperature as well as for insulators at zero Fermi-temperature. We discuss potential consequences of this observation for modelling the PES, as well as for solving the electronic structure problem. A particular feature of all our results is that they depend only weakly on the point spectrum which arises from the study of point defects in crystals, for example. This observation extends and strengthens the previous locality results of [Chen, Ortner. Multiscale Model. Simul., 14(1), 232–264 (2016)] and [Chen, Lu, Ortner. Archive Rat. Mech. Anal., 230, 701-733 (2018)]. Joint work with Christoph Ortner and Huajie Chen.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling of the Transformation Ratcheting of Nitinol Using Computational Crystal Plasticity

Author(s): *Jacob Rusch, *Marquette University*; John Moore, *Marquette University*; Sivom Manchiraju, *Ansys Inc.*;

Nitinol is a near-equiatomic nickel-titanium alloy used mainly in biomedical applications such as coronary stents, but it is also used in aerospace applications and some consumer goods. Nitinol is a unique material with unusual properties such as shape memory and superelasticity. Because of the unusual properties of Nitinol, it is a challenge to model the material accurately. In particular, it is difficult to model the thermal and mechanical mechanisms which drive plastic deformation and ultimately lead to failure due to fatigue. A microstructural model was developed by Manchiraju in 2011 (Manchiraju, 2011) which couples the martensitic phase transformation and plastic deformation. In addition to the martensitic phase transformation and plastic deformation, the inelastic deformation from the build-up of martensite during cyclic loading known as transformation ratcheting has been added into the existing implicit model. Results from the simulation are then compared to those seen experimentally. Manchiraju, S. (2011). Modeling the coupling between martensitic phase transformation and plasticity in shape memory alloys (Doctoral dissertation, The Ohio State University). Retrieved from https://etd.ohiolink.edu/

16th U.S. National Congress on Computational Mechanics
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Title: Conformings vs Weakly Conforming Comparison of the Double Adaptivity in Petrov Galerking Methods with Optimal Test Functions

Author(s): *Jacob Salazar Solano, *The University of Texas at Austin*; Leszek Demkowicz, *The University of Texas at Austin*;

We present the comparison between a conforming and a weakly conforming Petrov Garlerkin Method with optimal test functions. During the implementation of the modified double adaptivity algorithm of Cohen, Dahmen and Welpert [1] using duality theory for the a-posteriori error estimation for the inner adaptivity loop [3], within the setting of the Petrov-Galerkin Method with Optimal Test Functions [2], the inner loop convergence results hindered for high order polynomial spaces. Given the already proved track record of the weakly conforming (Discontinuous) Petrov Galerkin Method with optimal test functions, we expect the extra relaxation it provides to be the advantageous point with respect to the conforming version of the method. We present numerical results for a) the solution of the ultra weak variational formulation of the convection-dominated diffusion problem in 1D and 2D and b) modelling of ductile to brittle phase transitions. However the presented conclusions are expected to extend to virtually any well posed system of first order PDEs including singular perturbation problems. The ideal Petrov-Galerkin Method with Optimal Test Functions reproduces the stability of the original problem and guarantees optimal convergence for any well posed problem; the practical version of it approximates the Riesz (error) representation function Ψ using an enriched test space by means of increasing the polynomial order of the trial space. However, for singular perturbation problems, and test norms involving the perturbation parameter, resolution of Ψ is still challenging due to approximability issues. The revolutionary contribution of Cohen, Dahmen and Welper calls for determining an optimal discrete test space using adaptivity. The outer adaptivity loop is performed to refine the discrete trial space and the inner adaptivity loop allows for control of the error in Ψ. The adaptively determined enriched test space is “custom made” for the particular load and the trial space, and despite the fact that it does not imply the discrete stability, the ultimate method converges. References: [1] A. Cohen, W. Dahmen, and G. Welper, “Adaptivity and variational stabilization for convectiondiffusion equations”, ESAIM Math. Model. Numer. Anal., 46(5):1247–1273, 2012 [2] C. Carstensen, L. Demkowicz and J. Gopalakrishnan, “Breaking spaces and forms for the DPG method and applications including Maxwell equations”, Comput. Math. Appl., 72(3):494–522, 2016 [3] L. Demkowicz, T. Fuhrer, N. Heuer and X. Tian, ¨ “The Double Adaptivity Paradigm (How to circumvent the discrete inf-sup conditions of Babuska and Brezzi)” ? , The University of Texas at Austin, ICES report, 19-07, 2019

16th U.S. National Congress on Computational Mechanics
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Title: A Function Space Variational Autoencoder

Author(s): *Jacob Seidman, *University of Pennsylvania*; Paris Perdikaris, *University of Pennsylvania*; George Pappas, *University of Pennsylvania*; Victor Preciado, *University of Pennsylvania*;

Variational autoencoders have proved useful at creating low dimensional representations of higher dimensional datasets such as images. We extend this model to create latent representations of data sets where each data point resides in a space of functions of a continuous time variable. In this sense, we construct a variational autoencoder which can operate on infinite dimensional vector spaces of trajectories. This can be useful in scenarios where we have access to high frequency measurements of a dynamical system that are noisily embedded into a higher dimensional measurement space. After positing a simple generative model for the data from a latent space of functions, we are able to formulate a well defined Evidence Lower Bound (ELBO) objective function based on a likelihood derived from the white noise measure. By using Gaussian measures for our latent prior and variational family, we examine how the choice of these measures affects the model’s performance and leads to the emergence of some familiar quantities in our objective which act as regularizers. Finally, we perform some experiments that showcase the model's ability to recover low dimensional structures from curves embedded into high dimensional spaces.

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Title: Industrial Applications of Computational Mechanics to Support Applied Research and Product Development

Author(s): *James Sobotka, *Southwest Research Institute*; Ghadir Haikal, *Southwest Research Institute*;

To bridge the “Valley of Death” between universities/national labs and industry, Southwest Research Institute® employs computational mechanics as a tool to support applied research and product development. This presentation summarizes projects that have applied computational mechanics as a tool to solve problems in domains that include fracture mechanics, biomechanics, automated forging, gas-turbine engines, ballistics and explosives, rocket engine development, structural optimization, and prototyping using additive manufacturing. In these efforts, computational mechanics provides an essential tool to support collaborative efforts with industry. This work will also discuss how computational mechanics complements other tools to support a successful programs, including verification/validation, experimental testing programs, calibration, and software development. This presentation concludes by discussing attributes of successful advances in computational mechanics that are readily suitable for industrial applications.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multifidelity Failure Probability Estimation with Adaptively Designed Surrogate Models

Author(s): *James Warner, *NASA Langley Research Center*; David Cole, *Virginia Polytechnic Institute and State University*; Robert Gramacy, *Virginia Polytechnic Institute and State University*; Patrick Leser, *NASA Langley Research Center*; Geoffrey Bomarito, *NASA Langley Research Center*; William Leser, *NASA Langley Research Center*;

Estimating the probability of failure with Monte Carlo (MC) simulation is often intractable due to the large number of samples (and model evaluations) required to accurately resolve rare event probabilities. This challenge is exacerbated when the failure probability is small and/or an expensive, high-fidelity model is needed to model the system at hand. A common strategy to speed up MC simulation is to replace the high-fidelity model with a cheaper data-driven surrogate model. The downside of such an approach is that the resulting failure probability estimate is biased. Recently, multifidelity importance sampling (MFIS) was developed to leverage both the surrogate and high-fidelity model for efficient and unbiased failure probability estimates. While MFIS has shown the potential to yield substantial convergence improvements over MC, the efficacy of the approach is critically dependent on the accuracy of the surrogate model in the vicinity of the failure region. This work combines MFIS with an adaptively designed Gaussian Process (GP) surrogate model for low-variance, high-accuracy failure probability estimates. An entropy-based adaptive design strategy is introduced that tailors the accuracy of the GP model near the failure region and is shown to outperform existing contour-finding active learning methods. It is demonstrated that leveraging the tailored GP significantly improves the accuracy of MFIS on simple benchmark problems and can overcome some pathological cases where MFIS with a vanilla surrogate model fails (e.g., problems with multiple failure regions). Finally, a reliability analysis of a NASA spacesuit design under impact loading is used to highlight the efficiency and practicality of the approach.

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Title: Implicit Advection: Increased Robustness for Dynamical Cores

Author(s): *James Woodfield, *University of Reading / Imperial College London*; Hilary Weller, *University of Reading*; Colin Cotter, *Imperial College London*;

Can implicit time stepping satisfy the requirements for advection modelling on next generation dynamical cores? Many operational weather forecasting centres are aiming to move away from semi-Lagrangian advection schemes, in order to conserve mass. Many centres are choosing the flux-form semi-Lagrangian as an alternative. However, this method is expensive to implement on unstructured grids. Implicit time stepping methods could provide a potentially simpler option. In this talk, we will discuss whether implicit schemes can attain desirable properties for use in the atmosphere. We will be discussing some solving strategies associated with implicit time stepping schemes. The focus will be on attaining nonlinear stability whilst retaining mass conservation, accuracy, efficiency, order greater than one. One of the solving strategies associated with implicit schemes is a deferred correction technique proposed by P.K. Khosla and S.G. Rubin in 1974. We will examine the linear and non-linear properties of the Khosla and Rubin deferred correction technique, to determine whether this solving strategy is appropriate for use in atmospheric science. Another strategy is the use of linearised flux limiters, introduced by H.C. Lee in 1986. We will introduce these concepts from a theoretical perspective, but compare these strategies primarily with numerical experimentation.

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Title: Computational Investigation of Interactions Between Test Articles and the Medium Weight Shock Test

Author(s): Matthew Lear, *The Pennsylvania State University*; *Jason Sammut, *The Pennsylvania State University*;

In pursuit of continued advancement and protection against emerging threats, the U.S. Navy has an ever-increasing need for higher performance defense vehicles. Usage of modern materials, design, and manufacturing methods to address this need leads to novel problems, particularly in the area of shock resistance. Since all Naval structures must withstand “near-miss” shock events in accordance with MIL-DTL-901E, it is critical to effectively characterize how these modern methods respond to intense dynamic loading. Current modeling and computational tools provide the ability to greatly increase the capabilities and accuracy of analysis-driven shock design. Existing methods of shock design often involve unacceptable simplifications that can lead to significant over-design and substantial loss of performance as a result. Commonly used static load assumptions are insufficient to capture the true loading encountered by the intense, short-duration environments of shock events. This largely stems from a lack of availability of representative input loading for analysis, specifically from the standard shock qualification tests. This research addresses deficiencies in computational shock loads by replicating the Medium Weight Shock (MWS) test in a finite element simulation. An initial model was created from existing mechanical drawings of the MWS machine, and Abaqus/Explicit was used to simulate the contact and transient dynamics of the test setup. Iterative model validation and tuning was completed by comparing simulation results to multiple sets of existing test data for two separate mounted test components. A combination of shock parameters were analyzed to ensure accurate replication, including shock spectrum curves, pulse duration, and response magnitudes. The current MWS model accurately simulates test events for any component of interest and provides detailed structural response throughout the component. Full analysis is completed within a practical computation time, allowing future designs to be iteratively analyzed for shock response, and give confidence prior to qualification testing. This method can be extended to other Navy shock qualification test setups. Valuable insight into important behaviors of the MWS test setup were drawn from the model creation and validation processes. Among other discoveries, it was found that the interactions between the modal behaviors of the mounting structure and test component were responsible for primary features of shock spectrum results. The model opens the door for evaluations of current Navy shock qualification requirements, such as ensuring test structure mounting does not bias shock frequency content and that shock pulse characteristics of hammer contact sufficiently replicate those of underwater explosions.

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Title: Physics Aware Machine Learning for Structural Topology Optimization

Author(s): *Jaydeep Rade, *Iowa State University*; Ethan Herron, *Iowa State University*; Aditya Balu, *Iowa State University*; Soumik Sarkar, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Abstract: Traditional topology optimization methods are implemented as iterative processes, making them computationally expensive due to the finite element solve at each iteration of the optimization process. This computational time further increases when the design domain is scaled to 3D; even more when the resolution is increased. To address this issue, we have developed a deep-learning-based topology optimization that performs an end-to-end prediction of the optimal topology using the initial compliance of the design and target volume fraction for both 2D and 3D geometries. To generate the training data, we used the solid isotropic material with penalization (SIMP) method. We observed that the topology goes through a significant amount of transformation during the initial first five iterations of the SIMP method than in the later iterations. We have developed a pipeline of multiple deep neural networks to perform the different tasks in topology optimization. We used the intermediate compliance and topologies, which were saved during the data generation process, to predict the final optimal topology. The framework consists of three neural networks: (1) the compliance prediction network (CPN) that predicts the next iteration compliance, (2) the density prediction network (DPN) that predicts the next iteration density, and (3) the final density prediction network (FDPN) that uses the last output of the DPN to produce the final optimal topology. The CPN and DPN are coupled together and run iteratively, feeding their output as input to the next iteration. We cascade these three networks during inference. We compare the results obtained from our method with the ground truth obtained using the SIMP method. We also compared the various loss metrics between our method and a baseline approach using a single deep learning-based network prediction. Our resulting approach is much faster than traditional finite element-based topology optimization while generating similarly optimal geometries. In addition, our framework also predicts the total compliance value close to the ground truth value. References: 1. Aditya Balu, Sahiti Nallagonda, Fei Xu, Adarsh Krishnamurthy, Ming-Chen Hsu, Soumik Sarkar; A deep learning framework for design and analysis of surgical bioprosthetic heart valves, Scientific Reports, 9(18560), 2019. 2. Sambit Ghadai, Aditya Balu, Soumik Sarkar, Adarsh Krishnamurthy; Learning localized features in 3D CAD models for manufacturability analysis of drilled holes, Computer Aided Geometric Design, 62:263–275, 2018.

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Title: Quasi-Structured Quadrilateral Meshing in Gmsh -- a Robust Pipeline for Complex CAD Models

Author(s): *Jean-Francois Remacle, *Université catholique de Louvain*; Maxence Reberol, *Université catholique de Louvain*; Christos Georgiadis, *Université catholique de Louvain*;

We propose an end-to-end pipeline to robustly generate high-quality quadrilateral meshes for complex CAD models. A initial quad-dominant mesh is generated with frontal point insertion guided by a locally integrable cross field and a scalar size map adapted to the small CAD features. After triangle combination and midpoint-subdivision into an all-quadrilateral mesh, the topology of the mesh is modified to reduce the number of irregular vertices. The idea is to preserve the irregular vertices matching cross-field singularities and to eliminate the others. The topological modifications are either local and based on disk quadrangulations, or more global with the remeshing of patches of quads according to predefined patterns. Validity of the quad mesh is guaranteed by monitoring element quality during all operations and reverting the changes when necessary. Advantages of our approach include robustness, strict respect of the CAD features and support for user-prescribed size constraints. The quad mesher, which is available in Gmsh, is validated and illustrated on two datasets of CAD models.

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Title: Reducing Errors in Data Refinement

Author(s): *Jennifer Ryan, *Colorado School of Mines*;

This presentation focuses on techniques to reduce the errors when starting with coarse data and performing data refinement. The main mechanisms is to exploit superconvergence to obtain more accurate multi-resolution analysis. Specifically, we concentrate on enhancing the quality of passing of information between scales by implementing the Smoothness-Increasing Accuracy- Conserving (SIAC) Filtering combined with multi-wavelets. This allows for a more accurate approximation when passing information between meshes of different resolutions. This is possible for different types of data, although this presentation focuses on discontinuous Galerkin approximations. [1] J.K. Ryan, "Capitalizing on Superconvergence for more accurate Multi-Resolution discontinuous Galerkin Methods", Communications on Applied Mathematics and Computation, accepted (2021). [2] J. Docampo, G. Jacobs, X. Li, and J.K. Ryan, "Enhancing Accuracy with a Convolution Filter: What Works and Why!" Computers and Fluids, 213 (2020). [3] Bradley K. Alpert, A Class of Bases in L^2 for the Sparse Representation of Integral Operators, SIAM Journal on Mathematical Analysis 24, 246-262 (1993).

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Title: A Peridynamic Model of Degradation in Concrete

Author(s): *Jeremy Trageser, *Sandia National Laboratories*; Jessica Rimsza, *Sandia National Laboratories*; Reese Jones, *Sandia National Laboratories*; Joshua Hogancamp, *Sandia National Laboratories*;

The study of concrete is crucially important as it is one of the most widely employed materials. Unfortunately, concrete is notoriously difficult to model. Moreover, even before damage occurs, concrete exhibits many discontinuities which makes utilizing models employing spatial derivatives challenging. The nonlocal theory of Peridynamics [1] employs integral operators rather than differential operators to avoid issues posed by discontinuities. This work explores the applicability of peridynamics in simulating degradation of concrete due to water infiltration. Water infiltration in concrete results in the leaching of calcium and silica and leads to degradation of the mechanical properties of the concrete, e.g., a reduction of the elastic modulus and volumetric shrinkage. Moreover, as damage and fracture develop in the material, the permeability increases and leads to further water diffusion into the material. These features are implemented into the peridynamic framework and numerical studies were conducted. [1] Silling, Stewart. Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces. Journal of the Mechanics and Physics of Solids. (2000) 48:175-209. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2021-0199 A

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Title: Efficient Hydrocode Modeling of Airblast Propagation at Large Scaled Ranges

Author(s): *Jesse Sherburn, *US Army Engineer Research and Development Center*; Genevieve Pezzola, *US Army Engineer Research and Development Center*; Catherine Stephens, *US Army Engineer Research and Development Center*;

The ability to model explosively formed shock waves propagating through the air is of particular interest to engineers concerned with designing structures to resist blast. Accurate peak pressure and impulse values are critical to understanding blast loads and are required to validate computational modeling methods. When tied to experiments, computational modeling of explosive events can be an invaluable tool for an engineer. In some blast scenarios, the loading can come from large scaled ranges which can require substantial computational resources due to the large spatial scale required to propagate the blast wave. This is especially true if traditional Eulerian hydrocode flat mesh methods are used. The large spatial scale can be a hindrance to doing large parametric 3D studies with these methods. In this study, the hydrocode CTH [1] will be used to model various blast scenarios at large scaled ranges. An efficient method of modeling blast at large scaled ranges will be presented using the automatic mesh refinement (AMR) feature in CTH. AMR has the ability to maximize the mesh resolution in regions of interest. The method will be executed with a number of different equations of states as well as 2D and 3D scenarios. Two different explosive charge geometries will be used to show its flexibility and effectiveness to propagate blast loads out to large scaled ranges. Some experimental data will also be presented that will be used as validation for the method. [1] McGlaun, M. G., S. L. Thompson, and M. G. Elrick. 1990. CTH: A three-dimensional shock wave physics code. International Journal of Impact Engineering 10 (1-4):351-360. * Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

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Title: Deep Learning of Material Transport in Complex Neurite Networks

Author(s): Angran Li, *Carnegie Mellon University*; Amir Farimani, *Carnegie Mellon University*; *Jessica Zhang, *Carnegie Mellon University*;

Neurons exhibit complex geometry in their branched networks of neurites which is essential to the function of individual neuron but also brings challenges to transport a wide variety of essential materials throughout their neurite networks for their survival and function. While numerical methods like isogeometric analysis (IGA) have been used for modeling the material transport process via solving partial di fferential equations (PDEs), they require long computation time and huge computation resources to ensure accurate geometry representation and solution, thus limit their biomedical application. Here we present a graph neural network (GNN)-based deep learning model to learn the IGA-based material transport simulation and provide fast material concentration prediction within neurite networks of any topology. Given input boundary conditions and geometry con figurations, the well-trained model can predict the dynamical concentration change during the transport process with an average error less than 10% and 120~330 times faster compared to IGA simulations. The effectiveness of the proposed model is demonstrated within several complex neurite networks.

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Title: On Tailoring Fracture Toughness: Level-Set Topology Optimization Using an Interface-Enriched Formulation

Author(s): *Jian Zhang, *Delft University of Technology*; Fred Van Keulen, *Delft University of Technology*; Alejandro Aragón, *Delft University of Technology*;

Topology optimization has been widely used to optimize structures for mitigating structural failure. The most popular way is to consider stresses as objectives/constraints. However, instead of monitoring stress, one may is to use criteria based on linear elastic fracture mechanics. In this work, we propose a topology optimization procedure to design structures with tailored fracture resistance[1]. Instead of predefining the location of cracks, these are assumed to nucleate anywhere along the structural boundary, and their corresponding energy release rates are evaluated. While conventional methods use vast computational resources to simulate cracks at different locations separately, we adopt an analytical formulation based on the finite element solution of an uncracked domain and the topological derivative to calculate energy release rates[2]. An aggregate function is used to collect energy release rates into a single objective, and the corresponding sensitivity associated with design variables is derived analytically by using an adjoint formulation. The topology optimization approach used in this work, which uses a level set to represent the structural topology and the Interface-enriched Generalized Finite Element Method (IGFEM) to obtain the structural response, was introduced recently to solve compliance minimization problems[3]. The technique is showcased by means of several examples. An L-shaped bracket is provided to investigate the proposed optimization framework. Moreover, an optimized structure with anisotropy of fracture resistance is obtained by constructing a multiple-objective formulation. [1] Zhang, J., Van Keulen, F., and Aragon, A. M. Tailoring fracture toughness in brittle materials via level set topology optimization. Comput. Methods in Appl. Mech. Eng. Submitted for publication. [2] Silva, M., Geubelle, P.H. and Tortorelli, D.A. Energy release rate approximation for small surface-breaking cracks using the topological derivative. J. Mech. Phys. Solids (2011) 59: 925-939. [3] Van den Boom, S. J., Zhang, J., Van Keulen, F., and Aragon, A. M. An Interfaced-enriched Generalized Finite Element Method for level set-based topology optimization. Struct. Multidisc. Optim. (2021) 63: 1-20.

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Title: Physics-Informed Discretization-Based Learning: a Unified Framework for Solving PDE-Constrained Forward and Inverse Problems

Author(s): *Jian-xun Wang, *University of Notre Dame*; Han Gao, *University of Notre Dame*; Luning Sun, *University of Notre Dame*;

Numerical simulation has been playing an increasingly important role in understanding and predicting fluid phenomena. The traditional paradigm focuses on forward solutions with given modeling conditions (e.g., flow boundaries or mechanical parameters), some of which, however, are often unknown in many practical scenarios. On the other hand, indirect, sparse, and possibly noisy observations are usually available, which can be leveraged to estimate these unknowns, enabling modeling in an inverse fashion. Nonetheless, existing finite volume or finite element based numerical solvers have difficulties in assimilating data and solving such inverse problems because of considerable computational overhead for most nontrivial cases. In this work, we present a novel deep learning framework that enables us to solve forward and inverse problems in a unified manner, where sparse data can be naturally assimilated using discretization-based learning. The proposed method is demonstrated effective and efficient in simulating a number of PDEs with partially known boundary conditions.

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Title: Construction of a Nonlocal Model for Incompressible Flow at Low Reynolds Numbers

Author(s): *Jiangming Zhao, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

Abstract: Interactions between fluids and solids, such as the erosion corrosion and hydraulic fracture, are present in a variety of fields such as environmental, chemical and petroleum engineering. Classical models describe these problems using partial differential equations (PDEs), which makes it difficult to handle the evolution of material damage, fractures and discontinuities in general. The peridynamic (PD) theory is a nonlocal extension of the classical continuum mechanics, which employs integro-differential equations (IDEs) instead of PDEs. Cracks and other forms of damage can initiate and propagate naturally and autonomously in PD models. While the PD method has been used to deal with a myriad of mechanical and diffusion-type problems involving cracks and damage, its formulations and applications to fluid mechanics is few. A coupled model for both solid and fluid would contribute significantly to the study of fluid-solid interaction problems involving material damage. In this work, we construct a PD Navier-Stokes model for incompressible fluid flow from fundamental conservation principles, using an approach similar to that employed in [1,2]. Weight functions in the model are determined by matching PD and analytical solutions for problems with linear distribution of field variables. We verify the model against Couette and Poiseuille flows and the fluid flow past a regular lattice of cylinders at low Reynolds numbers. The PD solution matches analytical and finite element solutions very well. Finally, we couple the PD model for fluid flow with PD diffusion-advection and corrosion models to show the model's potential in several applications: mass transport in a flow field with obstacles, and flow accelerated corrosion. References: [1] F. Bobaru, M. Duangpanya, The peridynamic formulation for transient heat conduction, Int. J. Heat Mass Transf. 53 (2010) 4047–4059. https://doi.org/10.1016/j.ijheatmasstransfer.2010.05.024. [2] J. Zhao, Z. Chen, J. Mehrmashhadi, F. Bobaru, Construction of a peridynamic model for transient advection-diffusion problems, Int. J. Heat Mass Transf. 126 (2018) 1253–1266. https://doi.org/10.1016/j.ijheatmasstransfer.2018.06.075.

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Title: A Lagrangian Naturally Stabilized Meshfree Method

Author(s): *Jiarui Wang, *The Pennsylvania State University*; Michael Hillman, *The Pennsylvania State University*;

Over the past several decades, meshfree methods have proved advantageous in large-deformation problems such as manufacturing, fragment-impact, and natural disasters. However, instability in nodal integration of Galerkin meshfree methods is still an inherent obstacle that must be addressed for effective dynamic simulations [1]. Both stabilized conforming nodal integration (SCNI) [2] and direct nodal integration (DNI) [3] suffer from low energy modes of node-to-node oscillation, which can grow dramatically and destroy the simulation solution, particularly in high-strain-rate problems. While SCNI can alleviate the instability in DNI, severe oscillations can still occur when the surface to volume ratio of the domain is sufficiently low, or when the discretization is sufficiently fine. In this work, a Lagrangian naturally stabilized nodal integration (L-NSNI) method is proposed for meshfree modelling of dynamic problems. The Taylor’s expansion of strain and stress are employed, which finally lead to a supplement of internal energy to stabilize the original Lagrangian SCNI solution. As a result, the second order gradients of meshfree shape function are required and approximated by smoothed first order implicit gradients, which yields far less computational cost than the standard second order meshfree gradients. A novel stress update method is also proposed for the stabilization of material with high nonlinearity, where direct differentiation of stress terms in NSNI is non-trivial. The effectiveness of proposed methodology is demonstrated with several benchmark problems. References [1] Hillman, M., & Chen, J. S. (2016). An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics. International Journal for Numerical Methods in Engineering, 107(7), 603-630. [2] Chen, J. S., Wu, C. T., Yoon, S., & You, Y. (2001). A stabilized conforming nodal integration for Galerkin mesh?free methods. International journal for numerical methods in engineering, 50(2), 435-466. [3] Beissel, S., & Belytschko, T. (1996). Nodal integration of the element-free Galerkin method. Computer methods in applied mechanics and engineering, 139(1-4), 49-74.

16th U.S. National Congress on Computational Mechanics
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Title: Efficient Inverse Problem Learning with Precise Localization and Exploratory Sampling

Author(s): *Jiaxin Zhang, *Oak Ridge National Laboratory*; Victor Fung, *Oak Ridge National Laboratory*;

Solving inverse problems is a longstanding challenge in mathematics and the natural sciences, where the goal is to determine the hidden parameters given a set of specific observations. Typically, the forward problem going from parameter space to observation space is well established but the inverse process is often ill-posed and ambiguous, with multiple parameter sets resulting in the same measurement. Recently, deep invertible architectures have been proposed to solve the reverse problem, but these currently struggle in precisely localizing the exact solutions and in fully exploring the parameter spaces without missing solutions. In this work, we propose a novel approach leveraging recent advances in deep invertible models incorporated with gradient descent for efficiently and accurately solving inverse problems. Given a specific observation and latent space sampling, the learned invertible model provides a posterior over the parameter space; we identify these posterior samples as an implicit prior initialization which enables us to narrow down the search space. We then use gradient descent with backpropagation to calibrate the inverse solutions within a local region. Meanwhile, an exploratory sampling strategy is imposed on the latent space to better explore and capture all possible solutions. We evaluate our approach on three benchmark tasks and one real-world application from quantum chemistry and find it achieves superior performance compared to several state-of-the-art baseline methods.

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Title: Interplay Between Grain Shape and Grain Breakage in Crushable Sand Under Shear: A Multiscale Study Based on Physics Engine and Peridynamics

Author(s): *Jidong Zhao, *The Hong Kong University of Science and Technology*; Fan Zhu, *The Hong Kong University of Science and Technology*;

Natural sand grains often possess complex morphologies with varying aspect ratio, roundness and convexity. The morphologies of sand grains may evolve significantly through the breakage of particles under shear, compression or impact. Particle shape and breakage are known to be important factors underpinning many mechanical behaviors of sand such as packing, deformation and failure. Despite of great efforts made by mutli-disciplinary research communities involving civil, mining and chemical engineering as well as energy and pharmaceutical industries, the modeling irregular shape particles and particle breakage remains far from mature. A numerical framework that can incorporate irregular particle shapes while considering continuous particle breakage is highly desirable but unavailable. In current practice, however, particle shape and breakage have been commonly handled by adopting over-simplified, based upon diversified crushing criteria, and frequently incurring high computational cost. In this paper we introduce a novel numerical framework based on impulse-based dynamics (IBD), to simulate sand particles with irregular shapes, with proper consideration of continuous particle breakage. The IBD method, featured by its high computational efficiency and convenient integration of irregular particle shapes, has been commonly employed in physical simulation of robots and in the field of virtual reality, animation, games, but has gained relatively less attention from the engineering society. We demonstrate the predictive power of this IBD method with a simulation of one-dimensional compression on sand particles, where the particles were modeled using convex and non-convex polyhedrons with intertwined evolutions of both particle size and particle shape. The simulation results were validated with experimental observations with respect to particle size distribution, fractal dimension, and normal compression line. The interplay between evolution of particle size and particle shape during the crushing process is examined. The presented method provides a relatively efficient way to model sand particles with irregular shapes while considering particle breakage, offers insights into particle shape evolution under compression, and enables more in-depth study on micro-structural behavior of sand in the future.

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Title: Clot Growth Modeling Considering Physical Interactions Between Flow and Blood Cell Components

Author(s): *Jifu Tan, *Northern Illinois University*; Michael Hood, *Northern Illinois University*;

Platelets are one of the key blood cells that regulate bleeding and thrombus formation. Modeling thrombus formation can help us understand the dynamics of clot growth and evaluate the risk of embolism, which is critical for patients with heart attack or stroke history. However, modeling thrombus growth is very challenging. It involves many physics across different scales ranging from nanometer size membrane receptors to hundreds of micro size clots. The hydrodynamics, red blood cells, platelet activation and adhesion, blood coagulation pathways, and fibrin network formation all play important roles in thrombus formation. Moreover, the physical properties of platelets are time dependent, e.g., the bond strength increases with platelets activation; when fully activated, platelets also contract and stiffen the clot. In this paper, we developed a versatile thrombus formation model and studied the platelet deposition and clot growth in blood flow with cell suspensions using the immersed boundary method where the flow, platelet, and cell motion were coupled together. The fluid was solved by the lattice Boltzmann method. The cells were modeled as membranes using coarse grained molecular dynamics. The platelets were modeled as interactive particles with three different states: passive state (1), partially activated (2) and fully activated (3). Platelets with each state had distinctive adhesion strengths and can be transferred from less activated state to fully activated state. The formation of bonds between platelets also followed certain probability distributions, characterizing the stochastic nature of binding events. von Willebrand factor (vWF) modeled as coarse-grained polymer chains was found to help recruiting platelets and strengthen the clot structure. The clot growth process was studied considering different dimensionless numbers: Capillary number, activation state transition time ratio, and the ratio of platelet arriving time over platelet transition time. It showed that the clot structure simulated with the current model was heterogeneous with activated platelets in the core region and less activated platelets at the shell region. It is the dimensionless numbers that determine the clot growth process. The simulation results were also compared with in vivo experiments and agreed well with the experimental data.

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Title: A Bayesian Framework for Validation and Selection of Multiscale Plasticity Models with Quantified Uncertainty

Author(s): *Jingye Tan, *University at Buffalo*; Kathryn Maupin, *Sandia National Laboratories*; Danial Faghihi, *University at Buffalo*;

Key Words: Bayesian model selection, Bayesian validation, discrete dislocation dynamics, strain gradient plasticity
A class of multiscale models of size effect plastic deformation in polycrystalline materials consists of upscaling discrete dislocation dynamics (DDD) simulations to continuum strain gradient plasticity (SGP) models. However, an overriding challenge in predictive multiscale modeling is selecting a model among the enormous possible models with different fidelities, complexities, and computational costs. In this contribution, an adaptive computational algorithm is implemented to validate and select a family of hierarchical SGP models using the high-fidelity data furnished by DDD simulations. The algorithm leverages variance-based global sensitivity analyses, notion of model plausibility, and Bayesian model validation to systematically train and select an optimal valid SGP model, i.e., the simplest model that explains the data within the validation criteria. A statistical forward solver is also developed to characterize the effect of parameter uncertainty as well as grain morphological randomness (characterized by a phase-field grain growth model) on the plastic deformation prediction of the selected SGP model. The outcomes of this study indicate that the multiscale model prediction that goes beyond the available data requires taking advantage of physics-based models, along with coping with the stochasticity of the discrete simulations and uncertainties in model parameters and selection of the model itself. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: A Mixed Interface-Capturing/Interface-Tracking Approach to Thermal Multi-Phase Flows with Emphasis on Metal Additive Manufacturing Processes

Author(s): *Jinhui Yan, *University of Illinois at Urbana-Champaign*; Qiming Zhu, *University of Illinois at Urbana-Champaign*;

Accurate and robust thermal multi-phase flow simulations are the tools in demand to reveal the multi-scale and multi-physics phenomena in metal additive manufacturing (AM) processes. This paper presents a novel computational framework for thermal multi-phase flow simulations with emphasis on metal AM applications. The framework, built on level set method, features three contributions: (1) A new heat laser model with a simple geometry-based re-initialization technique, which maintains excellent signed distance property on unstructured meshes and eases the treatment of the multiple reflections during keyhole evolution in AM processes; (2) A variational multi-scale formulation for the coupled multi-phase Navier-Stokes, level set convection, and thermodynamics equations considering melting, solidification, evaporation and interfacial forces; (3) A recursive three-level preconditioning approach to achieve robust linear solvers. We first compare the geometry-based re-initialization with the Eikonal equation-based approach on two benchmark problems on level set convection and bubble dynamics. The results show the geometry-based approach attains equivalent and even better performance on key criteria. We then apply the developed framework to simulate two AM experiments, which have been recently conducted by Argonne National Laboratory with in-situ high-speed, high-energy x-ray imaging. The accuracy of the proposed framework is evaluated by comparing the simulated results against experimental measurements on various quantities. Excellent agreement is achieved.

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Title: Mesh Objective Fracture Modeling Using an Improved Smeared Crack Approach

Author(s): *Joel Upston, *University of New Mexico*; Howard Schreyer, *University of New Mexico*; Deborah Sulsky, *University of New Mexico*;

The smeared crack approach has been used extensively in the finite element method to implement cohesive failure models. There are several issues that have hindered its acceptance, for example, (i) accumulation of spurious shear stress, often resulting in locking, (ii) mis-oriented cracks and crack direction, and (iii) improper predicted load-deflection response (Rots and Blaauwendraad, 1989). Much work continues to address these issues due to the main advantage of the approach which is its algorithmic simplicity. Recent work (Burnett and Schreyer, 2019) for Mode I cracks has produced an efficient, explicit, mesh objective algorithm developed and implemented within a standard 4-node quadrilateral element. The techniques employed in this formulation include algorithms to preclude both spurious shear accumulation and mis-alignment of the stress field around the crack tip using a modified strain field in the cracked element, crack tracking, hourglass control, and so-called cross-over scaling. By analyzing the kinematics of a strong discontinuity within a finite element, we generalize the work of Burnett and Schreyer, 2019 to find the analytical strain correction term needed for Mode I, Mode II and mixed mode fracture. The analytical correction is found for arbitrary elements and general continuous shape functions. Using this proposed kinematic smeared crack approach we demonstrate in bilinear quadrilateral elements improvements that include simplified crack tracking, to make it computationally convenient to model multiple fractures where their locations are unknown a priori, and extend the method to four-point quadrature. Advantages of the method will be illustrated through demonstrated mesh-objective numerical examples that show agreement with known analytical solutions and other numerical solutions. References Burnett D.J. and Schreyer H.L. A mesh objective method for modeling crack propagation using the smeared crack approach. International Journal for Numerical Methods in Engineering,117(5):574–603, 2019. Rots J.G. and Blaauwendraad J. Crack models for concrete, discrete or smeared? Fixed,multi-directional or rotating? Heron, 34(1), 1989.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Uncovering Fetal Brain Folding Mechanisms via Medical Image Registration and Inverse Modeling

Author(s): Zhenlin Wang, *University of Michigan*; Blake Martin, *University of Michigan*; Yana Blinkouskaya, *Stevens Institute of Technology*; Krishna Garikipati, *University of Michigan*; *Johannes Weickenmeier, *Stevens Institute of Technology*;

During fetal development, the human brain undergoes large topological changes and volumetric growth. The corresponding folding of the outer cortex- also known as gyrification- is driven by the migration of neurons from the ventricular zone towards the cortex and the rapid dendritic arborization between individual neurons. The accumulation of neurons in the cortex and densification between neurons lead to primary folds that form consistently across all healthy brains around week 10; yet, the concise mechanistic mechanisms behind these folding patterns remain poorly understood. We developed an image registration-based approach to investigate this spatiotemporal evolution of microstructure and topology during gestation. Image registration is a powerful approach to quantify such large topological changes [1]. The registration approach minimizes the intensity difference between two medical images subject to regularization of the deformation field and surface area changes. We utilize the fetal brain atlas developed by Gholipour et al. which provides an averaged brain scan for each gestational week starting at week 21. We perform registration between consecutive weeks in order to determine the full-brain displacement field as it expands and folds. We then utilize the displacement field as input for an inverse optimization scheme to infer the growth field that best reproduces the registration data. Our growth model is based on the multiplicative split of the deformation gradient into an elastic and a growth part. We determine growth parameters and differentiate between tangential and normal growth parameters. Our work illustrates that early brain growth is primarily characterized by tangential surface growth in comparison to volumetric expansion. REFERENCES [1] Z. Whang, B. Martin, J. Weickenmeier, K. Garikipati. An inverse modelling study on the local volume changes during early morphoelastic growth of the fetal human brain. Brain Multiphysics (2021) 2:100023 [2] A. Pawar, Y.J. Zhang, C. Anitescu, Y. Jia, T. Rabczuk. DTHB3D Reg: dynamic truncated hierar- chical B-spline based 3D nonrigid image registration. Communications in Computational Physics (2018) 23:1–12. [3] A. Gholipour, C.K. Rollins, C. Velasco-Annis, A. Ouaalam, A. Akhondi-Asl, O. Afacan, C.M. Ortinau, S. Clancy, C. Limperopoulos, E. Yang, et al. A normative spatiotemporal MRI atlas of the fetal brain for automatic segmentation and analysis of early brain growth Scientific Reports (2017) 7:467.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Damage is an Important Dissipative Mechanism During Blood Clot Fracture

Author(s): *John Toaquiza Tubon, *Purdue University*; Vivek D Sree, *Purdue University*; Manuel K Rausch, *The University of Texas at Austin*; Adrian Buganza Tepole, *Purdue University*;

Pulmonary embolism is a significant source of morbidity and mortality world-wide. It arises from thrombus, or blood clot, first forming in our veins before breaking off and occluding the pulmonary arteries. Occlusion of the pulmonary arteries subsequently leads to ischemia of the downstream tissue, including the lungs. The embolization process may be described as mechanical fracture in response to hemodynamic forces. Thus, to understand pulmonary embolism and developed therapeutic and prognostic tools a fundamental understanding of blood clot's fracture properties is necessary. In our current work, we use mechanical test data on in-vitro blood clot to model fracture using a combination of a hyperelastic constitutive framework, a Mullin's type damage model, and a cohesive zone element. Specifically, we model a classic mode-I fracture experiments with a pure shear geometry in the implicit, nonlinear finite element software Abaqus. Through an inverse finite element analysis, we identify all hyperelastic, damage, and cohesive zone parameters to capture our mode-I experiments. Our work provides a comprehensive sensitivity analysis of above parameters, as well as an optimal set of these parameters that we identified for n=5 samples. Our work is a first step to identifying critical fracture properties of blood clot and may, down the line, be vitally important to understanding of a devastating and highly prevalent disease.

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Title: Assessing the Heterogeneous In Vivo Kinematics and Properties of the Human Aorta Using DENSE MRI to Improve Patient-Specific Computational Modeling and Clinical Diagnostics

Author(s): *John Wilson, *Virginia Commonwealth University*; Johane Bracamonte, *Virginia Commonwealth University*; Patrick Jones, *Virginia Commonwealth University*; Muhammad Islam, *Emory University*; John Oshinski, *Emory University*; Joao Soares, *Virginia Commonwealth University*;

Aortopathies such as aneurysms and dissections carry significant rates of morbidity and mortality, and their development and rupture-potential fundamentally depend on the patient-specific, heterogeneously evolving biomechanics of the aortic wall. While computational models offer significant potential for improving our understanding of pathologic aortic remodeling, there remains a fundamental lack of spatially-resolved in vivo mechanical data to inform and validate these models that ultimately must incorporate patient-specific properties for clinical utility. Unfortunately, current clinical imaging generally evaluates only basic aortic anatomy or simple homogenous metrics of aortic stiffness (e.g., pulse-wave velocity or distensibility). To address the need for more highly resolved clinical imaging of aortic mechanical function, we developed a novel application of Displacement Encoding with Stimulated Echoes (DENSE) MRI to quantify time-resolved regional aortic wall displacement and strain [1]. This presentation will summarize the methodology for acquiring DENSE images, post-processing the kinematic data to reduce noise and calculate the 2D Green strain tensor over 16 equally distributed sectors around the aortic wall, and the development of an inverse finite element method utilizing elastic foundation boundary conditions to quantify patient-specific aortic wall mechanical properties and spatially heterogeneous peri-vascular support (an often neglected source of mechanical heterogeneity) [2]. Experiments to validate DENSE-derived quantification of circumferential strain using in vitro polymer phantoms with independently trackable embedded nitinol wires will also be discussed. Results from three validation tests revealed that DENSE overestimates regional circumferential strain by 3% on average, but the difference reduces to 0.6% strain following mean-adjustment using a homogenized value of mean strain based on changes in aortic diameter from standard cine imaging. Results in 30 human subjects without structural aortopathy at three locations prone to pathology revealed heterogeneous distributions of wall strain and structural support unique for each location, with recurring patterns that aligned with known peri-vascular structures (e.g., vertebrae) that could be grouped by patient-specific metrics such as age and mean aortic displacement. These results suggest that normal distributions of heterogeneous aortic wall strain and peri-vascular stiffness may be established for both modeling purposes and for use as a comparative baseline for identifying and monitoring local pathology. Pilot testing in multiple aortopathies including aneurysms, dissections, hypertension, and Marfan’s Syndrome are currently underway, and early results may be presented as available. [1] Wilson JS, et al., J Cardiovasc Magn Reson, 21(1), 2019. [2] Bracamonte JH, et al., J Biomech Eng, 142(12), 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Patient-Specific Artery Geometry and ABM/FEA/CFD Computational Framework

Author(s): *John E. Yoo, *The University of Texas at Dallas*; Clark A. Meyer, *The University of Texas at Dallas*; Heather N. Hayenga, *The University of Texas at Dallas*;

The goal of this study was to explore a new method to quantifying the arterial mechanics based on patient-specific virtual histology-intravascular ultrasound (VH-IVUS) data. The ability to quantify the acute mechanical properties of an atherosclerotic artery in-vivo can help determine rupture risk. Systematically, understanding the mechanics driven mechanisms of growth and remodeling in an arterial plaque is unclear. Finite element analysis (FEA) has commonly been used to determine stress and strain within arteries, yet its application is limited. It has either been used for 2D modeling per VH-IVUS slice or linear 3D modeling [1][2]. To better recreate the artery, we fused the VH-IVUS data and the patient's artery centerline together to develop a nonlinear 3D presentation of the atherosclerotic artery. GIBBON [3] was used to create a volumetric mesh with material input and loads as input for FEBio [4], which performed the postprocessing and visualization output. Both FEBio and GIBBON are open source tools helping to further advance the research community's common agenda of innovation and availability. Better understanding the artery mechanisms will ultimately help create a better tool to predict growth and re-modeling of a patient-specific atherosclerotic artery. Utilizing open source tools allowed us to make custom changes to the source code. This enabled a way to combine all of the separate codes from reading the VH-IVUS images in MATLAB all the way to FEBio post processing. Secondly, having a 3D model with 1:1 material assignment to its volumetric mesh from VH-IVUS images influenced a more realistic model to better understand the wall mechanics. This software will have the capability to determine the arterial mechanics of any other patient's data thanks to its easily changeable input and output parameters. Such flexibility will help validate the current model's outputs in the future. This modeling platform proves it is feasible to calculate the wall mechanics based on patient-specific imaging in-vivo. Knowing the wall mechanics will help facilitate interventional cardiologist to assess atherosclerotic plaque stability. Moreover, it will help us better understand the impacting role of wall mechanics during plaque remodeling. [1] Timmins, Int J Cardiovasc Imaging, 33:13-24, 2017 [2] Teng, AHA Journals: Cardiovascular Imaging, 7: 461-470, 2014 [3] Moerman, JOSS, 3(22), 506, 2018 [4] Maas, et al, Journal of Biomechanical Engineering, 134(1), 2012

16th U.S. National Congress on Computational Mechanics
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Title: Subgrid Corrections in Finite-Element Models of Storm-Driven Coastal Flooding

Author(s): *Johnathan Woodruff, *North Carolina State University*; Casey Dietrich, *North Carolina State University*; Damrongsak Wirasaet, *University of Notre Dame*; Andrew Kennedy, *University of Notre Dame*; Diogo Bolster, *University of Notre Dame*; Zachariah Silver, *University of Notre Dame*; Sheppard Medlin, *University of Georgia*; Randall Kolar, *University of Oklahoma*;

Coastal flooding models based on the numerical solution of the 2D shallow water equations are widely used to predict the timing and magnitude of inundation during storms, both in real-time forecasting and long-term design. Oftentimes a constraint on computing time, especially in forecasting, limits the level of spatial resolution of the models and hence their accuracy. Fast flooding predictions that also include the highest-resolution datasets to represent flow pathways and barriers at the scales of critical infrastructure are therefore highly desirable. This need can be addressed in a computationally economical way via subgrid corrections, which use information at smaller scales to ‘correct’ the flow variables (water levels and current velocities) averaged over the model scale. Recent studies have shown a decrease in run time by 1 to 2 orders of magnitude, with the ability to decrease further if model time step were also increased. Traditionally, subgrid studies do not implement corrections in a finite element framework due to difficulties in defining averaged areas and wetting and drying schemes. In this study, subgrid corrections have been added to the ADvanced CIRCulation (ADCIRC) model, a widely used continuous-Galerkin finite-element based shallow water flow model. By pre-computing the averaged variables from high-resolution bathy/topo datasets, the model can represent hydraulic connectivity at smaller scales. This allows for a coarsening of the model, and thus faster predictions of flooding, while also improving accuracy. Subgrid implementation in ADCIRC permits changing a logic-based wetting and drying algorithm to a more desirable logicless algorithm, and requires averaging correction factors on both an elemental and vertex basis. This new framework further increases efficiency of the model, and is general enough to be used in other Galerkin finite element hydrodynamic models. The benefits of the sub-mesh corrections are demonstrated on a number of test cases, ranging from idealized test cases to a realistic setting of a larger domain in southwestern Louisiana. The larger Louisiana domain was run with forcing from Hurricane Rita (2005) to provide a realistic storm surge scenario. It is shown that subgrid ADCIRC can match the accuracy of the traditional model, while offering a 10 to 50 times increase in speed.

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Title: An Euler-Lagrange Model of the Transmission of Respiratory Ejecta Carrying SARS-CoV-2 in Enclosed Spaces

Author(s): *Joseph Wilson, *University of Colorado Boulder*; Shelly Miller, *University of Colorado Boulder*; Debanjan Mukherjee, *University of Colorado Boulder*;

The current COVID-19 pandemic has altered societal operations and norms in ways that likely will continue in the years to come. One common method of transmission of SARS-CoV-2 between humans is through respiratory ejecta when infected individuals cough, sneeze, talk, etc [1]. Occupied indoor spaces present a heightened risk of transmission of these respiratory ejecta [2]. Nursing homes house individuals considered to be high risk for COVID-19, and this population has suffered greatly in this pandemic. Many schools and businesses have been impacted from this pandemic as well, forcing these entities to remote learning and/or working. It is therefore important to understand how these respiratory ejecta particles propagate through an enclosed space and present a risk of transmission to an uninfected individual. Here we present a quantitative analysis of respiratory ejecta particle transport while accounting for full-scale indoor space configuration, ventilation, and HVAC flow information. Using the Lagrangian approach to describe respiratory ejecta particles, we quantify the viral exposure and infection transmission risk in enclosed spaces. With this model, we can classify exposure risk between individuals in both single room, and full-scale building configurations. References [1] Klompas, M., Baker, M. A., and Rhee, C., “Airborne transmission of SARS-CoV-2: theoretical considerations and available evidence,” Jama, 2020. [2] Lu, J., Gu, J., Li, K., Xu, C., Su, W., Lai, Z., Zhou, D., Yu, C., Xu, B., and Yang, Z., “COVID-19 outbreak associated with air conditioning in restaurant, Guangzhou, China, 2020,” Emerging infectious diseases, Vol. 26, No. 7, 2020, p. 1628.

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Chicago, IL, July 25-29. 2021

Title: An Efficient Multi-Temperature Kinetic Method for the RVE Generation of Particle-Reinforced Heterogeneous Materials

Author(s): *José L. P. Vila-Chã, *University of Porto*; Bernardo P. Ferreira, *University of Porto*; F. M. Andrade Pires, *University of Porto*;

Nowadays, the design and modeling of advanced materials rely on the knowledge that their macroscopic properties and mechanical response result from the interaction between heterogeneous structures spanning multiple lengths and time scales. Computational homogenization has emerged as an effective method for modeling heterogeneous materials by performing a homogenization procedure over a representative volume element (RVE) of the microstructure. Nevertheless, to accurately capture the macroscopic behavior, it is crucial that the RVE contains enough morphological and topological information of the microstructural constituents and is considered representative in an average sense (Hill, 1963). ? Regarding the design of particle-reinforced heterogeneous materials, the engineering design space's high dimensionality results in an overwhelming number of different designs, often leading to suboptimal and/or unexplored solutions. In Bessa et al. (2017), this challenge is tackled by proposing a unified data-driven framework for designing and modeling materials under uncertainty, relying on machine learning capabilities. After defining a finite set of microstructure morphology descriptors, this and similar approaches require the computation of an extensive material response database. Given that each design point is associated with one or more microstructure samples, it is mandatory to develop an efficient method to generate high-fidelity RVEs in an unsupervised and robust manner. ? This contribution presents a robust and efficient multi-temperature kinetic method for the RVE generation of particle-reinforced heterogeneous materials. Starting from the method proposed in Salnikov et al. (2015), several improvements are proposed. Notably, a coupled cell- Verlet lists to efficiently detect particles intersections, a multi-temperature quenching process to speed up the elimination of the particles overlap, and a dynamic time integration step to improve convergence and avoid solution instability. Several numerical examples demonstrate the proposed method's suitability to be integrated into a data-driven material design framework. References Bessa, M., R. Bostanabad, Z. Liu, A. Hu, D. W. Apley, C. Brinson, W. Chen, and W. K. Liu 2017. A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality. Computer Methods in Applied Mechanics and Engineering, 320:633–667. Hill, R. 1963. Elastic properties of reinforced solids: some theoretical principles. Journal of the Mechanics and Physics of Solids, 11(5):357–372. Salnikov, V., D. Choï, and P. Karamian-Surville 2015. On efficient and reliable stochastic generation of RVEs for analysis of composites within the framework of homogenization. Computational Mechanics, 55(1):127–144.

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Title: Stochastic Homogenization and Uncertainty Quantification: A Data-Driven Approach

Author(s): *José Pablo Quesada Molina, *Politecnico di Milano*; Stefano Mariani, *Politecnico di Milano*;

In recent years, machine learning (ML) tools have been applied to the broad majority of scientific fields, computational mechanics being one of them. In this specific field, ML methods have been devised to perform a number of descriptive, predictive and prescriptive tasks, leading to important advantages if compared to classical approaches [1]. Since the prediction of the effective mechanical properties of heterogeneous random media, like e.g. polycrystalline materials, can be computationally-intensive, data-driven approaches represent a viable alternative. In this context, the use of deep learning strategies based on artificial neural networks (NNs) has gained momentum due to their intrinsic capability of automatic feature extraction from large datasets. These algorithms do not require in fact to handle structured input data. In this work, we move from our previous results collected in [2]. By optimizing the architecture of convolutional NN-based models, we aim at predicting the scattering in the overall stiffness of polysilicon microstructures, representative of film morphologies typically found in inertial micro electro-mechanical systems. These microstructures are characterized by a small ratio between the dimension of the polycrystalline aggregate and the representative size of a single grain. As the length scale separation principle does not hold true, the homogenization procedure is to be performed over material representations referred to as statistical volume elements (SVEs). These SVEs are synthetically generated as microstructural images, obtained via regularized Voronoi tessellations, that are used to feed a Monte Carlo procedure to account for the scattering in their morphology. Each microstructure is associated to a ground-truth label, that accounts for the relevant overall stiffness and is obtained via finite element simulations. Having trained the NN with these data, the model is employed to predict the upscaled property of unseen images characterized by a different scale ratio, so that size effects in the apparent properties can be estimated. [1] F. E. Bock, R. C. Aydin, C. J. Cyron, N. Huber, S. R. Kalidindi, and B. Klusemann, “A review of the application of machine learning and data mining approaches in continuum materials mechanics,” Front. Mater. 6:110. [2] J. P. Quesada Molina, L. Rosafalco, and S. Mariani, “Mechanical Characterization of Polysilicon MEMS Devices: a Stochastic, Deep Learning-based Approach,” 21st International Conference on Thermal, Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems (EuroSimE), 2020, pp. 117-124.

16th U.S. National Congress on Computational Mechanics
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Title: Hybrid Optimization: Filling the Gap Between Topology and Shape Optimization with Machine Learning Techniques

Author(s): David Muñoz, *Universitat Politècnica de València*; Enrique Nadal, *Universitat Politècnica de València*; José Albelda, *Universitat Politècnica de València*; *Juan José Ródenas, *Universitat Politècnica de València*;

Topology Optimization algorithms try to distribute material over a predefined design domain, minimizing an objective function (compliance, total volume, etc.) under certain constraints (total mass, maximum von Mises stress, etc.). The SIMP method [1] and the Level-Set approach [2] are two of the most used approaches. In both algorithms, the number of optimization parameters is roughly equal to the number of elements (one density per element) or the number of nodes (one distance to boundary per node), respectively. Thus, the amount of design variables in topology optimization can be large. Shape Optimization algorithms optimize the component considering a reduced number of design variables, such as thickness, radii, etc., that define the boundary. However, the topology is fixed in these approaches and not suitable for modifications, although this may be mitigated by using topological derivatives [3]. In this work, we propose a hybrid optimization that combines both types of algorithms. In our strategy we start running a topology optimization process considering a relaxed convergence criterion. This process will provide a preform of the optimal component. Once the topology is roughly defined, a Machine Learning (ML) model is trained with the material distribution provided by the intermediate and last steps of the iterative topology optimization process. The ML algorithm is then able to infer information about the geometry a to provide a parametric definition of the geometry based on a reduced set of parameters, each of them associated to a "geometrical mode". Finally, this ML-based parametric model will be used by a standard parameter-based shape optimization algorithm. The combination of these two algorithms, provided by the use of the ML algorithm, can be appropriately tuned to reduce the overall computational cost of the process. ACKNOWLEDGEMENTS: The authors gratefully acknowledge the financial support of Ministerio de Economía, Industria y Competitividad (project DPI2017-89816-R) and Ministerio de Educación (FPU16 /07121). KEY WORDS: Topology Optimization, Shape Optimization, Geometry Reconstruction, Machine Learning REFERENCES [1] O. Sigmund. A 99 line topology optimization code written in Matlab. Structural and Multi-disciplinary Optimization. 21(2):120-127, 2001. [2] M.Y. Wang, X. Wang, D. Guo. A level set method for structural topology optimization. Computer Methods in Applied Mechanics and Engineering. 192(1-2):227-246,2003 [3] Novotny, A. A., Sokoowski, J. (2013). Topological derivatives in shape optimization. Interaction of Mechanics and Mathematics, 1427. https://doi.org/10.1007/978-3-642-35245-4-1

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Title: A Fast and Effective Sensitivity and Uncertainty Quantification for the Molten Pool in Metal Additive Manufacturing

Author(s): *Juan Sebastian Rincon, *The University of Texas at San Antonio*; Arturo Montoya, *The University of Texas at San Antonio*; Matthew Balcer, *The University of Texas at San Antonio*; Harry Millwater, *The University of Texas at San Antonio*; David Restrepo, *The University of Texas at San Antonio*;

Metal-based additive manufacturing (AM) has awakened the interest of the production industry due to its cost-effectiveness, availability to reproduce complex-shaped components, and the possibility to use metallic alloys powders with outstanding properties. Despite the transformative potential of AM, the full utility of this fabrication technology remains unrealized due to the lack of reproducibility and reliability in the process, and the uncertainty in mechanical properties of the fabricated parts. To overcome these issues, finite element method simulations validated with experimental testing, sensitivity analysis, and uncertainty quantification (UQ) have been stated as promising approaches to optimize the printing parameters. The purpose of this research is to develop and implement the hypercomplex finite element method (ZFEM) and a novel fast UQ method into a simulation model for the molten pool process in metal additive manufacturing. We implemented these methods in a 2D transient thermo-mechanical simulation using the Abaqus commercial finite element program. The enhancement with a hypercomplex formulation allows us to obtain arbitrary order sensitivity analysis with respect to initial conditions, load conditions, material properties, or shape with a single average sample. Consequently, ZFEM allows the identification of the relative importance of the manufacturing variables with an only run for each input parameter. The sensitivity information feed into a new fast UQ method. This new UQ approach uses the “moments” of the output variables to construct a stochastic model. In this method, the mean, variance, skewness, and kurtosis, aka “moments” are modeled assuming a 2nd order, 3rd, or 4th order Taylor series and the deterministic sensitivities of the quantity of interest. Using this approach, one can utilize the full fidelity of a finite element model, unlike other UQ methods like Monte Carlo sampling of simplified or surrogate models, which limits the accuracy, or polynomial chaos, or design of experiment approaches that limit the number of parameters considered. The significance of this research is clear, to understand the variations governing the AM process and to determine best practices for improvement, it is of paramount importance to determine the processing variables affecting the variability in deformation, residual stresses, material strength, and other properties. This research seeks to address this gap and to contribute to the efforts towards the qualification and certification of AM produced parts.

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Title: Weighted High-Order Gradient Collocation Method for Detecting Inverse Boundaries

Author(s): *Judy Yang, *National Yang Ming Chiao Tung University*; Hon Fung Samuel Lam, *National Yang Ming Chiao Tung University*;

In comparison with traditional mesh-based methods in solving inverse problems, the weighted reproducing kernel collocation method (RKCM) exhibits high accuracy and efficiency. However, it is known that the calculation of derivatives of reproducing kernel (RK) shape functions is computationally expensive, particularly, in solving strong-from equations with high-order derivative operators. In recent years, the gradient approximation has been introduced to construct implicit derivatives of RK shape functions synchronically, which allieviates the computation complexity greatly. In view of the advantage, this study first introduces the weighted high-order gradient RKCM to the inverse analysis. The weights on the boundary conditions are examined in the convergence study. Several configurations of multiply connected domains are provided to numerically investigate the stability and efficiency of the method. From the benchmark examples, the efficacy of the method in detecting the unknown boundary is demonstrated. References [1] J. P. Yang and H. F. S. Lam, Detecting inverse boundaries by weighted high-order gradient collocation method, Mathematics. 8(8) (2020) 1297. [2] A. Mahdavi, S. W. Chi, and H. Zhu, A gradient reproducing kernel collocation method for high order differential equations, Comput. Mech. 64 (2019) 1421-1454. [3] S. W. Chi, J. S. Chen, H. Y. Hu and J. P. Yang, A gradient reproducing kernel collocation method for boundary value problems, Int. J. Numer. Methods Engrg. 93 (2013) 1381-1402.

16th U.S. National Congress on Computational Mechanics
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Title: Multifidelity Multiobjective Optimization for Wake Steering Strategies

Author(s): *Julian Quick, *University of Colorado Boulder*; Ryan King, *National Renewable Energy Laboratory*; Peter Hamlington, *University of Colorado Boulder*;

Wake steering is a wind power plant control strategy where upstream turbines are intentionally yawed away from the incoming wind, thereby “steering” wakes away from downstream turbines. Trade-offs between the additional power and fatigue loads induced through this control strategy are the subject of continuing investigation. In this study, we present a multiobjective multifidelity optimization approach for exploring these trade-offs. Numerical simulations with different resolutions are used to model the system at multiple computational fidelities. Single-fidelity and multifidelity Bayesian optimization studies are performed, maximizing an acquisition function in each iteration, after some initial sampling of the system. The performance of single-fidelity and multifidelity approaches is compared in terms of computational cost and accuracy. Each optimization uses the expected hypervolume improvement acquisition function, which accounts for multiple objectives. In the multifidelity case, the acquisition function is weighted by the total cost of a proposed model evaluation. Our multifidelity approach identifies a Pareto front of optimal control strategies that balance competing power and loading objectives. Preliminary results suggest the multifidelity approach is twice as fast as the single-fidelity approach, and we expect this advantage to grow as we consider more expensive simulations.

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Title: An Efficient Implementation of Elastodynamics into Three-Dimensional Discrete Dislocation Dynamics Simulation of Finite Volumes

Author(s): *Junjie Yang, *Johns Hopkins University*; Yejun Gu, *Johns Hopkins University*; Tamer Zaki, *Johns Hopkins University*; Jaafar El-Awady, *Johns Hopkins University*;

To understand the mechanical responses of crystalline materials under shock loading conditions, it is important to characterize the collective behavior of dislocation networks under high strain rate. Most current discrete dislocation dynamics (DDD) simulations are based on the assumption of quasi-static loading conditions, hence, they are inadequate to study the material response under shock loading conditions. The analytical solution for the time-dependent stress field of a Volterra dislocation was first developed by Mura in 1963 [1] and recently implemented numerically by virtue of the retarded potentials technique [2]. Here, we develop a new efficient algorithm for large-scale three-dimensional (3D) discrete dislocation dynamics simulations utilizing the retarded potentials technique to numerically compute both the displacement and stress waves generated by evolving dislocation networks. This approach is thus compatible with finite volume simulations (e.g. [3]).

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Title: The Interface-Flux-Recovery (IFR) Method for Conservative and Stable Coupling Schemes in Geophysical Fluids and Mechanics

Author(s): *K. Chad Sockwell, *Sandia National Laboratories*; Kara Peterson, *Sandia National Laboratories*; Paul Kuberrry, *Sandia National Laboratories*; Pavel Bochev, *Sandia National Laboratories*;

Coupling schemes serve as the glue which holds multi-physics simulations together and are ideally efficient, stable, and conservative in terms of flux. However, satisfying all three of these properties at the same time is difficult in a coupling scheme, and in many cases stability and conservation take a higher priority. Dual Schur complement methods potentially provide an advantageous middle ground of the three properties in some cases. These methods are very efficient when the discrete operators involved in the Schur complement can be computed efficiently or efficiently stored. Moreover, dual Schur complement methods provide a partitioned solution strategy, allowing each model to use its own well developed solver strategy or preconditioner. In this talk, we present a Dual Schur complement coupling method, the Interface Flux Recovery (IFR) method aimed at handling a general set of interface conditions while maintaining conservation of flux. Previously designed dual Schur complement methods, such the Implicit Value Recovery (IVR) and Bulk Interface Flux Recovery (Bulk-IFR) methods, were specifically designed to handle the standard continuity conditions under explicit time-integration and the so-called bulk condition existing in air-sea systems, respectively. The IFR method provides a more general way to realize a partitioned coupling scheme for either condition considered in the IVR or Bulk-IFR cases, as well as heterogeneous integration, while maintaining a notion of conserved flux. The notion of conserved flux is very important for many earth modeling and engineering applications. We present the IFR framework and its flexibility in terms of interface conditions, and we present results on fluid-fluid coupling models related to earth modeling and engineering applications.

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Title: System Identification in Digital Twins of Human Musculo-Skeletal Systems.

Author(s): *Karan Taneja, *University of California, San Diego*; Xiaolong He, *University of California, San Diego*; J.S. Chen, *University of California, San Diego*;

In recent years, the concept of Digital Twin (DT) has come up to play a massive role in the efficient functioning of various Industry and Manufacturing sectors. Originally designed for the aerospace sector, the benefits of the framework were soon recognised for other arenas. One particularly exciting avenue for this concept is for healthcare where DTs of Human Beings can have applications for the prognosis of muscle injuries and diseases and rehabilitation of patients. A DT application in Human Musculo-Skeletal (MSK) systems requires multiple muscle parameters and muscle excitation signals, traditionally found by solving a system identification problem through optimisation. In this work, a framework for the system identification of a DT of a Human MSK system is proposed where the problem is solved using Physics Informed Deep Learning to identify the model parameters and muscle excitations, given the recorded motion data and the system of equations governing the movement of the Human MSK system. This framework is formulated by enhancing Deep Neural Networks (DNNs) with physics-based constraints such as residuals of the governing equations. Adding the physics-based residual as a regularisation term to the loss function of DNNs allows for a robust system identification procedure. The approach is further enhanced with modern machine learning architectures to yield a computationally efficient framework for system parameters and function identification. The future work in integrating various data streams of the subject including motion capture data (position, velocity, and acceleration) and wearable sensor data (kinetic and kinematic data of the muscle groups) for a better solution accuracy and connecting the system identification of the multi-body dynamics of the MSK DT to the patient specific muscle mechanical properties, is also highlighted.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: How to Capture Centimeter-Scale Local Variations in the Pore Space of Paper: A Benchmark Study Using µ-CT

Author(s): Matthias Neumann, *Ulm University*; Eduardo Machado Charry, *Graz University of Technology*; Ekaterina Baikova, *Graz University of Technology*; André Hilger, *Helmholtz-Zentrum Berlin*; Ulrich Hirn, *Graz University of Technology*; Ingo Manke, *Helmholtz-Zentrum Berlin*; Volker Schmidt, *Ulm University*; *Karin Zojer, *Graz University of Technology*;

Paper materials consist of a complex network of fibers. The formation process induces strong local variations in the microstructure of paper, as found for fiber-based microstructures in general [1]. For properties associated with the pore space of paper, the impact of local in-plane variations, e.g. due to regions where fiber accumulations occur, is not well established so far. Hence, paper and particularly its pore space is an elegant test bed for designing and performing a µ-CT-based microstructure acquisition that is capable of revealing sheet-representative in-plane variations up to the centimeter range and variations in the sheet cross-sections within a few micrometers. A framework to analyze local variations in the microstructure of paper sheets based on 3D image data is presented. To this end, a workflow to efficiently acquire a large set of highly-resolved tomographic image data is developed. In combination with statistical image analysis, this enables the quantification of local variations and pairwise correlations of morphological microstructure characteristics on length scales ranging from micrometers to centimeters. The microstructure characteristics considered in the present study are porosity, thickness, and mean geodesic tortuosity quantifying the length of the shortest transportation paths in the pore space [2]. The power of the presented framework is demonstrated by (i) quantitatively revealing the difference in terms of local structural variations between a model paper before and after unidirectional compression via hard-nip calendaring, as well as (ii) determining the field of view, which is required to reliably compute the considered microstructure characteristics. On the basis of our comprehensive data sets, relationships between structural differences and local densifications are elucidated. In particular, it is shown how calendering transforms local variations in sheet thickness into marked local mass density variations. The obtained results are in line with experimental measurements of macroscopic properties (basis weight, Bekk smoothness parameters, thickness, Gurley retention times) determined for the considered paper materials. [1] J. Dirrenberger, S. Forest, and D. Jeulin, Towards gigantic RVE sizes for 3D stochastic fibrous networks, Int. J. Solids Struc. 51, 359–376, 2014, doi: 10.1016/j.ijsolstr.2013.10.011. [2] M. Neumann, E. Machado Charry, K. Zojer, and V. Schmidt. On variability and interdependence of local porosity and local tortuosity in porous materials: A case study for sack paper. Methodol. Comput. Appl., 2021, doi:10.1007/s11009-0 19-09761-1.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Multiscale ECM Inhomogeneity in the Arterial Wall

Author(s): *Katherine Yanhang Zhang, *Boston University*;

The extracellular matrix (ECM) of an artery endows the tissue its load bearing and damage resistance capacities. This talk will present our recent findings on the ECM structural inhomogeneities and the important roles that they play in contributing to tissue mechanics and homeostasis. Our recent studies integrating multiphoton imaging and quantification, biomechanical characterization, and computational modelling showed that ECM structural inhomogeneity exists at multiple structural levels of the arterial wall. At the intralamellar level, varying fiber orientation distribution and undulation contributes to local ECM mechanical properties1. At the interlamellar level, transmural variation in in-plane fiber orientation distribution determines the anisotropic mechanical behavior of the elastin network2. Furthermore, the waviness gradient among the elastic lamellar layers plays an important role in maintaining tissue homeostasis3. Finally, structural inhomogeneity in transmural interlamellar fibers and the development and propagation of aortic dissection will be discussed4. Considering ECM structural inhomogeneity is important when studying the physiological function and failure of the arterial wall. The complex structural and mechanical interplay calls for new approaches that integrate imaging, mechanical characterization, and computational modeling. Reference: 1 Li, H., Mattson, J. M. & Zhang, Y. Integrating structural heterogeneity, fiber orientation, and recruitment in multiscale ECM mechanics. J Mech Behav Biomed Mater 92, 1-10, doi:10.1016/j.jmbbm.2018.12.023 (2019). 2 Yu, X., Wang, Y. & Zhang, Y. Transmural variation in elastin fiber orientation distribution in the arterial wall. J Mech Behav Biomed Mater 77, 745-753, doi:10.1016/j.jmbbm.2017.08.002 (2018). 3 Yu, X., Turcotte, R., Seta, F. & Zhang, Y. Micromechanics of elastic lamellae: unravelling the role of structural inhomogeneity in multi-scale arterial mechanics. J R Soc Interface 15, doi:10.1098/rsif.2018.0492 (2018). 4 Yu, X., Suki, B. & Zhang, Y. Avalanches and power law behavior in aortic dissection propagation. Sci Adv 6, eaaz1173, doi:10.1126/sciadv.aaz1173 (2020).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Immersogeometric Approach for Transmission Risk Assessment in Classrooms

Author(s): *Kendrick Tan, *Iowa State University*; Boshun Gao, *Iowa State University*; Cheng-Hau Yang, *Iowa State University*; Emily Johnson, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*; Alberto Passalacqua, *Iowa State University*; Baskar Ganapathysubramanian, *Iowa State University*;

Due to the on-going COVID-19 pandemic, closed, confined space are high risk areas to infection. There is an increasing push to have in-person teaching in the K-12 and university settings. Hence, there is a pressing need to evaluate the risk of airborne disease transmission within an enclosed environment such as a classroom, while accounting for the HVAC system, physical presence of humans, furniture and electronic equipment. In this context, high fidelity fluid/aerosol simulation is a practical approach to evaluate various seating and operating scenarios, identify risk factors, and rank order mitigation strategies. We report on a framework that integrates four distinct concepts to provide very detailed estimates of aerosol distribution in indoor environments: (a) a VMS based flow solver that accounts for the boundary and HVAC conditions, (b) a buoyant heat solver extension that models the thermal plumes created by heat released by humans and electronics, (c) a detailed microdroplet distribution model that accounts for the distribution of droplet size due to evaporation, coalescence and breakup, and (d) an octree based adaptive mesher that allows rapid exploration of a diverse array of configurations with complex geometries, We illustrate the ability of the approach to rapidly rank order various seating scenarios based on transmission risk.

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Title: A Fast and Scalable Computational Framework for Large-Scale and High-Dimensional Bayesian Optimal Experimental Design

Author(s): *Keyi Wu, *The University of Texas at Austin*; Peng Chen, *The University of Texas at Austin*; Omar Ghattas, *The University of Texas at Austin*;

We develop a fast and scalable computational framework to solve large-scale and high-dimensional Bayesian optimal experimental design problems. In particular, we consider the problem of optimal observation sensor placement for Bayesian inference of high-dimensional parameters governed by partial differential equations (PDEs), which is formulated as an optimization problem that seeks to maximize an expected information gain (EIG). Such optimization problems are particularly challenging due to the curse of dimensionality for high-dimensional parameters and the expensive solution of large-scale PDEs. To address these challenges, we exploit two essential properties of such problems: (1) the low-rank structure of the Jacobian of the parameter-to-observable map to extract the intrinsically low-dimensional data-informed subspace, and (2) the high correlation of the approximate EIGs by a series of approximations to reduce the number of PDE solves. Based on these properties, we propose an efficient offline-online decomposition for the optimization problem: an offline stage of computing all the quantities that require a limited number of PDE solves independent of parameter and data dimensions, which is the dominant cost, and an online stage of optimizing sensor placement that does not require any PDE solve. For the online optimization, we propose a swapping greedy algorithm that first construct an initial set of sensors using leverage scores and then swap the chosen sensors with other candidates until certain convergence criteria are met. We demonstrate the efficiency and scalability of the proposed computational framework by a linear inverse problem of inferring the initial condition for an advection-diffusion equation, and a nonlinear inverse problem of inferring the diffusion coefficient of a log-normal diffusion equation, with both the parameter and data dimensions ranging from a few tens to a few thousands.

16th U.S. National Congress on Computational Mechanics
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Title: Ablating Woven Thermal Protection System Materials Under High Shear Flow Conditions

Author(s): *Krishnan Swaminathan Gopalan, *Analytical Mechanics Associates*; Arnaud Borner, *Analytical Mechanics Associates*; Nagi Mansour, *Analytical Mechanics Associates*;

With the objective of developing a comprehensive spallation model for thermo-protective material, the Stochastic PArallel Rarefied-gas Time-accurate Analyzer (SPARTA) direct simulation Monte Carlo (DSMC) code [1] is used to perform boundary layer flows over woven thermal protection system (TPS) materials during various stages of chemical degradation. The purpose of this study is to compute the shear stress, pressure and heat flux on the TPS material resulting from high shear flow simulations at the micro-scale. Loss of structural integrity of thermal protection system (TPS) materials occurs due weakening caused by chemical reactions (mainly oxidation) along with the high mechanical and thermal stresses. This structural failure can result in removal of chunks of TPS materials (spallation), thus increasing the rate of ablation. Hence, the critical properties which contribute to these failure mechanisms such as the pressure, shear stress and heat flux are computed for the weave geometries. Further, the variation of these properties as the microstructure undergoes changes due to oxidation is also investigated. The detailed micro-structure of woven TPS material at the micro-scale will either be generated synthetically or obtained from X-ray micro-tomography [2]. The boundary layer flow properties are obtained directly from Computational Fluid Dynamics (CFD) simulations of entry missions. These flow properties are then used to determine the inlet and outlet boundary conditions in the DSMC simulations. We consider the case where the chemical degradation process mainly occurs due to the reaction with atomic oxygen. The Porous Microstructure Analysis (PuMA) software [3] is used to perform simulations of this oxidation process to generate the microstructure at various stages of material thinning. Flow simulations are then performed over these oxidized microstructures to compute the stresses on the material surface, which can further be used to develop predictive macroscale modelling of spallation and structural failure. [1] M. A. Gallis, J. R. Torczynski, S. J. Plimpton, D. J. Rader, T. Koehler, “Direct Simulation Monte Carlo: The Quest for Speed”, 29th Intl Symposium on Rarefied Gas Dynamics in Xi'an, China, AIP Conf Proc, 1628, 27 (2014). [2] Vanaerschot, A., Panerai, F., Cassell, A., Lomov, S. V., Vandepitte, D., & Mansour, N. N. (2017). Stochastic characterisation methodology for 3-D textiles based on micro-tomography. Composite Structures, 173, 44-52. [3] J. C. Ferguson, F. Panerai, A. Borner, N. N. Mansour, “PuMA: the Porous Microstructure Analysis software”, SoftwareX 7 (2018): 81-87.

16th U.S. National Congress on Computational Mechanics
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Title: Process Model for Multilayer Slide Coating of Polymer Electrolyte Membrane Fuel Cells

Author(s): *Kristianto Tjiptowidjojo, *University of New Mexico*; P. Randall Schunk, *Sandia National Laboratories*;

Slide coating is a precision method suitable for depositing multiple liquid-film layers simultaneously. Originally developed in the photographic film industry, it has been deployed for manufacturing of other products that benefit from multilayer coatings. One emerging application is the manufacture of polymer electrolyte membrane fuel cells (PEMFCs), which are used to produce electricity through electrochemical reactions of hydrogen and oxygen gas. The membrane-electrode assembly (MEA), in which key electrochemical reactions occur, consists of three layers which are typically deposited separately in serial fashion and then laminated together to form the three-layer MEA, i.e. three sequential steps of coat and dry. Adapting the process to simultaneous, multi-layer slide coating of all three -layers will save equipment cost and space while minimizing possible exposure to contaminants during transition between the steps. We are developing a three-layer slide coating model to aid the manufacturing process design of PEMFCs. Free surface and interlayer shapes are tracked using the Arbitrary Eulerian Lagrangian (ALE) method. The model accounts for rheology of each layer, which typically exhibit shear thinning behavior. Model predictions are used to investigate simultaneous coatability of catalyst inks and to determine the best layer-by-layer ink selection.

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Title: Modeling Multi-Neuron Growth with Dendritic Spines Using Isogeometric Collocation and Phase Field Model

Author(s): *Kuanren Qian, *Carnegie Mellon University*; Aishwarya Pawar, *Purdue University*; Ashlee Liao, *Carnegie Mellon University*; Victoria Webster-Wood, *Carnegie Mellon University*; Yongjie Jessica Zhang, *Carnegie Mellon University*;

Neural control of living muscle actuators has proven to enhance performance in biohybrid robots. To design and culture functional controllers using biological neurons, as well as to model neurodegenerative diseases, modeling multi-neuron interactions during growth is necessary. A robust neuron growth model that incorporates a broad range of factors that impact neuronal growth and generates important cell structures is therefore needed. Dendritic spines are small “mushroom-shaped” actin-rich protrusions along dendrites and play a crucial role in determining synaptic connection in complex neurite networks. The location and morphology of dendritic spines vary based on cell membrane characteristics and actin concentration, and dendritic spine growth involves an intricate balance between membrane forces and actin-generated force. Existing models on dendritic spines lack the coupling between intracellular concentration and dendritic spines characteristics [1]. Coupling dendritic spine growth with propagating actin waves in neurons during growth, we can simulate and control neural synaptic connection [2]. Using the isogeometric collocation method and phase-field models, this work models multi-neuron growth based on actin wave driven dendritic spines morphology. Developed based on the recent neuron growth model that considers both intracellular transport of tubulin and extracellular culture medium [3], we incorporate the effect of actin concentration driven dendritic spines growth to simulate realistic muti-neuron synaptic interactions. Modeling the dendritic spine growth in the neuron growth model allows us to study the behavior of synaptic connections, which is a crucial factor in understanding neural control, neurodegenerative diseases, and designing future biohybrid robots. [1] H. Alimohamadi, M. K. Bell, S. Halpain, and P. Rangamani, “Mechanical principles governing the shapes of dendritic spines,” bioRxiv, p. 2020.09.09.290650, Sep. 2020, doi: 10.1101/2020.09.09.290650. [2] V. Wasnik and R. Mukhopadhyay, “Modeling the dynamics of dendritic actin waves in living cells,” Phys Rev E Stat Nonlin Soft Matter Phys, vol. 90, no. 5–1, p. 052707, Nov. 2014, doi: 10.1103/PhysRevE.90.052707. [3] A. Pawar, A. Liao, K. Qian, V. Webster-Wood, A. W. Feinberg, and Y. Jessica, “Modeling Neuron Growth Using Phase Field Method,” In Preparation

16th U.S. National Congress on Computational Mechanics
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Title: Industrial Scale Simulations Using Immersogeometric Analysis on Octree Meshes

Author(s): *Kumar Saurabh, *Iowa State University*; Boshun Gao, *Iowa State University*; Masado Ishii, *The University of Utah*; Milinda Fernando, *The University of Utah*; Makrand Khanwale, *Iowa State University*; Biswajit Khara, *Iowa State University*; Sudeep Menon, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*; Hari Sundar, *The University of Utah*; Baskar Ganapathysubramanian, *Iowa State University*;

Efficiently and accurately simulating partial differential equations (PDEs) in and around arbitrarily defined geometries, especially with high levels of adaptivity, has significant implications for different application domains. A key bottleneck in the above process is the fast construction of a good adaptively-refined mesh for arbitrary geometry. In this work, we integrate the octree based mesh with immersogeometric analysis for highly efficient and accurate Large-Eddy Simulations (LES) of flows around complex geometries. We discuss significant algorithmic advances over existing methods that would serve towards achieving the community goal of overnight LES. Further, we compare and contrast the immersed approach with recently developed octree based carved out approach, where the object is carved out from the domain rather than immersed in it.

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Title: A Phase-Field Model of Plasticity

Author(s): *Kumar Vemaganti, *University of Cincinnati*; Pietro Pascale, *University of Cincinnati*;

In this work, we present a mesoscale phase-field model of elastic-plastic behavior as an extension of the model of plastic slip presented by Ambrosio et al [1]. In proposed model, we consider (a) a new strain energy density decomposition that is not directly correlated to the von Mises assumption, and (b) a new formulation of the surface plastic energy that accounts for the fact that plastic energy is consumed when gliding occurs across the slip bands. With this formulation the phase field distribution captures the nature of the activation process of slip planes and is capable of characterizing a wide range of plastic behavior, from very diffuse to highly localized, as evidenced by two- and three-dimensional numerical results. Our results also show that this mesoscopic model is able to capture the Hall-Petch effect, wherein the strength of some polycrystalline materials is inversely proportional to the square root of the average grain size. This means that the size effect does not necessarily need to be explained with models at microscopic scale but can be captured by mesoscopic models. The proposed model is also consistent with the classical theory of plasticity in terms of the postulate of incompressibility and yield criteria. Finally we show that the phenomena described by the model can be characterized by dimensionless parameters and we present related similarity laws. KEYWORDS: Phase-field model, Plasticity, Scaling, Size effect [1] Ambrosio, L., A. Lemenant, and G. Royer-Carfagni (2013). A variational model for plastic slip and its regularization via gamma-convergence. J Elast 110, 201–235.

16th U.S. National Congress on Computational Mechanics
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Title: Modeling the Interplay Between Heat Transfer and Crack Propagation in the Phase-Field Method

Author(s): *Lampros Svolos, *Los Alamos National Laboratory*; Haim Waisman, *Columbia University*; Hashem Mourad, *Los Alamos National Laboratory*;

Among fracture modeling methods, continuum damage formulations, such as the phase-field method, has gained significant attention in the past few years due to their ability to model multiple propagating cracks without the need to explicitly track each crack. However, accurately modeling heat transfer physics in continuum fracture methods is a fundamental science problem that is not yet well understood. In this talk, reliable damage models – which (i) degrade the thermal-conductivity in continuum crack descriptions, and (ii) introduce additional temperature-dependent crack driving forces – are proposed to capture the correct heat transfer physics across fracture surfaces. In particular, both an isotropic and anisotropic thermal-conductivity degradation approaches will be presented. The derivation of the former is based on a micro-mechanics void extension model of Laplace's equation, while the latter accounts for crack directionality and improves the near-field approximation of temperature and heat flux across cracks (compared with discontinuous crack solutions). In addition, preliminary results concerning the role of a damage-dependent specific heat quantity will also be discussed. A unified model which accounts for the simultaneous formation of shear bands and cracks is used as a numerical tool to investigate the behavior of the aforementioned proposed models. In this unified model, the phase-field method is used to model crack initiation and propagation and is coupled to a temperature dependent visco-plastic model that captures shear bands.

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Title: Machine Learning Discovery of High-Temperature Polymers

Author(s): *Lei Tao, *University of Connecticut*; Guang Chen, *University of Connecticut*; Ying Li, *University of Connecticut*;

The design and development of high-temperature polymers have been an experimentally-driven and trial-and-error process guided by experience, intuition, and conceptual insights. However, such an Edisonian approach is often costly, slow, biased towards certain chemical space domains, and limited to relatively small-scale studies, which may easily miss promising compounds. To overcome this challenge, we formulate a data-driven machine-learning (ML) approach, integrated with high-fidelity molecular dynamics (MD) simulations, for quantitatively predicting polymer's glass transition temperature (T_g) from its chemical structure and rapid screening of promising candidates for high-temperature polymers. Specifically, we collect a diverse set of nearly 13,000 real polymers from the largest polymer database, PoLyInfo. Among them, 6,923 experimental T_g values are available; while, the remaining 5,690 polymers do not have reported T_g values. We train the deep neural network (DNN) model with 6,923 experimental T_g values using Morgan fingerprint representations of chemical structures for these polymers. Interestingly, the trained DNN model can reasonably predict the unknown T_g values of polymers with distinct molecular structures, in comparison with MD simulations and experimental results. We find that this excellent transferability is attributed to the feature representation of Morgan fingerprints, which carry the chemical connectivity between neighboring repeating units in a polymer and the frequency of occurrence of different chemical substructures. With the validated ML model for high-throughput screening of nearly 1 million hypothetical polymers, we identify more than 65,000 promising candidates with T_g>200 oC, which is 30 times more than existing known high-temperature polymers (~2,000 from PoLyInfo). The discovery of this large number of promising candidates will be of significant interest in the development and design of high-temperature polymers. In short, our work demonstrates that ML is a powerful method for the prediction and rapid screening of high-temperature polymers, particularly with growing large sets of experimental and computational data for polymeric materials.

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Title: A Novel Surface Correction Technique for State-Based Peridynamics

Author(s): *Lei Wang, *Xiamen University*; Quan Gu, *Xiamen University*;

The state-based peridynamics is an effective method to solve problems including cracking, damage and crushing of structures. However, the solutions of peridynamics at the boundaries show inaccuracy and instability, which is possibly caused by the incomplete horizon of the material points at the boundaries, i.e., the so called surface effect. This paper proposed a novel technique to solve the inaccurate and unstable issue of peridynamics due to the surface effects. Three examples are presented to verify the proposed technique. Firstly, quasi static analysis for a two-dimensional elastic column is proposed under monotonic compression. Secondly, dynamic analysis for a two-dimensional soil column under earthquake base excitation is applied using multi yield surface plasticity model. Thirdly, pseudo-static pushover analysis for a three-dimensional concrete column is applied using the cap plasticity model. By contrasting and analyzing the results from using finite element method, peridynamics and surface correction, it is proved that surface correction technique is an effective solution to solve the problem of inaccuracy and instability of state-based peridynamics. Compared with other correction methods, surface correction is more simple and easier to implement, and it can be suitably applied to linear elastic and complex nonlinear material constitutive models.

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Title: HiDeNN-PGD: Reduced Order Deep Learning Network

Author(s): *Lei Zhang, *Peking University*; Ye Lu, *Northwestern University*; Shaoqiang Tang, *Peking University*; Wing Kam Liu, *Northwestern University*;

In this work, we propose a novel reduced order deep learning approach, called HiDeNN-PGD, for a class of PDEs, which is a combination of Hierarchical Deep-learning Neural Network (HiDeNN) [1] and Proper Generalized Decomposition (PGD) [2] and takes advantages of both methods. Similar with PGD, HiDeNN-PGD adopts the concept of separation of variables and considers the solution of PDEs as a summation of the products of multiple one-dimensional functions. But differently, each of these 1D functions is represented by structured deep neural networks (DNNs), i.e., the 1D HiDeNN. In these neural networks, the weights and biases are functions of the nodal positions, which allows the optimization of the nodal coordinates in each dimension. This is the spirit of r-adaptivity, and it increases the accuracy of the approximation and reduces the necessary number of modes for the separation of variables. Compared to HiDeNN, HiDeNN-PGD is a way to seek for a good balance between accuracy and efficiency. Based on function spaces, we mathematically analyze the relations among error bounds of several methods for PDEs including Finite Element Analysis (FEA), PGD, HiDeNN, DNN-based approaches and HiDeNN-PGD. The analysis shows that HiDeNN-PGD can reach the better accuracy than traditional PGD and FEA with the fixed regular mesh. 2D and 3D numerical examples for Poisson equation performed by these methods illustrate the accuracy of HiDeNN-PGD and verify our theoretical analysis. We also numerically explore the convergence rate of above methods with element size, degrees of freedom (DoFs) and number of modes. Reference [1] Lei Zhang, Lin Cheng, Hengyang Li, Jiaying Gao, Cheng Yu, Reno Domel, Yang Yang, Shaoqiang Tang, Wing Kam Liu. Hierarchical deep-learning neural networks: finite elements and beyond, Computational Mechanics 67(1): 207-230 (2021). https://doi.org/10.1007/s00466-020-01928-9 [2] David González, Amine Ammar, Francisco Chinesta, Elías Cueto. Recent advances on the use of separated representations. International Journal for Numerical Methods in Engineering 81(5): 637-659 (2010).

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Topology Optimization of Spinodoid Metamaterials with Seamlessly Tunable Anisotropy

Author(s): *Li Zheng, *ETH Zurich*; Siddhant Kumar, *Delft University of Technology*; Dennis Kochmann, *ETH Zurich*;

We present a two-scale topology optimization framework for the design of macroscopic bodies with an optimized elastic response, which is achieved by means of a spatially-variant cellular architecture on the microscale. The chosen spinodoid topology for the cellular network on the microscale (which is inspired by natural microstructures forming during spinodal decomposition) admits a seamless spatial grading as well as tunable elastic anisotropy, and it is parametrized by a small set of design parameters associated with the underlying Gaussian random field. The macroscale boundary value problem is discretized by finite elements, which in addition to the displacement field continuously interpolate the microscale design parameters. By assuming a separation of scales, the local constitutive behavior on the macroscale is identified as the homogenized elastic response of the microstructure based on the local design parameters. As a departure from classical FE2-type approaches, we replace the costly microscale homogenization by a data-driven surrogate model, using deep neural networks, which accurately and efficiently maps design parameters onto the effective elasticity tensor. The model is trained on homogenized stiffness data obtained from numerical homogenization by finite elements. As an added benefit, the machine learning setup admits automatic differentiation, so that sensitivities (required for the optimization problem) can be computed exactly and without the need for numerical derivatives - a strategy that holds promise far beyond the elastic stiffness. Therefore, this framework presents a new opportunity for multiscale topology optimization based on data-driven surrogate models.

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Title: A Computational Analysis of the Plasticity-Assisted Ionic Transport from the Atomistic to the Microscale

Author(s): *Liming Xiong, *Iowa State University*;

Many solid oxides, such as SrTiO3 or multilayered SrTiO3/MgO, containing a high density of built-in defects like dislocations, grain boundaries (GBs), phase boundaries (PBs), can be plastically deformable without cracking. These defects carry high local stresses and largely strain the materials locally. This is utilized to enhance the ion mobility and in turn, the material's ionic conductivity. However, evidenced by a large scatter in the enhancement level, the development of super ionic conductors through 'straining the solid oxides' is still at a "trial and error" stage. The limit of a strain-induced ionic transport enhancement is not converged yet due to the lack of a commonly agreed explanation on how ions hop nearby the complex defects, e.g., the dislocation pileup at a GB in SrTiO3, which spans from nano- to micro-meter level. It remains a challenge using single-scale techniques to fully address the atomistic ion jumping, the defect structure change together with the long-range stress field evolution in solid oxides under deformation. To meet this challenge, here we present a concurrent atomistic-continuum (CAC) computational framework to probe the coupling between the dislocation-mediated plastic flow and interstitial ion transport in materials under deformation. Our CAC model is shown to be applicable in determining: (i) the connection between the defect-induced stresses, the local structure distortion and the ion mobility; (ii) the decisive factor that dictates the ion transport in solid oxides with microstructure complexities; and (iii) the link between the loading, deformation localization, and the theoretical limit of a strain-induced ionic transport enhancement. The gained knowledge may support the search of (a) new methods for generating fast ionic transport channels through patterning the defects in solid oxides via a plastic engineering approach; and (b) new materials applied in low-temperature fuel cells, bio-chemical sensors, perovskite solar cells, Li-/Na- batteries.

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Title: A Spatiotemporal Nonlocal Homogenization Framework for Thermomechanical Response of Heterogeneous Materials

Author(s): *Linjuan Wang, *Beihang University*; Jifeng Xu, *Beijing Aeronautical Science and Technology Research Institute*; Jianxiang Wang, *Peking University*; Bhushan Karihaloo, *Cardiff University*;

The governing equations of heterogeneous materials given by the conventional homogenization theories usually have the same form as those of the constituents, that is, if the latter obey the principle of spatial location action, the former also exhibit the same behaviour. While this simple up-scaling transmission of the governing equations is successful in most cases, it is cannot describe complex dynamic responses of various heterogeneous materials. We develop a spatiotemporal nonlocal thermomechanical dynamic constitutive formulation for heterogeneous materials composed of conventional local thermoelastic constituents. In the mechanical sense, this formulation can correspond to the Mindlin equation, the Willis formalism, as well as the spatial non-local Eringen constitutive relation, and the peridynamic formulation. In the thermal sense, the governing equation of the average temperature can degenerate into the Jeffreys-type equation, Nunziato equation, Gurtin and Pipkin equation, peridynamic formulation, and dual-phase-lag (DPL) equation. The results on examples demonstrate that for static deformation and steady-state heat conduction, the spatiotemporal nonlocal is more accurate at capturing the variations of the average fields in regions of high gradients than the conventional homogenization schemes; for dynamic cases, the formulation can capture both the acoustic and optical branches of the dispersion relations. All the parameters in this formulation can be well determined from the geometrical and physical parameters of the constituents; thus it also sheds light on the physical mechanisms of the relevant theories in the context of heterogeneous materials.

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Title: Computational Analysis of the Effects of Geometric Irregularities and Post-Processing Steps on the Mechanical Behavior of Additively Manufactured 316L Stainless Steel Stents

Author(s): *Lisa Wiesent, *Ostbayerische Technische Hochschule Regensburg*; Ulrich Schultheiß, *Ostbayerische Technische Hochschule Regensburg*; Philipp Lulla, *FIT Production GmbH*; Thomas Schratzenstaller, *Ostbayerische Technische Hochschule Regensburg / Regensburg Center of Biomedical Engineering*; Christof Schmid, *Universität Regensburg*; Aida Nonn, *Ostbayerische Technische Hochschule Regensburg*; Ashley Spear, *The University of Utah*;

Advances in additive manufacturing enable the production of tailored lattice structures and thus, in principle, coronary stents. This study investigates the effects of process-related irregularities, heat and surface treatment on the morphology, mechanical response, and expansion behavior of 316L stainless steel stents produced by laser powder bed fusion and provides a methodological approach for their numerical evaluation. A combined experimental and computational framework is used, based on both actual and computationally reconstructed laser powder bed fused stents. This study was previously published in the scientific journal PLOS ONE [1]. Process-related morphological deviations between the as-designed and actual laser powder bed fused stents were observed, resulting in a diameter increase by a factor of 2-2.6 for the stents without surface treatment and 1.3-2 for the electropolished stent compared to the as-designed stent. Thus, due to the increased geometrically induced stiffness, the laser powder bed fused stents in the as-built (7.11 ± 0.63 N) or the heat treated condition (5.87 ± 0.49 N) showed increased radial forces when compressed between two plates. After electropolishing, the heat treated stents exhibited radial forces (2.38 ± 0.23 N) comparable to conventional metallic stents. The laser powder bed fused stents were further affected by the size effect, resulting in a reduced yield strength by 41% in the as-built and by 59% in the heat treated condition compared to the bulk material obtained from tensile tests. The presented numerical approach was successful in predicting the macroscopic mechanical response of the stents under compression. During deformation, increased stiffness and local stress concentration were observed within the laser powder bed fused stents. Subsequent numerical expansion analysis of the derived stent models within a previously verified numerical model of stent expansion showed that electropolished and heat treated laser powder bed fused stents can exhibit comparable expansion behavior to conventional stents. The findings from this work motivate future experimental/numerical studies to quantify threshold values of critical geometric irregularities, which could be used to establish design guidelines for laser powder bed fused stents/lattice structures. [1] L. Wiesent et al., “Computational analysis of the effects of geometric irregularities and post-processing steps on the mechanical behavior of additively manufactured 316L stainless steel stents,” PLoS One, vol. 15, no. 12, p. e0244463, Dec. 2020, doi: 10.1371/journal.pone.0244463.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Generative Ensemble-Regression: Learn Particle Dynamics from Observations of Ensembles with Physics-Informed Deep Generative Models

Author(s): *Liu Yang, *Brown University*; Constantinos Daskalakis, *Massachusetts Institute of Technology*; George Karniadakis, *Brown University*;

We propose a new method for inferring the governing stochastic ordinary differential equations by observing particle ensembles at discrete and sparse time instants, i.e., multiple "snapshots". Particle coordinates at a single time instant, possibly noisy or truncated, are recorded in each snapshot but are unpaired across the snapshots. By training a physics-informed generative model that generates "fake" sample paths, we aim to fit the observed particle ensemble distributions with a curve in the probability measure space, which is induced from the inferred particle dynamics. We employ different metrics to quantify the differences between distributions, like the sliced Wasserstein distances and the adversarial losses in generative adversarial networks. We refer to this approach as generative "ensemble-regression", in analogy to the classic "point-regression", where we infer the dynamics by performing regression in the Euclidean space, e.g. linear/logistic regression. We illustrate the ensemble-regression by learning the drift and diffusion terms of particle ensembles governed by stochastic ordinary differential equations with Brownian motions and Levy processes up to 20 dimensions. We also discuss how to treat cases with noisy or truncated observations. Apart from systems consisting of independent particles, we will also introduce how to tackle interacting particle systems with unknown interaction potential parameters, by constructing a physics-informed loss function. Finally, we will discuss the scenario of paired observations and prove a theorem for convergence in Wasserstein distance for continuous sample spaces.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Latent Variable Model and Data-Driven Design of Metamaterials: A New Synthesis

Author(s): *Liwei Wang, *Shanghai Jiao Tong University / Northwestern University*; Yu-Chin Chan, *Northwestern University*; Anton van Beek, *Northwestern University*; Daicong Da, *Northwestern University*; Faez Ahmed, *Massachusetts Institute of Technology*; Ping Zhu, *Shanghai Jiao Tong University*; Wei Chen, *Northwestern University*;

Metamaterials are emerging as a new paradigmatic material system that renders unprecedented and tailorable properties for a wide variety of engineering applications. However, the inverse design of a metamaterial and its multiscale system is challenging due to the high-dimensional topological design space, multiple local optima, and high computational cost. To address these hurdles, we propose a data-driven metamaterial design framework centered around the concept of the latent variable. We demonstrate that the use of latent variable models can greatly facilitate the representation, management, and utilization of a large metamaterial database to enable efficient microstructure and multiscale systems design. Specifically, we will present two latent variable models devised for data-driven metamaterial design, i.e., a modified variational autoencoder (VAE) and a multi-response latent variable Gaussian process (MR-LVGP). To enable an efficient design of free-form microstructures and heterogeneous multiscale systems, a deep neural network model consisting of a VAE and a regressor for property prediction is trained on a large metamaterial database to map complex microstructures into a low-dimensional and continuous latent space. Complex shape transformation is encoded in different moving directions in the latent space, rendering a natural interpolation method and a distance metric to measure shape similarity. Semantic structures of the latent space are identified to enable higher-level control of the mechanical properties. These mechanistic insights are combined with data-driven optimization algorithms to enable efficient microstructure design, metamaterial family generation, and assembly of multiscale metamaterial systems. For data-driven design of graded structures, a multi-response LVGP model is proposed for libraries of metamaterial microstructures with both qualitative microstructure concepts and quantitative volume fraction as mixed-variable inputs. The MR-LVGP model embeds the mixed variables into a continuous latent design space based on their collective effects on the responses, providing substantial insights into the interplay between different geometrical classes and material parameters of microstructures. With this model, we can easily obtain a continuous and differentiable transition between different classes that can render gradient information for multiscale topology optimization. We demonstrate its benefits through multiscale topology optimization for both static compliance and dynamic frequency optimization problems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Predicting the Influence of an Interface in Dynamic Brittle Fracture of PMMA

Author(s): *Longzhen Wang, *University of Nebraska-Lincoln*; Javad Mehrmashhadi, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

Recent experiments [1-2] in bonded PMMA layers have shown strong effects the interface toughness and location have on the crack path and propagation speed of a dynamic crack running perpendicular towards the interface. In this study, we use a peridynamic (PD) model to test whether the observed dependencies of crack behavior on the location of the interface relative to the pre-crack tip position are captured. The PD model follows a linear-elastic and brittle fracture constitutive model enhanced by softening the material near in the crack tip region that is triggered from the onset of the crack growth [3]. This enhancement is needed to approximately account for the effects heat generated at the crack tip has on the crack propagation speed in PMMA. We show that the PD model captures the main dynamic fracture characteristics observed in the bi-layer PMMA experiments: cracks branching or not at the interface, running along the interface before punching through into the second PMMA layer, crack speed accelerating before reaching the interface and dropping suddenly after passing the interface, etc. Keywords: Dynamic fracture, PMMA, peridynamics, interfacial failure Reference 1. Sundaram, B. M., & Tippur, H. V. (2016). Dynamic Crack Growth Normal to an Interface in Bi-Layered Materials: An Experimental Study Using Digital Gradient Sensing Technique. Experimental Mechanics, 56(1), 37–57. https://doi.org/10.1007/s11340-015-0029-x 2. Sundaram, B. M., & Tippur, H. V. (2016). Dynamics of crack penetration vs. branching at a weak interface: an experimental study. Journal of the Mechanics and Physics of Solids, 96, 312–332. 3. Mehrmashhadi, J., Wang, L., & Bobaru, F. (2019). Uncovering the dynamic fracture behavior of PMMA with peridynamics: The importance of softening at the crack tip. Engineering Fracture Mechanics, 219, 106617. https://doi.org/10.1016/j.engfracmech.2019.106617

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Integration of Patient-Specific Computational Modeling Frameworks into the Clinical Setting to Advance the Detection of Coronary Atherosclerosis Progression and Plaque Vulnerability

Author(s): *Lucas Timmins, *The University of Utah*; Caleb Berggren, *The University of Utah*; Jack Wang, *The University of Utah*; David Jiang, *The University of Utah*; David Molony, *Emory University*; Habib Samady, *Emory University*;

Acute coronary syndromes are a significant clinical problem, because of their frequency and the clinical challenge in stratifying risk for coronary lesions and identifying lesions that will undergo rapid progression and increased vulnerability. As mechanical loads have been postulated to play a central role in coronary atherosclerosis progression and plaque rupture, the development of image-based computational approaches to predict the in vivo coronary mechanical environment has been actively pursued. Towards this end, our laboratory is pioneering patient-specific computational modeling efforts to evaluate the in vivo fluid and solid coronary mechanical environments in patients enrolled in longitudinal clinical studies. Patient-specific coronary geometries are constructed from multi-modal imaging data and boundary conditions are derived from intravascular hemodynamic measures. Predicted fluid and solid mechanical metrics (e.g., wall shear stress, WSS; plaque structural stress, PSS) are associated with clinical measures of plaque progression, increased vulnerability, and rupture. In longitudinal clinical studies with >40 patients, we have demonstrated, for example, that high WSS is associated with increased plaque vulnerability [1] and that vulnerability increases in regions where high WSS co-localizes with high PSS [2]. More recently, we have focused efforts on advancing our computational models through the establishment of experimental frameworks to aid model validation and extract the material properties of plaque constituents. For example, deformable image registration methods have been applied to intravascular image data acquired in intact coronary tissue under varying deformation states to extract heterogeneous material properties from image defined plaque constituents. Collectively, these investigations seek to continually establish innovative computational approaches with broad application while maintaining direct clinical application to advance lesion prognostication and the detection of vulnerable plaques to guide patient management and treatment strategies towards minimizing adverse clinical events. [1] Samady, et al., Circulation, 2011. [2] Costopoulos et al., European Heart Journal, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: MPM Modeling of Large Deformations and Soil-Structure Interaction in Geotechnical In-Situ Testing

Author(s): *Luis Zambrano-Cruzatty, *Virginia Polytechnic Institute and State University*; Kaleigh Yost, *Virginia Polytechnic Institute and State University*; Alba Yerro, *Virginia Polytechnic Institute and State University*;

In geotechnical engineering, in-situ testing is a popular and efficient way to determine the geomechanical properties of soils. These parameters are then used to analyze complex problems such as soil-structure interaction (e.g., monopile foundations for offshore wind turbines) or advanced hazard modeling (e.g., run-out analysis of landslides). The cone penetration test (CPT) and the free fall penetrometer test (FFP) are widely used among the available in-situ methods. Both FFP and CPT testing consist of penetrating the soil with a probe. In the case of CPT, the penetration occurs at a low constant velocity of 2 cm/s. In contrast, FFP penetration occurs at transient velocities of 3m/s to 10 m/s. The hydro-mechanical coupling, loading rate, soil-structure interaction, and large deformations add complexity to analyzing the data collected in situ. Hence, numerical modeling can improve the understanding of these processes to develop new correlations between the tests and the soil parameters. We propose a numerical framework using the Material Point Method (MPM) to simulate CPT and FFP testing. It includes (1) a moving-mesh technique to keep a well-defined CPT/FFP device geometry, (2) a frictional contact algorithm used to describe the interaction of the soil and CPT/FFP device, and (3) a rigid body algorithm to enforce the incompressibility of the CPT/FFP device. It is shown that the behavior predicted by the MPM simulations of CPT and FFP tests are consistent with laboratory data even when using simple constitutive models. MPM simulations of CPT performed in layered soil profiles are shown to replicate the tendency of the CPT to smear boundaries between soil layers. For FFP simulations, parametric analyses are used to study the effect of soil parameters on the characteristics of the failure mechanism and deceleration profile. The numerical response of the FFP and CPT test are compared.

16th U.S. National Congress on Computational Mechanics
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Title: Predict Fracture Stress of Poly-Crystalline Graphene Using Deep Learning

Author(s): *MD Imrul Reza Shishir, *University of North Carolina at Charlotte*; Mohan Surya Raja Elapolu, *University of North Carolina at Charlotte*; Alireza Tabarraei, *University of North Carolina at Charlotte*;

Atomistic molecular dynamics simulations has been widely used to understand the mechanical properties of nanomaterials. To avoid the high computational costs associated with molecular dynamics simulations, data-driven computations can be used as an alternative. In this approach, experimental or computation data are used to build a machine learning model which can predict the material behavior at a considerably lower computational cost by eliminating atomistic modeling in every instance. Due to their ability to learn complex nature of data and make predictions, machine learning techniques are finding applications in various industries. In this study, we develop a deep neural network model to predict the fracture strength of polycrystalline graphene. Graphene, a monolayer of carbon atom with honeycombed latticed structure, displays fantastic properties which bring it a wide spectrum of applications. The data required for training our machine learning model is generated using molecular dynamics simulations. The molecular dynamics conducted in LAMMPS [1] are used to predict the fracture strength of polycrystallne graphene under uniaxial tensile loading. More than 2000 data points are generated using graphene sheets of different grain sizes with grain orientations. For each sheet, an atomic resolution image is created, and this image and its corresponding fracture strength are used as the input of deep learning model. Deep convolution neural network model is used to predict the fracture stress of polycrystalline graphene from the atomic resolution image. The results show that our model after training can predict the fracture strength of polycrystalline graphene with high accuracy. [1] Plimpton, Steve. "Fast parallel algorithms for short-range molecular dynamics." Journal of computational physics 117, no. 1 (1995): 1-19.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: 2D to 3D Volumetric Reconstruction of Human Spine for Diagnosis and Prognosis of Spinal Deformities

Author(s): *Mahsa Tajdari, *Northwestern University*; Farzam Tajdari, *Delft University of Technology*; Aishwarya Pawar, *Purdue University*; Jessica Zhang, *Carnegie Mellon University*; Wing Kam Liu, *Northwestern University*;

Abstract-The goal of this research is reconstructing patient-specific segmented 3-dimensional (3D) volumetric geometry of the human spine using 2-dimensional (2D) X-ray images. The X-ray images in anteroposterior and lateral views are segmented to identify the 2D contour around each vertebra using an active contour model based on gradient vector flow (GVF) snakes [1]. The 2D segmented contours of each vertebra are converted to 3D image segmentation result by implementing a Recurrent Neural Network (RNN) approach [2]. The generated 3D image is piecewise continuous and cannot be directly used for analysis. A 3D atlas spine model with segmented volumetric meshing for different regions of the vertebra (including the surface of each vertebra, the top and bottom surfaces of the individual vertebra, and volumetric segmented meshing) [3] is generated and registered to the 3D image segmentation result via Iterative Closest Point (ICP) algorithm which gives same meshing quality and geometric properties for different patients. The proposed model can track motion and physical changes of a patient's spine over a period of time by generating patient-specific geometry using X-ray images. Using the detailed 3D volumetric model, one can extract spinal geometric features that help surgeons to cluster spinal deformity based on the 3D features and design treatment path. The volumetric mesh can be implemented to analyze stress distribution on different regions of the spine and the extracted information may be used to predict spine curvature over years using machine learning methods. References: 1. M. Tajdari, A. Pawar, H. Li, F. Tajdari, A. Maqsood, E. Cleary, S. Saha, Y. J. Zhang, J. F. Sarwark, W. K. Liu. Image-based modelling for Adolescent Idiopathic Scoliosis: Mechanistic machine learning analysis and prediction. Computer Methods in Applied Mechanics and Engineering, 374:113590, 2021. 2. C.B. Choy, D. Xu, J. Gwak, K. Chen, S. Savarese. 3d-r2n2: A unified approach for single and multi-view 3D object reconstruction. European Conference on Computer Vision, 628-644, 2016. 3. Y. Yang, T. Yuan, T. Huysmans, W. Elkhuizen, F. Tajdari, Y. Song. Posture-invariant 3D Human Hand Statistical Shape Model. Journal of Computing and Information Science in Engineering, 1-31, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Non-Matching Interface Fluid–Structure Interaction Modeling for Compressible Flow Problems

Author(s): *Manoj R. Rajanna, *Iowa State University*; Emily L. Johnson, *Iowa State University*; Ning Liu, *Global Engineering & Materials, Inc.*; Jim Lua, *Global Engineering & Materials, Inc.*; Ming-Chen Hsu, *Iowa State University*;

Aircraft tail buffeting is an aeroelastic phenomenon characterized by random pressure oscillations impacting on the aircraft tail structures caused due to the unsteady airflow in the wake of the wing. This unsteady dynamic flow in the wake can damage aircraft tail structural components and can reduce its fatigue life. The numerical modeling of aircraft buffeting has been challenging due to the aerodynamic nonlinearities and complex aircraft structural components. To accurately model the buffeting phenomena, a high-fidelity fully-coupled framework for compressible flow fluid–structure interaction (FSI) modeling and simulation using non-matching interface discretizations is developed in this work. Finite element based Navier–Stokes equation of compressible flow and the isogeometric analysis (IGA) based rotation-free Kirchhoff–Love shell structural formulation are considered to model the physics involved. FSI methodology is developed to handle the different non-matching discretizations at the interface and a projection method is used for the transfer of kinematic and traction data between the fluid and structure subdomains. The method is validated for its accuracy through a benchmark problem and is applied to simulate flow around full-scale aircraft and the buffeting of its horizontal stabilizer. A novel hybrid FSI methodology in the application to aircraft buffet modeling is developed. The FSI framework is also extended to model the aircraft maneuvers based on arbitrary Lagrangian–Eulerian (ALE) approach to simulate realistic time-dependent flight maneuvers and study the unsteady loads and its effects acting on the horizontal stabilizer of the aircraft.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling the Viscolelastic-Damage Mechanics of Blood Clot

Author(s): *Manuel Rausch, *The University of Texas at Austin*; Gabriella Sugerman, *The University of Texas at Austin*; Sotirios Kakaletsis, *The University of Texas at Austin*; Berkin Dortdivanlioglu, *The University of Texas at Austin*;

Blood clot plays a diametric role in our bodies as it is both vital as a wound sealant as well as the source for many devastating diseases. In its physiological and pathological roles, the mechanics of blood clot play a critical part. These mechanics are non-trivial owing to blood clot's complex nonlinear, viscoelastic behavior. Casting this behavior into mathematical form is a fundamental step toward a better basic scientific understanding of blood clot as well as toward diagnostic and prognostic computational models. Here we identify a hyper-viscoelastic damage model that we fit to original data on the nonlinear, viscoelastic behavior of blood clot. Our model combines the classic Ogden hyperelastic constitutive law, a finite viscoelastic model for large deformation, and a non-local, gradient-enhanced damage formulation. By fitting our model to cyclic tensile test data and extension-to-failure data, we inform the model's nine unknown material parameters. We demonstrate the predictability of our model by validating it against unseen cyclic tensile test and stress-relaxation data. Together, our results will be an important step toward well-informed simulations of blood clot mechanics.

16th U.S. National Congress on Computational Mechanics
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Title: Symplectic Hamiltonian HDG Methods for Elastodynamics

Author(s): *Manuel Sanchez, *Pontificia Universidad Católica de Chile*; Bernardo Cockburn, *University of Minnesota*; Ngoc-Cuong Nguyen, *Massachusetts Institute of Technology*; Jaime Peraire, *Massachusetts Institute of Technology*;

We present a class of high-order finite element methods that can conserve the linear and angular momenta as well as the energy for the equations of linear elastodynamics. These methods are devised by exploiting and preserving the Hamiltonian structure of the equations of linear elastodynamics. We show that several mixed finite elements, discontinuous Galerkin, and hybridizable discontinuous Galerkin (HDG) methods belong to this class. We discretize the semidiscrete Hamiltonian system in time by using a symplectic integrator in order to ensure the symplectic properties of the resulting methods, which are called symplectic Hamiltonian finite element methods. For a particular semidiscrete HDG method, we obtain optimal error estimates and present, for the symplectic Hamiltonian HDG method, numerical experiments that confirm its optimal orders of convergence for all variables as well as its conservation properties.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Viscous Regularization Framework for the Compressible Euler Equations Originating from VMS and Variation Entropy Theory

Author(s): *Marco ten Eikelder, *Delft University of Technology*; Stein Stoter, *Leibniz University Hannover*; Ido Akkerman, *Delft University of Technology*; Yuri Bazilevs, *Brown University*; Dominik Schillinger, *Leibniz University Hannover*;

Variational multiscale (VMS) modeling is nowadays a popular approach for turbulence modeling [1]. Tiny turbulent eddies generally can not be represented by the computer mesh and the VMS method takes their effect into account via the fine-scale models. Shock waves are another physical phenomenon that is typically unresolved in a numerical simulation. Following this line of thought suggests to employ fine-models in a similar fashion for shock waves as for turbulence modeling. In this talk we present a theoretical finite element isogeometric framework for discontinuity capturing for the compressible Euler equations. The approach extends the mathematical discontinuity capturing framework proposed for scalar conservation laws [2]. The discontinuity capturing mechanism enters the variational formulation via the fine-scales in a VMS paradigm. The associated multiscale projector is based on variation entropy theory [3], which is a continuous generalization of the total variation diminishing concept. Apart from the standard fine-scale solutions, this approach also introduces fine-scale variation entropy terms. Analogously to the residual-based fine-scale models, we propose residual-based models for the fine-scale variation entropy terms which are based on so-called variation entropy conditions. The emerging viscous regularization possesses the following properties: (i) it is derived instead of augmented in an ad hoc fashion to the formulation, (ii) it is variationally consistent, (iii) it is active near contact discontinuities and in shock regions and renders inoperative elsewhere, (iv) higher-order convergence rates are obtained in smooth regions, and (v) it satisfies the general requirements for viscous regularization tensors. Several benchmark problems with higher-order isogeometric elements confirm the properties of the proposed methodology. [1] Y. Bazilevs, V.M. Calo, J.A. Cottrel, T.J.R. Hughes, A. Reali, and G. Scovazzi. Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows. Computer Methods in Applied Mechanics and Engineering, 197:173–201, 2007. [2] M.F.P. ten Eikelder, Y. Bazilevs, and I. Akkerman. A theoretical framework for discontinuity capturing: Joining variational multiscale analysis and variation entropy theory. Computer Methods in Applied Mechanics and Engineering, 359:112664, 2020. [3] M.F.P. ten Eikelder and I. Akkerman. Variation entropy: a continuous local generalization of the TVD property using entropy principles. Computer Methods in Applied Mechanics and Engineering, 355:261–283, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Computational and Experimental Study of Permeability Changes under Confinement in Fractured Porous Media

Author(s): *Maria Warren, *Sandia National Laboratories / Georgia Institute of Technology*; Mario J. Martinez, *Sandia National Laboratories*; Alec Kucala, *Sandia National Laboratories*; James E. Bean, *Sandia National Laboratories*; Scott T. Broome, *Sandia National Laboratories*; Jennifer Wilson, *Sandia National Laboratories*; Hongkyu Yoon, *Sandia National Laboratories*;

Discontinuous features of fractured deformable media pose significant challenges to analysis and control of coupled flow and transport processes relevant to subsurface energy recovery and storage, environmental and climate change, and nuclear waste disposal. As such, there is a significant body of work dedicated to modeling the coupling of fluid and solid mechanics within fractured porous media. Fully coupled monolithic schemes, though accurate, require a unified flow-mechanics solver and are computationally expensive. These limitations spurred the development of iteratively coupled methods, such as the unconditionally stable fixed stress scheme, to solve poromechanics problems. First, this work will discuss the implementation of the fixed stress scheme into the existing Sandia Sierra Multiphysics toolkit [1-3]. Then, benchmark poroelastic problems including the one-dimensional (1D) Terzaghi, 2D Mandel, and 3D Cryer problems are used to verify the implementation methods. The effects of material parameters, convergence criteria, and numerical solver are evaluated through these benchmark problems. This uniquely comprehensive study assesses how the fixed stress scheme tolerance affects the accuracy of pore pressures and solid skeleton displacement results for one-, two-, and three-dimensional problems. The results provide new considerations for selection of an appropriate fixed-stress tolerance given the physical properties of materials. The aforementioned benchmark problems are also used to analyze the numerical solver implemented in the simulation. This work shows significant differences in solution stability between two different GMRES (generalized minimum residual method) solvers available in Sierra Multiphysics toolkit. Finally, the fixed stress scheme implementation is validated using laboratory experimental results with fractured porous geomaterials where permeability changes have been measured under confined pressure conditions. Key aspects of material characteristics are described based on microCT and thin section images and simplified parameterization of fracture response under confinement are evaluated through comparison of simulation results with experimental data. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. References: [1] SIERRA Multimechanics Module: Aria User Manual – Version 4.58, SIERRA Thermal/Fluid Development Team. SAND2020-11537, October 20, 2020. [2] SIERRA Code Coupling Module: Arpeggio, User Manual – Version 4.58, S.R. Subia, J.R. Overfelt, and D.G. Baur. SAND2020-11532, October 20, 2020. [3] SIERRA/Solid Mechanics 4.58 User’s Guide, SIERRA Solid Mechanics Team, Computational Solid Mechanics and Structural Dynamics Department, Engineering Sciences Center. SAND2020-10045, October 20, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Dislocation Microstructure Evolution During Selective Laser Melting of 316L Stainless Steel

Author(s): *Markus Sudmanns, *Johns Hopkins University*; Andrew Birnbaum, *US Naval Research Laboratory*; Yejun Gu, *Johns Hopkins University*; Athanasios Iliopoulos, *US Naval Research Laboratory*; John Michopoulos, *US Naval Research Laboratory*; Jaafar A. El-Awady, *Johns Hopkins University*;

One major challenge in Additive Manufacturing (AM) of metallic components is developing the relationship between the microstructural evolution due to processing conditions involving thermo-mechanical stresses and the final and occasionally improved mechanical properties and performance of the manufactured part. Various studies attribute the enhanced mechanical properties of Selective Laser Melted (SLM) metallic parts to the formation of cellular dislocation structures, which are usually accompanied by solute segregation to the dislocation cell walls [1,2]. However, the formation of those cellular structures as well as their effects on the mechanical properties are still poorly understood. Furthermore, the role of solute segregation on microstructural evolution during the cooldown phase of SLM is still under discussion. Three-dimensional (3D) discrete dislocation dynamics (DDD) simulations can provide a unique understanding of the influence of solidification induced solute segregation on the evolution of dislocation ensembles. However, most investigations using DDD simulations have so far been limited to pure metals since no relevant approach towards considering the effect of solid solution atoms on the evolution of the dislocation microstructure in 3D DDD has been made. Here, we incorporate a recently developed theoretical model of solid solution strengthening in fcc alloys from [3] into 3D DDD simulations. Using 3D thermo-mechanical Finite Element (FE) simulations of a single SLM scan of 316L stainless steel we extract the emerging temperature and residual stresses during SLM processing. Considering the relevant thermo-mechanical boundary conditions, we then present bulk 3D DDD simulations of the dislocation and composition microstructure evolution during SLM manufacturing of 316L stainless steel accounting for solute segregation. These results provide an explanation for the formation of characteristic microstructure orientations observed experimentally after SLM processing and therefore establish a relationship between emerging cellular dislocation structures, solute segregation and the thermo-mechanical process conditions in experiments. [1] Wang, Y. M. et al., (2018). Nature Materials, 17(1), 63–70 [2] Krakhmalev, P. et al., (2018). Metals, 8(8) [3] Varvenne, C. et al., (2016). Acta Materialia, 118, 164–176

16th U.S. National Congress on Computational Mechanics
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Title: Harnack Inequality for Fractional Elliptic Equations in Nondivergence Form

Author(s): *Mary Vaughan, *The University of Texas at Austin*; Pablo Raúl Stinga, *Iowa State University*;

In this talk, we will define fractional powers of nondivergence form elliptic operators in bounded domains under minimal regularity assumptions. We will show that equations driven by such operators have applications in elasticity. The main result we will present is a Harnack inequality for solutions to a corresponding fractional Poisson problem. In order to overcome the nonlocality, we will characterize the fractional Poisson problem with a degenerate/singular extension problem.

16th U.S. National Congress on Computational Mechanics
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Title: A Posteriori Error Estimates for Biot System Using Enriched Galerkin for Flow

Author(s): Vivette Girault, *Sorbonne Université*; Xueying Lu, *The University of Texas at Austin*; *Mary Wheeler, *The University of Texas at Austin*;

We analyze the Biot system solved with a fixed-stress split, Enriched Galerkin (EG) discretization for the flow equation, and Galerkin for the mechanics equation. Residual-based a posteriori error estimates are established with both lower and upper bounds. These theoretical results are confirmed by numerical experiments performed with the Mandel’s problem. The efficiency of these a posteriori error estimators to guide dynamic mesh refinement is demonstrated with a prototype unconventional reservoir model containing a fracture network. We further propose a novel stopping criterion for the fixed-stress iterations using the error indicators to balance the fixed-stress split error with the discretization errors. The new stopping criterion does not require hyperparameter tuning and demonstrates efficiency and accuracy in numerical experiments. References: Girault, Vivette, Xueying Lu, and Mary F. Wheeler. "A posteriori error estimates for Biot system using Enriched Galerkin for flow." Computer Methods in Applied Mechanics and Engineering 369 (2020): 113185. Lu, Xueying, Vivette Girault, and Mary F. Wheeler. "Dynamic Adaptivity for Coupled Flow and Geomechanics in Unconventional Reservoirs Using A Posteriori Error Estimation with Enriched Galerkin Method." 54th US Rock Mechanics/Geomechanics Symposium. American Rock Mechanics Association, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Fiber-Reinforced Composites: Interface Failures, Convergence Issues, and Sensitivity Analysis

Author(s): *Maryam Shakiba, *Virginia Polytechnic Institute and State University*; Reza Sepasdar, *Virginia Polytechnic Institute and State University*;

In fiber-reinforced composites, cracks initiate around the fibers aligned transversely to the loading direction. The transverse cracks can potentially cause leakage in specific applications or progress to inter-ply delamination and catastrophic failure. Initiated micro-cracks can go undetected since the instantaneous loss in the composites' response is negligible. In this presentation, we study transverse crack propagation in a realistic representation of high-volume fraction unidirectional fiber-reinforced composites. First, the root of convergence difficulty in modeling interfacial debonding is investigated. It is shown that an inappropriate starting point of iterations in the Newton–Raphson method is responsible for the convergence difficulty. Based on the numerical cause of the convergence issue, we propose a novel and simple method to modify the Newton-Raphson method in order to get fast and easy convergence. The technique is robust, simple to implement in a finite element framework, does not compromise the accuracy of analysis, and provides fast convergence. Then, the effect of interfacial properties on the composite's failure response is quantified. A gradient-based method to calculate the sensitivity of the transverse failure response with respect to the distribution of the fiber/matrix interface properties is devised. The method is built upon the work by Shakiba et al.1 where an analytical sensitivity formulation based on the direct differentiation method was derived and implemented in a nonlinear cohesive interface-enriched generalized finite element method (IGFEM) solver. The analytical sensitivity results show that the sensitivity of the stress response in a transverse ply with respect to individual fiber/matrix interface cohesive properties follows a normal distribution before cracks initiate. The distribution of the sensitivities deviates suddenly from a normal distribution from cracks initiation to the formation. The numerical prediction of cracks initiation and extreme fibers sensitivities can be used as a failure risk indicator to increase the reliability of laminates' designs.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Optimization of Material Orientation in Flat Inflatable Structures

Author(s): *Masato Tanaka, *Toyota Motor North America, Inc.*; Katsuya Nomura, *Toyota Central R&D Labs., Inc.*; Tsuyoshi Nomura, *Toyota Central R&D Labs., Inc.*;

Additive manufacturing or so-called 3D printing demonstrates a great potential to construct optimized structures and manipulate spatially varying material orientation. Compared to traditional subtractive manufacturing processes, the 3D printing is capable of fabricating complex geometry with various advanced composite materials. Finding optimal distribution of material orientation is of great importance to minimize/maximize properties of the additively manufactured structures. Recently, 4D printing, a new 3D printing method, is receiving much attention since it provides printed objects with the ability to transform into a variety of their shapes, functions or stiffnesses over time according to environmental stimuli. This study addresses programming of material orientations for initially flat inflatable structures which can easily change their 2-dimensional shapes to 3-dimensional surfaces by a simple air pressure input. Such inflatable structures offer a path for light weight deployable structures in various engineering applications including soft robotics, medical equipment, architectural domes and aerospace habitats. In our study, the inflatable structures are modeled and analyzed by nonlinear shell finite element method. The shell element is based on the formulation of 3-node ``Mixed Interpolation of Tensorial Components'' (MITC3), which uses the assumed transverse shear strain fields in order to alleviate the so-called shear and membrane locking phenomena. We introduce displacement-dependent follower forces to model internal pressure acting upon the shell elements. In this study, the material model in the shell element is limited to transversely isotropic one, that is, only one preferred direction is considered. Our proposed orientation optimization method is founded on gradient-based topology optimization with Helmholtz filtering and Heaviside projection. The components of an orientation tensor are regarded as design variables in the material orientation optimization problem. This tensor representation of material orientations can remove nonlinear constraints and numerical instability during optimization which often appear in the angular or vector representations due to their cyclic behavior of trigonometric functions. The idea of a relaxed orientation tensor whose trace can be allowed to be less than one is also provided. The interpretation of the physical meaning of the relaxed orientation tensor is investigated. The formulation of adjoint method is also presented to derive the sensitivity of objective function with respect to the orientation design variables and some complicated computations of the derivatives are avoided using the highly accurate complex-step derivative approximation method. In our presentation, several numerical examples are provided to illustrate the performance of the proposed optimization method.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Hyperreduction for Discontinuous Galerkin Methods: Element- and Point-Wise Reduced Quadrature Formulations with Applications to Aerodynamics

Author(s): *Masayuki Yano, *University of Toronto*;

We consider model reduction of parametrized nonlinear partial differential equations with applications in aerodynamics. Our model reduction approach builds on the adaptive high-order discontinuous Galerkin (DG) method, reduced-basis spaces, and hyperreduction based on reduced quadrature rules found through an optimization procedure. We consider two distinct approaches to quadrature-based hyperreduction: an element-wise and point-wise formulations, which use a finite element and an individual quadrature point, respectively, as the working unit for hyperreduction. We analyze the characteristics of the two approaches in terms of the stability, online computational cost, and offline training cost. The element-wise formulation enables a decomposition that guarantees energy stability for any choice of non-negative quadrature weights; in the point-wise formulation, stability conditions must be included explicitly as constraints in the reduced quadrature construction. As regards online computational cost, the point-wise formulation provides more significant online reduction, both in theory and practice, particularly for high-order approximations with a large number of degrees freedom and quadrature points per element. Conversely, in the offline stage, the point-wise formulation requires the solution of a significantly larger optimization problem to find reduced quadrature rules. The two formulations are assessed using a series of aerodynamics problems governed by the Euler and Reynolds-averaged Navier-Stokes equations. While both formulations reduces computational cost by several orders of magnitude, the point-wise formulation provides more significant speed up with no apparent loss of stability in practice.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: The Importance of Time-Temperature Data Fidelity to Accurate Modeling of Additive Grain Structure: A Cellular Automata Study

Author(s): *Matt Rolchigo, *Lawrence Livermore National Laboratory*; Jim Belak, *Lawrence Livermore National Laboratory*; Benjamin Stump, *Oak Ridge National Laboratory*;

Accurate and high fidelity modeling of fluid and heat transport is necessary to accurately predict AM grain structures. While cellular automata (CA) models of nucleation and grain growth can efficiently simulate large regions of microstructure, the combined performance of process-microstructure simulations is limited by the more computationally expensive computational fluid dynamic (CFD) models. As part of the larger ExaAM project, the CA code ExaCA is being developed to take advantage of pre-Exascale computing architectures and simulate large scale microstructure development. In this study, we apply a novel method for one-way coupling of time-temperature history data to ExaCA, allowing calculations of multilayer grain structure independent from CFD models. We explore and compare CA results using two sparse forms of the time-temperature history. The first form lists the times at which each CFD node goes below the liquidus temperature for the final time, along with their cooling rates. The second form lists each time that each CFD nodes crosses the liquidus temperature, in addition to their cooling rates. The implications on code performance and accuracy using each data format will be discussed – use of the first form of data allows remelting to be ignored, simplifying the CA code and allowing fast, first order approximations of grain structure for many common AM melt pool conditions. Use of the second form is less efficient but needed to accurately model microstructure for more complex melt pool geometry. Future work regarding direct incorporation of ExaCA as a callable library within CFD and analytical heat transport models will be discussed as well. Work performed under the auspices of the U.S. DOE by LLNL under contract DE-AC52-07NA27344, and supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. DOE Office of Science and the NNSA.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Parallel Overlay Grid Tet Mesh Generation with Combined Snapping & Cutting with Automatic CAD Defeaturing

Author(s): *Matt Staten, *Sandia National Laboratories*; David Noble, *Sandia National Laboratories*; Corey McBride, *Sandia National Laboratories*; C. Riley Wilson, *Sandia National Laboratories*;

We present a new approach to massively parallel overlay grid tetrahedral mesh generation, by adding cutting into the Morph snapping algorithm [1], while maintaining the ability to automatically ignore CAD features smaller than a specified size. This presentation will include extending the algorithms for cutting and snapping to capture of CAD curves and vertices in a massively parallel environment. Overlay approaches to tetrahedral mesh generation began decades ago, but struggled to gain traction until recently [1,2,3]. Morph [1] and FTetWild [3] are the first approaches that removes the assumption of a “clean” geometry, required for industrial application. FTetWild takes a triangle soup as input, with overlaps/gaps between triangles, cutting in all triangles, coupled with mesh optimization to improve quality and remove small features while maintaining a set of geometry capture tolerances. Similarly, Morph has no assumption of a “clean” geometry, but from a different approach. Morph computes xyz intersection points between the vertices, curves, and surfaces of a CAD BREP (not a faceted representation of the CAD), and then snaps, cuts, and agglomerates each intersection point into an overlay grid that is already constructed with the final desired mesh refinement. Morph cuts in only the CAD features which are larger than a user set tolerance, avoiding the creation of unnecessarily small tets which must later be removed. This small feature tolerance is often set from a minimum time step required for a subsequent explicit analysis. Morph currently uses mesh optimization to maintain element quality, although we maintain the long-term goal of maintaining quality throughout cutting without mesh optimization. Morph runs in distributed memory parallel from step one, with the initial overlay providing the domain decomposition with strategic rebalancing. [1] M. L. Staten, D. R. Noble, C. R. Wilson, C. L. McBride, M. K. Bhardwaj. “Massively Parallel Tet Meshing With Size-Dependent Feature Capture on CAD Models,” Proceedings 27th International Meshing Roundtable, 2018. [2] B. Liang, A. Nagarajan, S. Soghrati, “Scalable Parallel Implementation of CISAMR: a Non-Iterative Mesh Generation Algorithm,” Comput Mech 64, 173–195, 2019. [3] Y. Hu, T. Schneider, B. Wang, D. Zorin, D Panozzo, “Fast Tetrahedral Meshing in the Wild," ACM Trans. Graph., Vol 39(4), Article 117, 2020. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. SAND2021-0711 A

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Discrete Modeling of Reinforced Concrete Panels and Columns Subject to Spherical Near-Field Air Blasts

Author(s): *Matthew Troemner, *Northwestern University*; Gianluca Cusatis, *Northwestern University*; Photios Papados, *Department of Defense*;

Unlike the direct structural loading of high-speed impacts, detonation events result in a pressure wave emanating through the surrounding medium which interacts with feature geometry. In the case of near-field air blasts, these pressure waves are highly spherical, introducing non-uniform and non-simultaneous loads on the subject surfaces. In this paper, the Lattice Discrete Particle Model (LDPM) is used to simulate the effect of spherical near-field air blasts on normal-strength reinforced concrete panels and columns. Concrete aggregate is modeled at true-to-life scale and an explicit-dynamic simulation without rate effect is used for processing of the lattice system of both concrete structures. Further, reinforcement is simulated with Timoshenko beam elements governed by J2 plasticity and with ductile damage and evolution parameters. For the case of reinforced concrete columns, the application of loading is performed via discrete pressure fields directly applied to the blast-facing surface. Fields are discontinuous and include both positive and negative pressure phases such to accurately emulate the behavior of spherical blasts. The selected pressure histories are of an order-of-magnitude realistic to a moderately-large near-field detonation. Loading for the reinforced concrete panels is also applied to the blast-facing surface, with load histories instead handled via an empirical CONWEP model included in commercial Abaqus/CAE packages. A discussion of results is provided for both structural cases, with the concrete panels also validated against full-scale laboratory experiments completed by Kumar et al. (2020). Kumar, V., et al. (2020). "Experimental and numerical investigation of reinforced concrete slabs under blast loading." Engineering Structures 206.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Model Reduction of Convection-Dominated Partial Differential Equations via Optimization-Based Implicit Feature Tracking

Author(s): *Matthew Zahr, *University of Notre Dame*; Marzieh Mirhoseini, *University of Notre Dame*;

Partial differential equations (PDEs) that model convection-dominated phenomena often arise in engineering practice and scientific applications, ranging from the study of high-speed, turbulent flow over vehicles to wave propagation through solid media. The solutions of these equations are characterized by local features or disturbances that propagate throughout the domain as time evolves or a system parameter varies. Numerical methods to approximate these solutions require stabilization and fine, usually adaptive, grids to adequately resolve the local features, which lead to expensive discretizations with a large number of degrees of freedom. Projection-based model reduction methods tend to be ineffective in reducing the computational cost of such problems due to a slowly decaying Kolmogorov n-width of the solution manifold. To avoid the fundamental linear reducibility limitation associated with convection-dominated problems, we construct a nonlinear approximation by composing a low-dimensional linear space with a parametrized domain mapping. The linear space is constructed using the method of snapshots and POD; prior to compression, each snapshot is composed with a mapping that causes its local features to align (same spatial location) with the corresponding features in all other snapshots. The parametrized domain mapping is chosen such that the local features present in the linear space deform to the corresponding features in the solution being approximated, effectively removing the convection-dominated nature of the problem. The domain mapping is determined implicitly through the solution of a residual minimization problem, rather than relying on explicit sensing/detection. We provide numerous numerical experiments to demonstrate the effectivity of the proposed method on benchmark problems from computational fluid dynamics.

16th U.S. National Congress on Computational Mechanics
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Title: Hex-Dominant Meshing with All-Hexahedral Boundary Layer

Author(s): *Maxence Reberol, *Université catholique de Louvain*; Christos Georgiadis, *Université catholique de Louvain*; Kilian Verhetsel, *Université catholique de Louvain*; Jean-Francois Remacle, *Université catholique de Louvain*;

We propose a robust approach to generate hex-dominant meshes of arbitrary CAD models with a layer of pure hexahedra on the boundary. An initial all-quadrilateral mesh is built on the model boundary. The quad mesh is extruded inside the volume on the CAD faces and irregular hexahedral configurations are used on the CAD corners and curves to join the extruded parts. Once a first hex layer is built, the rest of the volume is filled with a frontal hex-dominant mesher guided by a frame field. The all-quadrilateral mesh generation follows a unstructured approach: (1) points are inserted frontally by following a guiding field, (2) a triangulation is build from the points, (3) the triangles are combined to form a quadrilateral mesh or a quad-dominant mesh, which is then subdivided into an all quadrilateral mesh. The guiding field is made of a boundary-aligned smooth cross field and a size map. The number of irregular vertices in the mesh is reduced thanks to cavity remeshing [1]. The hexahedral boundary layer is made of extruded quads on the smooth parts of the surface and of irregular hexahedral configurations at the interfaces along the CAD curves. The irregular configurations, which are sometimes complicated and unintuitive, are found by enumerating all hexahedral configurations around vertices and choosing the ones which satisfy all the local topological constraints. In the remaining volume, the hex-dominant mesh is built by inserting points frontally according to a frame field, which are used to build a tetrahedral mesh. Then, a large proportion of the tetrahedra are combined into hexahedra [2] and pyramids are used to make conformal transitions between the hexahedra and the remaining tetrahedra. The robustness of our approach is demonstrated by generating hex-dominant meshes on various CAD models with complex CAD curve arrangements. [1] Bunin, G. (2006). Non-local topological clean-up. In Proceedings of the 15th International Meshing Roundtable (pp. 3-20). Springer, Berlin, Heidelberg. [2] Pellerin, J., Johnen, A., & Remacle, J. F. (2017). Identifying combinations of tetrahedra into hexahedra: a vertex based strategy. Procedia engineering, 203, 2-13.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Coupled Left Ventricular and Atrial FSI Simulations with Bioprosthetic Valves

Author(s): *Mehdi Saraeian, *Iowa State University*; Arian Jafari, *Iowa State University*; Remy Braun, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Transcatheter heart valve interventions have proven effective for unfavorable surgical candidates with valve disease. However, the success of this minimally invasive intervention depends on several factors such as the patient's anatomy as well as the fit of the valve design to the specific patient. Clinicians have limited resources to evaluate the outcome of such interventions. Computational models of the cardiovascular systems can provide specific feedback on the effectiveness of the valve in controlling the blood flow from the atrium to the ventricles. In addition, specific flow parameters can be investigated to optimize the outcome of the intervention. In order to enable such computational analysis, we have developed a four-chamber finite element model of the human heart using cubic-Hermite meshes and simulated the complete cardiac cycle using a lumped circulation model. Coupling the deformations of the heart captured from our biomechanics simulation, we perform the computational fluid-structure interaction (FSI) simulations using the immersogeometric method. In this method, the leaflets are modeled as thin shells using incompressible Fung-type material under tensile loading. Using this FSI framework, we propose to study the post-intervention hemodynamics behavior in the heart. The resulting analysis can help us design better transcatheter heart valves and provide clinicians with quantitative measures to analyze their options and intervene with a higher level of certainty for better patient care. References: 1. Fei Xu, Emily L. Johnson, Chenglong Wang, Arian Jafari, Cheng-Hau Yang, Michael S. Sacks, Adarsh Krishnamurthy, Ming-Chen Hsu; Computational investigation of left ventricular hemodynamics following bioprosthetic aortic and mitral valve replacement, Mechanics Research Communications, In Press, 2020. 2. Arian Jafari, Edward Pszczolkowski, Adarsh Krishnamurthy; A framework for biomechanics simulations using four-chamber cardiac models, Journal of Biomechanics, 91:92–101, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: High-Order Space-Time Flux Reconstruction Methods for Moving Domain Simulation

Author(s): *Meilin Yu, *University of Maryland, Baltimore County*;

Numerical simulation on moving domains poses big challenges on the development of high-order computational fluid dynamics (CFD) methods with the arbitrary Lagrangian-Eulerian (ALE) formulation. If the method of line is used to perform the moving-domain simulation, the time-derivative term and spatial flux terms are not discretized in a spatiotemporally uniform way. This can introduce geometric conservation law (GCL) errors into the numerical simulation. Even if high-order temporal and spatial discretization is used to handle every term, GCL errors can still be generated due to that the evaluation of the grid velocity and the Jacobian is not consistent with each other. To eliminate such type of errors, two approaches are usually adopted. One way is to solve the Jacobian from the GCL formula using the same scheme that solves the unsteady flows; and the other is to directly substitute the temporal derivative with the spatial ones. We note that no matter what approach is used, systematic errors due to the inconsistency between the grid velocity and time-dependent metrics can still exist if these terms are not handled with sufficient caution. To reduce the GCL-related errors, small time steps can be used in moving-domain simulation. However, this may substantially decrease simulation efficiency when solving complex moving mesh problems from industrial applications. The space-time formulation provides a uniform treatment of both space and time, and can resolve GCL automatically without involving grid velocity. Although some research has been conducted for the space-time discontinuous Galerkin (DG) method and streamline-upwind/Petrov-Galerkin (SUPG) method, more work is still needed to fully explore the numerical potential of this method. We have recently developed a nodal space-time FR method to solve hyperbolic conservation laws on stationary meshes. We found that the space-time FR method using Gauss-Legendre points is spatially superconvergent during long-term unsteady simulations; and is temporally superconvergent during both short-term and long-term unsteady simulations. In this work, we further develop this collocation based nodal space-time FR method for moving-domain simulation. The contribution of this study is that we develop the high-order nodal space-time FR method with the ALE formulation for the first time, and numerically demonstrate that this method is superconvergent in time for unsteady flow simulation.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Novel Time-Evolving Model for the In-Vivo Maturing Collagen in Engineered Tissues

Author(s): *Michael Sacks, *The University of Texas at Austin*;

To date, no known model for in-vivo maturing engineered tissues exists. The present study simulates the remodeling of a pulmonary artery (PA) conduit from 0 to 700 days in-vivo in an ovine animal model. It has been noted that the conduit maintained its gross dimensions, including length, diameter, and thickness, over the entire remodeling period. This indicating that the conduit was subjected to the same stress state throughout the maturation process. Only collagen fibers are considered to be mechanically relevant; cells and fluid constituents are ignored as being mechanically negligible. It was observed that collagen fibers underwent a continual increase in modulus and shift in recruitment distribution towards larger stretch values. Collectively, these phenomena suggest that the main remodeling events are at the collagen fiber level and include: 1) A rapid, near linear increase in collagen modulus that ceases at about one year. 2) A shift towards increased collagen fiber organization, 3) A shift towards increase in the mean collagen fiber slack stretch, and 4) There were no net total mass accretions or dissolutions with time or orientation; only a redistribution of fiber lengths. This is thus a soft tissue modeling problem, characterized by a shift in collagen fiber undulations to accommodate the increasing fiber stiffness in an effort to maintain the conduit dimensional stability. It was assumed that the current collagen fiber structure is the accumulation of all fibers created in past times, and that fiber formation and dissolution are separate processes. However, only changes in how these mechanisms result in a net shift in terms of a distribution of fiber lengths measured in the excised tissues evolve over time are identified and modeled. Unique to this model is the explicit simulation of the collagen fiber maturation process, which manifests itself as an increase in fiber modulus. Thus, following two key quantities are defined: Dc is the basal (i.e. not stress or strain dependent) rate of collagen fiber production, which is constant with time, and qc is collagen fiber survival function, which determines the rate of collagen fiber dissolution (i.e. removal). For the material model, we base it on a structural approach. The growth and remodeling phenomena observed in the present study are driven by an increase in collagen modulus due the underlying process. To the best of the author's knowledge, this is the first time collagen maturation model of a large artery implant has been developed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Grassmannian Diffusion Maps Based Manifold Learning for Uncertainty Quantification

Author(s): *Michael Shields, *Johns Hopkins University*; Dimitris Giovanis, *Johns Hopkins University*; Ketson dos Santos, *École polytechnique fédérale de Lausanne*;

In this work, we introduce a framework based upon Grassmann manifold projections and diffusion maps to unveil the essential geometric structure of high-dimensional model solutions. We then use these Grassmannian diffusion maps (GDMaps) to quantify uncertainties in high dimensional model responses. Specifically, the affinity between subspaces, represented by points on the Grassmann manifold, is determined using a suitable metric on the manifold and used to construct the transition probability matrix of a random walk on a graph connecting the points. The eigenfunctions of this matrix are used to obtain the Grassmannian diffusion coordinates that provide a compact representation embedded in a low-dimensional Euclidean space. This low-dimensional representation enables a variety of functions to be performed including uncertainty quantification, classification, and surrogate model construction. We demonstrate these applications on a variety of problems beginning with simple illustrations of random fields and low-dimensional problems that are straightforward to visualize. We then apply the framework to large computational models of materials systems and, more generally, to large data sets used for classification (e.g. for facial recognition).

16th U.S. National Congress on Computational Mechanics
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Title: Coupled Thermal-Fluid-Solid Simulations for High Fidelity Additive Manufacturing Predictions

Author(s): *Michael Stender, *Sandia National Laboratories*; Lauren Beghini, *Sandia National Laboratories*; Daniel Moser, *Sandia National Laboratories*; Bradley Trembacki, *Sandia National Laboratories*; Michael Veilleux, *Sandia National Laboratories*; Kurtis Ford, *Sandia National Laboratories*;

The desire to predict outcomes for additive manufacturing processes has motivated a great deal of development and study in computational mechanics and finite element simulation. Primary challenges associated with these simulations include resolving the large range of both spatial and temporal scales present in additive manufacturing at the part scale. Often, prohibitively large simulation runtimes, and/or sacrifices in the desired level of solution fidelity are required in these approaches. The goal of this work was to develop a high-fidelity multi physics approach for additive manufacturing simulation that incorporates relevant physics from both thermal-fluid simulations and solid mechanics. The developed simulation workflow produces high-fidelity results for additive manufacturing processes that are appropriate for small, critical regions of a build and for validation of lower fidelity and larger scale simulations. In this presentation, we share our strategy for the development of a thermal-fluid-solid coupled workflow for additive manufacturing simulation using the SIERRA simulation software suite. We discuss the development process and challenges associated with integrating thermal-fluid simulations of additive manufacturing that best capture temperature profiles, liquid and gas deformations and mass deposition with a solid mechanics framework that appropriately pre-dicts solid phase deformations and stresses. Accommodations are made to allow for different element classes, formulations, and mesh densities between thermal-fluid and solid mechanics simulations through an automated remeshing and mapping scheme. Results for several additive manufacturing examples will be presented and compared to results from a lower fidelity pro-cess model. Limitations and challenges associated with this approach will be discussed including strategies to resolve the complex surface topologies that can be present in additive manufacturing processes. Ultimately this methodology is capable of resolving extremely high-fidelity features of additive manufacturing and is useful for validation of lower fidelity models and exploring the intricacies of additive manufacturing processes. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An optimization-inspired solver for inequality constrained nonlinear solid mechanics applied to frictional contact, buckling, and phase-field fracture.

Author(s): *Michael Tupek, *Sandia National Laboratories*; Brandon Talamini, *Sandia National Laboratories*;

Robust and accurate solver strategies are essential for enabling rapid design turnaround times for nonlinear solid mechanics applications. Manually adjusting and tuning solver parameters and simulation setups can be both costly and tedious. The most challenging problems in this field typically involve nonlinear and non-convex material behavior (e.g. buckling and phase-field fracture) and/or inequality constraints (e.g. contact, friction and field bounds). We present progress on a hybrid augmented Lagrange trust region solver, combined with a globalized second order Lagrange multiplier update utilizing the Fischer-Bermeister function. Applied to constrained minimization problems, this solver is effective and superlinearly convergent for these various applications. However, there are also many solid mechanics applications which cannot be formulated as minimization problems, either because the energy to minimize is unknown (e.g. in legacy finite element codes), or because one does not exist (e.g. friction). We demonstrate some minor modification to our approach which allows these ‘quasi-optimization’ problems to also be solved effectively. Finally, we highlight the importance of finding stable solutions to the quasi-static equations of continuum mechanics and how this relates to second-order optimality. Using practically relevant examples, we show that the solver is accurate, efficient, robust, and consistently returns physically meaningful stable solutions. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Stress State in Cubic Shell Lattices for Lightweight Mechanical Metamaterials: Interplay Between Geometry and Mechanics

Author(s): *Michael Y. Wang, *The Hong Kong University of Science and Technology*;

With the vast advancements in approaches to modeling of cellular materials, analysis of their mechanical properties, testing methods, and AM processes, developing mechanical metamaterials with open-cell architecture and superior mechanical properties to satisfy multi-functional requirements for their diverse applications have become a paramount concern. Addressing this issue requires innovative techniques that can offer design and fabrication freedom in the determination of architecture and geometry of shell lattices beyond the simply known models of triply periodic minimal surfaces (TPMS). Essential for the design and optimization of shell lattices is to find the intrinsic relations between the geometry of shell surface and the mechanics of shells. In this paper, we focus on the cubic symmetric crystal system, which has unique geometric features that simplify the cubic unit cell into a fundamental domain. Within the fundamental design domain, we propose a versatile parametric model for cubic symmetric lattices, enabling geometric design of minimal surfaces, constant mean curvature surface families, as well as shape optimization, covering a broader design space than typical TPMS. A semi-analytical analysis tool based on the membrane theory of thin shells and advanced homogenization is developed as the guideline for the design of low-density cubic shell lattices, which links geometric features with mechanical behaviors. Key mechanical properties, including stiffness, yield strength and buckling strength, are analyzed through the proposed tool as well as finite element method. The novelty of this approach is that it explores new capabilities to design and fabricate shell lattices beyond the current technological boundaries. The proposed geometric and structural design methodology leads to generalized open-cell shell lattices with superior mechanical properties. Key References [1] J.U. Surjadi, L. Gao, H. Du, X. Li, X. Xiong, N.X. Fang, Y. Lu, Mechanical metamaterialsand their engineering applications, Adv. Eng. Mater. 21 (2019) 1800864 [2] L. Zhang, S. Feih, S. Daynes, S. Chang, M.Y. Wang, J. Wei, W.F. Lu, Energy absorption characteristics of metallic triply periodic minimal surface sheet structures under compressive loading, Addit. Manuf. 23 (2018) 505–515 [3] J.B. Berger, H.N.G. Wadley, R.M. McMeeking, Mechanical metamaterials at the theoretical limit of isotropic elastic stiffness, Nature 543 (2017) 533.

16th U.S. National Congress on Computational Mechanics
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Title: Die Shape Optimization Using Feedback Control; Solving the Inverse Problem

Author(s): *Michelle Spanjaards, *Eindhoven University of Technology*; Martien Hulsen, *Eindhoven University of Technology*; Patrick Anderson, *Eindhoven University of Technology*;

Extrusion is a widely used process to create products with a fixed cross-sectional profile. Many applications require cross-sections of complex shapes, where the dies contain sharp corners. Common requirement on the extrudate is dimensional precision. The dimensions of the extrudate, however, are highly influenced by extrudate swelling. When the extrudate has such a shape that it contains sharp edges, the material lines exiting from the corners will swell in two directions. Also, the sharp edge in the surface will be maintained over a large distance from the exit of the die. The swelling process involves complex dynamics influenced by many parameters, such as viscoelasticity and temperature. Therefore, the optimized shape of a die, to obtain an extrudate with desired dimensions and shape, is now often obtained through trial-and-error. We developed a transient 3D computational model for viscous and viscoelastic fluids, using the finite element method, to predict extrudate swelling for extrudates containing sharp edges. This model describes the corner lines of the domain separately to obtain the positions of these lines in the two swell directions. A 2D height function is used to describe the free surfaces of the extrudate, using the positions obtained from solving the material lines to expand the domain of the height function. A convergence study of a benchmark problem of a trumpet shaped object in an uniaxial extension flow is performed to validate the model [1]. A novel approach to solve the inverse problem of three-dimensional die design for extrudate swell is developed, using a real-time active control scheme. To this end, a feedback connection between the corner-line finite element method and the controller is envisioned. Advantages of this method are that there are no restrictions on the position of the elements, which allows for local mesh refinement, and that transient rheological phenomena can be taken into account. In this talk we show the validity of this method by showing optimization results for 2D axisymmetric extrusion flows of a viscoelastic fluid for different Weissenberg numbers. In 3D we first give a proof of concept by showing the results of a viscous fluid exiting dies with increasing complexity in shape. Finally, we show that this method is able to obtain the desired extrudate shape of extrudates of a viscoelastic fluid for different Weissenberg numbers and different amounts of shear-thinning. References: [1] M.M.A. Spanjaards, M.A. Hulsen, P.D. Anderson. Journal of Non-Newtonian Fluid Mechanics, 270:79-95, 2019

16th U.S. National Congress on Computational Mechanics
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Title: Numerical Analysis of Intergranular Fracture in Polycrystalline Materials

Author(s): *Miguel Vieira de Carvalho, *University of Porto*; Francisco Manuel Andrade Pires, *University of Porto*;

The increasing demand for new alloys with enhanced mechanical properties has motivated the development of advanced high-strength steels (AHSS) that simultaneously exhibit high strength and good ductility. The 3rd generation of AHSS often incorporates the so-called TRIP effect, which increases the strain hardening capacity of multiphase steels. One important aspect to consider when modelling the behaviour of this type of material is the initiation and posterior propagation of a crack [1]. In a polycrystalline material, this phenomenon is related to a variety of grain characteristics, with particular emphasis being placed on the difference between the elastic properties of adjacent grains, elastic anisotropy, grain orientation, stiffness and toughness mismatch and grain size distribution [2]. The influence of the microstructure properties on the microscopic failure mechanisms can be investigated with experimental activities. However, usually expensive equipment and careful preparation is required, which may limit the applicability of such methods. The use of numerical techniques opens the possibility to study a wider range of conditions while maintaining the costs of a given project controlled. Moreover, cohesive zone models handle correctly and elegantly crack initiation, branching, propagation and coalescence, as long as all possible crack paths are known a-priori, which is the case when considering intergranular fracture in polycrystalline materials. In this work, the impact of such interfaces on the overall mechanical response of multi-phase polycrystalline materials is studied, under a variety of loading conditions. A large-strain fully implicit, RVE-based multi-scale finite element code is used. The grain interfaces are modelled using cohesive elements, which are based on a traction-separation relationship [3]. [1] Akbari et al. On the effect of grains interface parameters on the macroscopic properties of polycrystalline materials. Computers & Structures, Vol. 196 (2018). [2] Benedetti, I. and Aliabadi, M.H. A three-dimensional cohesive-frictional grain-boundary micromechanical model for intergranular degradation and failure in polycrystalline materials. Computer Methods in Applied Mechanics and Engineering, Vol. 265, (2013). [3] Kyoungsoo Park, Glaucio H. Paulino and Jeffery R. Roesler. A unified potential-based cohesive model of mixed-mode fracture. Journal of the Mechanics and Physics of Solids, Vol. 57, (2009)

16th U.S. National Congress on Computational Mechanics
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Title: Calibration of Dislocation Slip and Deformation Twinning Material Parameters for HMX

Author(s): *Milovan Zecevic, *Los Alamos National Laboratory*; Marc Cawkwell, *Los Alamos National Laboratory*; Kyle Ramos, *Los Alamos National Laboratory*; Darby Luscher, *Los Alamos National Laboratory*;

The calibration of the beta-cyclotetramethylene tetranitramine (beta-HMX) plastic response is divided into three consecutive steps: (a) slip system determination, (b) dislocation slip parameters calibration, and (c) deformation twinning parameters calibration. (a) The viable set of slip systems for beta-HMX is proposed from the modeling of the Knoop indentation experiments (Gallagher et al 2015) with a crystal plasticity finite element model. The simulated Knoop hardness variation with the crystal orientation depends on the unknown model parameters: set of active slip systems, twinning, and hardening behavior. Due to the significant computational cost of simulations, we carefully analyze the simulation data and manually define five relevant guesses. The optimal material parameters from our analysis are: set of slip systems proposed by Barton et al (2009) omitting (101)[010] slip system and twin system, with a modified Voce hardening law. (b) A finite strain thermomechanical model developed by Luscher et al (2017) is used to model the high rate deformation of beta-HMX single crystals during plate impact experiments. The recorded particle velocity during impact experiments is simulated with a quasi 1D finite element model. We calibrate the dislocation slip parameters by modeling a subset of data having negative Schmid factor for the twin system, i.e., twinning is not active. (c) Since the particle velocity is the only recorded variable during the plate impact experiments, the twinning behavior in the model needs to have a visible influence on the velocimetry in order to determine the twinning material parameters from these experiments. Hence, we examine the relationship between the velocimetry during plate impacts and twinning behavior. In our previous work we showed that the velocimetry is not very sensitive to the twinning behavior using a pseudo slip twinning model. Here we perform a similar analysis using a phase-field model coupled with a quasi 2D finite element model of the plate impact experiments. N. R. Barton, N. W. Winter, J. E. Reaugh, Modelling Simul. Mater. Sci. Eng. 17 (2009) 035003 (19pp) H. G. Gallagher, J. C. Miller, D. B. Sheen, J. N. Sherwood, R. M. Vrcelj, Chemistry Central Journal (2015) 9:22 D. J. Luscher, F.L. Addessio, M.J. Cawkwell, K.J. Ramos, Journal of the Mechanics and Physics of Solids 98 (2017) 63–86

16th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Modeling of Injection-Caused Delamination on Aortic Walls Using DeepONet

Author(s): *Minglang Yin, *Brown University*; Ehsan Ban, *Yale University*; Enrui Zhang, *Brown University*; Bruno Rego, *Yale University*; Jay Humphrey, *Yale University*; George Karniadakis, *Brown University*;

Aortic dissections progress due to delamination of the intimal layer of the aortic wall. Increasing evidence shows that delamination of lamellar structures within the intima can be initiated by localized accumulations of glycosaminoglycans hyaluronan (GAGs), where negatively charged aggregates of GAGs imbibe more water and further pressurize the intramural space. Further in-vitro and in-silico studies on delamination of the aorta driven by quasi-static injection demonstrate that the differential propensity of dissection can be affected by local microstructure, i.e., spatial distributions of structural significant interlamellar struts that connect adjacent elastic lamellae. In particular, diverse histological microstructures may lead to differential mechanical behaviors during dissection (i.e., pressure-volume curves and displacement fields). In this study, we develop a data-driven surrogate model for the injection-driven delamination processes on walls with differential struts distribution using DeepONet, a powerful operator- regression neural network. The surrogate model is trained with limited in-silico data generated from a phase-field finite element model, where training data consists of a list of microstructural images and the corresponding field information. Specifically, given a spatial distribution of a strut map, the model is trained to predict the corresponding pressure-volume curve and field displacement. The results suggest that the surrogate model can extract the underlying functional relation between a distinctive microstructure and its mechanical properties, which can be reflected by accurate predictions of mechanical behavior for diverse walls. Furthermore, our DeepONet model can facilitate surrogate model-based analysis on quantifying biological variability, inverse design, and it has great potential for predicting mechanical properties based on experimental multi-modality data.

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Title: Mechanics of Brain Folding: Interplay of Differential Growth and Axonal Tension

Author(s): Poorya Chavoshnejad, *Binghamton University*; *Mir Jalil Razavi, *Binghamton University*;

Cortical folding is the most important stage of the normal development of human brain during the early stages of growth. This complex process influenced by multiple neurogenesis and axonogenesis events including cortical expansion and neuronal wiring. Primary cortical folding is notably preserved among individuals, while secondary and tertiary foldings which evolve after primary folding can vary widely across individuals. Despite variation in folding patterns, there are still a few specific types of regular shapes within individuals or across species. To date, the origin and the formation mechanism of variable or regular folding patterns have not been explored very well. This study aims to delineate how the interplay between differential growth and axonal tension mechanisms induces and regulates folding patterns in the developing human brain. To do so, image-based multiscale mechanical models based on the embedded non-linear finite element method are developed. Different growth and folding scenarios in the developed models including embedded axonal fiber bundles in the white matter are designed and studied. The results of the study show that the growth rate mismatch between the cortex and the subcortex layers is the main inducer of cortical folding. Gyrification of the cortex unexpectedly pulls areas with the high concentration of the stiff fiber bundles towards gyri than sulci. As the result, axonal fiber bundles break the symmetry and regulate the folding patterns. Distribution of axonal fiber bundles and their spacing are the determinant factors to control the locations of gyri and sulci. This study provides a deeper understanding of cortical folding and its morphogenesis that is the key to interpreting the normal development of the human brain during the early stages of growth.

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Title: Simulation of Multi-Physics Phenomena with a Hybrid FEM-Peridynamic Approach

Author(s): *Mirco Zaccariotto, *University of Padova*; Tao Ni, *University of Padova*; Federico Moro, *University of Padova*; Francesco Pesavento, *University of Padova*; Bernhard A. Schrefler, *University of Padova*; Ugo Galvanetto, *University of Padova*;

Crack initiation and propagation in materials is an important problem concerning many practical applications in which multi-physics phenomena can determine complex material behaviour. The theory of Peridynamics is particularly suitable for dealing with crack propagation in solid materials. Unfortunately, Peridynamics-based methods are not computationally efficient, due to the nonlocal nature of the approach, for this reason numerical coupling between Peridynamics and Finite Element Method has been widely studied to improve computational efficiency [1]. The present contribution is focussed on the solution of physically coupled problems in which Peridynamics is used to describe solid deformation and fracture, while classical FEM modelling reproduces another field (fluid, thermal, electrical, chemical, etc.). The proposed computational approach is applied to hydraulic fracture propagation in saturated porous media adopting classical Biot poroelasticity theory. We will show the accuracy of the method by comparing the simulation results with two analytical solutions. Furthermore, several examples will prove the capabilities of the multi-physics model in solving pressure- and fluid-driven crack propagation problems [2]. Cases in which stepwise crack advancement with pore pressure fluctuations is observed, consistently with previous experimental and numerical evidences, will complete the presentation. Finally, inspired by [3], the first results of electro-mechanical coupled simulated phenomena will demonstrate the flexibility of the proposed approach. U. Galvanetto and M. Zaccariotto would like to acknowledge the support they received from MIUR under the research project PRIN2017-DEVISU and from the University of Padua under the research projects BIRD2018 NR.183703/18 and BIRD2020 NR.202824/20. References [1] Ni, T., Zaccariotto, M., Zhu, Q.-Z. and Galvanetto, U., Coupling of FEM and ordinary state-based peridynamics for brittle failure analysis in 3D. Mech. Adv. Mater. Struc., 1–16. (2019). [2] Ni, T., Pesavento, F., Zaccariotto, M., Galvanetto, U., Zhu, Q.-Z. and Schrefler, B.A., Hybrid FEM and peridynamic simulation of hydraulic fracture propagation in saturated porous media, Comp. Meth. Appl. Mech. Eng. 366, nr.113101, (2020). [3] Wildman R. A. and Gazonas G.A., A dynamic electro-thermo-mechanical model of dielectric breakdown in solids using peridynamics, J. Mech. Mat. and Struct., 10(5), 613-630, (2015).

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Title: Numerical Integration of a Novel Directional Damage Model for Rate-Dependent Behavior of Brittle Rocks

Author(s): *Mitul Sisodiya, *University of Colorado Boulder*; Yida Zhang, *University of Colorado Boulder*;

The role of microcracks in the deformation and failure of brittle rocks has been well recognized. However, the direct inclusion of individual microcracks in modeling remains a difficult task due to the numerical difficulties and high computational costs involved. Continuum damage mechanics provides a useful tool to circumvent these difficulties by smearing the effect of microcracks on material degradation at a macroscopic level. For brittle rocks, continuum representation of damage through damage tensor is a popular approach that can capture to some degree the anisotropic nature of damage. However, damage tensors are limited to representing very specific and regular shapes of the directional distribution of microcracks (i.e. the density of microcracks inclined along different orientations) which may not be representative of the state of microcracking in rocks. To enrich the representation of microcrack distribution and the associated material anisotropy, we have developed a novel directional damage model [1] that can describe arbitrary shapes of the initial microcrack distribution density as well as its evolution. The notion of directional damage enters the model as a continuous internal state function (as opposed to the familiar concept of internal state variable), which poses unique challenges in the numerical implementation of the model. In this presentation, the numerical aspects of the model implementation are presented. Since the damage is a continuous function of direction, the representative element volume (REV) is internally discretized along different orientations, and the damage condition is judged along each direction for every time increment. At each material point and at every increment, damage only evolves along those directions where the damage condition is satisfied. To account for friction along crack surfaces, additional internal state functions such as mobilized shear resistance are introduced. The conjugated directional sliding-induced shear strain is also evolved in a similar fashion by evaluating at all directions against the frictional-sliding condition. Rate effect associated with subcritical crack propagation is incorporated in the directional damage evolution law through a Perzyna-type treatment. Both explicit and implicit integration algorithms are developed for different control scenarios. The gain of computational efficiency through vectorization of the code will be discussed. Finally, the spatial and directional evolution of damage in preliminary finite element simulations of constant-strain-rate compression and brittle creep tests on Basalt rock will be presented. 1. Sisodiya, M. & Zhang, Y. 2021 A directional microcrack damage theory based on continuous hyperplasticity. Submitted to Proceedings of The Royal Society A, under review.

16th U.S. National Congress on Computational Mechanics
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Title: Virtual Elements on Agglomerated Finite Elements to Increase the Critical Time Step in Explicit Three-Dimensional Elastodynamic Simulations

Author(s): *N. Sukumar, *University of California, Davis*; Michael Tupek, *Sandia National Laboratories*;

The virtual element element (VEM) [1] is a stabilized Galerkin method that is accurate and robust on general convex and nonconvex polyhedral meshes. In this study, we investigate the effect of shape quality of polyhedra in the estimation of the critical time step for explicit elastodynamic finite element simulations using the first-order three-dimensional virtual element method [2]. Low-quality elements are common when meshing realistic complex components, and while tetrahedral meshing technology is generally robust, meshing algorithms cannot guarantee high-quality meshes for arbitrary geometries or for non-water-tight CAD models. To deliver reliable simulations on such meshes, we consider finite element meshes with prismatic, pyramidal and tetrahedral elements that have poor element-quality (for example, tetrahedra with dihedral angles close to 0/180 degree, or slender prisms with triangular faces of poor quality), and agglomerate such `bad' elements with neighboring elements to form a polyhedral element. The VEM is used to solve the elastodynamic eigenproblem on each polyhedral element of the mesh, and we use the element eigenvalue inequality to obtain a conservative estimate of the critical time step. For a suite of illustrative finite element meshes with poor mesh-quality, we show that agglomeration and use of the VEM on the resulting polyhedra can substantially increase the critical time step (few orders of magnitude), which suggests that use of the virtual element technology on three-dimensional finite element meshes holds promise to improve the performance of explicit elastodynamic finite element simulations. References [1] L. Beirao da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. Mathematical Models & Methods in Applied Sciences, 23(1):199–214, 2014. [2] K. Park, H. Chi, and G. H. Paulino. On nonconvex meshes for elastodynamics using virtual element methods with explicit time integration. Computer Methods in Applied Mechanics and Engineering, 356:669–684, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Patient-Specific Prediction of IMR Recurrence after Mitral Valve Surgical Repair

Author(s): Harshita Narang, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*; *Natalie Simonian, *The University of Texas at Austin*;

We have previously developed a completely noninvasive method to produce open and closed MV geometries and compute MV leaflet deformation patterns from 3D in vivo images. We have applied this approach to ovine post-IMR MVs and determined that the kinematic behavior of the MV changes progressively. Each of these results strongly suggests that there is a relationship between pre-surgical MV state and post-surgical outcomes. To investigate this relationship in humans, we have developed models of 21 human MVs and investigated leaflet strains and deformations. Clinical rt-3DE images of the MV were obtained from 18 patients with IMR (11 without recurrence of IMR and 7 with recurrence) and 3 normal human MVs. These images were processed to obtain 3D midsurface representations of each valve in the fully open (end-diastolic) and fully closed (end-systolic) states, immediately pre- and post-surgery. In order to establish material point correspondence between the open and closed states of each valve, we applied a hyperelastic shape morphing technique in a finite element (FE) framework, where the open state geometry of the valve was morphed to match the closed state shape using globally applied pressure as well as a level-set penalization. Metrics including in-plane circumferential and radial strain, leaflet area, coaptation area, and orifice dimensions were then computed and compared between MVs with and without recurrence of MR at 6 months post-repair. We found that MVs with IMR had significantly lower magnitudes of compressive circumferential strain in the posterior leaflet and significantly higher radial strains across the whole MV than MVs without IMR . Patients who would later exhibit IMR recurrence were found to have significantly higher circumferential leaflet strain in the anterior commissure prior to surgery than those without recurrence ($p = 0.0228$). Pre-surgical circumferential strain in the A1 segment is likely predictive of patient-specific repair success through a logistic regression model ($p=0.0362$), as shown by a high area under the associated ROC curve of 0.832—in other words, a high rate of correctly identified recurrent MVs. The recurrent MVs also had significantly larger leaflet areas and annuli than the non-recurrent MVs and had reduced annular contraction at systole. Our model may also be extended to optimizing other repair methods such as minimally invasive leaflet clipping or augmentation.

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Title: Reinforcement Learning-Driven Adaptive Mesh Refinement for Second-Order Elliptic Boundary Value Problems

Author(s): *Natasha Sharma, *The University of Texas at El Paso*; Ramakrishna Tipireddy, *Pacific Northwest National Laboratory*; Samrat Chatterjee, *Pacific Northwest National Laboratory*;

Adaptive mesh refinement techniques have become an indispensable tool in achieving accurate and efficiently computed solutions to problems which require impractically fine uniform meshes to obtain an accurate approximation. The adaptive algorithm involves a recursive application of SOLVE-ESTIMATE-MARK-REFINE where in particular, the step `ESTIMATE' involves computing a posteriori error estimator based on only the numerical solution and the data of the problem. Over the years, several a posteriori error estimators have been developed and successfully applied but often times, the choice of estimator is ill suited for the problem at hand. In this talk, we present a learning algorithm that optimizes the choice of the a posteriori error estimator for the given problem. As a prototype, we apply this learning algorithm to linear elliptic boundary value problems with under resolved solutions and report on the performance of this method for several benchmark problems. This is a joint work with Ramakrishna Tipireddy (PNNL) and Samrat Chatterjee (PNNL).

16th U.S. National Congress on Computational Mechanics
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Title: Exploiting Tensor-Product Structure in High-Order Finite Elements on Next-Generation Architectures

Author(s): *Nathan Roberts, *Sandia National Laboratories*; Mauro Perego, *Sandia National Laboratories*;

A standard finite element stiffness matrix assembly algorithm in 3D requires O(p^9) floating point operations per hexahedral element; sum factorization techniques allow the reordering of operations to reduce the cost to O(p^7) for general geometries, and O(p^6) for axis-aligned hexahedral geometries. In higher dimensions, the savings from sum factorization are still more dramatic. We present a general framework for performing sum factorization in arbitrary dimensions. Our approach can be regarded (and indeed was developed) as a generalization of recent work by Mora and Demkowicz, and Badger et al., which described algorithms for particular cases in three dimensions. We implement our framework in the context of the Intrepid2 package within Trilinos. Because Intrepid2 supports Algorithmic Differentiation types provided by Sacado package, our implementation also supports these types, which can be used in sensitivity analysis, among other applications. We include performance results on CUDA platforms. References: 1. J. Mora, L. Demkowicz, Fast integration of DPG matrices based on sum factorization for all the energy spaces, Computational Methods in Applied Mathematics, 2019. 2. J. Badger, S. Henneking, L. Demkowicz, Sum factorization for fast integration of DPG matrices on prismatic elements, Finite Elements in Analysis and Design, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: A Three-Dimensional Generalized Finite Element Method for the Simulation of Wave Propagation in Fluid-Filled Fractures

Author(s): *Nathan Shauer, *University of Illinois at Urbana-Champaign*; Carlos Armando Duarte, *University of Illinois at Urbana-Champaign*; Fushen Liu, *Zhejiang University*; Peter Gordon, *ExxonMobil Research & Engineering*; Kenneth Desmond, *ExxonMobil Research & Engineering*;

Guided waves propagating along hydraulic fractures are commonly called Krauklis waves or Stoneley guided waves. In hydraulic fracturing, waves in fluid-filled fractures can be excited by a pressure pulse traveling back and forth in the wellbore. The pulse may be generated from a controlled source input such as in hydraulic impedance testing, or may be the by-product of a water hammer generated in the wellbore when pumping operations are rapidly shut down. The pressure pulse so created travels down the wellbore and back multiple times, and the interaction with open hydraulic fractures connected to the wellbore influences the frequency and attenuation of this traveling wave. Some authors have attempted to utilize this signal as a diagnostic of fracture size in the context of multi-stage horizontal stimulation. In the most direct approach, simple data analytics methods have been utilized to qualitatively rank fracture size and complexity among multiple stages, and to relate completion parameters (fluid and proppant volumes pumped, viscosity, stage, and cluster spacing, etc.) to features of the transient pressure pulse decay. In this presentation, a novel 3-D GFEM methodology to simulate waves in fluid-filled fractures (Krauklis waves) is proposed. This method is particularly appealing for the discretization of the fractures since it does not require the fracture faces to fit finite element faces. Additionally, analytical asymptotic solutions are used to enrich the fracture fronts, which increases the accuracy of the approximation. Mesh adaptivity around the fracture fronts is employed to further decrease discretization error while controlling the computational time. The rock is assumed to be a 3-D isotropic linear elastic material governed by the elastic-wave equations, and the fluid is assumed to be Newtonian and governed by a nearly incompressible Reynolds lubrication description. The elastic-wave equation is solved with a quadratic GFEM and the fluid-filled fracture equations are solved with a standard quadratic FEM. The methodology is verified with analytical solutions and compared with experimental results. Different fracture geometries are investigated to demonstrate the complex 3-D effects of the physical phenomenon and the robustness of the proposed GFEM methodology.

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Title: Guaranteeing Exact Structure Preservation and Consistency in Data-Driven Modeling

Author(s): *Nathaniel Trask, *Sandia National Laboratories*;

While physics-informed machine learning has emerged as a powerful tool for data-driven modeling, there are significant challenges related to both how to guarantee neural network PDE simulations converge, and how to guarantee desired physical properties hold to machine precision. In this talk we present recent work developing novel architectures taking advantage of the exterior calculus framework underpinning traditional mimetic forward simulation to extract data-driven models with a rigorous stability and accuracy theory. We will show how these tools may be used to extract data-driven multiscale finite element spaces which may be employed in traditional finite element codes.

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Title: Effective Machine Learning-Based Calibration of Finite Element Models for Progressive Damage and Failure Simulation of Fiber-Reinforced Composites

Author(s): *Navid Zobeiry, *University of Washington*; Johannes Reiner, *Deakin University*; Reza Vaziri, *University of British Columbia*;

Fiber-reinforced composites are widely used in a large range of applications thanks to their exceptional specific strength and stiffness. The properties of advanced composites can be tailored effectively to satisfy specific requirements by careful selection of raw materials, fiber architectures, lay-ups and processing parameters. This large design space comes at a cost. To certify composites for aerospace structural applications, industry must rely on the building-block approach for which comprehensive testing programs must be undertaken. Given that the foundation of the certification process is based on testing supported by analysis, designers and certification authorities require a high degree of confidence and robust assessment of damage evolution and failure in composite components. Finite element (FE) simulation of the structural response promises the possibility to reduce costs and efforts associated with these testing programs. However, despite tremendous efforts and partial success in establishing FE models and failure theories for advanced composites, the search for physics-based damage models, validated for industrial applications, is still ongoing. Owing to multiple interacting failure modes in fiber, matrix or interface, it is challenging to establish a robust and efficient modelling strategy. More importantly, it is vital to develop effective data reduction and calibration methods to capture the underlying physics of the material response with the least amount of complexity. To reduce experimental efforts, we present a recently developed data-driven approach for the characterization of FE damage models using theory-guided Machine Learning (ML) that relies on a limited number of experiments [1]. Integration of theory ensures physical consistency, allows for efficient integration of small experimental datasets, and mitigates the brittleness of ML models. For ML training, a highly efficient continuum damage FE model provides virtual data from over 10,000 simulations for a system of interconnected neural networks, designed based on theory of failure in advanced composites. We demonstrate and critically assess how ML can be used to find optimal input parameters for the FE simulation of progressive damage in carbon fiber-reinforced composites. The developed ML-based approach is a promising method to reduce experimental efforts required for effective calibration of FE models. Implementation of such a method in the building-block approach, can potentially reduce the cost and time associated with certification of aerospace composite structures, hence expediting the development and implementation of next generation of high-performance composites. [1] N. Zobeiry, J. Reiner, and R. Vaziri, “Theory-Guided Machine Learning for Damage Characterization of Composites,” Composite Structures, vol. 246, p. 112407, 2020.

16th U.S. National Congress on Computational Mechanics
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Title: Configurational Forces in Density Functional Theory Calculations Using Orthogonalized Enriched Finite Elements

Author(s): *Nelson David Rufus, *University of Michigan*; Vikram Gavini, *University of Michigan*;

Real-space all-electron Kohn-Sham DFT calculations can be efficiently performed using orthogonalized enriched finite element (FE) basis, wherein the classical (standard) FE basis are augmented with atom-centered numerical basis functions (enrichments) that are appropriately orthogonalized with respect to the underlying FE basis. Orthogonalized enriched FE basis improves the numerical conditioning of the basis as well as renders the overlap matrix block-diagonal, greatly simplifying its inversion. In this work, we extend the framework to compute configurational forces which arise from the variational derivative of the Kohn-Sham energy functional with respect to the position of the material point x. This allows us to compute the ionic forces as well as stresses in periodic systems. We establish the accuracy of the formulation, by comparing the computed forces and stresses for various benchmark systems with those obtained from finite-differencing the ground-state energy. We also benchmark our calculations against Gaussian basis for isolated systems and LAPW basis for periodic systems. We finally demonstrate the capability of this approach to obtain relaxed structures for large-scale systems. Funding Acknowledgment: DoE BES, Award Number DE-SC0017380

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization with Truncated Octahedron Mesh

Author(s): *Nikhil Singh, *Indian Institute of Technology Kanpur*; Anupam Saxena, *Indian Institute of Technology Kanpur*;

We present a structural topology optimization formulation using a truncated octahedral mesh. Truncated octahedrons, a special case of tetra-kai-decahedron, form a lattice in three-dimensions with cells sharing no more and no less than faces. Lack of point and edge connections in the lattice makes parent meshes comprising only of tetra-kai-decahedral cells ideal to be adopted for topology optimization. Possibility of singular solutions, e.g., three-dimensional checkerboards and point connections, which otherwise exist with say, hexahedral cells, are eliminated geometrically. The notion of implementing truncated octahedral meshes in topology optimization to eliminate singular solutions was first proposed in [1]. Geometrical analysis of a unit cell and the lattice structure required for mesh development is discussed. Intermediate solutions in an optimization problem are assessed using linear finite element (FE) analysis. To perform the analysis, an iso-parametric truncated octahedral element is defined. The FE analysis employs barycentric coordinates for convex polyhedral structures introduced in [2] as shape functions. For ease in analysis, analytical expressions of the shape functions are simplified for the specific (regular) case of a truncated octahedron. Further, expressions for the shape function derivatives are also evaluated. To evaluate the stiffness matrix, numerical integration is adopted from [3], where the number of integration points equals the number of vertices of the element. As there is no known method yet, for mesh generation using a truncated octahedral cell, a planar mesh, i.e. a mesh in which all element centroids lie on a plane is developed. To demonstrate topology optimization with regular truncated octahedral cells, two simple examples are presented using the density based SIMP (Solid Isotropic Material with Penalization) material model for a compliance minimization problem. References: 1. Saxena, Anupam. "Topology design with negative masks using gradient search." Structural and Multidisciplinary Optimization 44, no. 5 (2011): 629-649. 2. Warren, Joe. "Barycentric coordinates for convex polytopes." Advances in Computational Mathematics 6, no. 1 (1996): 97-108. 3. Rashid, M. M., and M. Selimotic. "A three?dimensional finite element method with arbitrary polyhedral elements." International Journal for Numerical Methods in Engineering 67, no. 2 (2006): 226-252.

16th U.S. National Congress on Computational Mechanics
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Title: Sobolev Training of Thermodynamic-Informed Neural Networks for Interpretable Elasto-Plasticity Models with Level Set Hardening

Author(s): *Nikolas Vlassis, *Columbia University*; WaiChing Sun, *Columbia University*;

We introduce a deep learning framework designed to train smoothed elastoplasticity models with interpretable components, such as the stored elastic energy function, yield surface, and plastic flow that evolve based on a set of deep neural network predictions. By recasting the yield function as an evolving level set, we introduce a deep learning approach to deduce the solutions of the Hamilton-Jacobi equation that governs the hardening/softening mechanism. This machine learning hardening law may recover any classical hand-crafted hardening rules and discover new mechanisms that are either unbeknownst or difficult to express with mathematical expressions. Leveraging Sobolev training to gain control over the derivatives of the learned functions, the resultant machine learning elastoplasticity models are thermodynamically consistent, interpretable, while exhibiting excellent learning capacity. Using a 3D FFT solver to create a polycrystal database, numerical experiments are conducted and the implementations of each component of the models are individually verified. Our numerical experiments reveal that this new approach provides more robust and accurate forward predictions of cyclic stress paths than those obtained from black-box deep neural network models such as the recurrent neural network, the 1D convolutional neural network, and the multi-step feed-forward models.

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Title: Influence of Particle Morphology on the Expansion Behaviour of LiNi0.8Mn0.1Co0.1O2 During Delithiation

Author(s): *Nils Wenzler, *ETH Zurich*; Federica Marone, *Paul Scherrer Institut*; Marco Stampanoni, *Paul Scherrer Institut*; Vanessa Wood, *ETH Zurich*;

High nickel content LiNiMnCoO2 (NMC) cathode materials bring the promise of an increase in battery energy density while reducing the use of cobalt, which is problematic to source and expensive. However, there continue to be stability and lifetime issues, arising partly from the lattice expansion and contraction upon deep delithiation and subsequent cracking of the material [1]. NMC particles typically consist of primary particles in the sub-micrometer range that are packed together in secondary particles with diameters of 5-25 micrometers. In this work we investigate the link between the lattice change and secondary particle volume change as well as the influence of the secondary particle morphology. For this we measure the volume change on two different length scales: The change of the lattice constants with in-operando XRD and the change in secondary particle volume with in-operando x-ray tomography [2]. While we found them to behave the same in principle, there is a difference in magnitude of initial expansion. Using coupled electro-chemical and mechanical 3D simulations, we are currently investigating the relationship between particle morphology, grain orientation and volume expansion. We aim to identify to which morphology parameters the secondary particle volume is sensitive to and explain the discrepancies between the two measurements. [1] Wangda Li, Collapse of LiNi1–x–yCoxMnyO2 Lattice at Deep Charge Irrespective of Nickel Content in Lithium-Ion Batteries, J. Am. Chem. Soc. 2019, 141, 13, 5097–5101 [2] Pietsch, P.et al.Quantifying microstructural dynamics andelectrochemical activity of graphite and silicon-graphite lithium ion battery anodes.Nat. Commun.7:12909 doi: 10.1038/ncomms12909 (2016).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Mixed Finite Element Method With Piecewise Linear Elements for the Biharmonic Equation on Surfaces

Author(s): *Oded Stein, *Massachusetts Institute of Technology*; Eitan Grinspun, *University of Toronto / Columbia University*; Alec Jacobson, *University of Toronto*; Max Wardetzky, *University of Göttingen*;

We present a convergence proof for a popular discretization of the biharmonic equation with Dirichlet and Neumann boundary conditions. The discretization of the biharmonic equation with Dirichlet and Neumann boundary conditions using piecewise linear Lagrangian finite elements in a mixed finite element method has been well-studied for domains in R2. Although extensions of such methods are popular for surfaces embedded in R3 approximated by polyhedral meshes, there is no comprehensive analysis of the mixed finite element method with piecewise linear Lagrangian finite elements for that setting. We provide a convergence proof of discrete solutions to the corresponding smooth solution of the biharmonic equation, and obtain convergence rates identical to the ones known for the planar setting. Our proof focuses on three different problems: solving the biharmonic equation on the surface, solving the biharmonic equation in a discrete space in the metric of the surface, and solving the biharmonic equation in a discrete space in the metric of the polyhedral approximation of the surface. We employ inverse discrete Laplacians and the mixed finite element spaces of Ciarlet and Raviart to bound the error between the solutions of the two discrete problems. We then generalize a flat strategy of Scholz using Ritz interpolations (with an estimate by Demlow for the L-infinity error of the Ritz interpolation) to bound the error between the solution of the discrete problem on the surface and the exact solution on the surface. Combined, these two steps yield error bounds on the order of h for the function, on the order of h^(3/4) for its first derivatives, and in the order of h^(1/2) for its Laplacian, where h is the edge length of the discrete polyheral mesh approximating the surface.

16th U.S. National Congress on Computational Mechanics
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Title: Patient-Specific Characterization of Hypoplastic Left Heart Mechanics

Author(s): *Oguz Ziya Tikenogullari, *Stanford University*; Matthias Peirlinck, *Stanford University*; Vijay Vedula, *Columbia University*; Ellen Kuhl, *Stanford University*; Alison Lesley Marsden, *Stanford University*;

Single ventricle physiology is a complex congenital heart condition which leaves a baby with only a single functional pumping chamber, and typically requires three surgeries for palliation starting immediately after birth. Hypoplastic left heart syndrome (HLHS) is a form of single ventricle physiology in which the right ventricle becomes the primary systemic pumping chamber, however long-term complications such as right heart failure, arrythmia, and other sequelae lead to high morbidity and mortality in this high-risk patient population. There is significant interest in testing and optimizing novel surgical and interventional approaches to improve outcomes for HLHS patients using cardiac mechanics modeling. However, the mechanical properties of single right ventricles in HLHS remain unknown. As a step towards futher modeling goals, we focus here on calibration of mechanical response using in-vivo clinical data and cardiac mechanics models. We segmented a patient-specific model from the clinical magnetic resonance imaging data of a 6-year-old HLHS patient after Fontan completion. The biventricular geometry was created in SimVascular from images obtained at end-diastole, and the anatomy was cut off above the mitral and tricuspid valves. We used the commercial finite element analysis software Abaqus to for finite element cardiac mechanics simulations of the patient-specific heart. This required the inclusion of rule-based fiber architecture and appropriate kinemetic boundary conditions which were imposed on base surface and endocardial ring of the left ventricle [1]. The passive mechanical properties are based on the Holzapfel and Ogden orthotropic hyperelasticity model. We tuned the subject-specific lumped parameter network [2] using clinical catheterization and MRI data. We computed the end-diastolic pressure volume relationship for the right ventricle using Sellier’s inverse method for stress-free volume estimation, and subsequently tuned the constitutive parameters to match the analytical diastolic filling Klotz relationship using sequential least squares programming [3]. This study lays the groundwork for future computational modeling studies of surgical interventions and growth simulations in HLHS. References: [1] Peirlinck, Mathias, et al. "Kinematic boundary conditions substantially impact in silico ventricular function." International journal for numerical methods in biomedical engineering 35.1 (2019): e3151. [2] Schiavazzi, Daniele E., et al. "Patient?specific parameter estimation in single?ventricle lumped circulation models under uncertainty." International journal for numerical methods in biomedical engineering 33.3 (2017): e02799. [3] Klotz, Stefan, et al. "Single-beat estimation of end-diastolic pressure-volume relationship: a novel method with potential for noninvasive application." American Journal of Physiology-Heart and Circulatory Physiology 291.1 (2006): H403-H412.

16th U.S. National Congress on Computational Mechanics
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Title: Space-Time Finite Element Methods in Moving Domains

Author(s): *Olaf Steinbach, *Graz University of Technology*; Peter Gangl, *Graz University of Technology*; Mario Gobrial, *Graz University of Technology*;

Space-time discretisation methods are well suited to handle moving domains, since the space-time domain is discretised at once, and no re-meshing as in time-stepping methods is required. Moreover, space-time methods allow for an adaptive resolution simultaneously in space and time, and for a parallel iterative solution in space and time. For the solution of parabolic evolution equations in moving domains we formulate and analyse space-time finite element methods. We assume that the velocity of the deformation is given, and that the deformation is volume preserving. As in the case of a fixed domain we are able to prove an inf-sup stability condition to ensure unique solvability. For the analysis of the finite element discretisation we introduce a discrete norm for which we can provide a discrete inf-sup stability condition, and a Cea type quasi-optimal error estimate. Applications include not only the time-dependent heat equation and the eddy current approximation of the Maxwell equations in rotating two-dimensional domains, but also flow problems including the Navier-Stokes system and its simplifications.

16th U.S. National Congress on Computational Mechanics
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Title: Overall Equilibrium in the Coupling of Peridynamics and Classical Continuum Mechanics

Author(s): Greta Ongaro, *University of Padova*; *Pablo Seleson, *Oak Ridge National Laboratory*; Ugo Galvanetto, *University of Padova*; Tao Ni, *Hohai University*; Mirco Zaccariotto, *University of Padova*;

Coupling peridynamics based computational tools with those using classical continuum mechanics can be very beneficial, because it can provide a means to generate a computational method that combines the efficiency of classical continuum mechanics with the capability to simulate crack propagation, typical of peridynamics. This talk presents an overlooked issue in this type of coupled computational methods: the lack of overall equilibrium. This can be the case even if the coupling strategy satisfies the usual numerical tests involving rigid body motions as well as uniform and linear strain distributions. We focus our investigation on the lack of overall equilibrium in an approach to couple peridynamics and classical continuum mechanics recently proposed by the authors. In our examples, the magnitude of the out-of-balance forces is a fraction of a per cent of the applied forces, but it cannot be assumed to be a numerical round-off error. We show analytically and numerically that the main reason for the existence of out-of-balance forces is a lack of balance between the local and nonlocal tractions at the coupling interface. This usually results from the presence of high-order derivatives of displacements in the coupling zone.

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Title: Poro-Hyperelastic Shear

Author(s): *Patrick Selvadurai, *McGill University*; Alexander Suvorov, *Moscow State University for Civil Engineering*;

The theory of fluid-saturated elastic materials, where the porous skeleton exhibits large elastic deformations was developed by many authors including MA Biot. The theory has applications to the study of soft biological tissues that can experience large strains in a fluid-saturated condition. We consider a porous hyperelastic skeleton that is saturated with an incompressible pore fluid the flow of which is governed by Darcy's law. The strain energy function characterizing the hyperelastic mechanics of the porous skeleton can be assigned a constitutive relationship that accounts for compressible behaviour. When the pore space is saturated with an incompressible fluid, the instantaneous response of the fluid-saturated porous medium will resemble that of an incompressible elastic solid. This presentation will examine the formulation of the poro-hyperelastic shear problem and the method of solution of the resulting non-linear partial differential equation for an unknown function characterizing the shear behaviour. Appropriate boundary conditions are also applied to the shearing problem of a layer of infinite extent and suitable boundary conditions are invoked on the surfaces of the poro-hyperelastic body that reflect the possibilities for fluid drainage. The solutions derived from the analytical study of the pro-hyperelastic shear problem are also compared with computational results derived from standard computational schemes. The theory of poro-hyperelasticity has recently been examined in a series of canonical benchmark problems, with analytical and computational approaches [1-4]. References [1] Selvadurai, A.P.S. and Suvorov, A.P. (2016) Coupled hydro-mechanical effects in a poro-hyperelastic material, Journal of the Mechanics and Physics of Solids, 91: 311-333. [2] Suvorov, A.P. and Selvadurai, A.P.S. (2016) On poro-hyperelastic shear, Journal of the Mechanics and Physics of Solids, 96: 445-459. [3] Selvadurai, A.P.S. and Suvorov, A.P. (2017) On the inflation of poro-hyperelastic annuli, Journal of the Mechanics and Physics of Solids, 107: 229-252 [4] Selvadurai, A.P.S. and Suvorov, A.P. (2018) On the development of instabilities in an annulus and a shell composed of a poro-hyperelastic material, Proceedings of the Royal Society, Mathematical and Physical Sciences Series A, 474 : Art. ID 20180239; https://dx.doi.org/10.6084/m9.figshare.c.4271114.

16th U.S. National Congress on Computational Mechanics
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Title: An Immersed Domain Formulation for Fluid-Structure Interaction with Contact

Author(s): *Patrick Zulian, *Università della Svizzera italiana*; Maria Nestolka, *Università della Svizzera italiana*; Lisa Gaedke-Merzhaüser, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*;

We present an immersed domain approach for the numerical solution of contact problems between multiple elastic structures immersed in a Newtonian fluid. Our approach is designed to simulate the full dynamics of immersed hyper-elastic anisotropic structures undergoing large deformations. A motivating application is the study of bio-prosthetic heart valves. In fact, our goal is to model the blood-valve interaction, the blood-aortic wall interaction, and the contact among leaflets during the valve closure. For simulating this coupled multiphysics model with the addition of the contact mechanics, we assemble and solve a large-scale nonlinear problem that is both challenging and computationally expensive. The key challenges in simulating such a system are due to the requirements of handling coupling conditions between solid and fluid and the contact conditions between solid surfaces that may come in contact. In particular, in a parallel-computing environment where the geometric data is arbitrarily distributed and unrelated this task is far from trivial. Our approach employs a parallel variational transfer algorithm for assembling the volumetric coupling between structure and fluid and contact conditions. In particular, we employ a discrete localized version of the L2-projection based on dual Lagrange multipliers. Our strategy is verified through numerical benchmarks and finally employed to model the dynamics of a bio-prosthetic heart valve placed in the aortic root.

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Title: MPI-Accelerated Level Set-Discrete Element Method Using Binning Algorithm

Author(s): *Peng Tan, *University of California, Berkeley*; Nicholas Sitar, *University of California, Berkeley*;

Discrete element method (DEM) is ideally suited for the study of mechanical behavior of particulate media. While serial DEM codes can readily handle models containing thousands of regularly shaped particles, the computational demands increase significantly once the problem size increases to 100's of thousands or millions of particles. Therefore, parallel implementation of DEM suitable for execution on modern high-performance clusters (HPC) is highly desirable and significant efforts have been extended in this direction (see e.g. Yan and Regueiro, 2016). In our study of the mechanical properties of naturally deposited sands we have adopted the Level-Set DEM (LS-DEM, Kawamoto et al., 2016) which is capable of capturing the kinematics and mechanics of a system of arbitrarily shaped 3D particles using level set function as geometric basis. In this application, the complex shape of the particles significantly increased the computational demands for interparticle contact detection, which dramatically increase the computational time using a serial implementation. In this paper, we present a parallel, binning algorithm, which has been implemented and optimized based on the existing LS-DEM framework using C++. The binning algorithm effectively reduces the computational complexity from O(n^2) to O(n). The code maps relationship between bins and particles with linked-list like data structure and manages MPI communication in two major domains: border/ghost exchange and across-block migration. Many performance-critical implementation details are managed optimally to achieve high performance and scalability, such as: minimizing communication overhead, maintaining dynamic load balance, handling particle migrations across block borders, transmitting particle objects between MPI processes efficiently, eliminating redundant contact information between adjacent computational sub-domains, etc. We performed a series of numerical experiments with varied problem size and domain decomposition on UC Berkeley HPC cluster using parallelism up to 64 cores for simulating 30000 three-dimensional particles. The newly developed code successfully accelerated the original sequential code by a factor of more than 10 and has demonstrated the potential to have negligible serial fraction and low parallel overhead for large, uniformly distributed assemblies of complex-shaped particles. We are currently exploring applications to problems approaching 100,000 particles? Kawamoto, R., Andò, E., Viggiani, G., & Andrade, J. E. (2016). Level set discrete element method for three-dimensional computations with triaxial case study. Journal of the Mechanics and Physics of Solids, 91, 1-13. Yan, B., & Regueiro, R. A. (2018). A comprehensive study of MPI parallelism in three-dimensional discrete element method (DEM) simulation of complex-shaped granular particles. Computational Particle Mechanics, 5(4), 553-577.

16th U.S. National Congress on Computational Mechanics
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Title: Why do Grains Produced by Additive Manufacturing Look So Strange?

Author(s): *Peter Voorhees, *Northwestern University*; Alexander Chadwick, *Northwestern University*;

The morphology of grains produced during metal additive manufacturing is very different from that produced by conventional processing and is central to controlling the properties of the final build. In order to understand and control the unusual morphology of grains produced by additive manufacturing, a phase field model is developed that follows the evolution of many thousands of grains in three dimensions. The model is developed in the high velocity limit where the interface is planar or has low amplitude cells, as observed during additive manufacturing of stainless steel 316L at high solidification velocities. The model employs a coupled set of driven Allen-Cahn equations that capture the evolution of the solid-liquid interface and anisotropic interfacial mobility. We combine this phase field model with an analytical model for the thermal field, but the model is also compatible with more sophisticated finite element models of the heat and mass flow during additive manufacturing. The advantage of the approach is that the evolution of the grains is driven by the physics of the motion and rotation of the trijunctions that occur at the junction of the solid-liquid interfaces and grain boundaries; it is not a rule-based model. Examples of the three-dimensional grain shapes, a comparison to experiment, the mechanisms controlling grain evolution, and the critical role of anisotropic interfacial mobility will be discussed.

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Title: Nonlocal Frameworks: Operators and Convergence

Author(s): *Petronela Radu, *University of Nebraska-Lincoln*;

The emergence of nonlocal theories as successful models for studying phenomena and behaviors in different areas of science (continuum mechanics, biology, image processing) has led the mathematical community to introduce and conduct investigations of integral operators and associated systems of equations. In this talk I will present some recent results on nonlocal frameworks systems based on some existing, as well as newly introduced, nonlocal operators. An in-depth study of properties of the operators includes a series of results on nonlocal versions of integration by parts theorems, Helmholtz-Hodge type decompositions, as well as convergence of operators to their classical equivalents as the interaction horizon vanishes.

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Title: Entropy Stable, Well-Balanced, and Subcell Positivity Preserving DG Methods for the Shallow Water Equations

Author(s): *Philip Wu, *Rice University*; Jesse Chan, *Rice University*;

High order schemes are known to be unstable in the presence of shock discontinuities or under-resolved solution features, and have traditionally required additional filtering, limiting, or artificial viscosity to avoid solution blow up. Entropy stable schemes address this instability by ensuring that physically relevant solutions satisfy a semi-discrete entropy inequality independently of discretization parameters. We review the construction of well-balanced high order entropy stable summation-by-parts discontinuous Galerkin (SBP-DG) schemes for the shallow water equations, and introduce a modification based on convex limiting which guarantees positive water height while preserving sub-cell resolution.

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Title: A Modified Bayesian Convolutional Neural Network for Breast Histopathology Image Classification and Uncertainty Quantification

Author(s): *Ponkrshnan Thiagarajan, *Michigan Technological University*; Pushkar Khairnar, *Michigan Technological University*; Susanta Ghosh, *Michigan Technological University*;

Convolutional neural network (CNN) based classification models show great promise for histopathological images. Despite the promise, it yields erroneous or overfitted results when the data is not sufficiently large or is biased. We show that Bayesian-CNN can alleviate these limitations of CNN but still suffers from inaccuracies, especially in negative predictions. In the present work, we propose to extend the Bayesian-CNN to improve its accuracy and the rate of convergence. We name the proposed model as modified Bayesian-CNN. The novelty of the proposed model lies in an adaptive activation function that contains a learnable parameter for each of the neurons. This adaptive activation function dynamically changes the loss function, which helps it to provide faster convergence and better accuracy. The uncertainties associated with the predictions are obtainable since the model learns a probability distribution on the network parameters. It reduces overfitting through averaging over an ensemble of networks, which in turn improves accuracy on the unknown data. The proposed modified Bayesian-CNN performs much better than CNN by nearly eliminating overfitting and reducing (about 28%) the number of false-negative predictions. The proposed model also performs better than Bayesian-CNN in reducing the number of false-negative predictions (about 12%) while slightly improving the accuracy. The proposed model associates high uncertainties with images, which have features of both classes. We have also used uncertainty quantification to further improve the accuracy of a subset of the test data. These findings have the potential to advance the state-of-the-art machine learning-based automatic classification for histopathological images. These findings have the potential to advance the state-of-the-art machine learning-based automatic classification for histopathological images.

16th U.S. National Congress on Computational Mechanics
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Title: Greedy Multiscale Strategies for Sparse Modeling and Emulation Tasks

Author(s): *Prashant Shekhar, *Tufts University*; Abani Patra, *Tufts University*;

Multiscale strategies have been effectively used for physics and data modeling tasks in several communities such as machine learning, signal processing and statistical learning. In this talk, we describe a novel multiscale kernel based greedy approach for generating sparse representations from noisy datasets. Besides data reduction, such representations also provide efficient models for reconstruction and generalization. Starting with introduction of the underlying approximation space for such models [1,2], we will provide a careful single scale and multiscale analysis of our proposed approach. This will be followed by theoretical bounds and recommendations for setting up algorithmic hyperparameters intelligently for optimal performance. We will also discuss approximation issues and recommendations concerning finite scale truncation. Besides data reduction and fast inference, through extensive experimentation, the proposed approach will also be shown to be more stable and robust with respect to sampling design, when compared with other standard surrogate models like Gaussian Processes. The presented claims and results will then be further justified with performance on simulation and remote sensing datasets, demonstrating a data reduction of almost 2 orders of magnitude. [1]: Shekhar, Prashant, and Patra, Abani. "Hierarchical approximations for data reduction and learning at multiple scales." Foundations of Data Science 2.2 (2020): 123. [2]: Shekhar, Prashant, and Patra, Abani. "Hierarchical regularization networks for sparsification based learning on noisy datasets." arXiv preprint arXiv:2006.05444 (2020).

16th U.S. National Congress on Computational Mechanics
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Title: A Fast Data-Driven Residual Strain and Stress Prediction in Stainless Steel 316L Laser Powder Bed Fusion Additive Manufacturing

Author(s): *Praveen Vulimiri, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

One of the key criteria for a successful build using laser powder bed fusion (LPBF) additive manufacturing (AM) is the residual stress and deformation induced by the manufacturing process. Excessive residual stress due to the repeated heating and cooling of the manufacturing process can cause the part to crack and delaminate from the build plate, creating build failure. It is therefore important to predict the residual strain and stress quickly and compensate for them during the design process to ensure a successful build. Current methods for part-scale simulation of the LPBF manufacturing process, such as detailed thermomechanical process simulations or inherent strain methods, however, require hours or longer for accurate prediction results, limiting the number of iterations which can be performed to determine the ideal geometry. In this work, a data-driven approach is introduced to predict residual stress and deformation using convolutional neural networks (CNN). Training samples are generated using various computer aided design (CAD) geometries simulated for LPBF manufacturing using the modified inherent strain method. The finite element mesh of each geometry is used as the input for the CNN, and the output is the residual stress/strain from the manufacturing process. The trained CNN will provide a similar residual stress/strain result as current methods in much shorter time. The time saved using the methods introduced in this work can be reinvested into the design process, further exploring the design space to determine the ideal geometry.

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Title: ICME-Based Modeling and Qualification for Additive Manufacturing of Ni-Based Superalloys

Author(s): *Qiaofu Zhang, *QuesTek Innovations LLC*; Abhinav Saboo, *QuesTek Innovations LLC*; Sam Sorkin, *QuesTek Innovations LLC*; Jiadong Gong, *QuesTek Innovations LLC*; Greg Olson, *QuesTek Innovations LLC*;

Additive manufacturing (AM) of Ni-based superalloys has attracted increasing interests and attention from academia and industry. Based upon QuesTek's Materials by Design® technology, an ICME (Integrated Computational Materials Engineering) framework was assembled to predict the complete process-structure-properties chain of Ni-based superalloys. Following the ICME framework, computational models were developed and integrated by QuesTek to effectively simulate the microstructure evolution during heat treatment, as well as the resulting mechanical properties as a function of test temperature, including both yield strength and ultimate tensile strength. These models were further applied to optimize the post heat treatment processes for AM-printed Ni-alloys. The developed ICME framework and models have been applied to various additive manufacturing cases, with results verified by both microstructural characterization and tensile tests of AM-printed specimens. Using the ICME framework and package, QuesTek applied the Accelerated Insertion of Materials (AIM) methodology to quantify the property distribution, resulting from material and process variation, of the AM-printed components, thus enabling design under uncertainty by accounting for both the mean and minimum properties. By integrating all the ICME and AIM models for additive manufacturing, QuesTek has developed its AQC (Accelerated Qualification and Certification) software package, intended to help accelerate the qualification of additively manufactured components and processes.

16th U.S. National Congress on Computational Mechanics
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Title: An Immersogeometric Formulation for Free-Surface Flows with Application to Marine Engineering Problems

Author(s): *Qiming Zhu, *University of Illinois at Urbana-Champaign*; Jinhui Yan, *University of Illinois at Urbana-Champaign*;

An immersogeometric formulation is proposed to simulate free-surface flows around structures with complex geometry. The fluid-fluid interface (air-water interface) is handled by the level set method, while the fluid-structure interface is handled through an immersogeometric approach by immersing structures into non-boundary-fitted meshes and enforcing Dirichlet boundary conditions weakly. Residual-based variational multiscale method (RBVMS) is employed to stabilize the coupled Navier-Stokes equations of incompressible flows and level set convection equation. Other level set techniques, including re-distancing and mass balancing, are also incorporated into the immersed formulation. Adaptive quadrature rule is used to better capture the geometry of the immersed structure boundary by accurately integrating the intersected background elements. Generalized-alpha method is adopted for time integration, which results in a two-stage predictor multi-corrector algorithm. GMRES solver preconditioned with block Jacobian matrices of individual fluid and level set subproblems is used for solving the coupled linear systems arising from the multi-corrector stage. The capability and accuracy of the proposed method are assessed by simulating three challenging marine engineering problems, which are a solitary wave impacting a stationary platform, dam break with an obstacle, and the planing of a DTMB 5415 ship model. A refinement study is performed. The predictions of key quantities of interest by the proposed formulation are in good agreement with experimental results and boundary-fitted simulation results from others. The proposed formulation has great potential for wide applications in marine engineering problems.

16th U.S. National Congress on Computational Mechanics
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Title: Sequential Decision Making for Adaptive Time Stepping in Solving Nonlinear Differential Equations

Author(s): *Ramakrishna Tipireddy, *Pacific Northwest National Laboratory*; William Rosenthal, *Pacific Northwest National Laboratory*; Vinay Amatya, *Pacific Northwest National Laboratory*;

Adaptive time stepping plays a crucial role in solving nonlinear differential equations due to numerical instabilities caused by the changes in the underlying physical phenomenon. Upon the introduction of instabilities, the time step needs to be reduced appropriately to capture the changes in physical processes. Current methods for adaptive time stepping involve fixed rule-based criteria set prior to start of the numerical simulation. However, such criteria may not be flexible to dynamically changing simulation environment due to uncertainties, unknown and unexpected physical processes and a computational scientist (human) may have to update and reset the rule-based criterion and rerun the simulation. In such situations a sequential decision making (SDM) framework consisting of agent based methods such as reinforcement learning (RL) methods offer flexibility where an agent would continuously interact with the simulation environment, compute the best policies, and perform actions (adaptive time stepping) that maximize the payoff in the long run. In this work, we present a reinforcement learning algorithm to compute the optimal policies that efficiently chooses the time step needed to avoid instabilities and reduce the computations cost. We illustrate the proposed algorithm on nonlinear ODEs such as Van der Pol oscillator and Lorenz equations.

16th U.S. National Congress on Computational Mechanics
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Title: Handling Neumann and Robin Boundary Conditions in an Immersed Boundary Method

Author(s): *Ramakrishnan Thirumalaisamy, *San Diego State University*; Amneet Bhalla, *San Diego State University*;

Moving boundary problems are ubiquitous in engineering and science applications. Several numerical methods are proposed to model these applications efficiently. Volume penalization (VP) approach is one such method in which an original problem posed on a complicated domain is reformulated into a new problem posed on a simple domain with the region of interest embedded into it. Cartesian grids are commonly employed to discretize this computational domain and this allows us to employ fast linear solvers. In most cases, the immersed interface does not align with the mesh. Therefore, imposing the desired boundary conditions on the interface is not straightforward. Sakurai et al. (2019) proposed a flux-based VP approach to impose inhomogeneous Neumann boundary conditions on the immersed surface through a flux-forcing function. This function is constructed analytically as the interfaces considered in their study is relatively simpler. In this presentation, we present a numerical approach to construct the flux-forcing function based on the signed distance function to handle arbitrarily complex interfaces. The proposed approach can handle both spatially constant and varying boundary conditions. We also extend the flux-based VP approach to handle spatially constant and varying Robin boundary conditions using numerically constructed flux-forcing functions. Using the method of manufactured solutions, we solve several two- and three-dimensional Poisson problems including problems with complex geometries to assess the convergence rate of this proposed approach. It is observed that the convergence rate of the proposed approach is between first and second-order for spatially constant boundary conditions and is first order for spatially varying boundary conditions.

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Title: An Image-Based Deep Learning Approach to Predict Crack in 2D Representations of Composites

Author(s): *Reza Sepasdar, *Virginia Polytechnic Institute and State University*; Maryam Shakiba, *Virginia Polytechnic Institute and State University*;

An image-based deep learning framework is proposed to predict the crack pattern in two-dimensional representations of composites, where the crack pattern depends on the microstructural geometry. The framework is trained to predict crack patterns based on an image of composites' microstructural geometric representation. The training data set (i.e., images of propagated cracks in the composite) is generated using an efficient interface-enriched generalized finite element framework. A fiber-reinforced composite is chosen as the material of interest in this study. During the training process, the deep learning framework uses images of the microstructural representations, stress contours at an early stage of damage initiation (ESoDI), and crack patterns. The stress distribution at ESoDI is an intermediate prediction in the proposed approach to guide the training. Hence, the framework includes two stacked networks, namely Generator 1 and Generator 2, that are trained sequentially. Generator 1 translates the microstructural geometry to the stress at ESoDI, while Generator 2 translates the pre-trained Generator 1 output to the crack pattern. A modified U-Net generator, a fully convolutional autoencoder, is utilized for both generators. The mean absolute error is used as the objective function in the training of the generators. Since translating the microstructural geometry to stress at ESoDI is a complicated task, an attention objective function is also proposed for the training of Generator 1 to further boost the prediction accuracy. The ultimate framework accuracy was evaluated to be 91% based on a test data set. The obtained high accuracy demonstrates that the proposed deep learning framework can accurately predict the crack pattern in microstructure-dependent composites.

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Title: Scientific Modeling of Aerosol Jet Deposition

Author(s): *Robert Secor, *Hirdeal LLC*; Ethan Secor, *Iowa State University*;

Aerosol jet printing is a relatively new microscale additive manufacturing process where solvated ink droplets are deposited via a carrier gas. Key deposition characteristics such as resolution and viable deposition rate are dependent on the interplay between droplet drying and process design before and after deposition. To augment current mechanistic understanding of printer operation, the GOMA multi-physics package is used to quantify details of droplet evaporation, solvent vapor diffusion, and gas conveyance during aerosol flow through the printer and after deposition. Boundaries between the aerosol phase and the drying sheath gas are tracked with ALE interface tracking techniques. Solvent evaporation and diffusion from individual droplets and accompanying size change on the micron scale are coarse-grained and tracked with a suitably modified residence time field. Knowledge discovery from detailed physics-and-chemistry-based calculations will be instrumental in aerosol jet printing advancements yielding improved resolution, throughput, and process reliability. References: Ethan B Secor, “Guided ink and process design for aerosol jet printing based on annular drying effects,” Flex. Print. Electron. 3 (2018) 035007.

16th U.S. National Congress on Computational Mechanics
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Title: A High-Order Material Point Methods for Structured and Unstructured (Triangular) Grids

Author(s): *Roel Tielen, *Delft University of Technology*; Matthias Möller, *Delft University of Technology*; Kees Vuik, *Delft University of Technology*;

The Material Point Method (MPM) has shown to be successful in simulating problems that involve large deformations and history-dependent material behavior. MPM can be considered as a hybrid Eulerian-Langranian method that combines the use of a set of particles, called material points, with a fixed background grid. The equations of motion are solved on this background grid within a variational framework, typically adopting piece-wise linear (Lagrangian) basis functions. Integrals resulting from the variational formulation are then approximated by using the material points as quadrature points. The use of piecewise-linear basis functions leads, however, to unphysical oscillations (so called 'grid crossing errors') in the numerical solution, due to the discontinuity of the gradient of these basis functions. Different strategies have been proposed to overcome these shortcomings. The use of quadratic B-spline basis functions (i.e. B-spline MPM [1]) or Powell-Sabin spline basis functions (i.e. PS-MPM [2]) within MPM completely removes grid-crossing errors, due to the higher continuity of the basis functions. The use of material points as integration points leads to a quadrature rule of which the quality is uncertain. The application of a Taylor Least-Squares (TLS) reconstruction [3] has shown to lead to more accurate integration, while conserving the total mass and momentum within MPM. In this talk, we discuss different versions of MPM using splines (e.g B-spline MPM and PS-MPM). Numerical results are presented for two-dimensional benchmarks showing order p+1 spatial convergence with these spline-based versions of MPM. Furthermore, quantities of interest (e.g. displacement and stresses) can be represented more accurately compared to standard MPM. Finally, we show how accurate integration, for example obtained with TLS reconstruction, further improves the overall accuracy of MPM. References [1] R. Tielen, E. Wobbes, M. Möller and L. Beuth, A High Order Material Point Method, Procedia Engineering, 175 (2017) pp. 265–272 [2] P. de Koster, R. Tielen, E. Wobbes and M. Möller, Extension of B-spline Material Point Method for unstructured triangular grids using Powell-Sabin splines. Computational Particle Mechanics (2020). [3] E. Wobbes, M. Möller, V. Galavi and C. Vuik, Conservative Taylor least squares reconstruction with application to material point methods, International Journal Numerical Methods in Engineering, 117 (2018) pp. 271–290

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Curvilinear Surface-ALE Formulation for Deforming Fluidic Membranes

Author(s): *Roger A. Sauer, *Gdansk University of Technology / Indian Institute of Technology Kanpur / RWTH Aachen University*;

This work presents a new continuum formulation for describing fluidic membranes, such as lipid bilayers. The formulation is based on an arbitrary Lagrangian-Eulerian (ALE) surface description defined in curvilinear coordinates [1]. Therefore, a curvilinear ALE surface coordinate is introduced that generally differs from the Lagrangian and Eulerian surface coordinates. The ALE coordinate introduces a frame motion, whose out-of-plane component is constrained to follow the material motion, while its in-plane components can be arbitrary. The new formulation is implemented within the finite element method using both classical and isogeometric surface elements [2,3]. The generalized-alpha method is used for time integration. The new formulation is illustrated by several analytical and numerical examples. They demonstrate the superiority of an ALE formulation over Lagrangian and Eulerian surface descriptions. [1] A. Sahu, Y.A.D. Omar, R.A. Sauer and K.K. Mandadapu (2020), Arbitrary Lagrangian-Eulerian finite element method for curved and deforming surfaces: I. General theory and application to fluid interfaces, J. Comput. Phys., 407:109253. [2] R.A. Sauer, T.X. Duong and C.J. Corbett (2014), A computational formulation for constrained solid and liquid membranes considering isogeometric finite elements, Comput. Methods Appl. Mech. Engrg., 271:48-68. [3] R.A. Sauer, T.X. Duong, K.K. Mandadapu and D.J. Steigmann (2017), A stabilized finite element formulation for liquid shells and its application to lipid bilayers, J. Comput. Phys., 330:436-466.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Adhesion Modulates Cell Morphology and Migration Within Dense Fibrous Networks

Author(s): *Rui Travasso, *University of Coimbra*; Maurício Moreira-Soares, *University of Oslo*; José Rafael Bordin, *University of Pelotas*; Susana P Cunha, *University of Coimbra*;

One of the most fundamental abilities required for the sustainability of complex life forms is active cell migration, as it is essential in diverse processes from morphogenesis to leukocyte chemotaxis in immune response. The movement of a cell is the result of intricate mechanisms that involve the coordination between mechanical forces, biochemical regulatory pathways and environmental cues. In particular, epithelial cancer cells have to employ mechanical strategies in order to migrate through the tissue's basement membrane and infiltrate the bloodstream during the invasion stage of metastasis. In this work we explore how mechanical interactions such as spatial restriction and adhesion affect migration of a self-propelled droplet in dense fibrous media. We have performed a systematic analysis using a phase-field model and we propose a novel approach to simulate cell migration with dissipative particle dynamics modelling. With this purpose we have measured in our simulation the cell's velocity and quantified its morphology as a function of the fibre density and of its adhesiveness to the matrix fibres. Furthermore, we have compared our results to a previous in vitro migration assay of fibrosarcoma cells in fibrous matrices. The results show good agreement between the two methodologies and experiments in the literature, which indicates that these minimalist descriptions are able to capture the main features of the system. Our results indicate that adhesiveness is critical for cell migration, by modulating cell morphology in crowded environments and by enhancing cell velocity. In addition, our analysis suggests that matrix metalloproteinases (MMPs) play an important role as adhesiveness modulators. We propose that new assays should be carried out to address the role of adhesion and the effect of different MMPs in cell migration under confined conditions.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Discontinuous Cohesive Reproducing Kernel Finite Volume Method for Brittle Fracture Simulation

Author(s): *Saili Yang, *The Pennsylvania State University*; Michael Hillman, *The Pennsylvania State University*;

Cohesive zone models are widely used in the simulation of the debonding process at the crack tip. For the traditional finite element based approach, additional elements are required to implement the cohesive zone law. In the intrinsic cohesive zone method [1], cohesive zone elements are inserted on every bulk element's surface at the beginning of the simulation, which changes materials' elastic behavior by increasing compliance, and greatly increases the number of degrees of freedom. Even though the extrinsic cohesive zone method [2] only employs elements where the crack is initiating and propagating, this adds to the global degrees of freedom dynamically and causes complication in implementation. Previously, a reproducing kernel finite volume method (RKFM) for elasticity has been proposed [3]. Based on this method, a cohesive zone RKFM is introduced in the current work. The traction over the cohesive zone is naturally applied as a flux term in the finite volume framework. A cell-conforming discontinuous kernel is proposed such that the strong discontinuity can be updated naturally under the flexible meshfree framework. Therefore, no additional degrees of freedom are required in this method, which reduces the computational complexity compared to finite-element based approaches, and no additional compliance is introduced. Several benchmark examples are presented to show the sufficiency of this method in yielding mesh-independent results, crack initiation, and dynamic branching. Validation of the method is also provided.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Towards Computational Modeling of Cardiac Valve Tissue: Rapid High Fidelity Valve Fiducial Localization Utilizing MicroCT Acquired Stereography

Author(s): *Sam Stephens, *University of Arkansas*; Neil Ingels, *University of Arkansas*; Jonathan Wenk, *University of Kentucky*; Morten Jensen, *University of Arkansas*;

Introduction: Advanced imaging techniques such as micro-CT and MRI have enabled high-resolution datasets of many tissues including heart valves [1] for enhancing the fidelity of computational models of these tissues. While high-resolution 3D imagery is viewed as the gold-standard, it may not always be necessary, such as when fiducial point localization is sufficient [2] without the need to image the underlying tissue. In such cases, it is useful to quickly localize fiducial points from few projection datasets. A technique to rapidly localize spherical fiducial points in 3D space utilizing rotating-sample micro-CT was developed and tested. Methods: Fiducial localization is achieved by imaging the sample from known angles and using point displacements within the resulting images. A test sample with known geometry was 3D printed and scanned with a Nikon X TH 225 ST micro-CT system. Three sharp peaks contained within the sample represent fiducial points. The locations of these points were determined based upon a subset of three micro-CT projections, each separated by 45 degrees, and the distances between points computed. The full set of 3142 projections was used to reconstruct the dataset into z-axis slices with an isotropic 25-micron voxel resolution. The reconstructed dataset was used to accurately measure the absolute point-to-point distances. Total scan time was 14 minutes, while the subset considered would require substantially less than a minute to acquire. Results: The calculated point-to-point distances were within 3% of those measured from reconstructed imagery, with a maximum error or 0.74mm. Discussion: This technique is useful when scan time is a significant concern, such as when tissue is subjected to stress or to prevent tissue desiccation. It is of particular utility when co-registration of displaced fiducial points must be made with a co-existing high fidelity scan of, for example, heart valve leaflets. Conclusions: Using a subset of only three projections represents a very short scan time, yet relatively good localization was still achievable. The use of more projections can improve upon the accuracy of these results without dramatically increasing scan duration. Optimization of inter-projection rotation angles and larger projection subsets will be investigated in future aspects of this project. References [1] Stephens SE, et al., (2017) High resolution imaging of the mitral valve in the natural state with 7 tesla MRI. PLoS One 12(8):e0184042 [2] Pierce EL, et al. Novel Method to Track Soft Tissue Deformation by Micro-Computed Tomography: Application to the Mitral Valve. Ann Biomed Eng. 2016;44(7):2273-2281

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Sparse Methods for Automatic Relevance Determination

Author(s): *Samuel Rudy, *Massachusetts Institute of Technology*; Themistoklis Sapsis, *Massachusetts Institute of Technology*;

Sparsity imposing techniques for linear regression have received significant attention over the past several years as tools for nonlinear system identification. In this talk we discuss several sparse variations of automatic relevance determination (ARD), an empirical Bayes formulation of linear regression that seeks to learn the diagonal covariance of the prior. We will begin with a review of the motivation for ARD via empirical Bayes and show analytically that it often fails to learn an accurate set of active terms when applied to orthogonal systems of linear equations with sparse solutions. We will subsequently discuss methods based in regularization or thresholding which seek to address the lack of parsimony observed in ARD solutions to sparse linear systems. The motivation and implicit assumptions behind each method will be discussed. We will show analytical estimates of the number of falsely added and missed terms for orthogonal problems that demonstrate favorable performance when compared to ARD and also include empirical results for each method on canonical examples from nonlinear system identification. This talk aims to present an overview of several methods, their similarities, and relative merits, rather than advocating a single technique.

16th U.S. National Congress on Computational Mechanics
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Title: A Self-Adapting LPS Solver for Laminar and Turbulent Flows

Author(s): *Samuele Rubino, *University of Seville*; Tomás Chacón Rebollo, *University of Seville*; Macarena Gómez Mármol, *University of Seville*;

In this work, we study the performance of a local projection-based solver in the Large Eddy Simulation (LES) of laminar and turbulent flows governed by the incompressible Navier-Stokes Equations (NSE). We focus on a high-order term-by-term stabilization Finite Element (FE) method that has one level, in the sense that it is de fined on a single mesh, and in which the projection-stabilized structure of standard Local Projection Stabilization (LPS) methods is replaced by an interpolation-stabilized structure. The interest of LPS methods is that they ensure a self-adapting high accuracy in laminar regions of turbulent flows, which turns to be of overall optimal high accuracy if the flow is fully laminar. An overview about known results from the numerical analysis of the proposed method is given, by highlighting the used mathematical tools. In the numerical study, we have considered two well known problems with practical applications: the 3D turbulent flow in a channel and the 3D recirculating flow in a lid-driven cavity. [1] T. Chacón Rebollo, E. Delgado Ávila, M. Gómez Mármol, S. Rubino: Assessment of self-adapting local projection-based solvers for laminar and turbulent industrial flows, Journal of Mathematics in Industry, Vol. 8:3, pp. 1-20, 2018. [2] N. Ahmed, T. Chacón Rebollo, V. John, S. Rubino: Analysis of a full space-time discretization of the Navier-Stokes equations by a Local Projection Stabilization method, IMA Journal of Numerical Analysis, Vol. 37(3), pp. 1437-1467, 2017. [3] T. Chacón Rebollo, M. Gómez Mármol, S. Rubino: Numerical analysis of a finite element projection-based VMS turbulence model with wall laws, Computer Methods in Applied Mechanics and Engineering, Vol. 285, pp. 379-405, 2015.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Phononic Crystals with Smooth Boundary Descriptions Using an Enriched Finite Element Method

Author(s): *Sanne van den Boom, *Delft University of Technology*; Reza Abedi, *University of Tennessee*; Fred van Keulen, *Delft University of Technology*; Alejandro Aragón, *Delft University of Technology*;

Phononic crystals (PnCs) are periodically arranged materials that interact with mechanical waves. They have increasingly gained interest because of their interesting properties such as bandgaps, i.e., ranges of frequencies for which waves cannot propagate. This effect has potential applications in many fields of engineering, including energy harvesting, elastic/acoustic filters, vibrationless environments for high-precision equipment, sound protection devices, and earthquake shields. In order to optimally utilize the potential of these metamaterials, computational design techniques such as topology optimization are invaluable. At the core of such optimization techniques lies an analysis technique that is both sufficiently accurate and efficient. However, as the commonly-used density-based approach leads to staircased or pixelized boundaries, and in most cases introduces gray values (i.e. intermediate material densities), highly refined meshes are needed to obtain sufficient accuracy in the analysis. Moreover, in the density-based topology optimization approach, design variables are directly coupled to the finite elements in the analysis mesh. Together, these properties mean that this approach is prohibitively expensive in both the analysis and the optimization problem. In this presentation we demonstrate the use of level-set based TO employing the Interface-enriched Generalized Finite Element Method (IGFEM) [1] for the computational design of PnCs. We illustrate the advantages of immersed boundary methods over density-based boundary descriptions for the frequency-domain analysis of PnCs. Furthermore we show that staircased and diffuse boundaries are also detrimental for the accuracy of the parameter retrieval method for phononic crystals. As an alternative to density-based topology optimization, we discuss the extension of the level-set based TO approach to design phononic crystals [2]. Furthermore, designs obtained with this approach are discussed. [1] van den Boom, S.J., Zhang, J., van Keulen, F., Aragón, A.M. An interface-enriched generalized finite element method for level set-based topology optimization. Struct Multidisc Optim 63, 1–20 (2021). https://doi.org/10.1007/s00158-020-02682-5 [2] van den Boom, S.J., Abedi, R., van Keulen, F., Aragón, A.M. On the importance of boundary smoothness in the computational design of phononic crystals. To be submitted

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Localized Viscoelastic Behavior Of The Porcine Urinary Bladder

Author(s): Tyler Tuttle, *Michigan State University*; *Sara Roccabianca, *Michigan State University*;

Mechanical characteristics of the bladder have been shown to differ between anatomical locations [1], yet no study has evaluated location-dependent viscoelastic behavior. Furthermore, inflammation in response to pathological conditions can lead to edema and localized increased tissue swelling [2]. In this study we aim to evaluate the effect of location and swelling on the viscoelastic response of the porcine bladder wall by using a combination of experimental testing and constitutive modeling. We performed two sets of multi-step uniaxial stress-relaxation experiments, applying to each sample an increasing value of strain, from 25% to 200% of the initial length, with a relaxation time of 45 minutes (for all steps except the first, which relaxed for 30 minutes). The first set of tests aimed to estimate the localized viscoealastic properties of the porcine bladder. We tested samples from five anatomical locations of the bladder, as previously described in [1]. All experiments were performed in modified Krebs-Henseleit buffer solution with an osmolarity of 300 mOsm/L (without Ca++ to prevent smooth muscle cells contraction). The second set of experiments aimed to measure how swelling due to changes in osmolarity of testing solution affects the viscoelastic properties of the porcine bladder. We tested samples in solutions of four different osmolarities, from 100 to 900 mOsm/L, as well as dry (all samples from the same anatomical location). Finally, to quantify the mechanical variation, we employed a modified Maxwell-Weichert model with nonlinear spring stiffnesses [3]. We observed that anatomical location affects mostly the elastic parameters within the model, and the solution osmolarity mostly affects the viscous parameters. Moreover, the samples tested in air showed the most differences in both elastic and viscoelastic parameters. The location-specific differences seen in elastic parameters support previous work [1] in suggesting the trigone is elastically different than other regions of the bladder, yet the lack of differences seen in viscoelastic parameters suggests that all regions may have similar time-dependent behavior. Our results also suggest that swelling in the bladder wall could change the time-dependent behavior of the bladder and it could contribute to pathological mechanically-driven remodeling in highly inflammatory conditions. Finally, the dramatic differences in parameters between dry and submerged samples underscores the importance of tissue hydration in mechanical testing. REFERENCES [1] Korossis, S et al., Biomaterials, 30(2):266–275, 2009. [2] Geppetti, P et al., Int. Suppl., 101:2–6, 2008. [3] Mastrigt, R, and J. C. Nagtegaal. MBEC 19(3):291–296, 1981.

16th U.S. National Congress on Computational Mechanics
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Title: Residual Stress and Performance Predictions for Electron Beam Welds: Influence of Imbedded Multi-Physics and Material Calibrations on Outcomes

Author(s): *Scott Smith, *Sandia National Laboratories*; Carl Herriott, *Sandia National Laboratories*; Michael Stender, *Sandia National Laboratories*;

Electron beam welds are often used in joining processes where large penetration depths are needed, little surface area to place a weld is available, and when maintaining a high level of the base-material's strength is critical for system performance. During the welding process, large deformations originate from the molten material in the cooling and joining processes. As a result of the large deformations in the heat-affected-zone of the weld, highly localized residual stresses develop - posing uncertainties for in-use and lifetime performance. Using a generalized pressure vessel geometry composed of forged stainless steel (SS) 304L, an electron beam weld is simulated as a fully-coupled thermo-mechanical problem aimed at accurately estimating the residual stresses and material properties resultant from the welding process to inform structural performance predictions. Particular attention is given to residual stress predictions as a function of the imbedded contact behavior of the liquid and solid 304L during the weld and the importance of using material calibrations that incorporate near-melt behavior on performance outcomes. In welding simulations, it is commonly assumed that the material at surfaces to be joined or any point in the weld (i.e., in the heat affected zone) behave in a fully-tied or compatible manner. Here, it will be shown that sliding and sliding-to-tied contact considerations that treat the expected friction and bonding between liquid and solid SS 304L notably influence model predictions. Additionally, residual stress and tensile performance predictions will be presented that display the influence of using legacy material parameters for a SS 304L material model compared to a re-calibrated model for SS 304L's behavior at near-melt temperatures that occur in electron beam weld processes. As an outcome and perspective, these findings will be summarized in a manner to develop a framework for future simulations to better aid in the reliable performance and surety of components joined via electron beam welds. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

16th U.S. National Congress on Computational Mechanics
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Title: A Homogenization Framework for Inelastic Layered Porous Materials

Author(s): *Shabnam J. Semnani, *University of California, San Diego*; Joshua A. White, *Lawrence Livermore National Laboratory*;

Many applications involving geomaterials, such as reservoir engineering, geothermal energy, and waste storage, entail tight coupling between multiphase fluid flow, transport, as well as thermo-mechanical and poromechanical deformations. Natural rocks are often highly heterogeneous and consist of fractures, solid and fluid phases that form complex structures at multiple scales. Explicit incorporation of multiple scales of fractures and heterogeneities into large-scale tightly coupled models is impractical and would cause tremendous computational costs. Therefore, efficient multi-scale strategies are necessary for capturing the impacts of sub-grid-scale processes on macroscopic behavior. In this work, we present a homogenization framework for inelastic multi-scale layered porous media. Subsequently, we demonstrate extension of the framework to coupled hydro-mechanical problems. We describe a homogenization strategy for computing both the mechanical and fluid flow constitutive behavior of fractured rock. Contrary to continuum-scale constitutive models, the present framework accounts for the coupling between planes of weakness and the matrix. In addition, the proposed approach allows for separate micro-constitutive laws and properties for each layer, explicit representation of layers with different properties and their distribution, as well as incorporation of imperfect bonding between the adjacent layers. Simulation results show that important features such as strength and permeability anisotropy are derived naturally from the small-scale description of the layered structure and fracture distribution. We show how the proposed material models can be readily incorporated into discrete-fracture-network or continuum simulations of reservoir systems, to provide an efficient way of capturing both small- and large-scale processes.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Binary Structure Applied to Fluid-Structure Interaction of the Rotating Body for Non-Newtonian Fluid

Author(s): *Shahin Ranjbarzadeh, *University of Sao Paulo*; Renato Picelli, *University of Sao Paulo*; Emilio Carlos Nelli Silva, *University of Sao Paulo*;

This paper proposes a topology optimization design method for fluid-structure interaction (FSI) problems of the rotating body considering Non-Newtonian fluid such as blood and polymer solution. The non-Newtonian fluid does not obey the Newtonian relationship between the shear stress and shear rate. Fluid-structure interaction of rotating body involving Non-Newtonian fluid has a wide range of mixing application in oil and gas, chemical, food industries, microfluidics, and bio-engineering. We solve a compliance minimization problem subject to volume constraints of structures under FSI loads considering Non-Newtonian low Reynolds number flow. The structure is considered to undergo small deformation. The TOBS (Topology Optimization of Binary Structures) method is applied to solve the material distribution problem. The TOBS approach uses binary f0,1g design variables, which can be advantageous when dealing with design-dependent physics interactions, e.g., in cases where fluid-structure boundaries are allowed to change during optimization. The COMSOL Multiphysics software is used to solve the fluid-structure equations and output the sensitivities using automatic differentiation. The TOBS optimizer provides a new set of {0,1} variables at every iteration. Optimization results show that rotating body and non-Newtonian fluid has a crucial influence on FSI design.

16th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Hyperelastic Structures with Anisotropic Fiber Reinforcement under Large Deformations

Author(s): *Shelly Zhang, *University of Illinois at Urbana-Champaign*; Heng Chi, *Siemens Corporation*; Zhi Zhao, *University of Illinois at Urbana-Champaign*;

Fiber-reinforced soft materials have emerged as promising candidates in various applications such as soft robotics and soft fibrous tissues. To enable a systematic approach to design fiber-reinforced materials and structures, we present a general topology optimization framework for the computational optimized design of hyperelastic structures with nonlinear and anisotropic fiber reinforcements under large deformations. This framework simultaneously optimizes both the material distribution in the matrix phase and the orientations of the underlying fiber reinforcements. The optimized distribution of fiber orientations is chosen from a set of discrete orientations defined a priori, and several fiber orientation interpolation schemes are studied. In addition, this work proposes an anisotropic material interpolation scheme, which integrates both matrix and fiber design variables (both with material nonlinearity) into the stored-energy function. To improve the computational efficiency of both optimization and nonlinear structural analysis, we derive a fully decoupled update scheme which performs parallel updates of the matrix and fiber design variables and employ the virtual element method (VEM) together with a tailored mesh adaptivity scheme to solve the finite elasticity boundary value problem. Design examples involving three objective functions are presented, demonstrating the efficiency and effectiveness of the proposed framework in designing anisotropic hyperelastic structures under large deformations.

16th U.S. National Congress on Computational Mechanics
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Title: Injury Databank of Pedestrian with Various Realistic Pre-Impact Poses for Integrated Active and Passive Safety Technology

Author(s): *Shi Shang, *Tsinghua University*; Quan Li, *Tsinghua University*; Bingbing Nie, *Tsinghua University*;

Researchers usually set the pedestrian pre-impact pose as a normal walking gait with the facing orientation perpendicular to the vehicle moving direction in mathematic simulations or PMHS experiments to evaluate pedestrian kinematics response and assess the injury in a vehicle crash. However, pedestrians being impacted by vehicles with various poses from stances without noticing the impending collision to different avoiding postures in real-world crash scenes. In this study, we establish an injury databank based on pedestrian pre-impact poses to provide references to the vehicle-equipped integrated active and passive safety system to adjust the vehicle to an impact scenario that would result in a minimum predicted pedestrian injury severity. Typical pedestrian pre-impact poses are captured and extracted from real-world crash videos and VR-based volunteer experiments. Head brain injuries, chest injuries, pelvis injuries, upper and lower extremity injuries, et al., obtained from corresponding impact scenarios are assessed by reconstructed MADYMO simulations. We determine the injury risk with Injury Severity Score (ISS), which is calculated based on the Abbreviated Injury Scale (AIS) of multiple injured body parts. This study provides novel insights on injury risk of the pedestrian with typical avoiding postures and for integrated active and passive safety system’s decision making.

16th U.S. National Congress on Computational Mechanics
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Title: An Adjoint-Based Super-Convergent Galerkin Approximation of Eigenvalues

Author(s): *Shiqiang Xia, *University of Minnesota*; Bernardo Cockburn, *University of Minnesota*;

In this talk, we present a new method for computing high-order accurate approximations of eigenvalues defined in terms of Galerkin approximations. We consider the eigenvalue as a non-linear functional of its corresponding eigenfunction and show how to extend the adjoint-based approach proposed in [1] to compute it. We illustrate the method on a second-order elliptic eigenvalue problem. Our extensive numerical results show that the approximate eigenvalues computed by our method converge with a rate of 4k + 2 when tensor-product polynomials of degree k are used for the Galerkin approximations. In contrast, eigenvalues obtained by standard finite element methods such as the mixed method or the discontinuous Galerkin method converge with a rate at most of 2k + 2. Numerical results for the classic L-shape domain and for the quantum harmonic oscillator are also presented to display the performance of the method. We also include the uncovering of a new adjoint-corrected approximation of the eigenvalues provided by the hybridizable discontinuous Galkiern method which converges with order 2k + 2, as well as preliminary results showing the possibilities of using the adjoint-correction term as an asymptotically exact a posteriori error estimate. [1] B. Cockburn and Z. Wang, Adjoint-based, superconvergent Galerkin approximations of linear functionals, J. Sci. Comput., 73 (2017), pp. 644–666.

16th U.S. National Congress on Computational Mechanics
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Title: High Fidelity Numerical Modeling of Dendritic Solidification and Microstructure Evolution in Metal Additive Manufacturing

Author(s): Kunal Bhagat, *University of Wisconsin-Madison*; *Shiva Rudraraju, *University of Wisconsin-Madison*;

Metal additive manufacturing (MAM) or 3D metal printing is increasingly gaining ground as a key area of advanced manufacturing. Additive techniques, especially in the context of metals, allow for design of components without the constraints of traditional casting and subtractive processes and for fabrication of complex geometries with optimal heterogeneous property distributions. However, one of the primary challenges to MAM is the lack of a good understanding of the effect of process conditions on the resulting mechanical properties, and thus the inability to achieve optimal property distributions. Especially important is the lack of sufficient control over the microstructure of the printed components. Recognizing that microstructure is the foundation of mechanical properties, this work presents high fidelity numerical models for simulating dendritic solidification and the ensuing microstructure evolution in MAM printed components. A detailed review of the evolution of sharp and diffuse interface models for solidification is discussed, and a range of numerical schemes involving classical FEM and isogeometric analysis (IGA) are presented. To achieve the ability to model dendritic evolution at close to realistic length scales, extensive numerical adaptivity and multiscale strategies are necessary. We present detailed h-, p-, and hp-adaptivity studies and corresponding optimal convergence results for various solidification models. In addition, we demonstrate multiscale extensions to classical solidification models to capture useful estimates about mesoscale grain-structure evolution. The numerical models presented involve a high-fidelity representation of the heat transfer, fluid flow and the thermo-mechanics that is intrinsic to MAM solidification processes.

16th U.S. National Congress on Computational Mechanics
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Title: Is Heterogeneous Cortical Growth Necessary to Recapitulate Cortical Thickness Patterns Seen in the Brain?

Author(s): *Shuolun Wang, *University of Notre Dame*; Nagehan Demirci, *University of Notre Dame*; Maria Holland, *University of Notre Dame*;

Cortical folding – the process of forming the characteristic gyri (hills) and sulci (valleys) of the cortex – is a highly dynamic process that results from the interaction between gene expression, cellular mechanisms, and mechanical forces. Like many other cells, neurons are sensitive to their mechanical environment. Because of this, cortical growth may not happen uniformly throughout gyri and sulci after the onset of cortical folding, which is accompanied by patterns of tension and compression in the surrounding tissue. Here, as an extension of our previous work (Holland et al., 2018), we introduce a biomechanically coupled growth model to investigate the importance of interaction between biological growth and mechanical cues during brain development. Our earlier simulations of cortical growth consisted of a homogeneous growing cortex attached to an elastic subcortex. Here, we let the evolution of cortical growth depend on a geometrical quantity – the mean curvature of the cortex – to achieve preferential growth in either gyri or sulci. As opposed to the popular pre-patterning hypothesis, our model treats inhomogeneous cortical growth as the result of folding rather than the cause. The model is implemented numerically in a commercial finite element software Abaqus/Explicit (2019) by writing a user-defined material subroutine (VUMAT). Our simulations show that gyral-sulcal thickness variations are a phenomenon particular to low stiffness ratios. In comparison with cortical thickness measurements of N = 28 human brains via a consistent sampling scheme, our simulations with similar cortical and subcortical stiffnesses suggest that cortical growth is higher in gyri than in sulci (Wang et al., 2020). References Abaqus/Explicit. Abaqus Reference Manuals. Dassault Systemes Simulia, Providence, RI, 2019. Maria Holland, Silvia Budday, Alain Goriely, and Ellen Kuhl. Symmetry breaking in wrinkling patterns: Gyri are universally thicker than sulci. Physical review letters, 121(22):228002, 2018. Shuolun Wang, Nagehan Demirci, and Maria A Holland. Numerical investigation of biomechanically coupled growth in cortical folding. Biomechanics and Modeling in Mechanobiology, pages 1–13, 2020.

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Title: Discovery of Deformation Mechanisms and Constitutive Response of Soft Material Surrogates of Biological Tissue by Data-Driven Variational System Identification

Author(s): Zhenlin Wang, *University of Michigan*; Jon Estrada, *University of Michigan*; Ellen Arruda, *University of Michigan*; Krishna Garikipati, *University of Michigan*; *Siddharta Srivastava, *University of Michigan*;

We present a novel, fully three-dimensional approach to soft material characterization and constitutive modeling with relevance to soft biological tissue. Our approach leverages recent advances in experimental techniques and data-driven computation. The experimental component of this approach involves in situ mechanical loading in a magnetic field (using MRI), yielding the entire deformation tensor field throughout the specimen regardless of the possible irregularities in its three-dimensional shape. Characterization can therefore be accomplished with data at a reduced number of deformation states. Its combination with powerful approaches to inverse modelling, specifically methods of model inference, would open the door to insightful mechanical characterization for soft materials. In recent computational advances that answer this need, we have developed new, data-driven inverse techniques to infer the model that best explains the physics governing observed phenomena from a spectrum of admissible ones, while maintaining parsimony of representation. This approach is referred to as Variational System Identification (VSI). We infer the physically best-suited and parsimonious mathematical models of their mechanical response. We demonstrate the performance of our methods in the face of noisy data with physical constraints that challenge the identification of mathematical models, while attaining high accuracy in the predicted response of the inferred models.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Damage Detection of Plates with Ultrasonic Signals Using Autoencoders

Author(s): *Soheil Sadeghi Eshkevari, *MIT Senseable City Lab*; Nur Sila Gulgec, *Thornton Tomasetti*; Badri Hiriyur, *Thornton Tomasetti*;

Ultrasonic technology has been widely used for nondestructive testing of structural components in recent years. The majority of existing methods are based on tracking statistical or hand-crafted characteristics of signals in time for structural health monitoring and damage detection. Despite its wide application, there are limited studies that exploit learning-based features for real-time damage detection. In this study, a machine learning-based algorithm extracts informative latent features from raw ultrasonic signals, and next, an ensemble of classifiers determine the structure status. For feature extraction, a convolutional autoencoder is implemented, which can substantially reduce signal dimension with the minimum reconstruction error. In the next step, a group of classifiers (including MLP-based, random forest, and SVM classifiers) determine the status of the structural component based on the low-dimensional feature by majority voting. This method is found exceptionally accurate in a real-world test experiment. Besides, the latent features are analyzed in terms of their physical interpretability. The analysis revealed that the convolutional neural network is a suitable setting for extracting meaningful low-dimensional information from a long signal due to its resemblance to wavelet transforms. In addition, we argue that a majority voting approach for classification based on multiple simple classifiers leads to the very high overall accuracy and recall measures.

16th U.S. National Congress on Computational Mechanics
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Title: AI-Enhanced Automated Computational Framework for Modeling Materials with Complex Microstructures

Author(s): *Soheil Soghrati, *The Ohio State University*; Ming Yang, *The Ohio State University*; Hossein Ahmadian, *The Ohio State University*; Salil Pai, *The Ohio State University*; Mohamad Mohamadsalehi, *The Ohio State University*; Mingshi Ji, *The Ohio State University*; Balavignesh Vemparala, *The Ohio State University*;

We present an integrated computational framework relying on a virtual microstructure reconstruction and parallel mesh generation algorithms for creating high-fidelity finite element (FE) models and simulating the failure response of materials. A NURBS-based virtual reconstruction algorithm is developed for synthesizing the material microstructure by packing arbitrary shaped inclusions, morphologies of which are extracted from digital data such as scanning electron microscopy (SEM) and micro-computed tomography images. A genetic algorithm (GA) based optimization phase is then utilized to replicate target statistical microstructural descriptors such as the volume fraction, spatial arrangement, and orientations of embedded inclusions. We also introduce a new AI-based approach relying on Deep Convolutional Degenerative Adversarial Networks (DCGAN) for the virtual reconstruction of complex biomaterial microstructures. Conforming FE meshes are then generated using a non-iterative meshing algorithm, coined Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR), which transforms an initial structured mesh into a high-quality conforming mesh. CISAMR can handle problems with highly intricate geometries, including material interfaces with sharp edges/corners and pre-existing cracks. We show the application of this integrated reconstruction-meshing framework, together with deep learning, for predicting the failure response of a variety of materials systems, including particulate composites and biomaterials. New CISAMR algorithmic aspects are also introduced, including the simulation of crack growth problems and handling sharp geometric features of the domain.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Bayesian Topology Optimization for Efficient Design of Origami Folding Structures

Author(s): *Sourabh Shende, *University of Cincinnati*; Andrew Gillman, *Air Force Research Laboratory*; David Yoo, *Air Force Research Laboratory*; Philip Buskohl, *Air Force Research Laboratory*; Kumar Vemaganti, *University of Cincinnati*;

Bayesian optimization (BO) is a popular method for solving optimization problems involving expensive objective functions. Although BO has been applied across various fields, its use in structural optimization area is in its early stages. Origami folding structures provide a complex design space where the use of an efficient optimizer is critical [1,2]. In this work for the first time we demonstrate the ability of BO to solve origami-inspired design problems. We use a Gaussian process (GP) as the surrogate model that is trained to mimic the response of the expensive finite element (FE) objective function. The ability of this BO-FE framework to find optimal designs is verified by applying it to well known origami design problems: chomper, twist chomper and square twist. We compare the performance of the proposed approach to traditional gradient-based optimization techniques and genetic algorithm methods in terms of ability to discover designs and computational efficiency. BO has many user-defined parameters and intuitions for these for structural optimization are currently limited. We study the role of hyperparameter tuning and the sensitivity of BO to the quality and size of the initial training set. Taking a holistic view of the computational expense, we propose various heuristic approaches to reduce the overall cost of optimization. We also demonstrate improvement in the convergence rate of BO by incorporating gradient information of the objective function in the modeling the GP surrogate model. Our results show that Bayesian optimization is an efficient alternative to traditional methods. For instance, the optimal design discovered by standard BO for 18-dimensional chomper, 38-dimensional twist chomper and 84-dimensional square twist show 17%, 12% and 50% improvement in the objective function values, respectively, compared with the gradient-based sequential quadratic programming (SQP) technique. Moreover, BO discovers these optimal designs with an order of magnitude fewer FE evaluations compared with genetic algorithm (GA) results. We also show that gradient-enriched BO framework can further speed up the optimization process by almost 6 times for the 84-dimensional square twist problem. Overall, Bayesian optimization is shown to be an attractive choice for the non-convex design space of origami fold mechanics. [1] A Gillman, K Fuchi, P R Buskohl. Truss-based nonlinear mechanical analysis for origami structures exhibiting bifurcation and limit point instabilities. Int. J. Solids Struct., 147:80– 93, 2018. [2] Andrew S. Gillman, Kazuko Fuchi, Philip R. Buskohl. Discovering Sequenced Origami Folding Through Nonlinear Mechanics and Topology Optimization. J. Mech. Design, 141(4):1–11, 2019.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Advanced Identification of Material Law for Micro- and Macro-scale Deformation of Alloys

Author(s): *Sourav Saha, *Northwestern University*; Ye Lu, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

Metallic alloys have been used for myriad of applications throughout the ages. Therefore, modeling the deformation of complex alloys with proper physical models is an extensive field of research. In particular, with the advent of metal additive manufacturing, where the spatial heterogeneity of microstructure leads to the local concentration of strain leading to fatigue failure, importance of modeling both the micro- and macro-scale deformation under service conditions with advanced material laws such as crystal plasticity has become extremely important. However, such material laws have a number of parameters to be calibrated before ready to be used. The calibration involves optimization of the modeling parameters against experimental data. However, directly using full field methods such as FEM or FFT for optimization is time-consuming. In this paper, the proper generalized decomposition (PGD)-based [1] calibration of material laws has been proposed and the performance of calibration is compared with traditional optimization methods such as the genetic algorithm. It is found that PGD-based calibration of material law is considerably faster (~speed up 10). The experimental data for calibration is taken from the recently concluded Air Force Research Laboratory Additive Manufacturing Challenges 3 and 4 where the microstructure characterization and mechanical tests are performed for Laser Powder Bed Fusion (LPBF) Inconel 625, a Ni-based superalloy. For microscale prediction verification, local grain average elastic strain tensor is predicted using PGD-calibrated material law and compared against High Energy X-ray diffraction data. The calibration involves different post-processing conditions and two different temperature levels (room and high). The proposed calibration method relies on developing a surrogate model taking data from more expensive computational algorithms such as finite element method or Fast Fourier Transform. A demonstration is also presented where the calibration method is combined with reduced order mechanistic method called Self-consistent Clustering Analysis (SCA) [2] which can lead to faster design method combining data science and mechanics. References 1. Lu, Y., N. Blal, and A. Gravouil. "Adaptive sparse grid based HOPGD: Toward a nonintrusive strategy for constructing space?time welding computational vademecum." International Journal for Numerical Methods in Engineering 114.13 (2018): 1438-1461. 2. Yu, C., Kafka, O.L. and Liu, W.K., 2019. Self-consistent clustering analysis for multiscale modeling at finite strains. Computer Methods in Applied Mechanics and Engineering, 349, pp.339-359.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Finite-Deformation Sharp Interface Model for Void Evolution Under Irradiation

Author(s): Anter El-Azab, *Purdue University*; *Sreekar Rayaprolu, *Purdue University*; Kyle Starkey, *Purdue University*;

Crystalline materials subjected to irradiation in nuclear reactors can develop voids. We formulated a thermodynamically consistent sharp interface theory for void evolution under irradiation, which includes vacancy and interstitial dynamics coupled with finite deformation mechanics. We include energy and entropy fluxes due to point-defect diffusion in the balance laws, which are neglected in other similar models. We explicitly account for the anisotropic interfacial energy, interfacial stresses and eigenstrain associated with vacancies and self-interstitials using the multiplicative decomposition of deformation gradient. We developed the driving forces for the interface motion and point-defect fluxes in the reference configuration, along with the defect reaction rates at the void interface. The coupled governing equations are solved using a total Lagrangian approach. Test cases are presented to validate our new sharp interface formulation.

16th U.S. National Congress on Computational Mechanics
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Title: A Generalized Peridynamic Framework for Modeling Corrosion Mechanics, Damage and Failure

Author(s): *Srujan Rokkam, *ACT Inc.*; Masoud Behazadinasab, *Brown University*; Max Gunzburger, *Florida State University*; Nam Phan, *Naval Air Systems Command*; Sachin Shanbhag, *Florida State University*;

We present a recently developed peridynamics (PD) framework for modeling corrosion damage phenomena, crack propagation and failure under synergistic effects of corrosion and mechanical loading [1]. By extending the non-local peridynamic theory to capture the damage processes induced by corrosion, we obtain a system of integro-differential equations that enables simulation of crack propagation in scenarios of stress corrosion cracking (SCC), corrosion fatigue (CF) and failure. First we introduce the developed PD framework and its extension to capture the multiphysics of corrosion in a non-local setting. Subsequently, the developed corrosion model is coupled with a recently developed finite deformation PD theory, making it suitable for studying effects of corrosion on mechanical behavior of ductile materials by invoking their elastoplastic behavior. We demonstrate applicability of the framework to both ductile and brittle engineering materials. The developed framework is able to capture corrosion initiated failure, ductile damage, as well crack path dynamics without the drawbacks of conventional theories. This research was funded by U.S. Navy/ Naval Air Systems Command (NAVAIR) through a STTR program, Contract No. N68335-15C-0032, awarded to Advanced Cooling Technologies, Inc. [1] Rokkam, S., Gunzburger, M., Brothers, M., Phan, N., and K. Goel, "A nonlocal peridynamics modeling approach for corrosion damage and crack propagation", Theoretical and Applied Fracture Mechanics, Vol. 101, pp. 373-387, 2019.

16th U.S. National Congress on Computational Mechanics
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Title: Condition Number Bounds for IETI-DP Methods that are Explicit in h and p

Author(s): Rainer Schneckenleitner, *Johannes Kepler University Linz*; *Stefan Takacs, *Austrian Academy of Sciences*;

For the solution of the linear system resulting from the isogeometric discretization of a multi-patch domain, domain decomposition approaches are a canonical choice since they can be based on the subdivision of the overall domain into patches. We consider the Isogeometric Analysis Tearing and Interconnecting (IETI) method, which is a variant of the FETI-method for Isogeometric Analysis. We will discuss convergence analysis, focusing on the dependence of the condition number of the preconditioned system on the spline degree p. Previously, a convergence theory has been provided that is accurate concerning the dependence of the condition number on the grid size. There, an auxiliary problem with linear basis functions was introduced. The proof uses the fact that the stiffness matrices of the original and the auxiliary problem are spectrally equivalent. The constants in this spectral equivalence are independent of the grid size but grow exponentially in p. In this presentation, we will see a direct convergence proof, i.e., a convergence proof that is solely based on the spline spaces of interest and that does not use such an auxiliary problem. This allows us to get rid of the exponential dependence in p. We will discuss the dependence of all estimates on p. Numerical experiments, which confirm our theoretical findings, will be presented.

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Title: Stabilized Finite Elements for a Logarithmic Reformulation of Viscoelastic Constitutive Laws

Author(s): *Stefan Wittschieber, *RWTH Aachen University*; Marek Behr, *RWTH Aachen University*; Leszek Demkowicz, *The University of Texas at Austin*;

The microstructure of flowing media in different applications such as blood handling devices or polymer melt processing is connected to viscoelasticity. In order to model these flows, the constitutive equation for Newtonian fluids is supplemented by an additional unknown for the deviatoric stresses. These stresses follow highly non-linear hyperbolic laws posing several challenges for a finite element analysis. Highly elastic flows suffer from the so-called High Weissenberg number problem, which describes a breakdown of either the non-linear iteration or the linear solver at a problem dependent Weissenberg number. The loss of positive definiteness of the conformation tensor (an intrinsic quantity of the constitutive equation) is connected to a breakdown in a computation. Developments in the 21st century have produced so-called logarithmic conformation formulations: The original constitutive equation is replaced by an equivalent representation to ensure the positive definiteness of the conformation tensor. Computations of a wider range of Weissenberg numbers became possible. The present work is based on a formulation proposed by Saramito [1] to represent the differential Oldroyd-B model. A non-singular behavior at zero Weissenberg number of the surrogate constitutive equation enables continuation techniques for cost-efficient steady state computations. In addition, derivatives of all non-linear terms are well-defined, which allows usage of the Newton-Raphson method. We develop established stabilized methods (including an Algebraic Sub-Grid Scale method [2], Galerkin/Least-squares [3], and Streamline-Upwind/Petrov-Galerkin) to address the remaining sources of numerical instabilities. These include instabilities coming from the convective nature of the momentum equation or constitutive equation, and from the choice for the interpolation spaces for velocity, pressure, and extra stresses. We compare the accuracy and robustness of the methods by means of a benchmark flow past a cylinder, and planar contraction. Available benchmark data in the literature agrees very well with our results. The design of stabilization parameters is further explored. The Algebraic Sub-Grid Scale method was found to be highly robust. [1] P. Saramito. On a modified non-singular log-conformation formulation for Johnson–Segalman viscoelastic fluids. Journal of Non-Newtonian Fluid Mechanics. Vol. 211, pp. 16-30, (2014). [2] T.J.R. Hughes, G.R. Feijóo, L. Mazzei, J.B. Quincy. The variational multiscale method — a paradigm for computational mechanics. Computer Methods in Applied Mechanics and Engineering. Vol. 166, pp. 3-24, (1998) [3] O.M. Coronado, D. Arora, M. Behr, M. Pasquali. Four-Field Galerkin/Least-Squares Formulation for Viscoelastic Fluids. Journal of Non-Newtonian Fluid Mechanics. Vol. 140, pp. 132-144, (2006).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Modeling Spall in Additively Manufactured Steel with Local-Nonlocal Coupling

Author(s): *Stewart Silling, *Sandia National Laboratories*; John Mitchell, *Sandia National Laboratories*;

Additively manufactured (AM) metals can have microstructures that are very different from conventionally processed materials. The AM microstructure can influence many aspects of the mechanical response of the material. In this study, we apply peridynamics to investigate the effects of microstructure on the failure of AM stainless steel. The failure is due to strong, dynamic tensile loading generated by reflections from shock waves. The 3D microstructure is defined using a Voronoi cell structure or with a synthetic microstructure generated by the SPPARKS code. A new peridynamic crystal plasticity model is applied to each grain, which has a randomly assigned orientation of its slip systems. Dynamic failure of the grains and grain boundaries is modeled with the recently developed Spall Kinetics Model. The splice method for local-nonlocal coupling allows a subregion containing the spall plane to be modeled with peridynamics, while the remainder of the body is modeled with the local theory. The compatibility of peridynamics with complex patterns of fracture is helpful in simulating the influence of microstructure on the material failure process. Results of simulations are compared with test data from shock wave experiments.

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Title: Multiphase Reactive Poromechanical Modeling Of Non-Operable Glioblastoma IDH Wild Type

Author(s): *Stéphane Urcun, *Arts et Métiers ParisTech*; Giuseppe Sciumè, *University of Bordeaux*; Pierre-Yves Rohan, *Arts et Métiers ParisTech*; Davide Baroli, *Aachen Institute for Advanced Study in Computational Engineering Science*; Ruairidh Howells, *Toulouse NeuroImaging Center*; Vincent Lubrano, *Toulouse NeuroImaging Center*; Wafa Skalli, *Arts et Métiers ParisTech*; Stéphane Bordas, *University of Luxembourg*;

More than one third of glioblastomas of WHO grade IV are still non-operable and the operable cases are almost hundred percent recurrent. The interplay between extra-cellular matrix and interstitial fluid flow could permit new fundamental understanding of invasion patterns. Multiphase poromechanical modelling, coupled with mechanobiology, is particularly suited to this framework for reproducing structural shaped infiltration. The physical quantities and the initial and boundary conditions of the model are given by patient specific multi-modal MRI sets. These are fully translated into the finite element framework of FEniCS by a pipeline from Nifti format to tetrahedral meshes, thus the model inputs and outputs can be readily measured and compared clinically. To monitor the whole invasion process and control the model dynamics, data sets of non-operable patients are used. Clinical measurements, multicellular spheroid cultures, ex-vivo mechanical tests and in-vivo perfusion give initial estimates of the parameters of the model, the patient MRI set is then used to tune them and to produce a patient-specific scenario.

16th U.S. National Congress on Computational Mechanics
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Title: A Machine Learning Based Data Compression Strategy for Transient Simulations.

Author(s): *Sujal Tipnis, *Ansys Inc.*; Rishikesh Ranade, *Ansys Inc.*; Jay Pathak, *Ansys Inc.*;

Transient simulations performed on large computational domains with fine meshes can generate tremendous amounts of spatio-temporal data for different solution field variables. Although accurate, the fine mesh solutions have prohibitive data storage requirements. On the other hand, coarse meshes alleviate data storage but fail to accurately capture the desired physics. As a result, it may be useful to solve on fine meshes but only store their coarser representations in memory. Coarsening can be achieved by linearly interpolating fine mesh solutions on uniform grids of low resolution. The issue with such a coarsening strategy is that its inverse is unknown and hence, reconstruction of the fine mesh solution is non-trivial. Moreover, the complexity of reconstruction is increased as the resolution of coarsened representation is reduced. In this work, we propose a machine learning based reconstruction methodology to transform coarsened representations to their corresponding spatio-temporal fine mesh solutions. The proposed approach uses a machine learning method which learns from sparse data sets and can predict on discrete spatio-temporal locations in the computational domain, thus scaling to unstructured, multi-resolution and non-uniform meshes. The network architecture has two input channels to accommodate the coarsened solutions and discrete points, which are coordinates of the mesh nodes and time instants. The output of the network is the solution at each of these discrete spatio-temporal locations. The proposed approach is demonstrated for flow over a cylinder in 3D for a Reynolds number variation ranging from Re = 1000 to Re = 30000, simulated using Ansys Fluent on a 1.7 million cell mesh, which serves as the fine mesh solution dataset. The coarsened representations are interpolations of this fine mesh solution. The approach is trained using a combination of this fine mesh solution dataset and their corresponding coarsened representations and inferred for an intermediate Reynolds number specific dataset. This methodology achieves great agreement with the intermediate data generated using Ansys Fluent, with an impressive compression ratio. This methodology has also been extended to transient structural simulations with similar implications.

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Title: Cardiac Motion Estimation from Cine Cardiac MR Images Based on Deformable Image Registration and Mesh Warping

Author(s): Brian Wentz, *University of Kansas*; Roshan Upendra, *Rochester Institute of Technology*; *Suzanne Shontz, *University of Kansas*; Cristian Linte, *Rochester Institute of Technology*;

Reliable assessment of myocardial function entails accurate characterization of parameters such as the myocardial motion, strain, torsion, and wall thickness. This information is helpful for understanding myocardial diseases, such as dilated cardiomyopathy or hypertrophic cardiomyopathy. Such diseases may result in an enlarged heart and electrical conduction disturbances of the heart or heart failure. Accurate cardiac motion estimation from cardiac magnetic resonance (CMR) images helps to assess the kinematic and contractile properties of the myocardium, which serve to directly quantify regional heart function. To estimate the cardiac motion, we perform image registration to find an optimal flow between consecutive 3D frames of a 4D cine CMR dataset. To this end, we propose a convolutional neural network-based 4D deformable registration technique for consistent motion estimation [1]. Our unsupervised deep learning framework employs a Laplacian-based operator as smoothing loss for deformable registration of 3D cine CMR images. Prior to registration, the images are corrected for slice misalignment, common during CMR image acquisition. We segment the left and right ventricles from the end-diastole image and generate corresponding surface meshes, then decimate them in Meshlab to reduce the number of triangular faces. A volume mesh of the cardiac geometry is then generated for the end-diastole frame based on the decimated surface mesh, then smoothed using the Mesquite Mesh Quality Improvement Toolkit. We employ the developed deformable image registration technique to warp the surface meshes of the left and right ventricles from end-diastole to remaining cardiac phases, hence propagating the end-diastole surface meshes throughout the cardiac cycle. LBWARP (i.e., a log barrier-based mesh warping method) [2] is then used to deform the volume mesh at end-diastole throughout the cardiac cycle based on the warped surface meshes at the corresponding cardiac phases. We compare the volume meshes generated via LBWARP with the corresponding volume meshes obtained directly by warping the end-diastole volume mesh using the displacement field yielded by the deformable image registration method. We assess the performance of these methods on the Automated Cardiac Diagnosis Challenge Dataset. References: [1] Roshan R. Upendra, Brian Wentz, Suzanne M. Shontz, and Cristian A. Linte, A convolutional neural network-based deformable image registration method for cardiac motion estimation from cine cardiac MR images, Computing in Cardiology, IEEE, 47: 1-4, 2020 [2] Suzanne M. Shontz and Stephen A. Vavasis, A mesh warping algorithm based on weighted Laplacian smoothing, in Proceedings of the 12th International Meshing Roundtable, p. 147-158, 2003

16th U.S. National Congress on Computational Mechanics
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Title: Implementation of the Drucker-Prager Model for Ordinary State-Based Peridynamics Using a Local Plastic Multiplier

Author(s): *Taiki Shimbo, *National Institute of Technology, Ishikawa College*; Tomoki Kawamura, *GODAI KAIHATSU Co., LTD*; Yutaka Fukumoto, *Nagaoka University of Technology*;

An earthquake often induces soil embankment failure due to the formation of several cracks caused by extension stress and shear stress in these embankments. To improve the earthquake-resistance, studying the process of crack initiation and propagation in embankments is crucial. We developed the seismic response analysis method for Ordinary State-Based Peridynamics (OSB-PD) [1]. However, the analysis method cannot treat an elastic-plastic material. To evaluate the fracture toughness of soil embankments and clarify the fracture mechanism, dealing with an elastic-plastic material is required in the numerical analyses. In general, a soil material is assumed to be a pressure-sensitive material with a dilatancy characteristic (volume expansion phenomenon induced by shear deformation). E.Madenci and S.Oterkus [2] proposed a numerical formulation of the von Mises elastic-plastic model for OSB-PD. In their formulation, a Non-local plastic multiplier is defined, and its value is obtained by a convergence calculation. In this study, the Drucker-Prager elastic-plastic model, one of the simplest models of a pressure-sensitive material, is applied to OSB-PD. We focus on the fact that a Local plastic multiplier obtained by an implicit return-mapping algorithm based on Local Continuum Mechanics is consistent with the Non-local plastic multiplier and propose a novel formulation without convergence calculation using the Local plasticity multiplier. Several analyses are performed to clarify the validity of this formulation. As a result, it is shown that Load vs. Load point displacements are consistent with quasi-static and elastic-plastic FEM. Furthermore, an analysis by using the Local plastic multiplier is about 1.5 times faster than previous methods on average. [1] T. Shimbo, R. Itto, K. Inaba, K. Araki and N. Watanabe, “Seismic response analysis for ordinary state-based peridynamics in a linear isotropic elastic material” Journal of Peridynamics and Nonlocal Modeling, 2, 185-204 (2020). [2] E.Madenci and S.Oterkus, “Ordinary state-based peridynamics for plastic deformation according to von Mises yield criteria with isotropic hardening”, Journal of the Mechanics and Physics of Solids, 86, 192–219 (2016).

16th U.S. National Congress on Computational Mechanics
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Title: Numerical Verification of Eigenvalue Analysis of Vibration of Elastic Circular Cylinder by Using Specific P-Wave Modes

Author(s): *Takahiro Yamada, *Yokohama National University*;

In various fields, elastodynamic problems appear as structural vibrations or elastic wave propagations. In standard transient analyses of elastodynamics, we need to introduce two types of approximations consisting of a finite element approximation in space and temporal discretization, which is often called a numerical time integrator. Numerical properties of numerical time integrators are well studied by Fourier analysis. On the other hand, spatial approximations are characterized by numerical solutions of eigenvalues and eigenmodes associated with free vibrations. For general problems with complex geometrical shapes and free surfaces, it is almost impossible to find exact solutions of eigenvalues and eigenmodes and hence quantitative evaluation by comparison with exact and numerical solutions is hardly performed. Day and Romero proposed an analytically solvable eigenvalue problem for linear elaticity[1], in which a simple hexahedral domain and boundary condition are employed. In this work, an eigenvalue problem possessing solvable solutions for more complex shapes is proposed for verification of the code and evaluation of numerical properties. In a homogenous and isotropic elastic material, elastic waves are propagated as P- and S-waves. In this work, cylindrical domains are employed and stationary modes of P-wave, which can be described by scalar potential, are considered as specific eigenmodes of vibration. The exact eigenmodes presented in this work are axisymmetric and expressed in terms of tensor products of trigonometric and Bessel functions. In this approach, all the exact eigenvalues and eigenmodes are not provided and a technique to find numerical solutions associated with specific exact ones is proposed. Numerical properties of several finite element approximations are investigated. Reference [1] Day, D. and Romero, L.: An analytically solvable eigenvalue problem for the linear elasticity equations. Technical Report SAND2004-3310, Sandia National Laboratories(2004).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Topology Optimization with Geometric Templates

Author(s): *Tareq Zobaer, *The Ohio State University*; Alok Sutradhar, *The Ohio State University*;

When topology optimization is used for obtaining a minimum compliance design under a specified volume constraint, it produces a density distribution that seeks an optimal path from the site of application of load to the supports. It only considers regions in the domain that minimizes the objective function while satisfying the constraint, which gives rise to rather non-intuitive structural designs. There are some situations where this is not always desirable. For instance, if one seeks to design a structure that makes use of some pre-manufactured components having a specified cross-section, calculating their optimal placement in the domain becomes the design problem. In this work, we present a density-based topology optimization method for linear elastic materials that achieve structural designs with geometric templates. In the optimization problem, the location and orientation of a number of these specific templates are determined. However, there may be some regions in the domain where the placement of this template is not feasible. Those parts are filled with density elements that do not need to conform to the given geometric template. Thus, the connection between the templates is established by density elements, which competes with the path for load transfer.

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Title: Image-Based Polygonal Lattices for Mechanical Modeling of Biological Materials: 2D Demonstrations

Author(s): Di Liu, *Syracuse University*; Chao Chen, *Syracuse University*; *Teng Zhang, *Syracuse University*;

Understanding the structure-property relationship of biological materials, such as bones, teeth, cells, and biofilms, is critical for diagnosing diseases and developing bio-inspired materials and structures. The intrinsic multi-phase heterogeneity with interfaces places great challenges for mechanical modeling. Here, we develop an image-based polygonal lattice model for simulating the mechanical deformation of biological materials with complicated shapes and interfaces. The proposed lattice model maintains the uniform meshes inside the homogeneous phases and restricts the irregular polygonal meshes near the boundaries or interfaces. This approach significantly simplifies the mesh generation from images of biological structures with complicated geometries. The conventional finite element simulations validate this polygonal lattice model with high accuracy. We further demonstrate that the image-based polygonal lattices generate meshes from images of composited structure with multiple inclusions and capture the nonlinear mechanical deformation. We conclude the paper by highlighting a few future research directions that will benefit from the functionalities of the polygonal lattices modeling.

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Title: Discovery of Defect Diffusion Mechanisms: Correlation and Uncertainty Quantification

Author(s): *Thomas Swinburne, *French National Centre for Scientific Research*; Danny Perez, *Los Alamos National Laboratory*;

Defect transport is a key process in materials science, but atomistic mechanisms are often too complex to enumerate a priori, complicating uncertainty analysis and observable convergence. I will describe an asynchronous, massively parallel accelerated sampling scheme[1], autonomously controlled by rigorous Bayesian estimators of statewise sampling completeness, which builds atomistic kinetic Monte Carlo models on a state space irreducible under exchange and space group symmetries. A combined Monte Carlo and analytic procedure is outlined which provides a novel convergence metric for defect transport coefficients, via a Kullback-Leiber divergence across the ensemble of diffusion processes consistent with the sampling uncertainty. The autonomy and efficacy of the method is demonstrated on a range of challenging materials science problems. [1] "Automated calculation and convergence of defect transport tensors" TD Swinburne and D Perez, NPJ Computational Materials, December 2020

16th U.S. National Congress on Computational Mechanics
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Title: A Globally Convergent Method to Accelerate PDE-Constrained Optimization Using On-the-fly Model Hyperreduction

Author(s): *Tianshu Wen, *University of Notre Dame*; Matthew Zahr, *University of Notre Dame*;

We present a numerical method to efficiently solve optimization problems governed by partial differential equations using projection-based reduced-order models accelerated with hyperreduction and embedded in a trust-region framework that guarantees global convergence. The proposed optimization framework adaptively constructs a reduced-order model from snapshots of the high-dimensional model and its sensitivity or adjoint at trust-region centers, which ensures training samples lie on the optimization trajectory and are not wasted in other regions of the parameter space. In addition, at each trust-region center, an empirical quadrature procedure is used to construct a sparse quadrature rule so nonlinear terms can be efficiently approximated on a sample mesh. Numerical experiments are performed on a number of shape optimization problems to verify the computational efficiency and global convergence of the method.

16th U.S. National Congress on Computational Mechanics
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Title: Solving Stochastic Inverse Problems for Property-Structure Relationship in Computational Materials Science

Author(s): Anh Tran, *Sandia National Laboratories*; *Tim Wildey, *Sandia National Laboratories*;

Determining process–structure–property linkages is one of the key objectives in material science, and uncertainty quantification plays a critical role in understanding both process–structure and structure–property linkages. In this work, we seek to learn a distribution of microstructure parameters that are consistent in the sense that the forward propagation of this distribution through a crystal plasticity finite element model matches a target distribution on materials properties. This stochastic inversion formulation infers a distribution of acceptable/consistent microstructures, as opposed to a deterministic solution, which expands the range of feasible designs in a probabilistic manner. To solve this stochastic inverse problem, we employ a recently developed uncertainty quantification framework based on push-forward probability measures, which combines techniques from measure theory and Bayes' rule to define a unique and numerically stable solution. This approach requires making an initial prediction using an initial guess for the distribution on model inputs and solving a stochastic forward problem. To reduce the computational burden in solving both stochastic forward and stochastic inverse problems, we combine this approach with a machine learning Bayesian regression model based on Gaussian processes and demonstrate the proposed methodology on two representative case studies in structure–property linkages.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Low Dimensional Polynomial Chaos Expansion Performance at Assessing Uncertainty in Creep Life Prediction of Grade 91 Steel

Author(s): *Timothy Truster, *University of Tennessee*; Amirfarzad Behnam, *University of Tennessee*; Varun Gupta, *ExxonMobil Upstream Research Company*; Ramakrishna Tipireddy, *Pacific Northwest National Laboratory*;

This talk examines time to minimum creep rate and its uncertainty with respect to a set of fourteen material parameters. The time elapsed to minimum rate correlates greatly to overall creep lifespan of materials and hence is an important quantity of interest. The microstructural model of Grade 91 steel includes both dislocation creep and grain boundary opening/sliding within a finite element model, and hence the simulations are relatively expensive and have several sources of nonlinearity. We will propagate uncertainty in the input material parameters of these two mechanisms and determine the aggregate uncertainty in the predicted time to minimum creep rate as well as the sensitivities of the parameters upon this prediction. The cost, stability, accuracy of the polynomial chaos expansion as a means for stochastic dimensional reduction using basis adaptation method is assessed against the classical Monte Carlo method.

16th U.S. National Congress on Computational Mechanics
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Title: Stochastic Gradient Descent from the Piecewise Deterministic Markov Processes Perspective

Author(s): *Ting Wang, *US Army Research Laboratory*; Kenneth W. Leiter, *US Army Research Laboratory*; Jaroslaw Knap, *US Army Research Laboratory*;

Modern machine learning as well as engineering problems increasingly rely on enormous amounts of data. Deterministic optimization tools, reliant on complete datasets for each iteration, are computationally prohibitive for large-scale machine learning. In comparison, stochastic gradient descent (SGD) based algorithms only require a small batch of data for each update and hence have become the standard tools for training large scale neural networks. Nevertheless, the theoretical understanding of SGD still lags far behind its wide applications. We propose the piecewise deterministic Markov process (PDMP) framework to study the SGD algorithms from the continuous time perspective. Specifically, we demonstrate that PDMP is a continuous time analogy of SGD. Motivated by this insight, we utilize the optimal control theory for PDMP to discover the near optimal learning rate for SGD, which leads to a class of PDMP-SGD algorithms we develop. Applications of PDMP-SGD algorithms for benchmarking examples will be demonstrated.

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Title: A Computational Photopolymerization Model for Volumetric Additive Manufacturing

Author(s): *Todd Weisgraber, *Lawrence Livermore National Laboratory*; Caitlyn Cook, *Lawrence Livermore National Laboratory*; Erika Fong, *Lawrence Livermore National Laboratory*; John Karnes, *Lawrence Livermore National Laboratory*; Kyle Champley, *Lawrence Livermore National Laboratory*; Maxim Shusteff, *Lawrence Livermore National Laboratory*;

Volumetric additive manufacturing (VAM) produces a complete 3D polymer part by exposing a rotating resin to a synchronized set of optimized images from computed tomography projections. This one-step process overcomes inhomogeneous layering effects in conventional stereolithography and increases the design space by allowing overhanging and freestanding structures. Part accuracy and feature resolution are a complex function of resin properties, light source, and the dose-based tomographic reconstructions. To explore sensitivity to process parameters, we have developed a VAM computational model based on a mathematical description of polymerization chemistry and transport at the continuum level. Dynamic light patterns from the optimized back-projection algorithm, identical to those in the physical system, are incorporated into the simulations. Resin optical properties and polymerization kinetics are characterized experimentally and inform the physical parameters in model. The disparate length and time scales involved in the process present unique computational challenges and we demonstrate our approach to producing accurate and efficient simulations. We demonstrate the ability to predict the local degree of polymerization and inhibition effects, and discuss the sensitivity of structure dimensional accuracy to the photochemistry and tomographic reconstructions. This work performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-818423

16th U.S. National Congress on Computational Mechanics
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Title: Combining Peridynamics and Digital Image Correlation Algorithms for Challenging Strain Calculations

Author(s): *Tomas Vaitkunas, *Kaunas University of Technology*; Paulius Griškevicius, *Kaunas University of Technology*; Darius Eidukynas, *Kaunas University of Technology*; Valdas Grigaliunas, *Kaunas University of Technology*; Adi Adumitroaie, *Kaunas University of Technology*;

Digital Image Correlation (DIC) is a powerful non-contact measurement technique for 3D full field displacement and strain on almost any material surface based on digital image processing and numerical computing. Like conventional finite element (FE) method, in DIC strains are derived from displacement field by applying numerical differentiation. Thus, the system can face strain evaluation difficulties in discontinuous displacement field, for example, material with cracks or non-homogenous material. Differentiation can also induce strain errors when displacement data is noisy or has low correlation. Several methods improving DIC differentiation algorithm (e.g., image FE discretization, subset split, non-local strain measure) were offered. A new formulation of continuum mechanics – peridynamics (PD), based on integral equation of motion, was developed by S. Silling in 2000. PD theory looks very promising to analyse strains in previously mentioned challenging situations. DIC and PD coupling was used by Li [1] and Turner [2] to improve strain calculation accuracy of DIC system in discontinuous displacement field: low correlation regions of DIC system were identified and simulated by applying PD to find possible damage and predict cracks. The PD material model is defined by specific parameters which depend on material properties, such as bulk, shear modulus, Poisson's ratio and fracture toughness. More precise material model identification could lead to more accurate PD simulation. In our study we first analyse another possibility of applying PD differential operator directly to continuous displacement field given from DIC system, for the case when the DIC displacement data is affected by errors (high noise, low correlation coefficient). The second part of the study investigates the possibility to use DIC measurements in order to calibrate the PD material parameters (as, for example, applied for the calibration of FE material model by Stander [3]). The PD model calibrated in this way could increase the accuracy of the PD simulation and thus the strain evaluation in challenging regions. [1] T. Li, X. Gu, Q. Zhang and D. Lei, Coupled Digital Image Correlation and Peridynamics for Full-Field Deformation Measurement and Local Damage Prediction, Vol.121, no.2, pp.425-444 (Computer Modeling in Engineering & Sciences, 2019) [2] D. Z. Turner, Peridynamics-Based Digital Image Correlation Algorithm Suitable for Cracks and Other Discontinuities, Vol. 141, no.2 (Journal of Engineering Mechanics, 2015) [3] N. Stander, K. Witowsky, C. Ilg, A. Basudhar, A. Svedin, I. Gandikota, A. Haufe, S. Du Bois, D. Kirpicev, DIC-based full-field calibration using LS-Opt, 15th International LS-Dyna Users Conference, 2018

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Title: The Role of Mesh Quality and Mesh Quality Indicators in the Virtual Element Method

Author(s): *Tommaso Sorgente, *Consiglio Nazionale delle Ricerche*; Silvia Biasotti, *Consiglio Nazionale delle Ricerche*; Gianmarco Manzini, *Consiglio Nazionale delle Ricerche*; Michela Spagnuolo, *Consiglio Nazionale delle Ricerche*;

Since its introduction, the Virtual Element Method (VEM) was shown to be able to deal with a large variety of polygons, while achieving good convergence rates. The regularity assumptions proposed in the VEM literature to guarantee the convergence on a theoretical basis are therefore quite general. They have been deduced in analogy to the similar conditions developed in the Finite Element Methods (FEMs) analysis. In this presentation, we experimentally show that the VEM still converges with almost optimal rates and low errors in the L2 and H1 norms even if we significantly break the regularity assumptions that are used in the literature. These results suggest that the regularity assumptions proposed so far might be overestimated. We also exhibit examples on which the VEM sub-optimally converges or diverges. Finally, we introduce a mesh quality indicator that experimentally correlates the entity of the violation of the regularity assumptions and the performance of the VEM solution, thus predicting if a dataset is potentially critical for VEM.

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Title: Phase-Field Fracture Modeling for Chemically Strengthened Glass

Author(s): Revanth Matty, *Michigan Technological University*; Shabnam Konica, *Michigan Technological University*; Benedict Egboiyi, *Corning Science and Technology Division*; *Trisha Sain, *Michigan Technological University*;

Due to the inherent existence of surface flaws (often termed as Griffith cracks), monolithic pieces of glass demonstrate extremely poor resistance against fracture. Chemical strengthening (CS) via ion-exchange process has emerged as a powerful technique of improving the fracture strength of brittle glass. In the ion exchange process, the original glass samples are immersed into a molten alkali salt bath at a temperature below the glass transition. During the time of immersion, the alkali ions (Li+ or Na+) from the glass, that are close enough to the surface are exchanged for those from the molten salt (such as K+). This process is governed by a thermally activated ion inter-diffusion, which results in residual compressive stress on the surface of the glass, provided that the ionic radius of the inward diffusing ions is larger than the ions leaving the glass. In the present work, we demonstrate experimentally that the fracture toughness of the CS glass is not a constant material property, instead depends on the residual stress parameters. Most importantly the toughness is observed to be a function of the existing initial crack/notch length relative to the depth of compressive layer. To explain the experimental fracture behavior observed in the CS glass, we use phase-field fracture theory to model the brittle crack propagation, under the presence of residual compressive stress. The residual compressive stress is incorporated as initial state variables to the model. Fracture toughness of the CS glass samples are estimated from phase-field fracture simulations, as a function of surface compressive stress, depth of compressive layer (DOL) and initial notch length. The predicted fracture toughness values agree well with the experimentally measured data, compared to Green's function based analytical predictions. Hence, the present study affirms the use of phase-field fracture theory for simulating crack propagation and estimating fracture strength in the CS glass. Simulations involving fatigue type of loading and high rate impact are also being performed to show the fracture behavior in the CS glass under these loading.

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Title: Stable, High-Order Solutions of the One-Dimensional Burgers' Equation using a Generalized Finite Element Method

Author(s): *Troy Shilt, *The Ohio State University*; Patrick O'hara, *Air Force Research Laboratory*; Jack McNamara, *The Ohio State University*;

There is an increased interest in the application of finite element methods (FEM) to fluid dynamics problems due to a desire to obtain computationally efficient, high-order solution of multiscale flows. The generalized finite element method (GFEM) is a promising approach towards this goal due to a high-degree of flexibility for incorporating high-order features into the finite element approximation space. Previous work by the authors has explored GFEM application to fluid dynamics problems. For example, it has been shown that properties of the GFEM naturally mitigate the effect of volumetric locking in Stokes flow, a regime where viscous forces are dominant. Additionally, recent work has considered the linear advection-diffusion equation. In this work connections were made between the GFEM and variational multiscale method, which demonstrated the GFEM formulation naturally addresses instabilities arising from the advection term through use of enrichments, and without suffering from assumptions made in classical stabilized methods. The next step in progression towards developing and understanding GFEM for fluid dynamics is focused on application to the Burgers' equation, which is form identical to the advection-diffusion equation, except the advection coefficient is replaced by the solution variable, resulting in a nonlinear term. Additionally, the Burgers' equation contains an inertial and dissipation range similar to turbulence in the Navier-Stokes equations. As such, numerical simulation of the Burgers' equation presents a challenge when inertial effects dominate the solution, which is analogous to challenges associated when numerically solving high Reynolds number problems in the Navier-Stokes equations. These highly advective problems often demand highly refined discretization to accurately resolve the multiscale behavior of the system, otherwise nonphysical, node-to-node oscillations arise. Specific examples to be presented include solution to a boundary layer and shock formation problem over a range of kinematic viscosities where the linear Lagrangian FEM is known to exhibit numerical instability. Here it is shown by using solution-tailored enrichments, that stable, high-order GFEM solutions are obtainable at far fewer degrees of freedom than typical FEM approaches. Specifically, generalizable exponential and hyperbolic tangent enrichments are used which effectively capture the formation of local, steep boundary layer / shock features, thus alleviating node-to-node oscillations which arise in coarse grid, linear FEM solutions. Improved convergence in the L2 and H1 integral norms is shown with a significant reduction in error levels in the GFEM when compared to linear FEM at similar element sizes.

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Title: Estimation of Arterial Viscoelasticity through Full-Wave Elastography

Author(s): *Tuhin Roy, *North Carolina State University*; Murthy Guddati, *North Carolina State University*;

Arterial stiffness is an important biomarker for many cardiovascular diseases and can be measured through Shear Wave Elastography (SWE). Arterial SWE utilizes the acoustic radiation force to excite the arterial wall, measures the resulting wave propagation characteristics, which are in turn used to estimate the arterial stiffness. Specifically, SWE data has been employed to estimate arterial wall elastic modulus by matching the phase-velocity dispersion curves. Although this approach can estimate the elastic modulus, it cannot accurately invert for viscoelastic modulus, since the phase velocity is not strongly influenced by arterial viscoelasticity. This problem can be addressed by simulating the full-wave response, which is influenced by the viscoelasticity of the arterial wall. To this end, we present a novel computational approach combining the Padé interpolation and semi-analytical finite element (SAFE) method to result in a highly efficient forward modeling approach. The SAFE formulation takes advantage of the cylindrical geometry of the artery and utilizes Fourier series expansion in the azimuthal direction, and Fourier transform in the axial direction as well as time. The radial direction is discretized with finite elements for the interior fluid and arterial wall and perfectly matched discrete layers (PMDL) for the exterior fluid-like tissue. Appropriate interface conditions are utilized to simulate fluid-structure coupling. The viscoelasticity is simulated with the help of fractional calculus models. The computation is performed on a sparse frequency grid and the solution is interpolated using Padé interpolation on a fine frequency grid, which is then transformed back to the space-time domain. In the end, the entire simulation of 3D response takes less than 0.5 minute on a standard desktop computer. The forward model is utilized in a gradient inversion framework aimed at estimating viscoelasticity, which is parametrized by the overall modulus and the fractional order. Various forms of the objective function are explored, including misfit in the space-time response as well as misfit in effective dispersion and attenuation in selected frequency ranges. The effectiveness of the resulting algorithm is illustrated with noise-laden synthetic data. Specifically, we show that, unlike dispersion based inversion focusing on propagating waves, the proposed full-wave approach can successfully invert the viscoelastic parameters. The talk will include the details of both forward and inverse modeling approaches, along with observations related to the choice of objective functions. It will also include comments related to uncertainty quantification as well as the extensibility of Full-Wave Elastography approach to experimental data.

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Title: High-Quality Material Data Acquisition for Data-Driven Computing using Manifold Learning-Based Data-Driven Identification Approach

Author(s): *Tung-Huan Su, *National Taiwan University*; Jimmy Jean, *National Chiao Tung University*; Chuin-Shan Chen, *National Taiwan University*;

Material databases play a pivotal role in data-driven computing mechanics (DDCM) paradigm. The accuracy and robustness of data-driven computing algorithms not only require large database of stress-strain states but also rely on the noisy level of the database [1, 2]. In this work, we develop a novel data-driven identification (DDI) approach for quality enhancement of material databases. Inspiring from the work of the local convexity data-driven computing aimed for against noise and outliers in material database [2], we employed the technique of locally convex reconstruction into the original DDI approach termed as the local convexity data-driven identification (LCDDI) method [3]. In the LCDDI method, accuracy of mechanical stress-strain states can be improved using the optimal material stress coupling term, which given by projecting the material stress-strain states onto the material manifold reconstructed based on the nearest material data. Hence, through cluster sampling of the improved mechanical states (i.e. stress-strain states), high-quality database of material states can be obtained. The effectiveness of the LCDDI method to build high-quality material database is illustrated through two numerical examples dedicated to homogeneous and heterogeneous linear elastic materials. References: [1] R. Eggersmann, L. Stainier, M. Ortiz, S. Reese, Model-free data-driven computational mechanics enhanced by tensor voting, Comput Method Appl Mech Eng 373 (2021) 113499. [2] Q. He, J.-S. Chen, A physics-constrained data-driven approach based on locally convex reconstruction for noisy database, Comput Method Appl Mech Eng 363 (2020) 112791. [3] T.H. Su, J.G. Jean, C.S. Chen, A manifold learning based data-driven identification approach for high quality material database, (2021) (in preparation).

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Title: Data Driven Approach for the Deformation of Multiwalled Carbon Nanotubes

Author(s): *Upendra Yadav, *Michigan Technological University*; Shashank Pathrudkar, *Michigan Technoligical University*; Susanta Ghosh, *Michigan Technoligical University*;

We present a data-driven machine learning model to predict accurately the complex rippling deformations of multiwalled carbon nanotubes (MWCNT) made of millions of atoms. MWCNTs are modeled and simulated using conventional Atomistic-physics-based models that are accurate but computationally prohibitive for such large systems. To counter this shortcoming we propose a machine learning model that comprises a novel dimensionality reduction technique and a deep neural network-based learning in the reduced dimension. The proposed nonlinear dimensionality reduction technique extends the functional principal component analysis to satisfy the geometric constraint of MWCNT. Its novelty lies in designing a function space that satisfies the constraint exactly, which is crucial for efficient dimensionality reduction. Owing to the dimensionality reduction and several other strategies adopted in the present paper, learning through deep neural networks is remarkably accurate. The proposed model accurately matches an atomistic-physics-based model whereas being orders of magnitude faster. The model extracts universally dominant patterns of deformation in an unsupervised manner. These patterns are comprehensible and explain how the model predicts, yielding interpretability. The proposed model can form a basis for an exploration of machine learning toward the mechanics of one- and two-dimensional materials.

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Title: Geomiso SEA: A Cloud-Based Software for Non-Linear Inelastic Static Isogeometric Analysis of Complex Multi-Patch Geometries with Shell Elements

Author(s): Panagiotis Karakitsios, *Geomiso Company*; Panagiotis Kolios, *Geomiso Company*; *Vasiliki Tsotoulidi, *Geomiso Company*; George Mprellas, *Geomiso Company*;

This paper introduces Geomiso SEA, a new hybrid software for applications on isogeometric shell analysis and 3D design of complex multi-patch geometries with NURBS and T-splines. T-spline-based isogeometric analysis with shell elements has attracted increasing attention in automotive and aerospace industries, as it efficiently handles complex geometries with patches, discontinuities and irregularities. It is worth mentioning that cubic T-splines can design any geometry no matter how complex it is. Geomiso SEA (www.geomiso.com) provides non-linear inelastic static isogeometric analysis with shell elements. It is not just a plug-in, but a both stand-alone and cloud-based program, with a hybrid graphical user interface, which is used to simulate spline models of complex structures, or machine components, for analyzing their strength and behavior. Geomiso SEA is applicable to real-world industrial problems and satisfies the rising industrial need for technical software of dual computer-aided design and computer-aided analysis nature. This unique solution for seamless integration of the industrial design of any complex multi-patch geometry with its computational real-time testing, appears to be preferable to traditional finite element programs. Numerical applications on both thick (Mindlin-Reissner) and thin (Kirchhoff–Love) shells are demonstrated with a comparison between Geomiso SEA and finite element software packages. We compare the accuracy of the numerical results, as well as the matrix assembly and solver time. Parametric investigations were also conducted on the effects of the polynomial degree of the basis functions and the number of control points, knot spans and Gauss points. It represents major improvements over finite element programs, such as higher accuracy, robustness, and stability level, combined with considerably reduced computational time. This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T2EDK-00328). Keywords: Isogeometric analysis, Shell theory, Kirchhoff-Love, Mindlin-Reissner, Splines, Smooth multi-patch method, Complex geometries, Industrial applications, Software, Cloud References [1] P. Karakitsios, G. Karaiskos, A. Leontaris, P. Kolios, Geomiso TNL: A software for non-linear static T-spline-based isogeometric analysis of complex multi-patch structures, 14th World Congress in Computational Mechanics (WCCM), ECCOMAS Congress (2020). [2] A. Karatarakis, P. Karakitsios, M. Papadrakakis, GPU accelerated computation of the isogeometric analysis stiffness matrix, Comput. Methods Appl. Mech. Engrg., 269 (2014) 334-355. [3] H. Casquero, X. Wei, D. Toshniwal, A. Li, T.J.R. Hughes, J. Kiendl, Y.J. Zhang, Seamless integration of design and Kirchhoff–Love shell analysis using analysis-suitable unstructured T-splines, Comput. Methods Appl. Mech. Engrg., 360 (2020) 112765.

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Title: Embedded Discontinuity Finite Element Method (ED-FEM) for Modeling Fiber Failures in Random Fiber Networks

Author(s): *Vedad Tojaga, *KTH Royal Institute of Technology*; Artem Kulachenko, *KTH Royal Institute of Technology*; Sören Östlund, *KTH Royal Institute of Technology*;

Paper materials are natural composite materials where fibers are almost randomly distributed in a fiber network. Mechanical properties of fiber networks are known to be strongly controlled by fiber-fiber interactions and single fiber properties. A fiber network is often modeled as a beam network where beam-to-beam interactions are treated as cohesive zones and single beams stretch indefinitely without breaking. The latter assumption is not physically correct and leads to an overprediction of the mechanical response of the beam network. In this work, we present a computational modeling framework for simulating beam failures and thereby closing the gap to physically based micromechanical modeling of paper and packaging products. Modeling beam failure is a challenging engineering problem. At the onset of failure, the tangent stiffness tensor projected in a direction normal to the surface of discontinuity (commonly referred to as the localization tensor) is singular, i.e. we have a bifurcation point and the problem is ill-posed. Another implication of ill-posedness for the numerical simulation after a spatial discretization is a pathological mesh dependency of the computed result. We use the ED-FEM where a failure process zone (FPZ) is introduced into a multi-scale continuum mechanics formulation (i.e. the material is split into a small scale and a large scale defining the FPZ and the bulk material, respectively), making the computed result mesh independent. The multi-scale nature of the ED-FEM enables an operator splitting implementation method as opposed to carrying out the computations of the nodal displacement vector and the displacement discontinuity vector simultaneously with the global loop where the global stiffness matrix would be singular at the onset of failure. We show that fiber failures and fiber-fiber bond failures can contribute to the observed elastoplastic stress-strain response of paper.

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Title: Predicting the Damages in the asculature of the Brain from Traumatic Brain Injuries with an MRI Based Computational Framework

Author(s): *Vickie Shim, *The University of Auckland*; Samantha Holdsworth, *The University of Auckland*; Taerin Lee, *Seoul National University*; Shaofan Li, *University of California, Berkeley*; Micheal Dragunow, *The University of Auckland*;

Traumatic brain injury (TBI) is a leading cause of death and long-term disability, which still does not have either accurate diagnostic tools or effective treatment options1. To date, the primary focus of TBI research has been on neurons. However, Recent studies suggested that it is damages to the vasculature rather than the neurons themselves that might lead to long term consequences. The aim of this study is to develop an MR image based computational framework that can predict the vasculature damage after TBI. TBI subjects were MR scanned with the High Angular Resolution Diffusion Imaging (HARDI) 2to overcome the limitations of conventional diffusion tensor imaging. We used this to model the brain tissue as an anisotropic material. Especially, the white matter fibre tract was incorporated using an orthogonal curvilinear material coordinate system. We defined the structure-based material coordinate system which is aligned to the white matter fibre tract direction from DTI results. The Euler angles that align the reference coordinate to the final material coordinate were computed at each and every voxel. These Euler angles were then fitted as a finite element field (a node based interpolation field)3. The brain vasculature was first extracted using a novel algorithm that constructs 3D geometry of the vessels, which was then embedded in the sold model of the brain. This allowed the position of the vessels to be expressed in the brain's material coordinate system, which then deformed according to the injury pattern after TBI. This was used to simulate the change in the blood flow rate due the changes in the vessel geometry and diameters after TBI. Our result showed that the changes in the brain tissue structure due to the loss of white matter fibre tracts after TBI have significant effects in the internal strain patterns in the brain. This in turn deformed the brain vasculature in a way that changed the overall blood flow rate in the brain. The brain has the dynamic energy requirements which is primarily dependent on its blood supply. Any disruption to this will have significant effects in the progression of traumatic brain injury. Our model will be used to characterise this effect more quantitatively with an aim of finding potential biomarkers and therapeutic targets for TBI. 1. Dragunow, M. Trends in Pharm. Sc. 41, 772-92 (2020) 2. Tuch et al. MR in Medicine 48, 577-82 (2002) 3. Shim et al. IEEE Access 8, 179457-65 (2020)

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Title: Domain Partitioning Material Point Method for Evolving Multi-Body Thermal-Mechanical Contacts and Fragmentation

Author(s): Mian Xiao, *Columbia University*; Chuanqi Liu, *Columbia University*; *WaiChing Sun, *Columbia University*;

We propose a material point method (MPM) to model the evolving multi-body contacts due to crack growth and fragmentation of the thermo-elastic bodies. By representing particle interface with an implicit function, we adopt the gradient partition techniques introduced by Homel 2017 to identify the separation between a pair of distinct material surfaces. This treatment allows us to replicate the frictional heating of the evolving interface and predict the energy dissipation more precisely in the fragmentation process. By storing the temperature at material point, the resultant MPM model is able to capture the advection-discussion in a Lagrangian frame during the fragmentation, which in return affects the structural heating and dissipation across the frictional interface. The resultant model provides a more realistic predictions of the crack growths and fragmentation than discrete element models that used homogenized stress of particles to predict fragmentation, while also not requiring dynamic adaptation of data structures or insertion of interface element and hence relatively easy to implement. A staggered algorithm is adopted to integrate the mechanical field and the thermal field separately in time.Several numerical experiments are employed to validate this formulation in terms of the modeling of thermal contact, the multi-body contact interactions with thermo-mechanical responses and the dynamic fracture responses. A three-grain crush simulation is performed to illustrate the capability of this work for capturing dynamic crack pattern, post-fracture iteration and the coupling between mechanical and thermal fields.

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Title: Modeling Cracks with Frictional Contact in Thermomechanics via Phase Field and Stabilized Variational Multiscale Method

Author(s): *Wan Wan, *The Pennsylvania State University*; Pinlei Chen, *The Pennsylvania State University*;

Fully coupled thermomechanical problems with interfaces have attracted considerable interest for various engineering applications. In this study, a computational framework is proposed for thermomechanical contact and debonding problems with proper thermal resistance at the interface. Using the Variational Multiscale (VMS) framework, we present a fully coupled thermomechanical formulation with an explicit expression of the pressure at the contact interface. The formulation considers the quasi-static balance of the momentum and the transient heat transfer problem in a fully coupled fashion. At the interface, two different contact constitutive models are utilized for tension and compression. For tensile problems, in the mechanical phase, a tensile debonding model is employed, whereas in the thermal phase, the displacement-dependent model is employed. For compressive problems, in the mechanical phase, a Coulomb frictional model is employed, while in the thermal phase, a pressure-dependent model is embedded. Because of the naturally derived interface stability terms that possess area- and stress-weighting, the proposed VMS formulation accommodates contact/debonding and contact/frictional sliding at the interface due to both thermal and mechanical loading without losing numerical stability. In addition, phase field method is applied to model cracks with frictional contact and is compared with the VMS method. The proposed method is applied to a class of numerical test problems, including a large scale structural dam problem with discontinuity at the interfaces, and good agreement with analytical and numerical data is achieved.

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Title: Sequential Optimal Experimental Design Using Reinforcement Learning with Policy Gradient

Author(s): *Wanggang Shen, *University of Michigan*; Xun Huan, *University of Michigan*;

Experimental data play a crucial role for developing and refining models in computational mechanics. Some experiments are more useful than others, however, and well-chosen experiments can provide substantial resource savings. Optimal experimental design (OED) thus seeks the most valuable experiments and their data. When multiple experiments can be conducted in sequence, common current design practices use suboptimal approaches: batch (open-loop) design that chooses all experiments simultaneously with no feedback of information, and greedy (myopic) design that optimally selects the next experiment without accounting for future consequences and changes. In contrast, the sequential optimal experimental design (sOED) formulation is free of these limitations, and achieves the true optimality with respect to the entire design horizon. With the goal of acquiring data for inferring unknown parameters in physical systems, we develop a rigorous Bayesian formulation for sOED using an objective that incorporates a measure of information gain. A sequential design problem thus involves finding good policies—that is, functions that instruct design choices depending on the current state. We develop numerical tools for finding the optimal policies, targeting finite horizon design problems while accommodating nonlinear models with continuous parameter, design, and observation spaces. We solve for (near-)optimal policies numerically via policy gradient methods from reinforcement learning. In particular, we directly parameterize the policies and value functions by neural networks—thus adopting an actor-critic approach—and improve them using gradient estimates produced from simulated design and observation sequences. The overall method is demonstrated on an algebraic benchmark and a sensor movement application for contaminant source inversion in a convection-diffusion field. The results provide intuitive insights on the benefits of feedback and lookahead, and indicate substantial computational advantages compared to previous numerical approaches based on approximate dynamical programming.

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Title: Multiple Projection Markov Chain Monte Carlo Algorithms on Submanifolds

Author(s): *Wei Zhang, *Zuse Institute Berlin*; Tony Lelievre, *Ecole des Ponts ParisTech*; Gabriel Stoltz, *Ecole des Ponts ParisTech*;

In this talk, we present two Markov Chain Monte Carlo (MCMC) algorithms for the sampling of probability distributions on submanifolds. The first one is a MCMC method in the state space based on the standard MALA method, while the second one is based on HMC and its generalizations in the phase space. Both algorithms are new in that they allow the use of set-valued maps in the proposal step. We show that the new algorithms indeed sample the target probability measure correctly, thanks to some carefully enforced reversibility property. We present illustrative numerical examples which demonstrate the interest of the new MCMC algorithms. This talk is based on the work: https://arxiv.org/abs/2003.09402

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Title: A Cell-Based Interpolation Scheme to Mitigate Cell-Crossing Errors in the Material Point Method

Author(s): *Wen-Chia Yang, *National Chung Hsing University*;

The material point method (MPM) consists of particles, representing sampling points on objects of interest, and predefined computational background grids to evaluate bulk behavior of the particles. Since information of objects is discretely encapsulated in these particles, MPM adopts them as integration points at grids and yields a particle-form formulation. Errors of the integration scheme are tolerable in general but can be significant when multi-linear shape functions are used in grids. In this case, error-induced artificial impact forces may appear at nodes when particles cross cell boundaries, and can destabilize simulation results, especially when nearly incompressible material is modeled. This study proposes a cell-based interpolation scheme to mitigate cell-crossing integration errors in MPM when multi-linear shape functions are used.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: High-Speed Simulation of the 3D Behavior of Myocardium Using a Neural Network PDE Approach

Author(s): *Wenbo Zhang, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*; Tan Bui, *The University of Texas at Austin*;

In-silico implementation of such complex 3D continuum soft tissue constitutive models to obtain the responses of varying boundary conditions and fibrous structures requires the solution of the associated hyperelasticity problem, which remains impractical in translational clinical time frames. To alleviate the associated substantial computational costs at the time of simulation, we have developed a neural network-based method that can simulate the 3D mechanical behavior of soft tissues. A physics-informed approach was employed to train the neural network (NN) surrogate model to give physically correct solution for a range of loading conditions by minimizing the potential energy (without any training dataset generated by finite element (FE) solver). We consider the parametric hyperelasticity problem of myocardium on domain ? with a prescribed displacement u0 on the Dirichlet boundary ?_u and a traction term t the Neumann boundary in the reference configuration. The displacement depended on the prescribed Dirichlet boundary condition. The displacement was parametrized using u(X) = UN(X) where N(X) are the finite element basis functions and U is the nodal displacement values, and the Dirichlet boundary conditions m(x) was parametrized by a vector M. Thus, solving parametric PDEs is essentially to find the parameter-to-state map U(M) that minimize the energy potential of hyperelasticity for all M. We used a fully connected neural network f_FCN along with a linear term TM as the surrogate model to approximate the parameter-to-state map. We considered a cube of nearly incompressible myocardium with dimensions 1.0 × 1.0 × 1.0. The training range was based on deformation over the entire physiological range. The NN had 1 hidden layer of 100 neurons. The results obtained with present NN matched closely with the finite element method which has 8000 nodes (20×20×20). The compute time for one prediction of the NN surrogate model was 0.02236 s, while the FE solver takes 6.5762 s for one step. In summary the present method was found to be an order of 100 times faster than the equivalent FE model (using the same mesh on the same machine). With the learnability of the neural networks, the architecture of the NNs can incorporate attributes such as spatially varying fiber structures. By shifting the computation expense from FE problem solving to NN training, the NN surrogate model can be used to give significantly fast predictions of complex 3D deformations in full kinematic space with population-based fiber structures by forward propagation in the neural network.

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Title: Towards a Generalized Engineering Theory for Hydrodynamic Slamming Emanating from Partitioned Fluid-Structure Interaction Analysis

Author(s): *Wensi Wu, *Cornell University*; Christopher Earls, *Cornell University*;

Theoretical study of hydrodynamic slamming phenomenology was first undertaken by von Karman in his 1929 report focused on the impact of seaplane floats during landing. This seminal work opened the door to theoretical investigations into the effects of slamming (characterized by highly concentrated, nearly instantaneous fluid pressures) on the structural behavior of watercrafts. Since this initial work, the physics of wave slamming has been explored theoretically, experimentally, and numerically to better understand the underlying hydrodynamic and hydroelastic effects that characterize the behavior of a deformable structure impacting a water free surface. In spite of all this effort, a general engineering theory in wave slamming has yet to be uncovered, to this day. The reasons for this emanates from the intricacy in interplay between complex fluid flows and nonlinear structural deformations (most existing theories are limited to rigid body deformations) that accompany the phenomenology of slamming. In the present work, the authors aim to develop of a somewhat general wave slamming theory, by examining the oblique impact of a flexible plate during water entry using an in-house developed Fluid-Structure Interaction (FSI) solver. The computational framework of the FSI solver is built upon an implicit, partitioned coupling of an open source computational fluid dynamics (CFD) software (OpenFOAM) with an open source computational structural dynamics (CSD) library (CU-BENs). Numerical experiments, focusing on three specific aluminum plate geometries (i.e. approximately rigid, moderately deformable, and very flexible), each subject to a range of impact velocities, are considered. The hydroelastic response obtained from FSI analyses of these cases are validated against experimental data, to assess the veracity of the FSI solver. Subsequent to validation, a series of numerical simulations are carried out in an effort to characterize the global behavior of impact forces that contribute to the plate’s out-of-plane deformation in relation to impact velocities. A generalized engineering theory for slamming is subsequently formulated.

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Title: Shock Capturing in Nodal Spectral Element Methods Via Riemann Solutions for Intra-Element Fluxes

Author(s): *Will Trojak, *Texas A&M University*; Tarik Dzanic, *Texas A&M University*; Freddie Witherden, *Texas A&M University*;

We will present a novel approach to shock capturing in high-order discontinuous spectral element methods which uses the techniques of invariant domain preservation to construct a scheme devoid of tunable parameters. The method can be understood as a generalization of the Lax-Friedrichs flux to a high-order staggered grid of flux and solution points. Several theorems will be presented that demonstrate the stability of the method with respect to convex sets of admissible solutions. The technique is further enhanced by a novel point-local shock sensor based on the entropy residual that is independent of grid spacing and polynomial order, which enables sub-element levels of resolution for discontinuous solutions even at very high orders. We will go on to show the effectiveness of this method in several numerical test cases that include smooth solutions, complex shock interactions, nonlinear meshes, and practical applications.

16th U.S. National Congress on Computational Mechanics
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Title: Unconditionally Stable Numerical Algorithms for Evolution of Point-Sources in Wave Propagation Problems

Author(s): *William Sands, *Michigan State University*; Andrew Christlieb, *Michigan State University*;

In this talk, we discuss our work on extending a new class of solvers for wave propagation to couple with systems described by moving point-sources. This new class of solvers is based on an implicit, dimensionally-split formulation that replaces traditional differential operators with certain integral operators that can be evaluated in an efficient and scalable manner. We propose a hybrid approach that blends these ideas with components of a boundary-integral representation to allow for a true representation of point-sources. Experimental results for the proposed method are provided which demonstrate its effectiveness.

16th U.S. National Congress on Computational Mechanics
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Title: Untangling Inelasticity and Phase Transition Kinetics in Sn Under Extreme Deformation Conditions

Author(s): *William Schill, *Lawrence Livermore National Laboratory*; Ryan Austin, *Lawrence Livermore National Laboratory*; Kathleen Schmidt, *Lawrence Livermore National Laboratory*; Jon Belof, *Lawrence Livermore National Laboratory*; Justin Brown, *Sandia National Laboratories*; Nathan Barton, *Lawrence Livermore National Laboratory*;

Ramp-driven compression-release experiments offer possibilities to explore material response under conditions distinct from those accessed by shock-driven loading conditions. For a material undergoing phase transformation, the problem of material model identification from experimental measurement is made substantially more complex by the need to untangle not only elasticity and plasticity, but also features introduced by the phase transformation. Tin exhibits a complex phase diagram within a relatively accessible range of temperature and pressures and the characterization of its phases is considered an open problem with significant scientific merit. Moreover, under extreme loading conditions, equilibrium phase transition modeling appears insufficient, suggesting the presence of important kinetic processes. Simulation results are compared to recent observations of Sn response in ramp-driven compression-release experiments. We employ Bayesian statistical techniques with a full forward model of the experiment to explore the interactions between inelasticity and phase transition kinetics in Sn. The degree to which these different kinetic processes can be distinguished given velocimetry data is discussed.

16th U.S. National Congress on Computational Mechanics
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Title: A Hybrid Reaction-Diffusion-Monte Carlo Method for Modelling Signal Transduction in Crowded Environments

Author(s): *Wylie Stroberg, *University of Alberta*; Santiago Schnell, *University of Michigan*;

Several decades of theoretical work has placed physical limits on the accuracy with which receptors on the surfaces of cells can infer local ligand concentrations. However, cells must also measure concentrations within the cytoplasm and cellular compartments in order to maintain homeostasis. Measuring intracellular concentrations of chemical species fundamentally differs from measuring the extracellular environment due to the high degree of macromolecular crowding inside of cells and subcellular compartments. Crowding influences both the rate at which ligands and receptors encounter one another, as well as the transition rates between transient contacting ligand-receptor pairs and the stably bound complexes. Modelling such interactions poses two challenges: 1. The model must capture the heterogeneity of the crowded subcompartments, and 2. The simulation must be efficient enough to generate robust statistics of relatively rare binding events. In this work, we combine particle-based reaction diffusion simulations with Monte Carlo sampling to efficiently determine the accuracy of a concentration-sensing receptor as a function of macromolecular crowding. Compared to particle-based reaction diffusion simulation alone, the hybrid method is shown to determine binding statistics to the same accuracy at less than 1/10th the computational cost. This method can be used to understand and quantify information processing by cellular signalling pathways in the crowded cellular interior.

16th U.S. National Congress on Computational Mechanics
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Title: Towards Fully Automatic 3D NEFEM Mesh Generation

Author(s): *Xi Zou, *Swansea University*; Rubén Sevilla, *Swansea University*; Oubay Hassan, *Swansea University*; Kenneth Morgan, *Swansea University*;

The preparation of geometric models to perform simulations is known to be a major bottleneck when dealing with complex geometries. This is caused by the excessive number of human hours required to transfer information from a computer aided design (CAD) model to a computer aided engineering (CAE) model suitable for simulation. CAD models frequently involve a level of detail much greater than that required to perform a computational simulation. Over the last two decades, a large research effort has been placed on the development of algorithms for de-featuring complex CAD models. However, de-featuring cannot be fully automatised. Firstly, it is usually not possible to know, a priori, the effect of de-featuring on the results of a simulation. Secondly, the required de-featuring is different for fluid dynamics, electromagnetics, acoustics, heat transfer or structural mechanics applications. Finally, de-featuring is dependent upon the level of approximation required. When small geometric features are present in a CAD model, traditional mesh generators will produce small, often distorted, elements, when the spacing specified by the user is much larger than the size of the small features. The NURBS-enhanced finite element method (NEFEM) addresses this problem by completely decoupling the concepts of geometric and solution approximation. These two concepts are tightly coupled in the large majority of available solvers through the isoparametric concept. With NEFEM, the geometric description of the boundary uses the B-rep available in the CAD model, whereas polynomial functions are used to approximate the solution. This new concept completely avoids the need for de-featuring and, at the same time, is able to use meshes where the size of the elements is entirely decided by the user and not by the presence of geometric features smaller than the specified spacing. This work will present a new mesh generation technique where boundary faces span across multiple surfaces and retain the exact B-rep. The surface mesh generation process will be detailed, including the new data structures that have been devised to store the information required by NEFEM elements. New algorithms, in particular, the local enhanced advancing front method, have been implemented to fulfil the creation of boundary faces that span across multiple surfaces. The creation of the volume mesh will be outlined, and several examples will be presented to show the potential of the proposed technique. [1] Sevilla et al. (2016) The generation of triangular meshes for NURBS-enhanced FEM. Int. J. Numer. Meth. Engng, 108: 941-968.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Fabric-Enriched Continuum Breakage Mechanics for Cemented Granular Materials in Surface-Reactive Environments

Author(s): *Xianda Shen, *Northwestern University*; Giuseppe Buscarnera, *Northwestern University*;

Cemented granular geomaterials are moisture-sensitive materials, which exhibit anisotropic mechanical properties as a function of deposition history, microscopic fabric, and loading paths. Their yielding and stress-strain response are modulated by the relative humidity of their environment. Here, a new fabric-enriched continuum breakage model is proposed to examine the humidity-driven weakening mechanisms and the relation between elastic and inelastic anisotropy in cemented granular materials exposed to varying environmental conditions. A microstructure model is formulated to capture the evolution of the solid-fluid interfaces by accounting for the grain breakage and cement disintegration. This microstructure model is then implemented in the framework of fabric-enriched continuum breakage mechanics (F-CBM), where the anisotropic behavior prior to yielding is introduced through a symmetric second-order fabric tensor embedded in the expression of the elastic energy potential. The anisotropic strain energy storage prior to grain crushing leads to the rotation and distortion of the yield surface of cemented granular materials. Parametric analyses are performed to assess the overall capability of the model to characterize the anisotropic inelastic processes in cemented granular solids under both wet and dry conditions. The water sensitivity of the continuum formulation is developed based on the measured water adsorption properties of both grain and cement phases. It is shown that the proposed model can accurately predict the strong correlation between anisotropic elasticity and breakage-damage processes in cemented granular materials. The deformability and strength of cemented granular materials are assessed by successfully capturing the moisture-weakening effects. It is shown that the reduction of moisture enhances the yield stress and increases the brittleness of the post-yielding response of cemented granular materials. When damage involving the skeleton is the dominant inelastic process, the size of the elastic domain contracts and the material exhibits augmented brittleness with the disintegration of cement. While breakage processes are predicted to dominate the response of lightly cemented granular materials, which results in hardening behavior. The formulated approach captures the breakage and damage processes of anisotropic cemented solids in surface-reactive environments. This work can be further extended to dynamically characterize the anisotropic response of cemented granular materials with water-sensitive mineral constituents by accounting for the evolution of microstructural anisotropy.

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Title: Multiscale Design of Nonlinear Materials with Reduced-Order Modeling

Author(s): David Brandyberry, *University of Illinois at Urbana-Champaign*; *Xiang Zhang, *University of Wyoming*; Philippe Geubelle, *University of Illinois at Urbana-Champaign*;

Recent progress in multiscale modeling and sensitivity analysis, together with advances in additive manufacturing, have allowed for the development of an integrated framework to design and manufacture microstructural geometrical features and constituent properties of heterogeneous media to deliver a desired stress-strain response. However, the prohibitive computational cost associated with multiple optimization iterations and costly evaluation of every nonlinear multiscale problem limits the application of this workflow, especially for cases that involve complex microstructure and different deformation modes. Here we present a multiscale reduced-order optimization method for efficient nonlinear microstructure material design. This method builds on the recent development of Interface-enriched Generalized Finite Element Method (IGFEM)-based reduced-order modeling techniques used to formulate a reduced-order representation of the microstructure problem. Model order reduction is achieved by partitioning the microstructure's volume and interface into a number of subdomains called 'parts', where a series of influence function problems based on the elastic properties of the microstrucrue are solved a priori to obtain the interaction coefficients between the different parts and between each part and the microstructure. Based on these interaction coefficients, and the assumption that the response in each part is uniform, a system of linear algebraic equations is derived to replace the microstructure problem with part-wise response as unknows. In addition, the sensitivities of the homogenized response on the material properties of the microstructural constituents are transferred to the sensitivities of the influence functions associated with each part. These sensitivities are conveniently calculated using IGFEM when solving the influence functions and do not change during the nonlinear material optimization process as the influence functions only depend on the elastic properties of the microstructure. The reduced-order evaluation of the homogenized response and its sensitivities with regards to the material properties of the different phases and interfaces defining the microstructure allows us to optimize very efficiently the microstructure's material properties with multiple initial states. From these initial states, we choose the best optimization results and further conduct a full IGFEM-based optimization to obtain the final optimization result. This two-step optimization process is demonstrated to deliver good results in the multiscale design of 3D particulate composites in the presence of both volumetric and interfacial damage.

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Title: Probing the Mechanical Principle of 3-Hinge Gyral Formation and its Role in Brain Networks

Author(s): *Xianqiao Wang, *University of Georgia*;

Soft tissues are complex materials with typical nonlinear, anisotropic, inhomogeneous behaviors subjected to large strains and stresses. Growth or atrophy of soft materials in media may lead to instability and formation of surface wrinkling, folding or creasing. The cortical folding of brain, characterized by convex gyri and concave sulci, has an intrinsic relationship to the brain's functional organization. Understanding the mechanism of convolution patterns can provide useful insight into normal and pathological brain functioning. However, despite decades of speculation and endeavors the underlying mechanism of the folding process remains poorly understood. In this work, formation of complex patterns on the surface of brain, during cortical folding phenomenon, is interpreted by both mechanical modeling and imaging. In the modeling part, non-linear finite element (FE) models based on finite growth are employed to present growth, folding and formation of "3-hinges" of the growing brain and in the imaging part all Human Connectome Project (Q3 release) data was used to reconstruct white matter surfaces from structural MR scans of 868 healthy subjects. Then, we developed a robust algorithm to detect gyri lines and also number and location of 3-hinges in the brain in both FE models and images. Results show that after growth, tertiary convolutions and the exact locations of 3-hinges are unpredictable. Results indicate that in all computational models, qualitative features of folds and 3-hinges are similar to each other, but location and type can be quite different. We can observe same variation of 3-hinges locations in different individual brains. We also extracted the dominant patterns of 3-hinges to create a comparison with those taken from brain imaging data. For the imaging part, the dominant patterns of 3-hinge patterns and their percentages in 68 brain subjects were extracted, and for computational part, 30 FE models were used. The comparison indicates that the "Y" shape 3-hinge is the most favorable pattern in real brains as well as in FE models, although the real brain prefers more convoluted 3-hinges. Our study provides a mechanism to explain why locations and patterns of some specific 3-hinges are consistent. The growth, instability and convolution of the growing brain is a dynamic process, and a small difference between two initial states can lead to different 3-hinges patterns at different locations. Therefore, the type and number of 3-hinge patterns in a developing brain could be a new metric to characterize folding of a primate brain.

16th U.S. National Congress on Computational Mechanics
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Title: A Superconvergent Hybrid-Variable Discretization Method for Hyperbolic Problems

Author(s): *Xianyi Zeng, *The University of Texas at El Paso*; Md Mahmudul Hasan, *The University of Texas at El Paso*;

We present recent progresses in a superconvergent hybrid-variable (HV) discretization method [1, 2] to solve nonlinear hyperbolic conservation laws in one and two space dimensions. The HV framework is characterized by using both nodal and cell-averaged approximations to the solutions to construct discrete differential operators, and it is proven to be superconvergent irrespective of mesh uniformity and requires no data post-processing. In this talk, we investigate two strategies to remove spurious oscillations that are essential to improve the robustness of the algorithm. In the first approach, the artificial viscosity is adopted to capture strong discontinuities that frequently occur in nonlinear conservation problems. To this end, our exploration begins with the investigation of using HV methods to solve the model advection-diffusion equation while confirming the universal superconvergence property; next, the previous analysis is utilized to construct artificial viscosities that efficiently suppress spurious oscillations. In the second approach, we focus on reducing the numerical dispersion by developing a compact HV computational framework [3]. Particularly, hybrid- variable low-pass filters are utilized to remove the high-frequency data nearby discontinuities. We study the accuracy and stability of the methods by both theoretical analysis and numerical verifications. [1] X. Zeng. A high-order hybrid finite difference-finite volume approach with application to inviscid compressible flow problems: A preliminary study. Comput. Fluids, 98, 2014. [2] X. Zeng. Linear hybrid-variable methods for advection equations. Adv. Comput. Math., 45, 2019. [3] M. M. Hasan and X. Zeng. Compact hybrid-variable methods for acoustics problems and Euler equations. In preparation..

16th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Optimisation of Lattice-Skin Structures

Author(s): *Xiao Xiao, *Inria*; Fehmi Cirak, *University of Cambridge*;

Lattice-skin structures comprised of a lattice and a thin-shell have been adopted in engineering for their favourable properties such as a high strength-to-weight ratio and functional advantages. The recent advancement of additive manufacturing techniques allows producing large components with designed geometric features reaching down to sub-millimetre scale, broadening industrial applications of lattice-skin structures. We introduce an approach for the infill and shape optimisation of lattice-skin structures within an isogeometric design and analysis framework. The lattice consists of unit cells with each containing a small number of struts, and it conforms to the thin-shell shape. The Kirchhoff-Love thin-shell is discretised with a subdivision surface [1], and the lattice containing a large number of struts is explicitly modelled as a pin-jointed truss. The conforming lattice is created with the spline surface interrogation using implicit matrix representations [2]. The lattice-skin coupling is enforced with a Lagrange Multiplier approach. A SIMP-like penalisation and filtering technique is proposed to optimise the lattice infill topology without the homogenisation of the lattice, such that it is also applicable to non-periodic lattices. The freeform deformation technique is applied to parametrise the lattice-skin geometry for shape optimisation. The shapes of two different structural forms are sequentially updated and the lattice-skin coupling is thus guaranteed in the optimisation process. [1] F. Cirak, Q. Long. Subdivision shells with exact boundary control and non-manifold geometry, Internat. J. Numer. Methods Engreg. 88 (2011) 897-923. [2] X. Xiao, M. Sabin, F. Cirak, Interrogation of spline surfaces with application to isogeometric design and analysis of lattice-skin structures, Comput. Methods Appl. Mech. Engrg. 351 (2019) 928-950.

16th U.S. National Congress on Computational Mechanics
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Title: A Machine-Learning Framework for Peridynamic Material Models with Physical Constraints

Author(s): *Xiao Xu, *The University of Texas at Austin*; Marta D'Elia, *Sandia National Laboratories*; John Foster, *The University of Texas at Austin*;

As a nonlocal extension of continuum mechanics, peridynamics has been widely and effectively applied in different fields where discontinuities in the field variables arise from an initially continuous body. An important component of the constitutive model in peridynamics is the influence function which weights the contribution of all the interactions over a nonlocal region surrounding a point of interest. Recent work has shown that in solid mechanics the influence function has a strong relationship with the heterogeneity of a material's micro-structure. However, determining an accurate influence function analytically from a given micro-structure typically requires lengthy derivations and complex mathematical models. To avoid these complexities, the goal of this paper is to develop a data-driven regression algorithm to find the optimal bond-based peridynamic model to describe the macro-scale deformation of linear elastic medium with periodic heterogeneity. We generate macro-scale deformation training data by averaging over periodic micro-structure unit cells and add a physical energy constraint representing the homogenized elastic modulus of the micro-structure to the regression algorithm. We demonstrate this scheme for examples of one- and two-dimensional linear elastodynamics and show that the energy constraint improves the accuracy of the resulting peridynamic model.

16th U.S. National Congress on Computational Mechanics
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Title: Computational Mechanics in the Upstream Oil and Gas Industry

Author(s): *Xiao-Hui Wu, *ExxonMobil Upstream Integrated Solutions Company*;

Computational mechanics has a wide range of important applications in the upstream oil and gas industry. From remote sensing of the subsurface structures using seismic waves to predicting reservoir performance from multiphase fluid flow in porous media, from understanding natural fracture distributions to predicting the shape, reach, and density of hydraulic fractures, computational mechanics plays a crucial role. The continuum mechanics models are used not only to make forward predictions, they are also used to solve large-scale inverse problems against limited data in order to better understand the subsurface and reduce uncertainty. In addition, computational mechanics is utilized to solve computational geometry problems in reservoir modeling. In this talk, an overview of the applications of computational mechanics in the upstream industry is presented, along with a discussion of practical computational challenges and potential research opportunities.

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Title: Seamless Coupling of Nonlocal and Local Energies via Varying Horizons

Author(s): *Xiaochuan Tian, *University of California, San Diego*;

We consider nonlocal integral models with a spatially varying horizon that allows the range of nonlocal interactions to be position-dependent. In particular, we focus on linear variational problems of such nonlocal models with heterogeneous localization on co-dimension one interfaces. Such nonlocal models not only lead to mathematically well-posed nonlocal problems with classical Neumann- and Dirichlet-type boundary conditions, but also allow a seamless coupling with local models. We will see that the coupling errors can be well controlled if the horizon function is slowly varying. However, in practice, we may want to use piecewise linear horizon functions, and in this case we can construct auxiliary functions to minimize the coupling errors. This is a joint work with Qiang Du and Yunzhe Tao.

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Title: Isogeometric V-rep: Efficient and Robust Integration

Author(s): *Xiaodong Wei, *École polytechnique fédérale de Lausanne*; Pablo Antolin, *École polytechnique fédérale de Lausanne*; Annalisa Buffa, *École polytechnique fédérale de Lausanne*;

We present an efficient and robust integration method to deal with volume representations (V-reps) in isogeometric analysis. In contrast to boundary representations (B-reps), the building blocks of V-reps are B-spline or NURBS (Non-Uniform Rational B-Spline) trivariates that generally involve trimming. While the related theories have been established in our precedent works [1,2], here we focus on the corresponding algorithms to generate quadrature meshes for trimmed trivariates, including: (1) decomposition of a trimmed element into a collection of cells where the standard Gauss quadrature rule can be applied, and (2) reparameterization of the involved trimming surface in each cell as a Bézier surface. In particular, we adopt the marching-cubes cases [3] as the base cases and develop a corresponding decomposition for each of them to minimize the number of the resulting cells. Such a cell can be a hexahedron, wedge, pyramid, or a tetrahedron. On the other hand, a general trimmed element is recursively subdivided until every subelement falls into one of the base cases. In the end, we present several 3D examples to show the robustness of the proposed method. [1] Antolin, P., Buffa, A. and Martinelli, M. Isogeometric analysis on V-reps: First results. Computer Methods in Applied Mechanics and Engineering, 355:976--1002, 2019. [2] Antolin, P., Buffa, A., Puppi, R. and Wei, X. Overlapping multi-patch isogeometric method with minimal stabilization. SIAM J. Sci. Comput., 43(1), A330–A354, 2021. [3] Lorensen, W.E. and Cline, H.E. Marching Cubes: A high resolution 3D surface construction algorithm. SIGGRAPH Comput Graph, 21:163--169, 1987.

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Title: Parametrically Homogenized Continuum Damage Mechanics (PHCDM) Models for Composites using Physics-Informed Machine Learning

Author(s): *Xiaofan Zhang, *Johns Hopkins University*; Yanrong Xiao, *Johns Hopkins University*; Daniel O'Brien, *US Army Research Laboratory*; Somnath Ghosh, *Johns Hopkins University*;

Parametrically Homogenized Continuum Damage Mechanics (PHCDM) models are developed for glass fiber reinforced epoxy composites undergoing progressive damage. Damage in composite materials exhibits different failure behaviors across various material length scales – microscopic damage phenomena such as fiber-matrix interfacial debonding and micro-cracking in matrix phase subsequently leads to macroscopic failure behaviors such as structural stiffness degradation and crack propagation. Detailed micromechanical models can be built in order to accurately capture the dependence of microscopic damage behaviors on the composite microstructure (e.g., fiber volume fractions, fiber distributions, etc.). However, these micromechanical models are computationally expensive thus limited to microscale problems. On the other hand, the existing continuum damage approaches feasible for structural analysis neglect those microstructural effects. To overcome these limitations, the developed Parametrically Homogenized Continuum Damage Mechanics (PHCDM) models present a multiscale modeling framework through parametric homogenization, data synthesis and physics-based machine learning, which enables direct micro-macro connection through energy equivalence. The macroscopic constitutive law is developed based on detailed study of the micromechanical models under various loading scenarios. The microstructural effects, denoted via Representative Aggregated Microstructural Parameters (RAMPs), are explicitly incorporated into some functional representations of the parameters in PHCDM models. Extensive machine learning and data-driven techniques are employed during the calibration of PHCDM models such as sensitivity analysis, dimension reduction, symbolic regression and artificial neural networks. The developed PHCDM models can be easily implemented via user-subroutines (UMAT/VUMAT) in any FEM packages and they provide insight on damage behaviors across different material length scales and microstructural features with affordable computational effort. These merits of PHCDM make it a great tool for material-by-design process as well as understanding the multi-scale phenomena in material failures. Finally, some macroscopic examples will be demonstrated in which PHCDM models are applied to predict damage behaviors at various material length scales. Reference: Xiaofan Zhang, Daniel J. O'Brien, Somnath Ghosh, Parametrically homogenized continuum damage mechanics (PHCDM) models for composites from micromechanical analysis, Computer Methods in Applied Mechanics and Engineering, Volume 346, 2019, Pages 456-485

16th U.S. National Congress on Computational Mechanics
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Title: Adaptive Basis for Multifidelity Uncertainty Quantification

Author(s): *Xiaoshu Zeng, *University of Southern California*; Gianluca Geraci, *Sandia National Laboratories*; Michael Eldred, *Sandia National Laboratories*; John Jakeman, *Sandia National Laboratories*; Alex Gorodetsky, *University of Michigan*; Roger Ghanem, *University of Southern California*;

Multifidelity Uncertainty Quantification (MF UQ) is emerging as an efficient tool for enabling predictive analyses of high-fidelity systems. MF UQ strategies, e.g. Approximate Control Variate (ACV) [1], have been introduced to alleviate the prohibitive computational cost of UQ by leveraging a large number of evaluations of inaccurate models in combination with a limited number of realizations for the target high-fidelity model. We have recently demonstrated [2] how the Adaptive Basis (AB) method [3], which provides a rigorous way to identify lower dimensional manifolds to represent the input-output mapping of a computer model, can also be used to enhance the correlation between models with a dissimilar input parametrization within a sampling MF UQ workflow. In this contribution, we plan to extend [3] by combining AB with MF UQ strategies based on both sampling, e.g. ACV, and surrogate approaches, e.g. MFNets, in order to derive more flexible methods which are both flexible and capable of handling scenarios in which multiple low-fidelity models are available simultaneously. In the former case, the AB method will be used to align the low dimensional manifolds of different models and thus enhance the correlation among them, while in the latter, the AB method will be adopted as a general model reduction technique in UQ to build surrogate models. Several numerical test cases, which range from verification test cases to model problems and simplified computational applications, will be presented and discussed to demonstrate the advantages of the proposed strategies with respect to both single fidelity and classical MF UQ approaches. [1] Gorodetsky, A.A., Geraci, G., Eldred, M.S., and Jakeman, J.D., A Generalized Approximate Control Variate Framework for Multifidelity Uncertainty Quantification, J. Comput. Phys., 408:109257, 2020. [2] Tsilifis, P. and Ghanem, R. Reduced Wiener Chaos representation of random fields via basis adaptation and projection. Journal of Computational Physics, 341, pp. 102-120, 2017. [3] Zeng, X., Geraci, G., Gorodetsky, A.A., Eldred, M.S., Jakeman, J.D., Ghanem, Roger, Uncertainty Quantification with Multifidelity Strategies based on Models with Dissimilar Parameterizations, 14th World Congress on Computational Mechanics (WCCM), ECCOMAS Congress 2020. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

16th U.S. National Congress on Computational Mechanics
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Title: Bayesian Neural Networks for Weak Solution of PDEs with Uncertainty Quantification

Author(s): *Xiaoxuan Zhang, *University of Michigan*; Krishna Garikipati, *University of Michigan*;

The mathematical treatment of physical systems that are described in terms of field variables leads to partial differential equations (PDEs). However, the large scale solutions of PDEs using state of the art discretization techniques remains an expensive proposition. In this work, a new physics-constrained neural network (NN) approach is proposed to solve PDEs without labels, with a view to enabling high-throughput solutions in support of design and decision-making. Distinct from existing physics-informed NN approaches, where the strong form or weak form of PDEs are used to construct the loss function, we write the loss function of NNs in terms of the residual of PDEs obtained through an efficient, discrete, convolution operator-based, and vectorized implementation. We explore an encoder-decoder NN structure for both deterministic and probabilistic models, with Bayesian NNs (BNNs) for the latter, which allow us to quantify both epistemic uncertainty from model parameters and aleatoric uncertainty from noise in the data. For BNNs, the discretized residual is used to construct the likelihood function. In our approach, both deterministic and probabilistic convolutional layers are used to learn the applied boundary conditions (BCs) and to detect the problem domain. Bboth Dirichlet and Neumann BCs are specified as inputs to NNs, and therefore a single NN can solve for similar physics; i.e., the same PDE, but with different BCs and on a number of problem domains. The trained BNN PDE solvers can make interpolation and also (to a certain extent) extrapolation predictions for BCs that they were not exposed to during training. Such NN solution frameworks assume particular importance in problems, where the PDEs need to be repeatedly solved numerous times with different boundary conditions and on varying domains. We demonstrate the capacity and performance of the proposed framework by applying it to different steady-state and equilibrium boundary value problems with physics that spans diffusion, linear and nonlinear elasticity. References [1] Xiaoxuan Zhang and Krishna Garikipati. Bayesian neural networks for weak solution of PDEs with uncertainty quantification. arXiv:2101.04879, pages 1-37, 2021.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Computational Periporomechanics for Modeling Dynamic Failure of Porous Media

Author(s): *Xiaoyu Song, *University of Florida*; Shashank Menon, *University of Florida*;

We present a stabilized computational periporomechanics model for dynamic analysis of saturated porous media. A fully implicit time integration scheme is exploited to solve the stabilized coupled mathematical model. The implemented computational model is validated against analytical and numerical solutions for 1D and 2D dynamic poromechanics problems. Numerical examples are presented to show the efficacy of the proposed periporomechanics model for dynamic failure analysis of porous media.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: DimensionNet: A Deep Learning Network for Discovering Dimensionless Numbers

Author(s): *Xiaoyu Xie, *Northwestern University*; Zhengtao Gan, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

It is challenging to identify optimal dimensionless number(s) for complex physical systems using classical dimensional analysis and similitude theory due to a large number of parameters and a lack of well-tested governing equations. To this end, we propose a dimensionally invariant deep neural network (DimensionNet)[1] to automatically discover the governing dimensionless numbers from data. The DimensionNet is composed of two neural networks: (1) a scaling network to discover an explicit form of dimensionless numbers, (2) a deep feedforward network to fit the nonlinear relationship between the dimensionless numbers and desired outputs. The DimensionNet leverages dimensional analysis principles and deep learning networks. It can reduce the physical dependency of dimensional input parameters and maintain high accuracy. Furthermore, the proposed DimensionNet significantly improves the explainability and interpretability of the deep learning network and can be applied to many physical, chemical, and biological systems. Reference: 1. Saha, S., Gan, Z., Cheng, L., Gao, J., Kafka, O. L., Xie, X., Li, H., Tajdari, M., Kim, H. A., & Liu, W. K. (n.d.). Hierarchical Deep Learning Neural Network (HiDeNN): An artificial intelligence (AI) framework for computational science and engineering. Computer Methods in Applied Mechanics and Engineering, 373, 113452.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Imposing Physical Constraints Softly on Augmented Gaussian Random Fields

Author(s): *Xiu Yang, *Lehigh University*;

We provide a rigorous theoretical foundation for incorporating data of observable and its derivatives of any order in a Gaussian-random-field-based surrogate model using tools in real analysis and probability. We demonstrate that under some conditions, the random field representing the derivatives is a Gaussian random field (GRF) given that its structure is derived from the GRF regressing the data of the observable. We propose an augmented Gaussian random field (AGRF) framework to unify these GRFs and calculate the prediction of this surrogate model in a similar manner as the conventional Gaussian process regression method. The advantage of our method is that it can incorporate arbitrary order derivatives and deal with missing data. Then we demonstrate an AGRF-based approach to softly imposing physical constraints in the form of inequalities. Especially, we will illustrate our method's efficacy at preserving positivity and monotonicity.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Spatial White Matter Stiffness Variations in the Mouse Brain

Author(s): *Xuesong Zhang, *Stevens Institute of Technology*; Johannes Weickenmeier, *Stevens Institute of Technology*;

Multiple sclerosis (MS) is a demyelinating disease caused by a neuroinflammatory response that leads to the demyelination of white and gray matter axons, neuronal and axonal degeneration, and ultimately death. Most white matter axon fibers in the brain are wrapped by myelin sheaths that provide not only structural integrity to the fiber but also lead to a 10-fold increase in signaling speed along axons. In addition to the electrical importance of myelin in central nervous system, myelin is considered to play a critical role in preserving the mechanical environment in white matter tissue. Previous work used experimental methods to quantify tissue stiffness in discrete white matter locations in the corpus callosum using atomic force microscopy [1]. These and other studies typically provide an average stiffness value for local corpus callosum (CC) subregions, such that the actual spatial heterogeneity of white matter stiffness across the entire CC remains unclear. The objective of this study is to address this knowledge gap using nanoindentation experiments in coronal brain slices from healthy mice and to rationalize our measurements and microstructural observations using a microstructural white matter investigative model. Our study investigated the white matter stiffness variation patterns in healthy 14-week-old mouse CC using the nanoindentation method. The results suggest spatial heterogeneity of mouse CC stiffness which is caused by heterogeneous distribution of myelin, cell density, and fiber orientation [2]. We observed that white matter stiffness is lowest at the center of the CC (1.52±0.6 kPa) and increases when moving outwards (3.28±0.69 kPa). Our computational model allows to vary myelin content and prescribe the indentation loading state. Via inverse modeling to minimize the difference between experiments and simulation, we determine myelin properties that best reproduce our experimental measurements. Future work will show whether and how these parameters vary spatially across the CC and how they correlate with histochemical analysis of tissue microstructure. Our approach of combining mechanical testing, histology, and computational modeling will provide new insight into the heterogeneous origin of white matter stiffness. References [1] Urbanski et al. Sci. Rep. 9 (2019). [2] Min et al. Sci. Rep. 6 (2016).

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Learning Frame-Independent, Nonlocal Constitutive Relations on Unstructured Meshes with an Embedding Neural Network

Author(s): *Xuhui Zhou, *Virginia Polytechnic Institute and State University*; Jiequn Han, *Princeton University*; Heng Xiao, *Virginia Polytechnic Institute and State University*;

Constitutive models are widely used for modeling complex systems in science and engineering, where first-principle-based, well-resolved simulations are often prohibitively expensive. For example, in fluid dynamics, constitutive models are required to describe nonlocal, unresolved physics such as turbulence and laminar-turbulent transition. In particular, Reynolds stress models for turbulence and intermittency transport equations for laminar-turbulent transition both utilize convection-diffusion partial differential equations (PDEs). However, traditional PDE-based constitutive models can lack robustness and are often too rigid to accommodate diverse calibration data. We propose a frame-independent, non-local constitutive model based on an embedding neural network that can be trained with data. The learned constitutive model can predicate the closure variable at a point based on the flow information in its neighborhood. It can take any number of points arbitrarily arranged, and thus it is suitable for unstructured meshes, which are typical for finite-element and finite-volume simulations. The merits of the proposed model are demonstrated on scalar transport PDEs on a family of parameterized periodic hill geometries.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Extended FIVER Framework for Modelling Laser-Fluid Coupling and Laser-Induced Cavitation

Author(s): *Xuning Zhao, *Virginia Polytechnic Institute and State University*; Wentao Ma, *Virginia Polytechnic Institute and State University*; Ben Zhao, *Virginia Polytechnic Institute and State University*; Olivier Coutier-Delgosha, *Virginia Polytechnic Institute and State University*; Kevin Wang, *Virginia Polytechnic Institute and State University*;

The absorption of the laser by fluid and solid materials plays a significant role in many engineering and biomedical applications that use laser for material modification and fabrication. In this talk, we present a coupled photo-thermal-mechanical model of laser absorption in compressible multiphase fluid flows, including laser-induced cavitation. The proposed computational framework couples the three-dimensional compressible Navier-Stokes equation with a nonlocal laser absorption equation, and solves both equations on the same unstructured, non-boundary conforming finite volume grid. The computational framework is an extension of the recently developed FIVER (“a Finite Volume method with Exact multi-material Riemann solver”) framework, which features the use of level set and embedded boundary methods for tracking material (fluid-fluid and fluid-solid) interfaces, and the solution of local, one-dimensional multi-material Riemann problems for enforcing interface conditions. This talk will start with a brief review of the key model equations and numerical algorithms adopted by FIVER, as well as recent efforts on verification and validation. Next, the physical models of laser absorption and laser-induced heating will be presented. Then, the model of phase change induced by the laser will be introduced, including mass transfer and heat transfer between liquid and vapor. The development and verification of an embedded boundary method for solving the laser absorption equation on the unstructured non-boundary conforming fluid grid will be discussed in detail. Computational models and methods for tracking the interaction of laser with liquid-gas interfaces will also be discussed. Several numerical experiments involving laser absorption by bubbly flows and laser-induced bubble creation will be presented to assess the capability and performance of the computational framework. Key Words: fluid-solid interaction, laser absorption, embedded boundary method, cavitation, laser-induced phase transition.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Fluid-Structure Interaction Using FEM Based on VOF and IGA Methods

Author(s): *Yamato Yoshida, *Chuo University*; Kazuo Kashiyama, *Chuo University*; Hiroshi Hasebe, *Nihon University*;

Fluid-Structure Interaction is one of the important research topic in the field of civil engineering. In conventional FEM, the shape of structure drawn by Spline function in CAD is analyzed approximately based on the shape function that is used in FEM. Therefore, applying Isogeometric analysis[1] for the structure analysis is seemed to be very effective. Isogeometric analysis can analyze the shape of structure without the shape error by using Spline function as the shape function. In addition, Isogeometric analysis can express the analysis domain with fewer elements than FEM. The purpose of our research is to precisely analyze the fluid-structure interaction when the fluid force such as a tsunami acts on the complicated shape structure. In this research, we applied Isogeometric analysis to structure vibration analysis when the fluid force acted on the cylindrical cantilever that is assumed an elastic body, and compared with the result of FEM. As the fluid analysis method, the stabilized FEM based on VOF method was applied, the fluid force calculated by FEM was given as the external force in structure analysis. As the structure analysis, Isogeometric Analysis based on NURBS function was applied. For temporal discretization, the Newmark ? method was applied. REFERENCE [1] T.J.R.Hughes, J.A.Cottrell and Y.Bazilevs, Isogeometric analysis : CAD, finite elements, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering, Vol.194, pp.4135-4195, 2005.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Meshfree Methods for Problems with the Integral Fractional Laplacian

Author(s): *Yanzhi Zhang, *Missouri University of Science and Technology*; Yixuan Wu, *Missouri University of Science and Technology*;

In this talk, I will introduce the recently developed meshfree methods based on the radial basis function to solve problems with the integral fractional Laplacian. The proposed methods take advantage of the analytical Laplacian of the radial basis functions so as to accommodate the discretization of the classical and fractional Laplacian in a single framework and avoid the large computational cost for numerical evaluation of the fractional derivatives. Moreover, our methods are simple and easy to handle complex geometry and local refinement, and their computer program implementation remains the same for any dimension d. The effects of classical and fractional Laplacian will also be discussed.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Recent Advances in Improving the Material Point Method for Promoting Simulation-Based Engineering Science

Author(s): *Yonggang Zheng, *Dalian University of Technology*; Zhen Chen, *University of Missouri*; Hongwu Zhang, *Dalian University of Technology*; Hongfei Ye, *Dalian University of Technology*;

The material point method (MPM) [https://en.wikipedia.org/wiki/Material_point_method] has evolved for almost three decades since the first research project on it was funded by Sandia National Laboratories in the early 1990. The MPM takes advantage of both the Eulerian and Lagrangian spatial discretization methods, while avoiding the shortcomings of each, in order to better simulate multi-phase (solid-fluid-gas) interactions involving failure evolution under extreme loading conditions. The use of the single-valued mapping functions between material points and background grid nodes in the MPM results in a natural no-slip contact/impact treatment within an interfacial zone of finite size such that no inter-penetration would occur. The slip and penetration conditions could also be implemented based on the real physics involved in the interfacial failure evolution without invoking master/slave nodes at the contact surface of zero thickness as assumed in the finite element method (FEM). Furthermore, the MPM and FEM could be effectively combined in a single computational domain with a flexible discretization pattern for large-scale simulation, because both discretization methods are based on the same weak formulation of continuum mechanics. Much research has been conducted over the last two decades in the world to eliminate the limitations of the original MPM, such as the cell-crossing and moving quadrature point errors. To promote Simulation-Based Engineering Science as pioneered by Professor Oden and other leading scholars, a systematic effort [1-3, among others] has being made to improve the MPM, with the recent results to be presented in this symposium. References [1] Lu, M., Zhang, J., Zhang, H., Zheng, Y., and Chen, Z., “Time-discontinuous Material Point Method for Transient Problems,” Computer Methods in Applied Mechanics and Engineering, Vol. 328, pp. 663-685, 2018. [2] Tao, J., Zheng, Y., Zhang, H., and Chen, Z., “Axisymmetric Generalized Interpolation Material Point Method for Fully Coupled Thermomechanical Evaluation of Transient Responses,” International Journal of Computational Methods, Vol. 17(04), No. 1950003 (24pp), 2020. [3] Liu, Y., Ye, H., Zhang, H., Zheng, Y., “Coupling Lattice Boltzmann and Material Point Method for Fluid-Solid Interaction Problems Involving Massive Deformation,” International Journal for Numerical Methods in Engineering, Vol. 121, pp. 5546-5567, 2020.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Micromechanics-Informed Phase Field Model for Brittle and Ductile Fracture Accounting for Unilateral Constraint

Author(s): *Yongxing Shen, *Shanghai Jiao Tong University*; Yangyuanchen Liu, *Duke University*; Cheng Cheng, *Shanghai Jiao Tong University*; Vahid Ziaei-Rad, *Shanghai Jiao Tong University*; Shuo Yang, *Shanghai Jiao Tong University*;

We present a direction-dependent model for the unilateral constraint involved in the phase field approach to fracture. The construction of this phase field model is informed by micromechanical modeling through the homogenization theory, where the representative volume element (RVE) has a planar crack in the center. The proposed model is made closely match the response of the RVE, including the frictionless self-contact condition. This homogenization approach allows to identify a direction-dependent phase field model with the tension–compression split obtained from cracked microstructures. One important feature of the proposed model is that unlike most other models, the material degradation is consistently determined without artificial assumptions or ad hoc parameters with no physical interpretation, thus, a more realistic modeling is resulted. With standard tests such as uniaxial loadings, three-point bending, simple shear, and through-crack tests, the proposed model predicts reasonable crack paths. Moreover, with the RVE response as a benchmark, the proposed model gives rise to an accurate stress–strain curve under shear loads, more accurate than most existing models. Extension to the case of elastoplastic solid will also be presented. More information can be found in our publication, Engineering Fracture Mechanics 241 (2021) 107358.

16th U.S. National Congress on Computational Mechanics
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Title: Evaluation of Crack Propagation Analysis by Local Approach under Ultra Low Cycle Fatigue

Author(s): *Yoshitaka Wada, *Kindai University*; Kaito Ueda, *Kindai University*;

It is important for piping to predict unstable failure in a structure due to excessive cyclic load caused by a huge earthquake. The J-integral is used as a fracture mechanics parameter which is applicable to elastic-plastic problems. However, J-integral cannot be effective under cyclic loading. Fatigue crack growth rate in the low cycle fatigue is evaluated by ?J which is defined by the stress and strain ranges in a given cycle. The applicability of ?J has not been verified yet under extremely low cycle loading. A generation phase analysis requires several parameters by experiment during fracture of a compact tension (CT) specimen. Crack length and its front shape are the most important for load and load line displacement evaluation. In this study, we evaluate crack propagation with different crack propagation manners, which are simultaneous propagation of crack front, individual propagation by nodal release on a crack front and individual propagation in the mid-part of specimen under plane strain. A material of the specimen is SUS316. The FE model is 1/4 of actual CT specimen. Load control is used in experiments, however, displacement control is performed in the generation phase analysis. The approximation curve, which is determined by the experiment and represents the relationship of crack length and load line displacement, is for determinations of nodal release as crack propagation. In the ?J evaluation, the best result, which is the lowest deviation from the experiment, is obtained by generation phase analysis. Critical CTOD can be corrected by stress triaxiality under the monotonic loading [1]. Additionally, stress triaxiality and equivalent plastic strain are reciprocal relations in the cracked pipe fracture [2]. The relationship between stress triaxiality and incremental equivalent plastic strain along a crack front are well examined. The incremental equivalent plastic strain exhibits some critical condition of fracture. As a result of an evaluation, the crack propagation condition is defined by the COD, equivalent plastic strain and stress triaxiality as a local approach manner. The effectiveness of three-parameter approach will be discussed in detail. REFERENCES [1] K. Hang et al., The effect of constraint on CTOD fracture toughness of API X65 steel, Eng. Fract. Mech., Vol. 124-125, pp. 167-181,2014. [2] N. Miura et al., Benchmark Analysis for Ductile Fracture Simulation -Description of Problems and Comparison of Results-, 12th WCCM and 6th APCOM, 1 page.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Adaptive Surrogate Autoregressive Flow for Parameter Estimation with Expensive Computational Models

Author(s): *Yu Wang, *University of Notre Dame*; Fang Liu, *University of Notre Dame*; Daniele Schiavazzi, *University of Notre Dame*;

Development of fast inference procedures where the parameters of a numerical models can be efficiently learned from data is a cornerstone for the next-generation computational physiology. Sampling-based inference approaches such as Markov chain Monte Carlo (MCMC) may lead to an intractable computational burden when the computational cost of each pointwise likelihood evaluation is high. Unlike MCMC, new approaches combining variational inference with invertible auto-regressive transformations [1] are characterized by a computational cost that grows only linearly with the dimensionality of the latent variable space [2], providing a more efficient approach for density estimation. Moreover, the cost of computing an expensive likelihood may be mitigated by using pre-trained surrogate model which remains fixed during the inference process. However, this approach might generate significant bias with catastrophic consequences, particularly when the surrogate is insufficiently accurate around the true posterior modes. To improve the computational speed without sacrificing accuracy, we propose a nested optimization strategy that alternatively updates the parameters of a collection of auto-regressive transformations and the weights of a deep neural network surrogate. We provide a number of experiments including closed form posterior distributions, high-dimensional posteriors with correlated parameters and lumped parameter models of the human cardiovascular system. Finally, we focus on the performance of the proposed approach for situations where the underlying model lacks identifiability, and where introducing a mean field approximation is simply not acceptable in light of the posterior dependency among parameters. Reference: [1] George Papamakarios, Theo Pavlakou, and Iain Murray. Masked Autoregressive Flow for Density Estimation. arXiv preprint arXiv:1705.07057, 2017. [2] Danilo Rezende and Shakir Mohamed. Variational Inference with Normalizing Flows. In International Conference on Machine Learning, pages 1530–1538. PMLR, 2015.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Physics-Informed Machine Learning Method for Large-Scale Data Assimilation Problems with Application to Groundwater Modeling at the Hanford Site

Author(s): *Yu-Hong Yeung, *Pacific Northwest National Laboratory*; David Barajas-Solano, *Pacific Northwest National Laboratory*; Qizhi He, *Pacific Northwest National Laboratory*; Alexandre Tartakovsky, *University of Illinois at Urbana-Champaign*;

We develop a physics-informed machine learning approach for large-scale data assimilation and parameter estimation and apply it for estimating transmissivity and hydraulic head in a two-dimensional steady-state subsurface flow model of the Hanford Site given synthetic measurements of said variables. The synthetic data are generated using the hydraulic conductivity field and boundary conditions that were estimated in the previous Hanford Site calibration study. In our approach, we extend the physics-informed conditional Karhunen-Loéve expansion (PICKLE) method to modeling subsurface flow with unknown flux (Neumann) and varying head (Dirichlet) boundary conditions that are typical for large-scale systems like the Hanford Site. We demonstrate that overall, the proposed PICKLE method is comparable in accuracy to the standard maximum a posteriori (MAP) parameter estimation method, but is significantly faster than MAP for large-scale problems. Both methods use a mesh to discretize the computational domain: In MAP, the parameters and states are discretized on the mesh, which is also used to evaluate the Jacobian matrix in the inverse problem; therefore, the number of the parameter estimations depends directly on the mesh size. In PICKLE, the mesh is used to evaluate the residuals of the governing equation, while the parameters and states are approximated by the truncated conditional Karhunen-Loéve expansions with the number of parameters controlled by the smoothness of the parameter and state fields, but not by the grid size. We demonstrate that once trained for one set of values of the Dirichlet boundary condition (i.e., for one river stage), the PICKLE method provides accurate estimates of the hydraulic head for different Dirichlet boundary conditions (i.e., different river stage).

16th U.S. National Congress on Computational Mechanics
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Title: An Asymptotically Compatible Treatment of Traction Loading in Linearly Elastic Peridynamic Fracture

Author(s): *Yue Yu, *Lehigh University*; Huaiqian You, *Lehigh University*; Nathaniel Trask, *Sandia National Laboratories*;

Meshfree discretizations of state-based peridynamic models are attractive due to their ability to naturally describe fracture of general materials. However, two factors conspire to prevent meshfree discretizations of state-based peridynamics from converging to corresponding local solutions as resolution is increased: quadrature error prevents an accurate prediction of bulk mechanics, and the lack of an explicit boundary representation presents challenges when applying traction loads. In this paper, we develop a reformulation of the linear peridynamic solid (LPS) model to address these shortcomings, using improved meshfree quadrature, a reformulation of the nonlocal dilitation, and a consistent handling of the nonlocal traction condition to construct a model with rigorous accuracy guarantees. In particular, these improvements are designed to enforce discrete consistency in the presence of evolving fractures, whose a priori unknown location render consistent treatment difficult. In the absence of fracture, when a corresponding classical continuum mechanics model exists, our improvements provide asymptotically compatible convergence to corresponding local solutions, eliminating surface effects and issues with traction loading which have historically plagued peridynamic discretizations. When fracture occurs, our formulation automatically provides a sharp representation of the fracture surface by breaking bonds, avoiding the loss of mass. We provide rigorous error analysis and demonstrate convergence for a number of benchmarks, including manufactured solutions, free-surface, nonhomogeneous traction loading, and composite material problems. Finally, we validate simulations of brittle fracture against a recent experiment of dynamic crack branching in soda-lime glass, providing evidence that the scheme yields accurate predictions for practical engineering problems.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Effects of Heart Failure with Preserved Ejection Fraction on Left Ventricular Function and Coronary Perfusion

Author(s): Lei Fan, *Michigan State University*; *Yuexing Sun, *Michigan State University*; Lik Chuan Lee, *Michigan State University*;

Approximately half of heart failure patient suffer from preserved ejection fraction (EF) [1]. However, heart failure with preserved ejection fraction (HFpEF) remains to be poorly understand without effective therapies due to the complex and multifactorial mechanisms. Because of difficulties in determining the effects of each confounding factor in HFpEF in experimental and clinical studies, a computational framework that couples the systemic circulation of left ventricular (LV) and coronary perfusion with flow regulation in a closed loop lumped parameter system is developed to investigate the effects of HFpEF on the LV mechanics and coronary perfusion for the first time [2]. The LV is modeled using a time-varying elastance model. Coronary flow network consisting of 400 vessels is coupled in the model and flow in each vessel of the network is described by a three-element Windkessel model. The intramyocardial pressure (IMP), which is applied to each vessel, is defined as a combination of two mechanisms, e.g., time-varying elasticity and ventricular cavity-induced extracellular pressure, which are controlled by two prescribed parameters, respectively. Flow regulation that includes the myogenic, shear, and flow regulation responses is taken into account, in which myogenic and shear responses are modeled based on the transvascular pressure, and flow regulation response is controlled by a vasodilator signal. A linear relationship between a vasodilator signal (F_meta) and LV pressure-volume loop area (PVA) is prescribed to update F_meta from 0 to 1. The model is calibrated based on the clinical measurements under normal condition and the calibrated model is then applied to simulate HFpEF. Based on the developed model, it can be concluded that 1) the model predicted results under normal and HFpEF cases are validated against clinical measurements in terms of the LV pressures and volumes, LV EF, the ratio of two peaks in mitral valve flow rate and total coronary flow under passive and regulated conditions [3]; 2) from normal to HFpEF, the changes of pressures reduce passive coronary flow but the increased F_meta due to the elevated PVA rises regulated coronary flow, leading to reduced coronary flow reserve; 3) in sensitivity analysis, results suggest that an increase in either the LV relaxation rate, preload and afterload can increase the vulnerability of myocardium to ischemia. References: [1] Pfeffer, M. A. et al., Circ. Res.,124.11: 1598-1617, 2019. [2] Fan, L., et al., Am. J. Physiol. Heart Circ., 2020. [3] Walter, J. P., et al., Eur. Heart. J. 19: 990-1003, 1998.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: Optimization of Chiral Metamaterials via Deep Neural Networks

Author(s): *Yun-Che Wang, *National Cheng Kung University*; Chun-Wei Liu, *National Cheng Kung University*; Tsai-Wen Ko, *National Cheng Kung University*;

Metamaterials with particularly designed microstructure may exhibit unconventional physical properties, such as negative index of refraction (NIR), negative Poisson's ratio (NPR) or negative thermal expansion coefficient (NTEC). By introducing rotational degrees of freedom at each material point, deformation-mode couplings between tension/compression and torsion or bending can be obtained, as predicted by the non-centrosymmetric Cosserat mechanics for chiral materials. Such couplings are of great importance to the development of novel sensors. Traditionally, the design of metamaterials relies on human experiences through trial and error. By using deep convolution neural networks, such as VGG, we have developed a methodology to create metamaterials with desired chiral microstructures. The geometric data of chiral microstructures are provided, along with effective mechanical properties, to train the DNN model. The effective properties are from finite element calculations, as well as experimentally measured data. The geometry of chiral samples for DNN training is generated from a generative adversarial neural network. With our successfully trained DNN model, the inverse problem of searching a microstructure geometry for a given set of chiral properties can be solved efficiently. Optimization of chiral microstructure for maximum deformation mode coupling is hence accomplished with the trained DNN model, and verified by experimental data and brute force finite element calculations.

16th U.S. National Congress on Computational Mechanics
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Title: Non-Local Reformulation for the Transport of Fluids in Heterogeneous Unsaturated Porous Media

Author(s): Haitao Yu, *Tongji University*; *Yuqi Sun, *Tongji University*;

This paper aims to develop a nonlocal formulation for the transport of fluids in heterogeneous unsaturated porous media. Firstly, a new nonlocal governing equation for the transport of fluids is proposed based on the concepts of peridynamcis. In the proposed nonlocal transport model of fluids, the nonlocal flux of fluid at one material point is expressed by averaging all the local flux in its support domain. It is also demonstrated that the new nonlocal flux of fluids ensures the mathematical consistency between the nonlocal model and the classical continuum transport model when nonlocal effects between material points are ignored. Secondly, a non-local Gauss's formulation is presented by transforming the pressure and velocity boundaries in classical transport model into the non-local fictitious boundary layers, and this formulation unifies the variational framework and boundary conditions of nonlocal model and classical continuum transport model. Further, a penalty method is employed to eliminate the zero-energy mode oscillation inherently observed in the nonlocal model Further, there is no need special technique to treat the interface problem for the transport of fluids in heterogeneous unsaturated media. Finally, several numerical examples are illustrated to validate the proposed method by providing comparisons with available analytical solutions and experimental data. Results show that the proposed method can well simulate the transport of fluids in heterogeneous unsaturated media.

16th U.S. National Congress on Computational Mechanics
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Title: HexGen and Hex2Spline: Polycube-Based Hexahedral Mesh Generation and Spline Modeling for Isogeometric Analysis Applications in LS-DYNA

Author(s): *Yuxuan Yu, *Carnegie Mellon University*; Xiaodong Wei, *École polytechnique fédérale de Lausanne*; Angran Li, *Carnegie Mellon University*; Jialei Liu, *Carnegie Mellon University*; Jeffrey He, *Northwestern University*; Yongjie Zhang, *Carnegie Mellon University*;

In this paper, we present two software packages, HexGen and Hex2Spline, that seamlessly integrate geometry design with isogeometric analysis (IGA) in LS-DYNA. The software packages are open-source and can be found in the following Github link (https://github.com/CMU-CBML/HexGen_Hex2Spline). Given a boundary representation of a solid model, HexGen creates a hexahedral mesh by utilizing a semi-automatic polycube-based mesh generation method. Hex2Spline takes the output hexahedral mesh from HexGen as the input control mesh and constructs volumetric truncated hierarchical splines. Through B\'{e}zier extraction, Hex2Spline transfers spline information to LS-DYNA and performs IGA therein. We explain the underlying algorithms in each software package and use a rod model to explain how to run the software. We also apply our software to several other complex models to test its robustness. Our goal is to provide a robust volumetric modeling tool and thus expand the boundary of IGA to volume-based industrial applications. REFERENCES [1] Y. Yu, X. Wei, A. Li, J. Liu, J. He, Y. J. Zhang: HexGen and Hex2Spline: Polycube-based hexahedral mesh generation and spline modeling for isogeometric analysis applications in LS-DYNA. In Preparation. [2] K. Hu, Y. J. Zhang: Centroidal Voronoi tessellation based polycube construction for adaptive all-hexahedral mesh generation. Computer Methods in Applied Mechanics and Engineering, 305, 405–421 (2016) [3] X. Wei, Y. J. Zhang, T.J.R. Hughes: Truncated hierarchical tricubic C0 spline construction on unstructured hexahedral meshes for isogeometric analysis applications. Computers and Mathematics with Applications,74(9), 2203–2220 (2017)

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: An Efficient Benchmark Case for Scale-Resolving Simulation with Curved Walls

Author(s): *Z.J. Wang, *University of Kansas*; Eduardo Jourdan, *University of Kansas*;

Flow between rotating concentric cylinders, or the Taylor Couette flow, has been studied extensively because of its rich physics, ranging from axisymmetric steady laminar flow, to fully developed turbulent flow. In the present study, we advocate the use of this problem as a benchmark case for scale-resolving simulation, such as large eddy simulation (LES) and direct numerical simulation (DNS). The problem is attractive because of its simple geometry, simple boundary conditions, and complex physics involving wall-shear induced and centrifugal instability. Unlike the well-known fully developed channel flow, this problem has a curved wall boundary, and it is unnecessary to add a source term to the governing equations to sustain the fully developed turbulent flow. A p-refinement study for Re = 4,000 is performed first to establish DNS data, including the time history of enstrophy, which can be used as an accuracy and resolution indicator to evaluate numerical methods, and is orders of magnitude faster than using the mean flow quantities and Reynolds stresses to evaluate solution quality. Finally, an hp-refinement study was performed to establish the relative accuracy and efficiency of high-order schemes of various accuracy.

16th U.S. National Congress on Computational Mechanics
Chicago, IL, July 25-29. 2021

Title: A Flexible High-Fidelity Thermal CFD Framework for Quenching Processes

Author(s): *Ze Zhao, *University of Illinois at Urbana-Champaign*; Jinhui Yan, *University of Illinois at Urbana-Champaign*;

Simulation of water quenching is challenging. Conventional numerical methods rely heavily on empirical parameters, such as heat transfer coefficient. In this talk, we present a flexible and first-principle-based computational fluid dynamics framework for large-scale quenching processes. We first develop a thermal fluid model based on multi-phase Navier-Stokes and thermodynamics equations considering evaporation to directly solve the fluid motion and temperature in the quenching tank. In the model, the volume-of-fluid method is employed to handle the gas-liquid interface, and variational multi-scale formulation (VMS) is utilized as a large eddy simulation (LES) model for the multi-phase turbulence in the quenching tank. The model can resolve the multi-scale and multi-physical phenomena (e.g., heat transfer, convection, multi-scale boiling) in water quenching in great detail, leading to more accurate temperature predictions inside quenched structures than conventional approaches. We then deploy the thermal fluid model to an immersogeometric discretization to enable direct simulations of complex structures with different quenching angles and dipping speeds in one universal background fluid mesh. To demonstrate the modeling capability and accuracy of the proposed framework, we simulate a set of real-world quenching problems and thoroughly validate the simulated results against experimental measurements. The results indicate that the proposed framework will be a valuable tool for quenching research and heat-treating in general.

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Title: Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites

Author(s): *Zhenze Yang, *Massachusetts Institute of Technology*; Chi-Hua Yu, *National Cheng Kung University*; Markus Buehler, *Massachusetts Institute of Technology*;

Materials-by-design is a new paradigm to develop novel high-performance materials. However, finding materials with superior properties is often computationally or experimentally intractable because of the astronomical number of possible combinations in the design space. Especially for composite materials, the heterogeneity and structural complexity often hinder us from calculating materials properties and searching for optimal designs at low costs. Fortunately, with recent advances in artificial intelligence (AI) or machine learning (ML), new approaches and perspectives are provided to solve the puzzles. This study reports leveraging deep learning methods to bridge the gap between a material's microstructure – the design space – and its physical performance. Specifically, it will answer research questions about how to use AI for fast predictions on physical fields of composite materials like stress or strain directly from the input materials geometry. Using a game-theory based conditional generative adversarial neural network (cGANs), an end-to-end deep learning approach is developed to give accurate predictions on not only physical fields data but also derivative global properties such as modulus and recoverability. Furthermore, the proposed approach offers extensibility by predicting complex materials behaviors regardless of component shapes, boundary conditions and geometrical hierarchy, providing new perspectives of performing physical modeling and simulations. We show that the method outperforms conventional numerical methods such as finite element analysis (FEA) and is able to vastly improves the efficiency of evaluating physical properties of hierarchical materials directly from the geometry of its structural makeup. In addition, the idea of geometry-to-field translation can also be applied to other areas in the sciences, such as density functional theory fields, fluid mechanical fields, or electromagnetism. Preliminary results will be discussed.

16th U.S. National Congress on Computational Mechanics
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Title: Design of Graded Porous Bone-Like Structures via a Multi-Material Topology Optimization Approach

Author(s): *Zhi Zhao, *University of Illinois at Urbana-Champaign*; Shelly Zhang, *University of Illinois at Urbana-Champaign*;

The rapid growth of additive manufacturing offers high freedom to fabricate materials and structures with intricate geometric configurations. Due to the development of this technique, the design of lightweight porous systems (e.g., bone-like infills) has been of growing interest over the last few years. In this work, we present a density-based topology optimization formulation to design bone-like structures with not only multiple levels of porosities but also different material properties. The proposed framework allows for flexible controls of local geometric features (e.g., local porosity and material distribution) in the optimized topologies via a novel multi-material topology optimization approach, which generalizes the concept of multiple materials. Namely, each material can have not only distinct material property but also a different level of local porosity, or a combination of both. Through numerical examples, we demonstrate that the proposed formulation is effective in generating graded porous structures with smooth transitions. Various material constitutive models are investigated, and their influences on the topology and performance of the final design are studied. We further investigate the interactions among material properties, multiple porosity levels, and structural stiffness. Additionally, the improving robustness of the optimized graded porous designs is demonstrated numerically. This study aims to contribute to the topology optimization field by proposing an effective multi-material design framework to optimize the distributions of not only multiple levels of porosity but also different types of materials.

16th U.S. National Congress on Computational Mechanics
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Title: Hierarchical Modeling for Uncertainty Quantification

Author(s): *Zhiheng Wang, *University of Southern California*; Roger Ghanem, *University of Southern California*;

In this presentation we will describe a novel procedure that simultaneously accounts for uncertainty due to statistical errors (lack of data), modeling error, and numerical errors. We present a formulation to contribution of these distinct errors to various quantities of interest (QoI). We focus our attention on QoI that pertain to tails of probability distributions. The approach is grounded in polynomial chaos formalism, and relies on the formulation of the polynomial chaos coefficients themselves as random variables. By combining KDE approximations of probability density functions with directional derivatives in Gaussian spaces, we construct composite maps that connect these QoIs with the various sources of error. The approach is useful both for diagnostics and for design and resource allocation. We demonstrate our approach on a number of problems of interest in science and engineering.

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Title: Crack Estimation in Miter Gates Using A Machine Learning-Based Global-Local Modeling Method

Author(s): *Zihan Wu, *University of California, San Diego*; Travis Fillmore, *Coastal and Hydraulics Laboratory, ERDC, USACE*; Manuel Vega, *University of California, San Diego*; Zhen Hu, *University of Michigan-Dearborn*; Michael Todd, *University of California, San Diego*;

Miter gates facilitate the navigation of cargo transportation along with the inland waterways network by helping ships transition between different water elevations. However, the aging of these steel gates brings multiple forms of damage, such as cracks, corrosion, and quoin block deterioration. Current structural health monitoring strategies are mostly focused on the damage identification from high-fidelity finite element (FE) models using inverse methods, which usually demands high computational costs and does not allow for real-time damage diagnosis. To overcome the computational challenge while maintaining accuracy, this research proposes a machine learning (ML)-based global-local modeling method for crack diagnosis of miter gate. Considering that a reference solution is nearly inaccessible for a large FE model of a miter gate, the framework is validated on an idealized problem, where the true solution is known. A local and global substructuring FE model is first developed, which consists of coupled global and local FE models. The global FE model captures the global behavior of the miter gate, and the local model predicts the localized response with high accuracy by modeling the crack using the extended Finite element method (XFEM). Based on simulation data collected from the global-local coupled FE models, first a neural network (NN) based autoencoder is employed as a nonlinear data compression method, which maps the high-dimensional coupling variables between the global and local substructures into low-dimensional latent variables. Following that, Gaussian process (GP) surrogate models are constructed in the latent space to efficiently and accurately predict the response for any given load and damage conditions. Finally, the GP surrogate models are used in conjunction with an NN-based autoencoder to replace the local FEM substructure in the coupled global-local analysis. The ML-based global-local modeling method enables for efficient and accurate prediction of stress intensity factors (SIF) over time, which is essential for the crack diagnostics of miter gate using Bayesian methods. The results show the efficacy of the proposed framework in performing crack diagnosis using Bayesian method and the developed ML-based global-local modeling method.

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Title: Multiscale Reduced Order Discrete Damage Theory for Fracture of Composite Materials

Author(s): *Zimu Su, *Vanderbilt University*; Caglar Oskay, *Vanderbilt University*;

In this study, we propose a reduced-order multiscale computational framework for failure analysis of composite materials subjected to static and fatigue loading. The multiscale approach is applied on both spatial and temporal domains. At the microstructural scale, the proposed model relies on discrete cohesive-interface representation of fracture, which is consistently bridged to continuum representation of damage at the macrostructural scale. The key feature of the proposed approach is that the microstructural fracture process is modeled using a novel reduced-order modeling strategy. At the macroscopic scale, the mesh size dependence that emanates from continuum damage representation is alleviated by introducing a length scale operator, which effectively adjusts the size of the microstructural volume as a function of the macroscopic element size in order to keep fracture energy consistency. To alleviate the computational cost of predicting failure evolution under cyclic loading, an adaptive multiple time scale time integrator is incorporated. The length scale operator for mesh-size objectivity is ensured effective under fatigue loading by employing a non-additive cyclic cohesive law for microscopic fracture. In this law, the static damage and fatigue damage respectively control cohesive stiffness and strength, thereby ensuring that localized energy dissipation is dictated by strain softening even in the fatigue regime. The performance of the proposed model is demonstrated in the context of three-dimensional open-hole unidirectional and cross-ply fiber-reinforced laminates subjected to tensile static and fatigue loading. The numerical examples display the capabilities of the proposed model in capturing multiple failure mechanisms, including transverse matrix cracking, splitting, delamination and fiber fracture. The failure responses subjected to static and fatigue loading show mesh-size independence in the presence of multiple failure modes.

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Title: Autonomous Finite Elements (AFE) – Are They Precursors of a Paradigm Shift?

Author(s): *Zohar Yosibash, *Tel-Aviv University, Israel*;

Finite element analysis requires a qualified analyst to generate the necessary input data, verify the output and post process the analysis results for a meaningful conclusion. The required expertise and labor efforts precluded the use of FEA in daily medical practice for example. Recent scientific advancements such as low dose CT scans, machine learning, and high order FEA which allows an inherent verification methodology of the numerical accuracy, make it possible to provide a fully autonomous process for assessing bone strength and fracture risk. This autonomous process, that we refer to as autonomous streamline, named autonomous finite element (AFE) analysis, introduces a paradigm shift in the use of FEA. We describe a novel AFE [1] for patient-specific analysis of human femurs: it involves an automatic segmentation of femurs from CT-scans by convolution neural networks, an automatic mesh generation and application of boundary conditions based on anatomical points, a high-order FE analysis with numerical error control, and finally an automatic report with a clear assessment of bone fracture risk. One specific application of AFE is the determination of the risk of fracture for patients with tumors of the femur and whether a prophylactic surgery is needed [2,3]. References: [1] Yosibash Z, Myers K, Trabelsi N, Sternheim A, "Autonomous FEs (AFE) - A stride toward personalized medicine", Comp. Math. Appl., 80(11), pp. 2417-2432, 2020. [2] Sternheim A, Giladi O, Gortzak Y, Drexler M, Salai M, Trabelsi N, Milgrom C and Yosibash Z, “Pathological fracture risk assessment in patients with femoral metastases using CT-based finite element methods. A retrospective clinical study”, Bone, 110, pp. 215-220, 2018. [3] Sternheim A, Traub F, Trabelsi N, Gortzak Y, Dadia S, Snir N, Gorfine M and Yosibash Z., “When and where do patients with bone metastases actually break their femur? A CT-based finite element analysis of patients”, Bone & Joint Jour., 102-B, No. 5, pp. 638-645, 2020.