

Monday, May 20th
Session 1: Fluids (CFD)
Lydia Mendelssohn Theatre 10:30 AM – 12:10 PM
Chair: Mauro Rodriguez

Computational modeling of magnetic particle margination within blood flow through LAMMPS

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Keywords: Magnetic particle, Blood flow, LAMMPS, Fluid–structure interaction

Abstract: We develop a multiscale and multiphysics computational method to investigate the transport of magnetic particles as drug carriers in blood flow under influence of hydrodynamic interaction and external magnetic field. A hybrid coupling method is proposed to handle red blood cell (RBC)-fluid interface (CFI) and magnetic particle-fluid interface (PFI), respectively. Immersed boundary method (IBM)-based velocity coupling is used to account for CFI, which is validated by tank-treading and tumbling behaviors of a single RBC in simple shear flow. While PFI is captured by IBM-based force coupling, which is verified through movement of a single magnetic particle under non-uniform external magnetic field and breakup of a magnetic chain in rotating magnetic field. These two components are seamlessly integrated within the LAMMPS framework, which is a highly parallelized molecular dynamics solver. In addition, we also implement a parallelized lattice Boltzmann simulator within LAMMPS to handle the fluid flow simulation. Based on the proposed method, we explore the margination behaviors of magnetic particles and magnetic chains within blood flow. We find that the external magnetic field can be used to guide the motion of these magnetic materials and promote their margination to the vascular wall region. Moreover, the scaling performance and speedup test further confirm the high efficiency and robustness of proposed computational method. Therefore, it provides an efficient way to simulate the transport of nanoparticle-based drug carriers within blood flow in a large scale. The simulation results can be applied in the design of efficient drug delivery vehicles that optimally accumulate within diseased tissue, thus providing better imaging sensitivity, therapeutic efficacy and lower toxicity.

Modeling and sensitivity analysis of PEM fuel cells by using CFD technique

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Keywords: CFD, PEM fuel cell, fuel cell modelling, numerical simulation

Abstract: The main objective of this article is to observe the effect of the parameters, active area of the catalytic layer, conductivity of the electrolyte and porosity of the catalytic layer, on the performance of PEM fuel cell, employing computational fluid dynamics (CFD) technique. A systematic mathematical model is developed to study the effect of these parameters. The model is applied to an isothermal, steady state, laminar flow and single phase comparing the simulated and experimental polarization curve. The results compare well with the experimental polarization data obtained at 80°C for ohmic and activation regions. The best match with the experimental data is obtained when the active area of the catalytic layer is 1300cm²/mg, conductivity of the electrolyte is 5 S/m and porosity of the catalytic layer is 0.4.

Inertial collapse of cavitation bubble near an interface

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Keywords: Cavitation bubble, Inertial collapse, Shock wave, Impact load

Abstract: Erosion of solid surface by the damage during collapse of cavitation bubble has been studied for many years. High shock pressure and high-velocity liquid jet produced during the bubble collapsing near an interface (e.g. a rigid boundary, a free surface, another bubble) have high potential to give the impact loads to the neighboring solid surfaces. In naval hydraulic applications, the repeated impact loads to the surface lead to undesired equipment failure while in medical applications, the damage is desired in non-invasive ultrasound therapy tools used for cancer tissue ablation. Understanding cavitation-induced damage is necessary to develop mitigation/enhancement strategies in naval hydraulic applications and medical therapy tools. When the liquid undergoes vaporization and the subsequent rupture in the liquid nucleates cavitation bubbles forming a bubble cloud. Bubbles respond to the pressure gradient in the flow by oscillating in volume. During the collapse, rarefaction/compression waves are produced, which interact with the original bubble in a cloud and communicate the presence of another bubble. These effects can break the symmetry of the bubble surroundings and leads to the non-spherical collapse of bubble with formation of re-entrant jet and emission of a shock wave with high pressure. The impact load from this shock can damage neighboring surfaces.

However, the nonlinear interactions between the bubbles and the wide range of spatial and temporal scales pose a significant challenge in experimentally and computationally studying bubble clouds. To gain fundamental understanding of bubble-bubble interactions, we consider the simplified geometric configuration involving a single bubble inertially collapsing near an interface, which is a rigid boundary and another bubble with an initial bubble radius ranging from one to infinite (e.g., flat free surface) size. The 3D compressible Navier-Stokes equations for gas-liquid flows are solved numerically using a solution-adaptive high-order accurate method. As bubble collapses, pressure waves produced during the collapse interacts affecting bubble collapse morphology and resulting emitted shock waves. Thus, we vary driving pressure, initial distance between the primary bubble and secondary interface and initial bubble size ratio to determine the effect on the bubble-bubble interactions and resulting shock waves. Different regimes classifying the different bubble morphologies and jet types are also presented.

Computational simulation of thrombus formation in vivo and in vitro

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Keywords: Blood flow, thrombosis, computational mechanics

Abstract: The incidence of blood wetted device thrombosis resulting in stroke or device-exchange surgery is a persistent problem for both clinical and medical community. The objective of this study was to gain improved understanding of the initiation and progression of thrombosis in vivo and in vitro. A spatio-temporal mathematical model for simulating the formation and growth of a thrombus is developed, where blood is treated as a multi-constituent mixture comprised of a linear fluid phase and a thrombus (solid) phase. The transport and reactions of 10 chemical and biological species are incorporated using a system of coupled convection-reaction-diffusion (CRD) equations to represent three processes in thrombus formation: initiation, propagation and stabilization. A computational fluid dynamics (CFD) simulation was performed using our thrombosis model. The patterns of deposition predicted by simulation agreed well with experimental observations. Furthermore, thrombus accumulation was found to increase with decreased flow rate, and can be completely suppressed by the application of anticoagulants and/or improvement of surface chemistry. The use of this simulation tool over a range of hemodynamic, hematological, and anticoagulation conditions would assist physicians to personalize clinical management to mitigate the risk of thrombosis. It may also contribute to the design of future blood-wetted medical devices that are less thrombogenic.

Improved upper bounds on the energy dissipation rate for shear flow with injection and suction

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Keywords: undefined

Abstract: Improved upper bounds on viscous energy dissipation rates of wall-driven shear flow subject to uniform injection and suction rates are computationally determined. The so-called 'background' variational formulation is implemented via a time-stepping numerical scheme to determine optimal estimates. Shear flow Reynolds numbers range from 50 to 40000 with injection angles up to 2° . The computed upper bounds for pre-selected angles of injection at high Reynolds numbers significantly improve the rigorously estimated ones. Our results suggest that the steady laminar flow is nonlinearly stable for angles of injection greater than 2° .

Monday, May 20th
Session 1: Polymer Mechanics
Koessler Room, League 10:30 AM – 12:10 PM
Chair: Alan Wineman

A Constitutive Model of Viscoelastic Polymers undergoing Microstructural Changes

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Keywords: viscoelastic, polymers, constitutive model

Abstract: Polymers undergo inelastic deformations when subjected to mechanical loadings. Macroscopic mechanical response of materials, which are often quantified in terms of stresses and deformations, depend upon the microstructures of the materials. When after being deformed and released the specimens do not regain their original dimensions, the materials are assumed to have undergone microstructural changes during deformations. In this study, a viscoelastic model that describes the overall (macroscopic) response of polymers and accounts for the effect of microstructural changes in the polymer microstructures is presented. The model is derived within a multiple configuration approach. It is assumed that due to mechanical loadings, the polymer microstructures are evolving between two natural configurations, which are stress free. The first configuration is associated with the initial microstructures of the polymer, and the second configuration is associated with the complete microstructural changes. The polymers under consideration are in the glassy state, and thus small deformation gradient problems are considered. However, the materials still can exhibit nonlinear viscoelastic responses, which are incorporated in the nonlinear constitutive equations. Experimental tests on polymers under a constant rate ramp loading and creep-recovery at several different stress levels and loading duration are used to examine the responses predicted by the model.

Thermodynamics response of thermoplastics in the glassy state: Evaluating internal heating during monotonic and cyclic deformation

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Keywords: Thermodynamics, Polyether ether ketone, Polycarbonate, shear, mechanical flow, thermal dissipation

Abstract: A newly developed method to characterize internal heating/storage during quasi-static deformation is used to study the shear response of polycarbonate (PC) and Polyether ether ketone (PEEK) during large-deformation monotonic and cyclic shearing. This characterization is done in the glassy range of these thermoplastics and is used to better understand the material response.

As one of the few homogenous deformation modes that can be easily reversed, shear can provide a clear picture of how a material responds during histories of complex loading. Yet, like most deformations, there is a possibility of strain localization (e.g., development of localized shear bands and necking), which makes the deformation inhomogeneous during testing. Fortunately, by digital image correlation (DIC), one can follow the deformation of the material and verify/frind conditions of homogenous deformation. It turns out that both PC, which is a fully amorphous thermoplastic, and PEEK, which is a semi-crystalline thermoplastic, show ranges of homogenous deformation. Within these regions, the response of both PEEK and PC show a strong similarity. In particular, fully reversing the load during cycling (i.e., centering the cycle at zero) shows a typical hysteresis loop with a clear kinematic strain hardening slope (i.e., modulus). This modulus is typically considered the signature of the internal back-stress. Studying the effect of plastic strain on this modulus shows a softening of the kinematic hardening modulus for larger cycling amplitudes. As this softening occurs both in amorphous and semi-crystalline systems, it might be a result of untangling of the elements that describe the back-stress in the amorphous polymer. A possible way to characterize this change is to use a special back-stress model that includes back-stress yield-controlled softening.

The shearing was done using a double shear sample that one side provided the deformation using DIC, and on the other side it was equipped with a thermocouple to evaluate the temperature change. The temperature change was used to extract the internal material heat storage/heating. This, in combination with the mechanical characterization, in a single test provided a picture of the thermo-mechanical response of both PC and PEEK. The combined results provide a thermodynamic picture of material response that can aid in developing better thermodynamically consistent models.

MODELLING THE MECHANICS OF CRYSTALLIZABLE SHAPE MEMORY POLYMERS

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Keywords: Shape Memory Polymer, SMP, Mechanics, Polymer, Smart material, Hyperelastic, Viscoelastic

Abstract: MODELLING THE MECHANICS OF CRYSTALLIZABLE SHAPE MEMORY POLYMERS

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ABSTRACT

Shape memory polymers(SMPs) are a class of soft active materials that have the ability to retain one or multiple temporary shapes and exhibit deformation as a response to stimuli. The deformed polymers in their temporary shape can be brought back to its original configuration by the application of suitable triggers. This shape memory behavior can be triggered using various stimuli. For example, changes in temperature (cooling process) can be used to fix a temporary shape in the polymer and subsequently changing the temperature again, i.e., heating the material will make the polymer go back to its original shape. SMPs can also be designed to show shape memory behavior as a response to exposure to light of specific wavelengths. The temporary shapes involved can be very complex but SMPs can recover large amounts of elongations as compared to other smart materials. These materials have a wide area of applications ranging from biomedical devices, aerospace engineering, morphing structures, smart adhesives, etc. Hence, there is a need to model their behavior.

Crystallizable shape memory polymers (CSMPs) is a thermally-activated subclass of SMPs and their temporary shape is fixed by a crystalline phase while their return to the original shape is due to the transition of this crystalline phase. We develop constitutive equations to model the thermo-mechanical behavior of CSMPs using a framework that is based on the theory of multiple natural configurations. The polymer is purely amorphous at an elevated temperature above the glass transition temperature and is considered hyperelastic and viscoelastic. The viscoelastic behavior is simulated using a rate type model. Viscoelasticity is only modelled in the amorphous phase and it depends on time, temperature and itself. After the onset of crystallization, the semi-crystalline phase formed is modelled as a hyperelastic material based on the mixture theory and theory of multiple natural configurations. This model does not account for the anisotropy in the crystalline phase and assumes isotropic behavior.

We have applied this model to different boundary value problems of constant stress and constant strain during uniaxial extension to study the mechanical behavior of the polymer under different conditions.

A diffusion coupled constitutive model for thermo-oxidation behavior in polymers

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Keywords: Multiphysics, thermo-oxidative, polymer, reaction-diffusion coupling

Abstract: A diffusion coupled constitutive model for thermo-oxidation behavior in polymers

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High temperature oxidation in polymers is a strongly coupled, highly nonlinear and complex process which limits the use of polymeric materials in several aerospace and defense application as it causes significant performance degradation. The coupled diffusion-reaction process that occurs during thermo-oxidation together with the macromolecular network behavior and finite viscoelasticity of a polymer require a time, temperature and oxidation dependent constitutive law to predict the mechanical response of the material. The objective of the present research is to develop a thermodynamically consistent continuum level theory and implement in finite elements, to describe the coupled thermo-chemo-mechanical process that occurs predominantly at high temperature due to oxidation in polymers. The thermo-oxidation phenomenon is a coupled reaction-diffusion of oxygen occurring within polymers at high temperature in oxygen-rich environment, resulting in the formation of volatile products. Under the application of external loading, this chemo-mechanical process can have severe impact on the material's response and life. Further, the driving forces for these various processes are time-dependent and highly complex in nature. In the present work, we develop a thermodynamically consistent thermo-chemo-mechanically coupled constitutive framework of polymer undergoing high temperature oxidation. A rate of reaction parameter is introduced based on the volume fraction of oxide formation to quantify the extent of oxidation within the bulk polymer. From a thermodynamic point of view, it is shown that the coupling between mechanical deformation and chemical reaction happens in both way; the oxidation reaction gets influenced by the mechanical stress and the rate of reaction eventually alters the deformation response of the material. The constitutive equations are developed in a finite deformation setting to capture locally large deformation of the polymer macromolecules. The kinematics considered the irreversible shrinkage strains generated in the core of the bulk samples due to oxide formation at the exposed surface. Several numerical simulations have been performed to study the combined effect of chemistry and mechanics, and to validate with experimental results.

A general result for the magnetoelastic response of isotropic suspensions of iron and ferrofluid particles in rubber, with applications to spherical and cylindrical specimens

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Keywords: Magnetorheological elastomers; Ferrofluid inclusions; Magnetostriction

Abstract: In this talk, I will present an approximate solution for the effective free-energy function describing the homogenized (or macroscopic) magnetoelastic response of magnetorheological elastomers comprised of non-Gaussian rubbers filled with isotropic suspensions of either iron or ferrofluid particles. The solution is general in that it applies to $N = 2$ and 3 space dimensions and any arbitrary (non-percolative) isotropic suspension of filler particles. By construction, it is exact in the limit of small deformations and moderate magnetic fields. For finite deformations and finite magnetic fields, its accuracy is demonstrated by means of direct comparisons with full-field simulations for two prominent cases: (i) isotropic suspensions of circular particles and (ii) isotropic suspensions of spherical particles.

With the combined objectives of demonstrating the possible benefits of using ferrofluid particles in lieu of the more conventional iron particles as fillers and gaining insight into recent experimental results, the proposed homogenization-based constitutive model is deployed to generate numerical solutions for boundary-value problems of both fundamental and practical significance: those consisting of magnetorheological elastomer specimens of spherical and cylindrical shape that are immersed in air and subjected to a remotely applied uniform magnetic field. It is found that magnetorheological elastomers filled with ferrofluid particles can exhibit magnetostrictive capabilities far superior to those of magnetorheological elastomers filled with iron particles. The results also reveal that the deformation and magnetic fields are highly heterogeneous within the specimens and strongly dependent on the shape of these, specially for magnetorheological elastomers filled with iron particles. From an applications perspective, this evidence makes it plain that attempts at designing magnetostrictive devices based on magnetorheological elastomers need to be approached, in general, as structural problems, and not simply as materials design problems.

Monday, May 20th
Session 1: Additive Architected and 2D Materials
Michigan Room, League 10:30 AM – 12:10 PM
Chair: Serife Tol

A design methodology for 3D auxetic lattice materials with enhanced stiffness and Poisson ratio

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Keywords: auxetic, lattice material

Abstract: Auxetic materials have potential engineering applications like novel actuators, morphing structures, sandwich panel cores, bio-implants, textile and footwear, et al. Significant progress has been achieved in this area during the last three decades in aspects of design and manufacturing. However, most of the 3D auxetic lattice materials do not have high stiffness and strength, which becomes a critical problem and an obstacle for their engineering adoption. In this work, we present a new design methodology towards developing 3D auxetic lattice materials with significantly enhanced stiffness and auxetic performance. This new methodology is expected to deliver a new class of 3D auxetic lattice materials for future applications.

Defects in truss-lattice materials: the impact of coordination number and anisotropy in their elastic properties

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Keywords: Defects, imperfections, architected materials, additive manufacturing

Abstract: The pursuit of new materials with properties superior to the current state of the art, has led many investigators to examine the behavior of materials with a truss-lattice microstructure which accommodates member sizes in the range of micro- and nanometers. Aided by the immense progress in 3D additive manufacturing techniques, such as self-assembly (bottom-up techniques), material scientists have been enabled to fabricate novel materials with complex architectures which can attain unique, unprecedented and tunable properties. However, defects of various forms and concentrations are unavoidable in any fabrication process, and it is anticipated that the application of self-assembly techniques to larger three-dimensional volumes will increase the concentration of defects. Of particular interest for the self-assembly of truss-lattice materials is the influence of struts that are missing from the network, in various defect forms such as missing blocks (clusters) or randomly missing members. In this study, the dependence of the elastic properties on the concentration and distribution of missing struts is investigated for several three-dimensional lattice-truss materials of varying coordination number. This work constitutes a systematic experimental and numerical approach to examine and identify the mechanical elastic regime of defected architected metamaterials. The experimental part of this project is conducted with a two-photon lithography approach, an advanced additive manufacturing technique capable of printing struts with sub-micron cross-sectional dimensions, while the numerical part utilizes finite element simulations accounting for the randomness of the damage spatial distribution through exhaustive Monte Carlo simulations. Focusing on a variety of elastic mechanical properties (Young's, bulk and shear modulus), their evolution is monitored as the total defect percentage increases in magnitude, providing a comprehensive picture of the defected architected metamaterials elastic property space. Finally, this work thoroughly explores the connection between defected truss-lattices and well-established homogenization techniques for composite mediums, elaborating on the applicability of the latter methods to accurately describe the response of defected lattice-based materials.

3D printing and finite element simulation of model composites with stiff and soft phases – effect of architecture on mechanical properties

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Keywords: 3D printing, finite element method, interpenetrating phase composite, matrix-inclusion composite, discontinuous phase composite

Abstract: Composite materials with stiff and soft phases have numerous applications in different industries and are widely found in nature. One of the main factors that determine mechanical properties of composites is the architecture of phases. Thus, understanding the effect of geometrical arrangements on the overall composite behavior holds great promise in the design of new composites with enhanced properties. In this study, the influence of architecture on the overall mechanical behavior of two-phase composites with stiff and soft phases is investigated. Two-phase composites with different geometrical arrangement of phases were studied including an interpenetrating phase composite with two continuous phases, a matrix-inclusion composite with one continuous phase, and a discontinuous phase composite with no continuous phases. These composites were fabricated by additive manufacturing and their mechanical performance was studied both experimentally, using compression testing and digital image correlation, and numerically by a finite element analysis. To better understand the role of stiff and soft phase on the overall mechanical response of the composites, similar one-phase cellular structures consisting of only the stiff phase were also studied. These cellular structures were modeled using finite element method by isolating the stiff phase in the model composites while the soft phase was replaced by air. Model composites developed in this study can also be used to help shed light on the nanoarchitecture of bone. Bone is a natural nanocomposite consisting mainly of collagen and hydroxyapatite. However, no full consensus has been reached on the architecture of these two phases in the bone at the nanoscale. These model composites were also simulated using properties of collagen as the soft phase and hydroxyapatite as the stiff phase. The resulting mechanical pro

Monday, May 20th
Session 2: Fluids (FSI)
Henderson Room, League 2:00 PM – 3:40 PM
Chair: Ying Li

Rayleigh collapse of a bubble near a soft object

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Keywords: bubble dynamics, soft matter, cavitation, multi-component flows

Abstract: Understanding the mechanics of bubble dynamics and shock wave propagation in viscoelastic media is important for various applications involving the high-strain rates of soft matter, particularly in the context of cavitation-induced damage. In the high-strain rate regime, the rheology of soft matter is not well understood, and such insights are invaluable in biomedical applications. Applications of interest include histotripsy, a therapeutic ultrasound treatment that uses high-amplitude and high-frequency ultrasound waves to destroy tissue. The local and transient pressure changes lead to the formation of cavitation bubbles that grow and collapse under high strain rates and producing shock waves upon collapse that propagate in the surroundings. Although not fully understood, the damage mechanism induced on the nearby object combines the effect of the incoming pulses and cavitation (bubble oscillation and collapse) produced by the high tension. The constitutive models describing the soft material are non-trivial and include effects such as (nonlinear) elasticity, history (stress relaxation) and viscosity. Thus, the influence of the bubble dynamics and shock on the material and the response of the material to the bubble and shock are poorly understood.

To simulate and understand this phenomenon, an in-house, solution-adaptive, high-order accurate shock- and interface-capturing method is used to solve the 3D equations for conservation of mass, momentum, energy in a Eulerian framework. This method incorporates evolution equations for the elastic stresses and stress relaxation variables to solve multi-component flows including Zener-like viscoelastic media. In this approach, the evolution equations are evaluated by taking the Lie objective time derivative of the constitutive relation that models the material of interest using strain rates. A 3D canonical problem is considered which involves the Rayleigh collapse of a vapor bubble in a liquid next to a linear viscoelastic object. Scaling relations for the maximum compressive and tensile stresses exhibited in the object will be presented for different bubble collapse distances and shear moduli of the soft object.

Simulating large-amplitude motions of membranes in inviscid flow

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Keywords: fluid-structure interaction, membrane, flutter, vortex sheet

Abstract: We present the dynamics of thin extensible membranes that have negligible bending stiffness. We fix the membrane at both ends and align it with a uniform inviscid background flow. This is a benchmark fluid-structure interaction that has previously been studied mainly in the small-deflection limit, to identify the flutter behavior of membranes. More recent work has also considered applications of thin membranes to shape-morphing airfoils. First, we characterize growth rates and frequencies at small amplitude with respect to the membrane's mass ratio and pretension. We find general agreement with previous work in the locations of divergence and flutter, but with an increased range of unstable motions. Our method is able to compute stable large-amplitude motions over a wide range of parameter space. In our model, large-amplitude motions are stable only at moderate-to-large stretching modulus. We describe how the membranes' motions and frequencies change as they transition from small- to large- amplitude motions.

Dynamic self-assembly of wet hair

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Keywords: self-assembly, capillarity, elasto-capillarity, fluid-structure interaction

Abstract: Reconfigurable materials can enable advanced optical, wetting, frictional and mechanical reconfiguration. We report various patterns formed by draining liquid from hair bundles. Hair-like fibers arranged in triangular bundles self-assemble into various cross sections when immersed in liquid then removed. The combinations of their length and the kinetics, represented by the drain rate, lead to various polymorphic self-assemblies: concave hexagonal, triangular, circular or inverted triangular patterns. Cylindrical fiber assemblies twist at finite drain rate. The equilibrium of these shapes is predicted by elastocapillarity: the balance between the bending strain energy of the hairs and the surface energy of the liquid. Shapes with larger strain energy, such as the inverted triangular bundles, are obtained at the higher liquid drain rates. These polymorphic self-assembly phenomena are reversible by re-wetting and draining, and can have applications in multi-functional dynamic textures.

Monday, May 20th
Session 2: Polymer Mechanics
Koessler Room, League 2:00 PM – 3:40 PM
Chair: Jon Estrada

Porous material deformation characterized by 3D light field imaging

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Keywords: Heterogenous material, Open-cell foam, 3D light field imaging, Volumetric particle tracking

Abstract: Elastomeric foam materials, a special class of heterogeneous materials consisting of an elastic polymer phase and a gaseous phase, are extensively employed in applications such as cushioning and impact protection. Recent experimental work has demonstrated extensive coupling between deviatoric and volumetric response in visco-elastomeric open-cell elastomeric foams, with concomitant marked increase in hysteresis. Both the coupled response and increase in dissipation may prove to be important design variables for using these specialized heterogeneous materials in practice, but these responses are poorly captured by commonly-used foam constitutive models. Furthermore, the processes responsible for both these effects remain unconfirmed. To understand how deviatoric-volumetric coupling and enhanced dissipation arise from open-cell foam microstructures at a mechanistic level, quantification of the deformation behavior at the microstructural scale will be elucidative. This work presents an experimental platform for full-field imaging of a transparent, 3D-printed open-cell foam architecture for use with fully 3D deformation tracking at the resolution of individual matrix elements. Light field imaging and topology-based particle tracking (TPT) are employed to reconstruct time-resolved fully-3D displacement fields from tracker particles embedded in the polymer matrix. In the light field imaging technique, a microlens array is used to simultaneously capture many viewpoints in a single image, providing z-resolution (i.e. depth information) at the cost of lateral resolution. Since TPT can resolve highly heterogeneous fully 3D displacement fields from low resolution 3D imaging, in contrast to digital volume correlation, this single-sensor imaging technique is suitable to reconstruct the complicated motion fields associated with foam microstructures under coupled loading. Thus, the dominant mechanisms of volumetric-deviatoric coupling and elevated hysteresis can be quantified directly from experimental measurements.

High-strain rate compressive behavior of open-cell polyurethane foams

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Keywords: polymeric foams, high strain rate, impact, cell morphology, compressive response, energy absorption

Abstract: Polymeric foams are used for impact protection due to their ability to absorb large amounts of strain energy. In this work, the compressive response of open cell polyurethane foams currently used as liners in the advanced combat helmet is examined across strain rates. A traditional load frame is used to investigate the quasistatic behavior, and two different modifications of a conventional Kolsky (split-Hopkinson) bar configuration are used to probe the dynamic response. A unique, independent method not relying on strain gage signals is presented that leverages full-field imaging to map the velocity on each side of the sample and used to extract the dynamic stress-strain response; and the results are compared with traditional strain gage measurements. X-ray tomography is used to examine the global morphological characteristics of the foam, as well as quantify cell distribution and orientation statistics that are linked to macroscopic behavior. The foams are found to be strongly rate dependent, where the characteristic properties vary logarithmically with strain rate. Specifically, two orders of magnitude increase in strain rate result in a threefold increase in the critical stress and specific strain energy. An analytical expression is presented to describe the rate dependency. Full-field kinematic data from digital image correlation taken during loading is used to extract a nonlinear Poisson's ratio as a function of strain, which is found to be strain rate insensitive. A tangent Poisson function is used to explore the foam's auxetic behavior. These findings provide insight on physically-based constitutive modeling of foams, crucial to predictive brain injury simulations, as well as motivate the need to probe local heterogeneous behavior across strain rates moving forward.

An artificial neural network approach to improve the material properties estimation from nanoindentation of rough surfaces

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Keywords: Indentation, Surface roughness, Artificial neural network

Abstract: Nanoindentation is a materials characterization technique that can measure mechanical properties and is increasingly used to characterize elastic, viscoelastic, and poroelastic properties of soft materials. Sample surface roughness decreases the accuracy of nanoindentation measurements by, for example, underestimating the Young's modulus and increasing variability in the data. However, even careful sample preparation like polishing and microtoming cannot always produce a smooth surface suitable for nanoindentation, particularly for complex, soft materials like soft tissue. This study aims to improve the accuracy of nanoindentation tests of samples with rough surfaces by combining finite element (FE) analysis with machine learning through an artificial neural network (ANN) approach. We hypothesized that the ANN can identify the changes in load-indentation curve caused by sample surface roughness and differentiate those from the changes related to variations in material properties. A parametric FE study of indentation of a rough surface was performed for a Neo-Hookean material. Surface roughness was modeled by a sine function representing the dominant height and frequency of random asperities, and roughness characteristics and the material parameter, c , were systematically changed. The results from the parametric study were used to train an ANN using load-indentation data as inputs and the Neo-Hookean material parameter and roughness characteristics as outputs. A Bayesian regularization algorithm with 10 hidden neurons trained the network. To evaluate the performance of the ANN and validate this approach, a set of simulations using roughness characteristics and material parameters outside the training set was used. Load-indentation data were fed into the trained network and estimated values were compared with the inputs of the FE model. The trained network improved the accuracy of material parameter estimation and successfully predicted the load-indentation data input into the FE model. To further evaluate this approach, we will use the ANN to characterize the material properties of polydimethylsiloxane (PDMS) with different artificially-generated levels of surface roughness. The proposed approach will improve the nanoindentation data analysis when a smooth sample surface cannot be achieved.

Manufacturing of Unidirectional Glass-Fiber Reinforced Composites via Frontal Polymerization

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undefined, undefined, undefined, undefined

Keywords: frontal polymerization, dicyclopentadiene, glass fiber-reinforced composites, reaction-diffusion model, homogenized

Abstract: This study conducts a numerical investigation to explore frontal polymerization of dicyclopentadiene (DCPD) as a faster and low-energy alternative to manufacture unidirectional glass fiber-reinforced composites. The focus is to examine the effects of the fiber volume fraction on key parameters of the front such as the front velocity, maximum temperature and characteristic length scales. The results are compared to the results of a similar study involving carbon fiber composites.

The governing system of coupled partial differential equations, describing the reaction-diffusion process, is solved using Multiphysics Object Oriented Simulation Environment (MOOSE), an open source finite element solver with mesh adaptivity to capture the sharp temperature and cure gradients associated with the front. The model is based on homogenized thermal properties of the composite. A series of simulations with varying fiber volume fractions are carried out to study its effects on the key characteristics of the polymerization front. The transient solutions are complemented by a faster, semi-analytical solver based on the assumption that the front propagates at a constant velocity once steady-state conditions are reached.

The results of the transient simulations show that increasing the glass fiber volume fraction leads to a decrease in the front velocity and temperature, eventually leading to the front being quenched due to a critical deficiency of DCPD in the system. We also observe that increasing the fiber volume fraction leads to longer characteristic lengths. This can be attributed to the fact that the thermal conductivity of the system increases with more concentration of the fiber. Comparing our results to the study on carbon fiber composites, we observe that the front velocity and length scales associated with carbon fiber composites are greater than glass fiber composites however, the front temperature is greater for the latter as compared to the former. The solutions obtained from the steady-state solver match well with the transient solutions with respect to the velocity of the polymerization front, thereby validating the steady state-state solver.

Modeling of Thermal Instabilities Driven by Frontal Polymerization of Composites

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Keywords: frontal polymerization, thermal instability, finite element, thermo-chemical modeling

Abstract: Frontal polymerization (FP) was recently proposed as a faster, more energy-efficient way to manufacture fiber reinforced polymer matrix composites. FP uses heat from the exothermic polymerization of the monomer to generate a self-propagating polymerization front. In most cases, the polymerization front propagates in a steady fashion. However, under some conditions, the front experiences thermal instabilities, which do affect the quality of the manufactured composite parts. In this study, we perform numerical simulations of the FP-driven instabilities in dicyclopentadiene (DCPD) and in carbon-fiber DCPD-matrix composites. In particular, we solve the coupled, nonlinear, transient, partial differential thermo-chemical equations via the Multiphysics Object Oriented Simulation Environment (MOOSE) finite element solver. MOOSE combines an implicit Euler time stepping scheme and the preconditioned Jacobian-free Newton-Krylov scheme to solve the nonlinear system of equations at each time step. In the case of frontal polymerization in composites, the thermo-chemical model relies on the homogenized thermal properties of the unidirectional composite, with the reduction in the source term associated with the exothermic reaction proportional to the fiber volume fraction. With the aid of 1-D transient simulations, we investigate how the initial temperature and degree of cure of the resin and the carbon fiber volume fraction affect the amplitude and wavelength of the thermal instabilities. We also extract the range of process conditions in which the instabilities are predicted to appear.

Monday, May 20th

Session 2: Additive Architected and 2D Materials

Michigan Room, League 2:00 PM – 3:40 PM

Chair: Ignacio Arretche

Numerical Modeling and Design for a 3D Printing Process based on Frontal Polymerization

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Keywords: frontal polymerization, 3D printing, design, thermo-chemo-mechanical model

Abstract: Frontal polymerization (FP) is a novel polymer and polymer composite manufacturing process, which utilizes the heat from the exothermic polymerization of the monomer to create a self-propagating polymerization front. A 3D printing technique that uses FP to simultaneously cure the printed material as it is deposited has also been recently introduced for free-standing polymer components. During this printing process, the polymerizing front follows the printing nozzle and rapidly transforms the viscoelastic filament into a stiff thermoset, thereby eliminating the need for post curing process and providing high printing accuracy compared to traditional direct ink writing. The process is also being considered for the 3D printing of particle- and nanofiber-filled polymeric-matrix composites for multifunctional applications.

In this talk, we present a coupled thermo-chemo-mechanical model specially developed to model the evolution of temperature, degree of cure, and strain fields during the FP process. The semi-analytical model is first validated against experimental measurements and then used to probe the front characteristics under different experimental settings. We then focus on the development of a design diagram for FP-based 3D printing, where the objective function consists in maximizing the printing efficiency (i.e., in achieving maximum printing velocity) while keeping the desired printing accuracy by limiting the deformation of the printed filament. The design space contains parameters that characterize the settings of the printer (ink temperature, extruding pressure, length and diameter of the nozzle), the nature of the ink (initial degree of cure, filler type and loading), and the printing environment (ambient temperature and air flow). The constraints are associated with equilibrated printing for which the front velocity equals the printing speed, the printing accuracy achieved by limiting the deflection of the deposited filament, and the capability of the printer.

Structures engineered to mitigate thermally induced stresses in metallic materials

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Keywords: thermal expansion, materials design, mechanics

Abstract: Fracture, the breakdown of materials, often arises due to undesired stress concentrations. Stress concentration can be caused by impact, pressure, and high temperatures, among other factors. Operating in high temperatures is common in internal combustion engines, batteries, computers, and additive manufacturing. Specifically, heat can cause materials to expand, which can cause stress concentrations, especially if the structure has sharp corners. In this work, we aim to provide guidelines on how to design metallic materials subjected to thermal boundary conditions. Computational analysis is used to investigate how geometrical configurations, near critical areas of high stress, affect the magnitude of thermally induced stress and strain under uniform heating conditions. Results show that tuning the curvature and concavities of sharp corners can mitigate the generation of potentially destructive thermal stresses, thereby suppressing the onset of permanent deformation and damage. Additionally, this study shows that the use of gradient materials (with varying values of coefficient of thermal expansion) can redistribute thermal stresses, improving the structural performance of metallic materials in high temperature environments. In the future, this combined computational mechanics and optimization approach will enable materials-by-design of complex architectures to tackle demanding engineering challenges.

Evaluation of a celestial structure constructed using additive manufacturing placed in a wind tunnel

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Keywords: three D manufacturing, wind tunnel, finite element nonlinear analysis

Abstract: A one foot celestial sphere is manufactured using Vera white plastic within the three D facility, analyzed using nonlinear finite element analysis and placed in a wind tunnel. The results show the effect of wind on this structure up to a velocity of 150 mph.

Fatigue crack growth at weak interfaces: mechanisms relevant for an additive manufactured alloy IN 718

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Keywords: Fatigue, Interface, Cohesive Zone

Abstract: We report on a study motivated by experiments on crack growth in additively manufactured IN 718. The material was made by a direct metal laser sintering process such strongly unidirectional microstructure was produced with grains elongated normal to the build plane. Grains internally possess a high dislocation density and a preferential alignment of the $\langle 001 \rangle$ direction with the grain elongation direction.

Fatigue crack growth experiments with the crack initially oriented parallel to the build plane demonstrate that crack deflection locally at grain boundaries plays a significant role. This finding motivates a computational study of the processes occurring when a fatigue crack interacts with weak interfaces (grain boundaries) and the solid beyond that interface (adjacent grain), as well as for configurations with an interlayer (low yield strength grain) between two domains of higher yield strength. This study asks the specific research question of how plastic strain gradients would influence the crack-interface interaction and the subsequent crack growth response. The computational study considers a modified boundary layer model with cohesive zone elements on the symmetry line of the model representing the main crack. The model is segmented into several domains to which yield strength values are assigned individually. Such domains are separated by cohesive interfaces orthogonal to the main crack. The constitutive model for the solid domains is a conventional mechanism-based strain gradient formulation. The cohesive zone elements follow a constitutive model allowing for cyclic degradation of the cohesive strength. The overall fatigue crack extension, the crack lengths along the interfaces, and the number of crack delay cycles at the interfaces are the key outcomes of the computations.

The finite element computations lead to the following main findings:

- (1) Computations with plastic strain gradients lead to less plastic strains than for cases where strain gradients are ignored, particularly where the plastic zone interacts with interfaces (grain boundaries).
- (2) Crack deflection conditions depend on the interplay between the interface (grain boundary) strength, yield strength mismatch between the domains (grains) on each side of the interface (grain boundary), and plastic strain gradients.
- (3) Plastic strain gradients play a key role in crack extension for an interlayer with a width (grain size) smaller than the plastic zone size.

A multiscale modeling framework to estimate fatigue life distribution

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Keywords: Multiscale model, fatigue, additive manufacturing

Abstract: In this work we explore a multiscale modeling framework designed to capture the heterogeneity and stochasticity observed in additively manufactured metal, and its impact on fatigue life. To generate the model, a microstructure is sampled from a known distribution at each material point in the part scale model. The collection of microstructures represents one possible part realization, and the minimum estimated fatigue life of a microstructure, based on a given part-scale loading condition, represents one point of the part-scale fatigue life distribution. The microstructure response is computed using a data-driven reduced order model and one-way coupling. A series of these realizations can then be used to estimate component level variability and chance of failure. If the distributions of microstructures are related to, e.g., build strategy this can be used to estimate the differences in failure likelihood between different processing routes. Specifically, at the micro-scale, voids were imaged in 3D using x-ray computed tomography at Argonne National Lab's Advanced Photon source. These voids, from LENS-build metal, are used as defect populations within a poly-crystal plasticity model where 3D grains are generated from diffraction images (EBSD, micro-Laue diffraction) or grain-growth models. This work is presented in the context of lifetime assessment for additive manufacturing, though the framework is broadly applicable to materials with defect-driven heterogeneity.

Monday, May 20th

Session 3: Fluids (FSI)

Henderson Room, League 4:10 PM – 5:50 PM

Chair: Sameh Tawfick

A novel deep learning model for fluid-structure interaction

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Keywords: Wake-body interaction, deep learning, convolutional neural network, POD

Abstract: This work introduces a novel machine learning model for unsteady fluid-structure interaction systems by incorporating low-dimensional physics. Of particular interest is to predict the long time series of unsteady flow dynamics using the learned low-dimensional model. We consider convolutional neural networks (CNN) to learn fluid-body interaction dynamics, which assembles layers of linear convolutions with nonlinear activations to extract low-dimensional features. We first project the high-fidelity time series data from the finite element Navier-Stokes solver to a low-dimensional subspace using proper orthogonal decomposition (POD). The time-dependent coefficients of the POD subspace are mapped to the flow field via a CNN with nonlinear rectification, and the CNN is trained using stochastic gradient descent method to predict the POD time coefficients when a new flow field is fed to it. The mean flow field, the POD basis vectors and the trained CNN are used to predict the long time series of the flow fields and the flow predictions are quantitatively assessed with the full-order (high-dimensional) simulation results. Our predictions via POD-CNN process maintain a remarkable accuracy throughout the long time series for the entire fluid domain including a highly nonlinear near wake region.

High-Order Fluid-Structure Interaction Simulations with Adaptive Meshing

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Keywords: Computational Fluid Dynamics, Flow-Structure Interaction and Adaptive Meshing

Abstract: This work proposes an adaptive approach for solving the fluid structure interaction problem using high-fidelity numerical methods. A high-order partitioned approach is applied to couple the fluid and the structural subsystems, where the fluid subsystem is discretized using a discontinuous Galerkin finite-element method while the structures solver uses a continuous Galerkin discretization. High-order time integration schemes, developed by Van Zuijlen et al. [1] are used by the coupled solver to march forward in time.

The space-time mesh of the fluid subsystem is adapted using output-based methods. The error estimates for the unsteady outputs are evaluated by calculating the uncoupled, unsteady adjoint of the fluid subsystem [2]. A one dimensional cantilevered Euler-Bernoulli beam placed in a uniform flow is used to validate the coupled solver. The effect of high order and adaptivity on the accuracy of fluid structure simulations will be demonstrated by predicting flutter over a pitching/plunging NACA 0012 airfoil. The benefits of the adaptation will be examined by comparing the convergence of engineering output of interests on the adapted mesh to that on a uniformly refined one.

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Large Amplitude Flapping of an Inverted Elastic Foil: Application to Energy Harvesting

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Keywords: flapping dynamics, inverted foil, splitter plate, vortex-vortex interaction

Abstract: An elastic foil interacting with a uniform flow with its trailing edge clamped, also known as the inverted foil, exhibits a wide range of complex self-induced flapping regimes such as large amplitude flapping (LAF), deformed and flipped flapping. In particular, the LAF is of interest for its applications in the development of energy harvesting devices. Here, we perform three-dimensional numerical experiments assuming spanwise periodicity to realize the role of vortex structures and the vortex-vortex interactions on the LAF response at Reynolds number $Re=30,000$ using a LES model. To understand the role of the counter-rotating periodic vortices generated and the interaction between them on the LAF, we investigate the dynamics of the inverted foil for a novel configuration wherein we introduce a fixed splitter plate at the trailing edge to suppress the vortex shedding from trailing edge and inhibit the interaction between the counter-rotating vortices. Unlike the vortex-induced vibration of an elastically-mounted circular cylinder, we find that the inhibition of the interaction has an insignificant effect on the transverse flapping amplitudes, due to a relatively weaker coupling between the counter-rotating vortices emanating from the leading edge and trailing edge. However, the inhibition of the trailing edge vortex reduces the streamwise flapping amplitude, the flapping frequency and the net strain energy of foil. To further generalize our understanding of the LAF, we next perform low-Reynolds number ($Re \in [0.1, 50]$) simulations for the identical foil properties to realize the impact of vortex shedding on the large amplitude flapping. Due to the absence of vortex shedding process in the low- Re regime, the inverted foil no longer exhibits the periodic flapping. However, the flexible foil still loses its stability through divergence instability to undergo a large static deformation. From our study on the effect of foil aspect ratio without side effects, we find that the foil aspect ratio has a minor impact on the LAF response at high Reynolds number. Finally, we introduce an analogous analytical model for the LAF based on the dynamics of an elastically mounted flat plate undergoing flow-induced pitching oscillations in a uniform stream. This study has implications on the development of novel control mechanisms for energy harvesting and propulsive devices.

Monday, May 20th

Session 3: Damage and Failure of Quasi-Brittle Composites

Koessler Room, League 4:10 PM – 5:50 PM

Chair: Anthony Waas

Design of New Materials and Structures to Maximize Strength at Probability Tail:
A Neglected Challenge for Quasibrittle and Biomimetic Materials

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Keywords: failure probability, size effect, nacre, imbricated, quasibrittle, biomimetics

Abstract: Similar to nacre (or mother-of-pearl), imbricated lamellar structures are widely found in natural and man-made materials, and are of interest for biomimetics. These staggered imbricated structures are known to be rather insensitive to defects and have strength and fracture toughness an order-of-magnitude higher than their constituents. Their deterministic behavior has been intensely studied, while statistical studies have been rare and no theoretical basis for the probability density function (pdf) of strength has yet been formulated. This lecture presents a theoretical and numerical study of the pdf of strength and of the corresponding statistical size effect. After reasonable simplifications of the shear bonds, a lamellar axially loaded lamellar shell is statistically modelled as a fishnet pulled diagonally. A FE model is developed and used in many millions of Monte Carlo simulations of strength. An analytical model for failure probability of the fishnet is developed and matched to the computed statistical histograms of strength of fishnet structures of various sizes. Based on fresh results at Northwestern, post-peak progressive softening of fishnet links is considered and its effect on the strength probability distribution is analysed on the basis of order statistics. It appears that, with increasing size, the pdf of strength slowly transits from Gaussian to Weibull distribution but the transition is different from that previously obtained at Northwestern for quasibrittle materials of random heterogeneous mesostructure. An important practical implication is that the staggered lamellar architecture not only enhances the mean strength but also contributes an additional major strength increase at the failure probability level of 10^{-6} , which is what matters for structural safety.

SURROGATE BASED OPTIMAL STEERED FIBER- PATHS FOR MAXIMIZED BUCKLING PERFORMANCE IN COMPOSITE LAMINATES, INCORPORATING MANUFACTURABILITY CONSTRAINTS

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Keywords: Optimization, Surrogate Model, Steered Fiber

Abstract: Automated Fiber Placement (AFP) technology has revolutionized composites manufacturing and is quickly replacing traditional hand-layup manufacturing. Among others, the notable advantage of AFP is that the designer is no more restricted to the use of straight fiber paths, which means it is possible to have fiber paths designed for optimizing structural performance. The scope of this work is to identify the manufacturing parameters and associated constraints imposed by these parameters on the manufacturability of steered fiber structural panels, using currently available AFP machines. Deriving optimal paths to maximize the buckling load of square laminated plate under compressive in-plane loads is the main goal. AFP is a robotic manufacturing technology to manufacture CFRP laminates by using slit tapes of pre-preg material. AFP is suitable for manufacturing large structural parts (wing skin panels, ribs, fuselage sections etc.) that can have curvatures. AFP is an additive manufacturing modality, so the benefits of AFP include minimal scrap, reduced cost and increased time efficiency of the manufacturing process. In addition to these, AFP opens up the design space for structural design engineers allowing optimal steered fiber paths that can be derived for specific structural performance of selected structural configurations.

In this study a 4-layer symmetric square panel of T800/3900 composite laminate is considered, simply supported on all the edges and under the influence of compressive in-plane loads. The objective is to maximize the buckling load of this panel subject to constraints on transverse stiffness of the panel. Design variables are identified to model center lines of each tow of the AFP machine, modeled using Bezier splines. Tow width, fiber continuity and radius of curvature constraints are explicitly included as design constraints on the mathematical formulation of the optimization problem.

A combination of Genetic Algorithm (GA) and surrogate modeling techniques are proposed to be implemented in conjunction with an FEA model to derive the optimal fiber path. These proposed methods applied to a single lamina problem posed with similar constraints have shown feasible results.

Fracturing Behavior and Size Effect of Discontinuous Fiber Composite Structures

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Keywords: Composites, Discontinuous Fiber Composites, Size Effect, Quasibrittleness

Abstract: This study investigates the mode I intra-laminar fracture and size effect in Discontinuous Fiber Composites (DFCs). Towards this goal, the results of fracture tests on geometrically-scaled Single Edge Notch Tension (SENT) specimens are presented and critically discussed for three platelet sizes. The results clearly show a decrease in nominal strength as the specimen size increases. This effect becomes more important as the structure size increases. It is found that, when the specimen is sufficiently large, the structural strength scales according to Linear Elastic Fracture Mechanics (LEFM) and the failure occurs in a very brittle way. In contrast, small specimens exhibit a more pronounced pseudo-ductility with a limited scaling effect and a significant deviation from LEFM. To characterize the fracture energy and the effective length of the fracture process zone, an approach combining equivalent fracture mechanics and stochastic finite element modeling is proposed. The model accounts for the complex random mesostructure of the material by modeling the platelets explicitly. Thanks to this theoretical framework, the mode I fracture energy of DFCs is estimated for the first time and it is shown to depend significantly on the platelet size. In particular, the fracture energy is shown to increase linearly with the platelet size in the range investigated in this work. Another important conclusion of this work is that, compared to traditional unidi-rectional composites, DFC structures exhibit higher pseudo-ductility and their strength is, by far, less sensitive to notches, defects and cracks. However, this aspect can be used advantageously in structural design only upon the condition that proper certification guidelines acknowledging the more pronounced quasibrittleness of DFCs is formulated. The size effect analysis presented in this work represents a first step in this direction as it allows the assessment of the severity of a defect or notch in DFCs.

Computational and Analytical Modeling for the Fracture of Micro-Architected Glass

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Keywords: Interlocking, Suture, Micro-architecture, Bio-Inspired, Fracture, Contact, Cohesive Zone Model

Abstract: Brittle materials such as glasses and ceramics are generally very stiff and hard but have very low toughness. Recent studies have demonstrated that bio-inspired interlocking micro-architectures or sutures within a brittle material can increase its ductility and fracture toughness remarkably. These interlocking micro-architectures are generated by creating weaker interfaces in the bulk. The interface is designed such that it partitions the bulk into jigsaw shaped interlocking teeth. Under tensile loading, the crack is guided through the weak interface and the teeth get engaged through interlocking, which is the key to higher toughness. Despite showing tremendous promise to improve material properties there is a lack in computational and analytical models for these interlocked systems. Besides, sufficient information about interface properties is not available from experiments.

In the present work the interface properties and the coefficient of friction, are inversely identified from experimental data by developing a finite element model involving mixed mode cohesive zone technique for the weak interface, frictional contact for the teeth interlocking. The experimental data used is available in the literature. In the present work, a novel approximate analytical model is also derived for the opening-mode fracture at the interface and complete pullout response of the interlocking teeth. The analytical model also incorporates the cohesive zone technique, non-Hertzian contact mechanics.

In the analytical model, the contact and the cohesive forces are obtained in terms of the displacements at the boundary of the compact tension specimen. Subsequently, these forces are used in the moment equilibrium equation for the compact tension specimen to determine the applied load. The proposed numerical-analytical model was derived using a non-Hertzian contact solution at the contact points between the tabs approximating them as disks, and kinematic unzipping modeled as independent of resultant forces apart from some minor corrections due to elastic deformations. The numerical-analytical model endowed with the inversely identified interface properties could match accurately with our finite element prediction and the published experimental results.

The proposed experimentally validated, computational model and numerical-analytical model of this interlocking behavior would enable performance optimization of the interlocking micro-architecture system.

Monday, May 20th

Session 3: Additive Architected and 2D Materials

Michigan Room, League – 4:10 PM – 5:50 PM

Chair:

Metamaterial concepts for low-frequency elastic wave focusing

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Keywords: Locally resonant metamaterials, low-frequency elastic wave focusing, gradient-index lens, bandgap-based mirror

Abstract: Elastic wave propagation in artificially structured metamaterials and phononic crystals (PCs) has recently received a growing attention. Due to their unique characteristics such as bandgaps and the ability to reduce the phase and group velocities metamaterials/PCs can manipulate and control waves propagating in structures yielding unprecedented applications in various disciplines. Among others, metamaterial/PC-based elastic wave focusing can benefit structure-borne wave energy harvesting and sensing applications by concentrating the wave energy at the harvester/sensor locations. However, the PC-based elastic lens and mirror concepts that have been explored for enhanced energy harvesting are suitable for relatively high-frequency waves (e.g. tens of kHz), which are very much outside the typical ambient structural frequency energy spectrum. In order to reduce the design frequency of such phononic crystal-based lens and reflector/mirror designs is to increase their size, which would yield very large dimensions to operate at ambient vibration frequencies (~hundreds of Hz). In this work, we explore locally resonant (LR) metamaterial concepts to enable low-frequency elastic wave focusing. To this end, we propose a gradient-index LR lens, a bandgap-based elastic mirror and a graded wave amplifier. The LR lens is designed in a similar way to its PC counterpart by tailoring the refractive index profile of the LR unit cell distribution. However, the key factor in the LR lens design is setting the local resonance frequency of the unit cells to a low frequency and achieving the refractive index variation hence focusing through altering the dispersion characteristics below the local resonance frequency by the mass ratio of the resonators. The low-frequency bandgap is exploited in the LR mirror concept. A LR parabolic mirror is designed by LR unit cells arranged in the form of a parabola to focus plane waves. In our last concept, a graded high-refractive-index metamaterial is presented to focus elastic wave energy through wave compression. In addition to enhanced structure-borne wave energy harvesting, these LR focusing concepts can be implemented in civil, aerospace, and mechanical systems to localize elastic wave energy.

Design of mechanical metamaterials for simultaneous vibration isolation and energy harvesting

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Keywords: mechanical metamaterial, vibration isolation, energy harvesting

Abstract: Through finite element analysis and a 3D printing assisted experimental study, we demonstrate a design of mechanical metamaterials for simultaneous mechanical wave filtering and energy harvesting. The mechanical metamaterials comprise a square array of free-standing cantilevers featuring piezoelectric properties being attached to a primary structural frame. A complete bandgap has thus been created via the strong coupling of the bulk elastic wave propagating along the structural frame and the distributed local resonance associated with the square array of piezoelectrically active cantilevers. Operating within the stop-band, external vibration energy has been trapped and transferred into the kinetic energy of the cantilevers, which is further converted into electric energy through mechano-electrical conversion of its integrated piezoelectric elements. Therefore, two distinct functions, vibration isolation and energy harvesting, are achieved simultaneously through the designed mechanical metamaterials.

Manipulating vibration response of 3D printed metastructures through lattice topology:
simulation and experimental validation.

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Keywords: metastructures, band gaps, vibration response, architected materials

Abstract: Architected metamaterials have the ability to manipulate elastic wave propagation through their design, which holds promise for many engineering applications. Through variations in their geometry and material composition, they have been able to achieve desirable dynamic properties such as band gaps, negative refraction, and enhanced energy absorption. A major challenge in vibration suppression is to achieve broadband low frequency band gaps without increasing the mass or scale of the system. Great efforts to address this problem have introduced a wide variety of metamaterial design spaces. We take particular interest in a metastructure design platform that combines a 3D periodic polymeric lattice with embedded steel resonators. The wide band gaps of these metastructures are bounded between acoustic and optical modes, which makes them highly suitable for achieving low frequency vibration mitigation. Furthermore, it has been shown that substantial tailoring of the metastructure's response can be achieved through small manipulations of the lattice geometry. Here, we study the effects of different lattice topologies on the metastructure's vibration response. We demonstrate how band gap frequencies can be manipulated by the lattice properties, and we interpret the band gap frequencies in terms of local static effective properties of the lattice material. This gives us a way to estimate band gap range and inform the design of the metastructure to tailor mitigation to the desired frequency range. We fabricate these multi-material metastructures using commercially available 3D printing techniques. We experimentally validate our finite element simulations using impact excitation and frequency transmission tests. We study axial, bending and torsional polarizations of vibration mitigation of finite metastructures, and investigate how different lattice topologies affect their attenuation efficiency.

Turning Planar Rigid Panels into Complex Freeform Shapes

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Keywords: flexible surface, complex microstructural morphology

Abstract: Contemporary architecture prominently features curved and complex surfaces, both as a means to provide aesthetically pleasing structures and to make efficient use of space. With the currently available conventional construction materials, i.e. steel, concrete, wood, aluminum, and glass, it is challenging and costly to form complex freeform shapes. Current approaches to construct such freeform complex shapes are based on modular methods, which require fabricating molds, casting individual modules, and assembling of the modules, which are not only labor intensive and costly operation but also generating large amount of waste. In this study, we consider an alternative approach to create flexible freeform surfaces from relatively stiff and thick panels through relief cutting, or kerfing. The flexibility and moldability are based on reducing the second moment of area of the solid plates in order to induce large out-of-plane deformations. Using the kerfing technique allows for generating flexible structures with complex geometries from mass-produced panels of standard shape and size. Kerfing creates continuous cut patterns, which minimizes waste and eliminates the need for mold casting. When using kerfing method to achieve the desired surface topology, the stresses, strains, and displacements in the surface will depend on the kerf pattern, cut density, and constituent behavior. From investigating the unit-cell responses of different kerf patterns (square and hexagon) with different cut densities we have information on the deformation behaviors, i.e., maximum stretch and distortion in each unit-cells. This information will guide the design of kerf freeform panels. The overall responses of the kerf panel also depend on the materials used in the panel. In this study, we only consider linear elastic and linear viscoelastic material behaviors for the kerf materials, and examine the overall deformations in the complex freeform shapes under different loading histories.

Mechanics of Kirigami Based Structures

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Keywords: kirigami, hyperelastic materials, finite element, experimental data

Abstract: The ancient Japanese art of paper cut, kirigami, was employed to silicone rubber doped with carbon nanotubes to create structures with large stretchability and variable Poisson's ratio capabilities. The high order Ogden hyperelastic models (3rd and 4th orders) were the ones more suitable for tensile tests. The CNT addition did not affect the overall stiffness, but the strength seems to be highly dependent of the CNT/silicone interaction. A soft material surrounding a very stiffness material could lead to a weak interface due to the high shear stress developed. This phenomenon is also related to the CNT spatial distribution around the silicone rubber matrix. AFM observations seems to indicate formation of clusters dispersed in a homogeneous way. The kirigami configuration associated to the CNT addition to silicone rubber lead to large deformations, up to 900 %, which is far beyond Ogden's instability. Based on experimental data curve fit, the best results for stress intensity decrease around the Kirigami's "crack" tip seems to be around 0.30 wt. % CNT.

Tuesday, May 21st

Session 1: Fluids (Cavitation and High Rate)

Henderson Room, League 10:30 AM – 12:10 PM

Chair: Jon Estrada

The interaction between mechanics and fluid permeation on the cavitation of polymer gels

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Keywords: polymer gels, swelling, cavitation, volume phase transition,

Abstract: The concomitant action of mechanical loading and absorption of swelling agents (solvent uptake) arises in a variety of contexts involving solids. This special kind of interaction between mechanics and chemistry underlies many interesting phenomena undergone by polymeric solids and gels. Among these, we mention environmental stress cracking and anomalous diffusion in polymeric solids and volumetric phase transitions in gels.

In this paper, we investigate the role played by the interaction of mechanics and absorption of a swelling agent on the occurrence of multiphase equilibria and cavitation in polymeric solids and gels. More specifically, we consider an initially dry and intact, i.e., not hollow, elastic sphere undergoing a spherically-symmetric deformation and investigate swelling induced by the combined action of mechanical loads, defined in terms of the ambient pressure and a normal traction, and the absorption of a swelling agent. The swollen sphere is viewed as a two-component body composed of two incompressible constituents, the elastic solid and the swelling-agent. The state of the swollen sphere is, therefore, fully characterised by the distribution of the swelling agent and the radius of a central hole, which is zero if the swollen sphere remains intact. When the ambient chemical potential of the swelling agent is fixed and chemical equilibrium prevails at the interface between the solid and the environment, we describe two types of intact states, namely uniform equilibrium states and states for which the sphere is divided in two regions, the inner one dry and the outer one uniformly swollen, separated by a sharp boundary. For these states, we also investigate the possibility of cavitation---i.e., the sudden appearance of a central traction-free cavity. Of importance in the analysis presented here is the notion of net-free-energy potential, the definition of which requires the specification of the chemical potential of the environment and the prescription for the constitutive equation for the free-energy density.

Non-spherical analysis of laser-induced bubble collapse in soft matter

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Keywords: Bubble dynamics, Soft matter

Abstract: Bubble dynamics in soft matter are of interest for the applications of high-strain rate rheometer or therapeutic ultrasound. When a bubble collapses inertially, it often deviates from a spherical shape. This non-sphericity causes difficulty in the rheometer where we characterize the surrounding soft material by comparing the bubble collapse and a cavitation model. In therapeutic ultrasound, the non-sphericity during inertial bubble collapse is an important factor to predict tissue damage. For these reasons, we investigate the non-spherical dynamics of inertial bubble collapse in soft matter. We first conduct the experiments of laser-induced bubble collapse in an agarose gel. Since the temporal and spatial resolutions of a high-speed camera are limited, we also investigate the laser-induced bubble collapse in an analytical approach. We use a non-spherical model where the bubble surface is expressed by a superposition of spherical harmonics. The time history of mean bubble radius is obtained by the Rayleigh-Plesset model, where compressibility, heat diffusion and vaporization are taken into account to precisely predict the inertial bubble collapse. Then, we solve an equation for non-spherical mode amplitudes via one-way coupling of the mean bubble radius. The initial conditions are set to when the bubble has its maximum radius, and we analyze the laser-induced bubble collapse by comparing the model and experiments. Although it is difficult to quantitatively measure the non-spherical shape of a bubble in experiments, our analysis and experiments show some agreements. The solutions of the non-spherical model show that the mode two is the most unstable during the inertial bubble collapse. In our experiments, a bubble often splits into two during the collapse, which agrees with our expectation. In this case, the initial amplitude of mode two is important to determine whether the bubble splits or not. We also investigate the viscoelastic effects of the surrounding soft matter on the laser-induced bubble collapse. The non-spherical analysis shows that the viscosity stabilizes and shear modulus suppresses the non-spherical mode. In addition, viscoelasticity reduces the maximum bubble radius and makes the bubble collapse less violent. As a result, a bubble in soft matter with higher concentration keeps its spherical shape more. The same behavior is observed in our experiments using agarose gels with different concentrations.

The poker-chip experiment explained

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Keywords: Cavitation, Poker-chip experiments, Finite deformations

Abstract: The internal nucleation of cavities/cracks in elastomers, a phenomenon commonly referred to as cavitation in the literature, was first reported by Busse (1938) and Yezley (1939) and later made more prominent by the work of Gent and Lindley (1959). All of them conducted tension tests on thin disks of rubber (“poker-chips”) bonded to plane metal end-pieces and observed the sudden appearance of cavities/cracks in the mid-plane of the rubber disks. Gent and Lindley, in their landmark study, attributed this phenomenon to the unstable elastic growth of pre-existing defects in elastomers. However recent experiments by Poulain et al. (2017), analogous to the classical experiments by Gent and collaborators but carried out at higher spatio-temporal resolution (of 1 micron in space and 60 ms in time), along with the analysis of Lefevre et al. (2015) made it clear that elasticity alone is insufficient to explain the cavitation event and that cavitation is fundamentally a by-product of fracture.

In this talk, I will examine the poker-chip experiments in the light of a recently developed macroscopic field theory (Kumar et al., 2018) that has the capability to explain, describe and predict the nucleation and propagation of fracture and occasional healing in elastomers in a unified manner. The theory rests on two central ideas. The first one is to view elastomers as solids capable to undergo finite elastic deformations and capable also to phase transition to another solid of vanishingly small stiffness: the forward phase transition serves to model the nucleation and propagation of fracture while the reverse phase transition models the possible healing. The second central idea is to take the phase transition to be driven by the competition between a combination of strain energy and hydrostatic stress concentration in the bulk and surface energy on the created/healed new surfaces in the elastomer. After outlining the numerical implementation of the theory, comprehensive 3D comparisons between the theory and the poker-chip experiments will be presented to definitively explain these classical experiments.

Tuesday, May 21st

Session 1: Damage and Failure of Quasi-Brittle Composites

Koessler Room, League 10:30 AM – 12:10 PM

Chair: Dianyun Zhang

Investigating anomalous fracture mechanisms at the nanoscale in quasi-brittle materials

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Keywords: Linear elastic fracture mechanics (LEFM), Length-scale effects, Non-local effects, Entropic effects , notch-insensitivity

Abstract: The overarching objective of this paper is to investigate the validity of applying continuum-based linear elastic fracture mechanics (LEFM) methodology at the nanoscale, which is often employed by researchers to model fracture processes at the “discrete” atomic scale. The potential sources of error in the application of LEFM at the nanoscale are: (a) Length-scale effects that lead to notch insensitivity, (b) non-local effects due to long range inter-atomic forces, (c) entropic effects due to random thermal motion of atoms, and (d) anomalous behavior of cohesive traction-separation law due to crack size effect. Each of these effects will be presented and discussed in detail. The material selected for this study is monolayer graphene, primarily because extensive data, both experimental and analytical, already exist for this material in the literature for model validation. Further, an atomistic J-integral is implemented as a nano-scale fracture metric to investigate flaw-tolerance at the nanoscale reported by many researchers, and to develop a methodology to predict the initiation fracture toughness of the material. For this purpose, a bond-order based potential (ReaxFF) available in LAMMPS molecular dynamics (MD) software is utilized to accurately pinpoint bond separation. Predictions obtained using the atomistic J are compared with LEFM predictions for the case of a single (zig-zag) graphene sheet with a center-crack under tensile loading at room temperature, and show significant deviations from LEFM and from standard cohesive zone models (CZM) for nanoscale cracks. Future work entails extending this methodology to quasi-brittle thermoset polymers.

A gradient damage model for polydisperse polymer networks

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Keywords: Polydisperse polymer networks, Equal force, Incompressible, Gradient damage

Abstract: A common underlying assumption for the majority of constitutive models for polymer networks is that all the chains admit the same length, i.e. the same number of Kuhn segments. However, all synthetic polymers are polydisperse in that they contain polymer chains of unequal length, characterized by a chain length distribution functions. The chain length distribution originates from randomness of the polymerization process.

Experiments and theoretical works have shown that the mechanical and mechanochemical properties, as well as the damage and fracture behaviors of a polymer networks depend on the distribution of the chain lengths between crosslinks. For this reason, a proper constitutive model should take into account the chain lengths distribution. Some constitutive models have been developed, in which the idealized networks of different chain lengths are assembled following an equal strain assumption corresponding to a parallel arrangement of chains having different lengths. However, such schemes result in large values of force and even diverged values of force for chains that their prescribed end-to-end length is beyond their contour length. One can try to remedy this problem either by restricting the end-to-end length to be less than the contour length, or by deactivating such chains accounting for chain rupture at some finite stretch. Another approach suggests the equal force assumption, corresponding to a series arrangement of chains where the subchains carry the same force between crosslinks.

In this contribution, we adopt the assumption of equal force and derive an eight-chain model of non-Gaussian randomly jointed chain with arbitrary chain length distribution, accounting for the extension of the Kuhn segments. To simulate the rupture of polymers by scission of bonds in the chain backbone, we resort to a gradient damage model that has the capability of addressing the crack nucleation, path selection, and discontinuous propagation. The polymer networks is modeled as incompressible materials. We validate the gradient damage model through comparison of the simulated critical loading for crack nucleation of a 3D hyperelastic bar under tension and the theoretical prediction. We demonstrate the modeling capability of the proposed model to crack propagation in polymer networks at large strains through representative 3D simulations.

Strength and Cohesive Behavior of Thermoset Polymers at the Microscale: A Size-Effect Study

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Keywords: Cohesive Fracture Mechanics, Size Effect, Micromechanics, Composites

Abstract: This study investigated, experimentally and numerically, the fracturing behavior of thermoset polymer structures featuring cracks and sharp u-notches. It is shown that, even for cases in which the sharpness of the notch would suggest otherwise, the failure behavior of cracked and pre-notched specimens is substantially different, the failure loads of the former configuration being about three times lower than the latter one. To capture this interesting behavior a two-scale cohesive model is proposed. The model is in excellent agreement with the experimental data and its predictions allow to conclude that (a) residual plastic stresses cannot explain the very high failure loads of notched structures; (b) the strength of the polymer at the microscale can be from six to ten times larger than the values measured from conventional tests whereas the fracture energy at the microscale can be about forty times lower; (c) the pre-notched specimens investigated in this work failed when the stress at the tip reached the microscale strength whereas the cracked specimens failed when the energy release rate reached the total fracture energy of the material. The foregoing considerations are of utmost importance for the design of microelectronic devices or polymer matrix composites for which the main damage mechanisms are governed by the strength and cohesive behavior at the microscale.

Effect of size and randomness in matrix properties on mechanical response of fiber-composite RVEs

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Keywords: RVE, ICME, fiber-reinforced polymer composite, crack-band model

Abstract: Representative Volume Element (RVE) is a geometrical representation that is typically used to numerically model the mechanical response of a material having heterogeneous microstructure, such as fiber-reinforced polymer composites. We address the effects of the appropriate RVE size and fiber packing on the tensile response of fiber reinforced composites, in the context of Integrated Computational Materials Engineering (ICME). Using micromechanics, different sizes of RVEs with random packing of fibers that preserve a fixed volume fraction are subjected to mechanical loading programs, using commercially available finite element analysis software ABAQUS. Salient features of the response are analyzed to determine the effects of fiber packing within the RVE and RVE size on the details of crack path, maximum load and overall fracture toughness. Damage accumulation/cracking in the matrix component of the RVE is modeled using the Bazant-Oh crack band model. Depending on the constituent fiber and matrix properties, the minimum RVE size requirement is established. Moreover, since local fracture properties (strength and toughness) in a realistic fiber-composite are not uniform, analysis is also performed taking into account variability in the matrix fracture properties within the RVE. For a given RVE size, matrix fracture properties are assumed to be normally distributed and are quantified in terms of the mean and variance. The influence of the matrix property variance on the overall response is also studied.

Tuesday, May 21st

Session 1: Additive Architected and 2D Materials

Michigan Room, League 10:30 AM – 12:10 PM

Chair: Grace Gu

Cracking and spalling of the oxide layer developed in high-burnup zircaloy-4 cladding under normal operating conditions in a PWR

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Keywords: oxidation, cracking, spalling

Abstract: In this paper, the evolution of cracks from the surface of a thick oxide layer on zircaloy-4 cladding has been analyzed for the normal operation of pressurized-water reactors. The conditions for the propagation of radial cracks towards the interface, channeling along the axis of the cladding, and the possible subsequent spalling of the oxide have been studied. The analysis was conducted by first calculating how the stresses in the oxide developed during operation, using a numerical model that incorporates multiple mechanisms such as creep, swelling and oxidation. These calculations demonstrate that the circumferential stresses within the oxide increase as oxidation proceeds, and as the cladding expands under the effect of fuel swelling. Although the intrinsic growth stresses of the oxide are compressive, tensile stresses can eventually develop in the outer region of the oxide. Within this regime, the energy-release rate for the radial propagation of a crack was determined using the J-integral, along with the calculated stress profile. By assuming a suitable value of toughness for the oxide, it is possible to determine the depth to which such a radial crack can grow. A second fracture-mechanics calculation was then conducted to explore the conditions under which such a surface crack can subsequently channel along the axial direction of the cladding. A third fracture-mechanics analysis considered the possibility of oxide spalling. This showed the possibility of spalling from the radial cracks, leaving a thin layer of the oxide adhered to the metal that could result in a local cold spot responsible for hydride formation.

Characterizing the interaction in atomically thin layered materials

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Keywords: Adhesion, Atomically thin layered materials, Atomic force microscopy, Graphene

Abstract: We combine conductive atomic force microscopy (CAFM) and molecular dynamics (MD) simulations to reveal the interaction of atomically thin layered materials (ATLMs) down to nanoscale lateral dimension. We glue the tip of a conductive atomic force microscope with a nanosized graphite pillar and apply a bias voltage and shear loading to reliably produce high-quality mono- and few-layer graphene features of different shapes and sizes on a substrate surface. The setup also allows quantifying, for the first time, the effect of layer number and electric field on the dielectric constant of ATLMs with few-layer down to monolayer thickness. Our CAFM-assisted electrostatic technique shows that high-quality mono- and bilayer graphene is reliably produced at significant yields by the shear type of bond breaking between layers, whereas the normal type of bond breaking exhibits a very stochastic process mainly due to the coexistence of local delamination and interlayer twist. Our dielectric constant measurements also reveal a very weak dependence on the layer number and the electric field (up to our experimental limit of 0.1 V/\AA), which is in contrast with theoretical reports. Owing to unexpectedly large variations in the screening ability of pristine monolayer graphene under ambient conditions, we further demonstrate that the effective dielectric constant of monolayer graphene can be engineered to provide a broad spectrum of dielectric responses (3.5-17) through oxidation and thermal annealing, thus confirming its much higher chemical reactivity than bilayer and few layers. We also implemented 3D spatial charge distribution of layered materials into molecular dynamics simulations to further reveal the anisotropic nature of the van der Waals interactions in the layered materials for accurate control of the number of exfoliated flakes. The experimental observations and atomistic simulations showed that the shear exfoliation technique exhibits a very promising and controllable behavior during the exfoliation process by eliminating the interlayer spacing variations and consequently suppressing the interlayer twist angles.

The route towards graphene composites

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Keywords: 2D materials, mechanics, Moire, atomicforce microscopy, indentation

Abstract: The synthesis of precisely engineered nanostructures will enable the discovery of new classes of multi-functional materials and change the way structures are designed. Graphene is a 2D material known for its extremely high strength. Its integration into composites requires clear understanding of its structural and interfacial characteristic at multiple length scales. I will present the route towards graphene-crystalline materials composites, bridging physics to manufacturing. I will introduce a model material, namely graphene-Pd heterostructure, to study graphene-metal composites. Mathematical models guide our understanding of the kinetics of graphene synthesis and its atomic registration on ultrathin catalyst towards the precise control of its structure. The mechanics and physics of graphene-Pd heterostructures are characterized at multiple length scales by combining atomic imaging, spectroscopy and mechanical testing. A machine learning approach is proposed to scale up the manufacturing of these new materials for applications ranging from gilding-based coatings to flexible electronics.

Moire Mechanics in 2D Materials

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Keywords: 2D materials, dislocations, strain engineering, buckling

Abstract: Moiré patterns are commonly observed in layered systems of 2D materials such as graphene, h-BN, MoS₂, etc, or when 2D materials are grown on crystalline metal substrates. These patterns are connected to a variety of interesting properties in 2D material heterostructures, from superconductivity to superlubricity. To understand moiré patterns, we introduce the concept of interlayer or van der Waals (vdW) dislocations, and show that arrays of these defects constitute the moiré patterns associated with regions of commensurability and incommensurability between the layers. We note that moiré patterns and the defects appearing therein are electronic structure objects formed by weak interactions between the layers, locked into place by strong in-plane interactions in the constituent layers, and can thus be understood as topological states. We explain several experimentally observed moiré phenomena, including the distinct moiré patterns formed by various combinations of 2D materials on the same metal support layers, as well as point and line defects in moiré patterns. Using this understanding of moiré mechanics in 2D materials, we then explore two novel mechanics observations in layered transition metal dichalcogenide systems. First, we show that predefined moiré patterns in MoS₂ bilayers can be used to template buckling modes when the layers are compressed laterally, either under uniaxial or biaxial loading. Since the moiré patterns are predefined by assigning a rotation angle between layers, it is possible to pre-program a buckling mode shape and periodicity, and thus a periodic strain distribution, simply by changing the relative rotation. Second, we show that in finite sized MoS₂ flakes on much larger MoS₂ substrates, moiré effects are responsible for the possibility of spontaneous coupled deformation including both stretch and rotation. This effect gives rise to small rotation angles between grains in polycrystalline layers of MoS₂, as well as the potential for strain-tunable electronic properties in nanoscale devices. By advancing the understanding of these systems in terms of the moiré mechanics, the work recasts and extends the emerging field of vdW heterostructures.

Toward an Intrinsic Cutting Energy

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Keywords: elastomer, fracture, cutting, failure

Abstract: Cutting and tearing of elastomeric solids cannot be quantitatively related. During the tearing of soft elastomers, large deformation occurs due to crack-blunting. Conversely, during cutting a razor blade imposes its radius throughout the failure process. Typically cutting is also associated with frictional effects between the material and the blade which vary as a function of the amount of material cut. However, by implementing an unusual Y-shaped cutting geometry inspired by the 1978 work of Lake and Yeoh, we can mitigate frictional effects while controlling the rate of fracture propagation. For a series of silica-reinforced and silica-free model silicone networks, find that cutting fracture energy increases nonlinearly with large blade radii. The nonlinearity scales with the material's constitutive response (strain stiffening). Interestingly, as the blade radius decreases, the cutting energy plateaus to a constant value that is a function of material properties. The plateau value decreases with decreasing the angle between the two legs of the 'Y' geometry, corresponding to a decrease in the applied cutting contribution. Its onset appears to be governed by a length scale that may be associated with the size of a fracture process zone. Given these observations, we evaluate the potential of the Y-shaped geometry for characterizing an "intrinsic" cutting energy that may have implications for the prediction of elastomeric tearing.

Tuesday, May 21st

Session 2: Fluids (Cavitation and High Rate)

Henderson Room, League 2:00 PM – 3:40 PM

Chair: Shelby Hutchens

Strain hardening effects of soft viscoelastic materials at extreme loading rates

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Keywords: cavitation, viscoelastic, high strain rates, strain hardening effects

Abstract: Cavitation is a well appreciated high-rate phenomenon in hydrodynamics and biology. Recently, our group showed that inertial microcavitation rheometry (IMR) can be used to characterize the mechanical behavior of viscoelastic materials at high loading to extreme loading rates as the cavitation bubble collapse is very sensitive to the constitutive equations of the surrounding medium. Specifically, Estrada et al. [J.Mech.Phys.Solids, 112: 291-317, 2018] demonstrated the IMR experiments to probe viscoelastic mechanical properties of soft materials, where time-resolved data for the temporal evolution of bubble radius is fitted to the prediction of the governing equations of bubble dynamics, combined with the neo-Hookean Kelvin-Voigt constitutive model for surrounding soft medium. Here we improve the accuracy and computation speed of the above data post-processing method where we decouple the set of governing equations into two subsystems. In the first subsystem, we can solve for the time-resolved bubble pressure p , bubble vapor mass fraction C and bubble inside temperature T accurately, without requiring any information about the constitutive relation of the surrounding material. Once solved, the bubble pressure p is substituted into the second subsystem, where we can solve for the surrounding soft material constitutive relations through a weighted least square fitting procedure, which is 98% faster than our original method developed in Estrada et al.

Vorticity Dynamics of Shock-Driven Interfaces

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Keywords: Vorticity dynamics, shock-driven interfaces, vortex-sheet

Abstract: A perturbed interface separating two fluids of different densities is unstable under the influence of an impacting shock wave. Such interaction is found both in nature and in engineering applications, spanning from the formation of supernovae from dying stars, to the collapse of cavitation bubbles near solid objects, as well as biomedical and High-Energy-Density-Physics applications. The growth of the interfacial perturbation is due to the baroclinic vorticity generated along the interface from the passage of the shock wave, and consists of different stages. In this work, we propose to investigate the vorticity dynamics of the interface, in order to identify the mechanisms responsible for the flow evolution in each stage. The use of a vortex-sheet approach allows us to isolate the governing physics of the interfacial dynamics, and offers a detailed description of the vortical structures developing along the interface. A parametric study is being performed, enabling a scaling analysis of the quantities of interest.

Prediction of Shock Levels to Packaged Products Cushioned with Foam Having Arbitrary Shapes

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Keywords: Cushion Curves, Shock Fragility, g-Factor, Nonlinear Strains

Abstract: Abstract:

Products in packages can be subjected to large forces when dropped. Large forces are the result of large decelerations. The packaging industry defines the shock fragility of a product as the largest deceleration or "g-factor" it can take without damage. The more fragile the product, the lower its g-factor. A cushion is often designed for the product using test results from controlled drops performed by foam manufacturers. This information is published as "cushion curves", which relate the peak deceleration experienced by a free falling weight, when flat dropped onto a block shaped pad of cushion material, to the drop height, impact area and cushion thickness. An adequate design is considered to be one where the cushion curve g-level is less than the product's fragility.

Cushions in packages are rarely pads. Popular designs incorporate ribs, cutouts and other features which result in shapes that have variable geometry. What is needed is a design method that can handle these cases. In this paper, closed cell foams are modeled as trapped air that undergoes a polytropic process when rapidly compressed. The resulting nonlinear stress-strain curve is used in an iterative finite element analysis to predict g-levels for arbitrary shapes. The predictions for pad shaped cushions are shown to predict the actual g-levels from cushion curves very well.

Evolution of perturbed interfaces subjected to large rarefactions

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Keywords: Hydrodynamic Instability, Vorticity

Abstract: In phenomena ranging from the expulsion of stellar core material during supernova explosions to the degradation of the ignition hot spot during inertial confinement fusion implosions, interfaces separating gasses of different densities are accelerated by strong rarefactions. Depending on the respective signs of the acceleration, the density gradient, and the pressure gradient, interfacial perturbations may be hydrodynamically unstable and thus experience significant growth. Although instability analysis is well established for constant-acceleration, incompressible, and small-perturbation-amplitude scenarios, predicting instability growth when departing from these conditions is more challenging. Our objective is to investigate interfacial perturbation growth driven by the transient accelerations, density changes, and pressure gradients imparted by the passage of a rarefaction wave from a relatively heavy gas to a relatively light gas. Previous analysis based on one-dimensional gas dynamics used to quantify the acceleration and dilatation experienced by such interfaces is extended to explore two-dimensional physics such as the effects of vorticity. The incorporation of such two-dimensional effects enables an in-depth study of the interface morphology and the growth of the hydrodynamic instability well into the nonlinear regime. A key result is the growth of the perturbation after the passage of the rarefaction wave, which is shown to scale with the baroclinic vorticity deposited onto the interface during the wave/interface interaction phase. All modeling results are compared to simulations using an in-house, high-order accurate hydrodynamics code.

This work is supported by the United States Department of Energy under grant DE-NA0003864 and by the LLNL under subcontract B614207.

Tuesday, May 21st

Session 2: Damage and Failure of Quasi-Brittle Composites

Koessler Room, League 2:00 PM – 3:40 PM

Chair: Marco Salviato

Defect Severity Quantification for Failure in Unidirectional Composites under Transverse Tension and Longitudinal Compression

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Keywords: Manufacturing defects, defect severity, transverse cracking, fiber microbuckling

Abstract: Composite materials are manufactured by a variety of processes that produce microstructural compositions depending on the process histories. In spite of efforts to achieve perfect microstructures, real manufactured composites contain defects in the forms of nonuniform fiber distributions, fiber misalignment, matrix voids, etc. Such defects affect the composite's performance, such as structural integrity and durability, when exposed to service environments. In many cases, the early failure events are significantly affected by the defects, and inadequate account of these effects leads to inaccurate assessment of damage progression and ultimate failure. Furthermore, evaluating the goodness of the manufacturing process requires that the defects are quantified in terms of their severity with respect to the performance metric. A concept for defect severity quantification will be proposed that generalizes the geometric size characterization and allows incorporation of the parameters governing the particular failure mode under consideration. Two failure modes in unidirectional composites will be taken to illustrate implementation of the defect severity measures: a) transverse cracking and b) longitudinal fiber microbuckling.

Progressive Failure Prediction of a Curved Composite Flange

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Keywords: progressive damage, microstructure, delamination

Abstract: The use of Polymer Matrix Composites (PMC) is increasing in several industries due to their attractiveness relative to weight savings. However, manufacturing of these PMC involves a resin curing process, and the elevated temperatures are usually applied on the composite to accelerate the cross-linking process. Because of the mismatch of the thermo-mechanical properties of the constituent fiber and resin, residual stresses can build up inside the composite, which influence the failure behavior of the composite after the curing process. The goal of this research is to investigate the effect of processing on the inter-laminar strength of a curved composite beam under flexural loading through an integrated multiscale progressive damage model.

In this research, L-shaped plain-weave textile composite specimens were fabricated using the Resin Transfer Molding (RTM) technique, and the inter-laminar strengths were characterized through four-point bend tests based on ASTM D6415. A global-local modeling framework was established to predict the progressive failure response of the curved beam. A textile-architecture based mesoscale model was implemented in the area under pure bending, while the regions away from the loading points were homogenized as an orthotropic solid. A multi-physics processing model was first employed to determine the spring-in angle and residual stress distribution after the curing process. Then, a failure model based on the Smeared Crack Approach (SCA) was implemented to predict the progressive damage response of the curved beam subject to four-point bending. Particularly, the through-thickness damage progression is examined, and it is shown that a good correlation is obtained through the use of SCA, implemented through a UMAT in the commercial Finite Element (FE) software Abaqus. The current effort is to determine the effect of processing and textile architecture on the resulting composite inter-laminar strength.

Damage mechanisms for nonwovens in textiles

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Keywords: Damage mechanisms, nonwoven, in-situ experiment, wavelet analysis, FEA simulation

Abstract: Fabric abrasion, especially pilling is a problem in textile industry. Pills on the fabric surface are the result of damage to the garment, which cause unappealing appearance. One of the requirements for the use of fabric in many applications is high abrasion resistance. In order to study the evolution of damage process during usage, and further investigate the relation between macro and micro mechanisms of abrasion, we performed in-situ experiments on nonwoven fabric. At macroscopic scale, different morphology of fabric have been identified when fabric rubs against a non-fiber abradant as well as against a fiber abradant. At the microscopic scale, four abrasion mechanisms at the individual fiber level have been identified. In addition, the correlation between two types of pills and six types of precursors have been found. Further, in-situ deformation of individual fiber has been designed and investigated. To evaluate abrasion of nonwoven fabrics with minimal human interpretation, we apply two-dimensional, discrete-wavelet transforms to the images of nonwoven fabrics. We describe the degree of damage in terms of a gray-value ratio that is extracted from the details of the wavelet characterization, and show that this parameter correlates well with an independent qualitative assessment of the damage.

To further optimize the parameters (fiber materials, fiber diameter, fiber orientation, bond spacing and bond orientation) and propose the next-generation design of fabric with better damage resistance, we developed damage models in ABAQUS for both fabric and individual fibers. A conditional random walk approach was developed to generate the distribution of fibers. Different material properties for the bonding sites and individual fibers were considered in the model. Property variations in individual fiber were generated by MATLAB and VUSDFLD user subroutine in ABAQUS. Two quantification parameters: degree of damage and degree of fuzziness were proposed to evaluate the damage and to guide the design of fabric.

Multiscale fatigue modeling of composites

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Keywords: Multi-scale analysis, composite, fatigue, failure

Abstract: Compared to ductile metals, composite materials, such as fiber reinforced composites (FRC) and textiles, have higher fatigue durability. Despite this, failure due to fatigue continues to be a challenge because in composite material ultimate failure due to cyclic loading is often sudden and catastrophic. Predicting and preventing this is a difficult task, and it is currently a topic of much research in literature. Experimental approaches are usually, limited due to a large amount of data required to characterize the behavior of a given material system. As a result, current composite material systems are often over-designed with a substantial fatigue safety factor. Numerical approaches can provide an alternative to an extensive testing regime; however, these approaches are also plagued by large data requirement. Hence, there is a need for a numerical approach that will require the least amount of test for parameter identification and can predict fatigue degradation in all possible material configurations.

In this paper an experimental procedure for determining fatigue in-situ matrix properties, to be used in a micro-mechanics framework, is described. The procedure utilizes only a tensile [+/- 45]^{2s} test to back out complete equivalent matrix stress-strain behavior. Quasi-static test on interrupted fatigue tests were conducted to obtain equivalent matrix response as a function of the number of cycles and stress ratio. The result of the test procedure is an easy to implement formulation of matrix stress-strain, in a multi-scale framework.

Crack Propagation Behaviour of Polyurethane Thermoplastic Elastomers in Cyclic Fatigue

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Keywords: Cyclic fatigue , Crack propagation, Thermoplastic Elastomers, Digital Image Analysis
, Pure Shear

Abstract: Requirements of waste reduction and environmental sustainability caused a renewed interest for thermoplastic elastomers (TPE's). TPE's are an interesting class of re-processable materials with intermediate properties between those of conventionally vulcanized elastomers and thermoplastics, such as, flexibility, high reversible extensibility, easy shaping and fast processing. Although TPE's have seen a fast diffusion in the last 20 years, few studies have appeared on the cyclic behaviour in fatigue (Mars and Ellul 2017). TPE's are typically composed by at least two components at the operating temperature: a hard and solid component and an elastomeric soft component (J.W.C Van Bogart, A. Lilaonitkul 1979). The presence of phase separation (at the submicron scale) between those two components provides physical crosslinking and dissipative mechanisms so that TPE's can be used without any chemical crosslinking and in the unfilled state.

In this study we investigate the crack propagation in cyclic fatigue of two commercial polyurethane/ester block copolymers (SP1 and SP2) and we compared their resistance in fatigue to that of natural rubber (NR) (Demassieux 2016). The fatigue resistance of the material is characterized by the crack propagation rate per cycle (dc/dn) in a pure shear sample as function of the applied energy release rate G in each cycle (Thomas 1959). Interestingly, while in monotonic loading the two materials have a similar Young's Modulus (9-15 MPa) and a similar stress-strain behaviour below 100% (Fig.1), in cyclic fatigue, the crack propagation rate for SP1 is considerably higher than that of SP2 and comparable to the values obtained for unfilled NR (see Fig.2). Moreover, in rubber like materials the highly stretched area ahead the crack tip, called process zone, plays a very important role in preventing crack propagation and can be more or less effective in shielding the crack bonds depending on material composition and morphology. The high toughness of SP2 is confirmed also by the appearance of huge blunting at the crack tip that can be a signal of more homogeneous stress distribution. In order to investigate on which additional or different dissipation mechanisms are active in SP2 ahead the crack tip, when it operates under cyclic stress condition, we are currently investigating the local zone near the crack tip, using the recent technique of Digital Image Correlation.

Tuesday, May 21st

Session 2: Data-Driven Modeling

Michigan Room, League 2:00 PM – 3:40 PM

Chair: Phani Motamarri

Multi-fidelity Modeling of Combustion Dynamics

Cheng Huang, Karthik Duraisamy

Keywords:

Abstract: A multi-fidelity framework is established and demonstrated for prediction of combustion instabilities in rocket engines. The major idea is to adapt appropriate fidelity modeling approaches for different components in a rocket engine to ensure accurate and efficient predictions. Specifically, the proposed framework integrates projection-based Reduced-Order Models (ROMs) that are developed using bases generated on truncated domain simulations. The ROM training is performed on truncated domains, and thus does not require full order model solutions on the full rocket geometry, thus demonstrating the potential to greatly reduce training cost. Geometry-specific training is replaced by the response generated by perturbing the characteristics at the boundary of the truncated domain.

Modeling turbulent flows using sparse regression with embedded invariance

Sarah Beetham, Jesse Capecelatro

Keywords:

Abstract: Turbulence is ubiquitous in science and industry; additionally, it is nearly always multiphase. Given current computational capabilities and the wide range of time- and length-scales of industrial systems, direct numerical simulation (DNS) is prohibitively costly. Thus, some degree of modeling must be employed. Current state-of-the-art modeling for turbulent multiphase flows is predominantly based on extensions to single-phase models, making it largely unsuccessful beyond the dilute limit. In this talk, we demonstrate the promise of using sparse regression with embedded invariance to determine tractable, compact models for challenging turbulent flows. Specifically, we present the formulation of models using this technique for two classes of flow with increasing difficulty: (1) single-phase free shear turbulence and (2) turbulent flow over periodic hills.

System identification of the partial differential equations governing pattern-forming physics

Zhenlin Wang, Xun Huan, Krishna Garikipati

Keywords:

Abstract: We present a contribution to the field of system identification of partial differential equations (PDEs), with emphasis on discerning between competing mathematical models of pattern-forming physics. The motivation comes from developmental biology, where pattern formation is central to the development of any multicellular organism, and from materials physics, where phase transitions similarly lead to microstructure. In both these fields there is a collection of nonlinear, parabolic PDEs that, over suitable parameter intervals and regimes of physics, can resolve the patterns or microstructures with comparable fidelity. This observation frames the question of which PDE best describes the data at hand. This question is particularly compelling because knowledge of the governing PDE immediately delivers insights to the physics underlying the systems. While building on recent work that uses stepwise regression, we present advances that leverage the variational framework and statistical tests. We also address the influences of variable fidelity and noise in the data.

Exact exchange-correlation potentials from electron densities

Bikash Kanungo, Paul M. Zimmerman, and Vikram Gavini

Keywords:

Abstract: Exchange-correlation (xc) functionals, the cornerstone of the success of density functional theory (DFT), encapsulate the quantum many-electron interactions in terms of a mean-field. Although known to be unique functionals of the ground-state electronic charge density, $\rho(r)$, the exact form of these functionals - expressed either as energy ($\text{Exc}[\rho(r)]$) or potential ($v_{xc}[\rho(r)] = \partial \text{Exc}[\rho(r)] / \partial \rho(r)$) - are unknown, thereby necessitating the use of approximate functionals. The existing xc functionals, despite their success in predicting wide range of materials properties, exhibit notable failures - underpredicted bandgaps, incorrect bond-dissociation curves, wrong charge-transfer excitations, to name a few. To this end, the inverse DFT problem of evaluating the xc potential ($v_{xc}(r)$), corresponding to given density ($\rho_{\text{data}}(r)$), can provide a powerful tool in our understanding as well as testing of the existing and future xc functionals. More importantly, it paves the way for a machine-learned xc functional, .i.e., one that uses the $\rho_{\text{data}}(r) \leftrightarrow v_{xc}(r)$ data to learn the functional form of $v_{xc}[\rho]$.

This work presents a numerically robust and accurate method for inverse DFT calculations. We cast it as a PDE-constrained optimization problem, with $v_{xc}(r)$ as the control variable and the Kohn-Sham eigenvalue problem as the PDE-constraint. The method employs a finite-element basis—a complete basis—to discretize the problem, and, thereby, eliminates the spurious oscillations resulting from incomplete basis sets employed in previous efforts. The exact xc potentials are obtained using correlated ab-initio ground-state densities for diatomic and polyatomic systems, to unprecedented accuracy. Notably, as is the case with exact xc potentials, we obtain good agreement between the Kohn-Sham HOMO level and negative of the ionization potential.

Prediction of effective material properties in multi-component crystalline solids with a data-driven approach

Xiaoxuan Zhang, Krishna Garikipati

Keywords:

Abstract: Many important multi-component crystalline solids undergo mechano-chemical phase transformations, in which the compositional redistribution is coupled with a crystal structural change. Capable of rapidly calculating the macroscopic behavior of this class of material based on their detailed microscopic structures is of paramount importance for accelerating new material design and discovery. However, evaluation of macroscopic material properties purely based on direct numerical simulation (DNS) is computationally very expensive and thus impractical for material design when a large number of microstructures need to be tested. To address this challenge, we present a data-driven approach, which combines deep neural networks (DNNs) with DNS, to predict the effective elastic material properties of a family of 2D multi-component crystalline solids, whose microstructures are numerically generated by solving a coupled, higher-order diffusion and nonlinear strain gradient elasticity problem. DNNs are trained with these synthetically generated data to reduce the dimensionality of the problem. Numerical examples, including studies on hyperparameters, accuracy, and convergence, are presented to demonstrate the effectiveness of our approach.

Tuesday, May 21st

Session 3: Fluids (Cavitation and High Rate)

Henderson Room, League 4:10 PM – 5:50 PM

Chair: Jin Yang

High-speed needle-mediated cavitation

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Keywords: cavitation, elastomer, hydrogel, dynamic

Abstract: Temporary cavitation occurs when a projectile impacts a soft material causing a large radial expansion of the wound tract immediately after the projectile passes. Though cavity size is known to scale with the kinetic energy of the projectile, the fracture-governed damage accompanying this large deformation remains poorly understood. Using a custom designed table-top ballistic cavitation device, we replicate the temporary cavity phenomenon in several soft tissue simulants on a small scale by applying a fast, high-pressure pulse of air through a needle. Temporary cavities produced via air pulse (characterized by energy density, loading rate, and needle size) isolate the damage accompanying large and dynamic stretches from that associated with more complicated impact dynamics. We compare the response between the tissue simulants, noting especially the differences in damage morphology and extent under varying rate and energy of loading conditions.

A Comparative Study of the Dynamics of Laser and Acoustically Generated Bubbles in Viscoelastic Media

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Keywords: cavitation dynamics, viscoelastic media, nucleation mechanisms

Abstract: Here we present results from experiments comparing the first-cycle growth and collapse dynamics of acoustically and laser-nucleated single bubbles in water and agarose gels of varying stiffness. Experiments were carried out in a custom-built spherical vessel which allowed both acoustically and laser-nucleated bubbles to be generated at its center. During all experiments the vessel was filled with degassed, deionized water and an opening at the top of the vessel allowed for the insertion of gel samples to its center. Acoustically nucleated bubbles were generated using acoustic pulses delivered from spherically focused transducer elements embedded in the vessel wall. The nucleating acoustic pulses had a center frequency of 1 MHz, a total duration of <2 acoustic cycles, and generated a peak rarefactional pressure at the focus of 24 MPa. Laser-nucleated bubbles were generated using a pulsed Nd:YAG laser (532 nm, 6 ns) with a pulse energy of 5 mJ/pulse, focused to the center of the vessel through an embedded laser window. Bubbles were nucleated by both mechanisms in water and agarose gels with stiffnesses ranging from 1.3 kPa to 570 kPa. The dynamics of the generated bubbles were measured via optical imaging using a high-speed camera that allowed for maximum effective frame rates of up to 17 Mfps.

The maximum radii of generated bubbles decreased as the stiffness of the media increased for bubbles nucleated by both mechanisms, but the maximum radii of laser-nucleated bubbles decreased more rapidly than acoustically nucleated bubbles as the gel stiffness increased. For water and low stiffness gels, the collapse times of the bubbles were well predicted by a Rayleigh cavity, but bubbles collapsed more quickly as the stiffness of the gels increased. The growth and collapse phases of the bubbles occurred symmetrically (in time) about the maximum radius in water but not in gels, where the duration of the growth phase decreased more rapidly than the collapse phase as gel stiffness increased. Slight nucleation-mechanism-dependent differences in development of the asymmetry in the growth and collapse durations were observed which indicated that the duration of the growth phase decreased more rapidly for the laser-nucleated bubbles than the acoustically nucleated ones as the gel stiffness increased. No such differences were apparent for the collapse durations.

Modeling ultrasound-induced single bubble cavitation in water and agarose gel

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Keywords: cavitation, viscoelastic materials, ultrasound, tissue fractionation

Abstract: Models of cavitation in soft matter are needed to understand the mechanics of ultrasound-induced tissue fractionation. However, predicting bubble dynamics in viscoelastic materials remains challenging due to parametric uncertainties and the dearth of validation data. Based on data from recent single-bubble experiments, we model a single cycle of bubble growth and collapse under ultrasound forcing for a variety of initial conditions. Results obtained for water are then extended to 0.3% agarose gel which is modeled with a finite deformation Kelvin Voigt constitutive equation. Experimental uncertainties are discussed. Threshold simulations are then used to determine bounded ranges for parameters that cannot be measured experimentally such as nucleus size and peak negative pressure.

Stress Relaxation Response of Shock wave Impacted Brain Tissue

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Keywords: Brain, Fractional Zener, bTBI, Blast, Shock wave, Compression, TBI

Abstract: In recent years, there has been an escalation of blast-induced traumatic brain injuries (bTBI) caused by improvised explosive devices (IEDs) during global conflict. Blast injuries are attributed to the blast wave and has the capability to cause life-threatening injuries and fatalities. However, the mechanical behavior of brains subjected to shock wave impact is still unknown. Thus, hindering improved countermeasure development to mitigate bTBI. This study aims to understand the stress relaxation response of shock wave impacted brain tissue. Unconfined compression experiments were conducted with postmortem porcine brain tissue at a linear rate of 5 and 50 mm/min to a strain of 20%. The tissue was allowed to relax for two minutes, after being compressed to 20% strain. The fractional Zener (FZ) constitutive model was applied to obtain the material properties of the brain tissue. Optimized FZ coefficients for brains impacted and unimpacted by a shock wave are compared. The results show that fresh porcine brains, less than 8 hours postmortem, are softer after shock wave impact.

Tuesday, May 21st

Session 3: Mechanics of Fracture and Failure in Solids

Koessler Room, League 4:10 PM – 5:50 PM

Chair: Krishnaswa Ravi-Chandar

Quasi-Continuum Analysis of Networked Materials

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Keywords: Quasi-continuum method, soft materials, fracture

Abstract: The skeleton of many natural and artificial structures may be abstracted as networks of elements interacting in a non-linear fashion. Examples include rubber, gels, soft tissues, and lattice materials. Understanding the multiscale nature of deformation and failure of networked structure holds key for uncovering origins of fragility in many complex systems including biological tissues and enables designing novel materials. However, these processes are intrinsically multiscale and for large scale structures it is computationally prohibitive to adopt a full discrete approach.

Here, we introduce a new adaptive numerical algorithm for solving polymer networks using an extended version of the Quasi-Continuum (QC) method. In regions of high interest, for example near defects or cracks, each polymer chain is idealized using the worm like chain model. Away from these imperfections, the network structure is computationally homogenized, using Hill-Mandell's principle, to yield an anisotropic material tensor consistent with the underlying network structure. Overall, only a fraction of the network nodes is solved at each time step. We illustrate the accuracy and efficiency of the method by applying it to study the fracture of large scale polymer network problems

An adaptive ensemble hybridization of phase field models for brittle and ductile failures

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Keywords: phase field, deep learning, adaptive model, partition of unity

Abstract: This paper presents a new adaptive model in which a diverse collections of deep learning and multiscale models, each of different speed and forward prediction capacity, are used to predict the same materials responses in a space-time continuum domain. The key idea is use phase fields as the weight functions to partition multiple incremental energy functionals. Meanwhile, the driving force are derived based on norms that measure error estimation, bifurcation, fracture criterion and speed. As such, the appropriate model will be chosen to predict the material behaviors at the right place at the right time. As an example, we apply this idea to formulate this multi-model framework to predict two common classes of material failures, brittle fracture and strain localization. A multi-fold cross-validation exercise is conducted to examine the speed, robustness and accuracy of the multi-model predictions.

Dynamic ductile fracture characterization with peridynamics: A Sandia Fracture Challenge study

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Keywords: Peridynamics; Ductile fracture; Blind prediction; Sandia Fracture Challenge

Abstract: Prediction of crack initiation, propagation, and ductile fracture can be very challenging in metallic materials with complex geometries. Damage accumulation along the plastic loading path governs the fracture initiation in ductile materials. Over the past two decades, peridynamics, a nonlocal theory, has been exploited for simulating dynamic problems involving fracture, mostly due to its capabilities in naturally representing discontinuities without any complicated numerical treatments. Peridynamics, however, has been mostly applied to modeling fracture in brittle materials; robustness of the theory in simulating ductile fracture has largely remained unexplored. Correspondence material modeling provides a setup to immediately use the (well-established) local constitutive relations within the context of peridynamics. Recently Foster et al. (2018) proposed a new correspondence framework to incorporate classical finite deformation material models. Tupek et al. (2013) also introduced a constitutive damage modeling approach for peridynamics to take advantage of the classical damage models. A material model corresponding to the finite strain elastoplasticity theory of Simo (1988) and a damage model corresponding to Johnson-Cook model (1985) have been implemented in Peridigm, an open-source massively-parallel computational peridynamic code. This framework has been applied to the Sandia Fracture Challenge 2017. The model was first calibrated with the data provided by Sandia National Laboratories. Then, a blind prediction was performed on the challenge geometry and results were compared with the experiments.

Effect of film topology on the impact resistance of nanocellulose films with helicoidal microstructures

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Keywords: Bouligand structure, cellulose nanocrystals, Coarse-grained molecular dynamics, ballistic performance

Abstract: Many impact tolerant biological structures contain helicoidal, or Bouligand, microstructures, which are characterized by their sequentially twisting layout of uniaxially arranged fiber planes. Even though this structural pattern is common in biology and known to display exceptional mechanics, much related to how its resilience to dynamic loading manifests remains unclear. This inability to fully understand the mechanisms that drive deformation and failure in materials with helicoidal structures limits the capacity to accurately design materials with efficiently balanced properties inspired from biology. Cellulose nanocrystals (CNCs) are excellent building blocks for hierarchical nanomaterials. They have received much attention due to their impressive mechanical properties and tunable surface chemistries. CNCs readily self-assemble into all-cellulose nanocomposites that naturally adopt helicoidal microstructures, emerging as an efficient platform for translating their superior properties to macroscopic products. Therefore, this work investigates the effects of structure and surface chemistry on the ballistic performance of CNC films with helicoidal microstructures using an experimentally validated coarse-grained molecular dynamics model for CNCs by subjecting them to loading similar to laser-induced projectile impact tests. Impact resistance was characterized by the ballistic limit velocity and dissipated projectile energy with respect to film pitch angle (the angle between fiber orientations of successive layers) and interfacial energy. Independent from the specific in-plane ordering of CNCs, helicoidal films with moderate pitch angles (18-42°) exhibited the highest impact tolerance. Improved ballistic performance was achieved through more intra-CNC sliding, larger in-plane cracks, and dissipative through-thickness twisting cracks. Reducing the interfacial strength between CNCs further enhances energy dissipation during impact, which can be conveniently accomplished through surface modifications. However, decreasing CNC fiber lengths, but preserving in-plane structure, lowers the impact tolerance by allowing premature fiber separation and disrupting energy propagation away from the projectile. Similarly, for CNC films with fibers shorter than the critical shear load transfer length, in-plane randomness can significantly reduce the energetic barrier for fiber dislodgement and film splitting, resulting in substantially lower ballistic velocity limits.

Coupling of Thermal and Mechanical Behaviors: An Energy Landscape Perspective

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Keywords: metallic glass, thermal hysteresis, mechanical yield and softening, energy landscape

Abstract: The mechanical performance of metallic glasses (e.g. the shear banding, softening, aging-rejuvenating crossover, brittle-to-ductile transitioning, etc) are known sensitive to the surrounding environments. However, the development of an effective structure-property model is very challenging because of the strong disordered atomic nature in amorphous materials. In this talk we will present a novel model built upon the perspective of potential energy landscape (PEL). The intrinsic energy variations in metallic glasses can be attributed to the competitions between the elementary activations and relaxations in the PEL. In particular, whether glasses will undergo aging or rejuvenation depends on whether the activation barrier is smaller or larger than the relaxation energy. Stemmed from such the dependence of activation barrier on PEL, a self-consistent equation in describing the coupling effect between the intrinsic energy dissipation and external stimuli has been derived. Without the necessity of empirical parameters, such PEL-based model can simultaneously capture both the thermal hysteresis and the mechanical yield and softening phenomena in metallic glasses.

Wednesday, May 22nd

Session 1: Biomechanics

Henderson Room, League 10:30 AM – 12:10 PM

Chair: Rhima Coleman

A New Robust 3D Constitutive Model for the Passive Properties of Left Ventricular Myocardium

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Tomonori Kawamura, University of Pennsylvania, United States,
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Keywords:

Abstract: Myocardium exhibits complex behavior that demands a comprehensive 3D constitutive formulation in order for its mechanical properties to be captured in a computational model. Current modeling efforts remain limited in that they are not based on full 3D deformation datasets, do not use optimal loading paths, and have not been able to define the optimal form of the strain energy function and determine its associated material parameters. To this end, we employed a novel numerical-experimental methodology to determine the optimal form of the strain energy function for passive ventricular myocardium. Full 3D structural-mechanical measurements were obtained from cuboidal specimens cut out from the left ventricles of Dorset sheep. We modeled the myocardium as an orthotropic material with material directions f (myofiber), s (sheet or cross-fiber), and n (normal to the fiber-sheet plane), using an initial form by Holzapfel and Ogden [1]. The model was fitted both a set of simple shear loading paths [2], and a set of optimally selected paths consisting of simple shear and pure shear [3], using a finite element tetrahedral mesh whose elements were assigned spatially varying material directions. Model parameters were estimated with nonlinear least-squares in order to fit all optimal paths simultaneously regression, via a trust-region-reflective algorithm. While the model fit the simple shear paths well, it was unable to fully capture the mechanical anisotropy in the optimal paths. Further examination revealed that the optimal paths caused both relative stretching and shearing of fiber, sheet, and normal directions in the myocardium, which could be explained by interactions (shearing in particular) between myofibers and their surrounding collagen matrix. The initial model was extended accordingly to reflect these coupling modes. We used this extended model to successfully fit the optimal datasets for multiple specimens with $r^2 = 0.80-0.99$ and used the fitted parameters to accurately predict the myocardium response in other paths outside of the optimal set. This extended constitutive model has particular relevance in the simulation of myocardium in non-physiological states like myocardial infarction. Ultimately, development of more robust models in this manner will make them better suited for clinical evaluation and for simulating treatment of cardiac diseases.

Viscoelastic Model of Human Myocardium

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Introduction

Across species, myocardial tissue has been shown to exhibit viscoelastic behaviour [1,2]. Significant hysteresis at low shear rates, stress relaxation, and frequency dependent stiffness have all been observed experimentally. Despite this long history of experimental evidence, the myocardium is typically modelled as a hyperelastic material [3]. New viscoelastic models have been proposed [4], but these lack the capacity to account for these varying viscoelastic factors that are encountered experimentally.

In this study, we develop a viscoelastic model for human myocardium. The model – based on a nonlinear viscoelastic anisotropic generalized power law – is demonstrated to capture the viscoelastic features of myocardial tissue across shear relaxation, cyclic shear and biaxial experiments. The model is also shown to exhibit behaviours observed in animal studies, including frequency dependent stiffness and transitional nonlinearity.

Integrating the new model into a patient-specific heart model, the behaviors of the hyperelastic and viscoelastic models are compared within the myocardium, focusing specifically on passive inflation and active contraction. Quasi-static and transient cardiac models are considered, demonstrating the impact of these assumptions on the behaviour of biventricular heart models.

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Analyzing the role of viscoelasticity in the residual stress in soft tissues: a case study on human aortas

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Residual stress is a crucial and well-recognized property in understanding the functional mechanical properties of soft tissues. Its existence is crucial in homogenizing the in vivo stresses in tissues and organs, thus also proving its importance in computational studies of biological tissues and organs. The primary example used to study residual stresses is the gradual opening of arterial tissues after being cut longitudinally. However, vast majority of such analyses consider only the elastic component of the tissues, yet the gradual opening of the artery indicates the significant role of viscoelasticity in this time-dependent process. In this study, we built a finite element model using the geometry and data from the study by Holzapfel et al. [1] using the constitutive model and the material parameters for human aorta from Niestrawska et al. [2]. We extended the elastic model for viscoelasticity by embedding the inside a fractional derivative and develop a computationally efficient approach for evaluating the viscoelastic fraction. We determined the degree of viscoelasticity based on the fraction of elastic vs viscoelastic component, and the order of the fractional derivative. These two values were determined by matching the change in opening angle over the course of 18 hours and by simulating the biaxial mechanical testing from Holzapfel et al. [2] and matching the resulting hysteresis. Although the hysteresis exhibited in the physiologic range is small in arterial tissues, matrix of the artery is mostly elastic, approximately 40% of the matrix is viscoelastic. Most of the viscoelastic effects are due to the collagen fiber networks, while the residual strains are in the range of the matrix, below the range where collagen fibers start bearing stresses. This suggests that the residual stresses are much smaller than conventional estimates, and that viscoelasticity is important to understand the functional mechanical properties of such soft tissues.

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Wednesday, May 22nd

Session 1: Mechanics of Fracture and Failure in Solids

Koessler Room, League 10:30 AM – 12:10 PM

Chair: Ahmed Elbanna

Poroelastic effects on fracture of polymer gels

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Keywords: fracture, diffusion, gels

Abstract: Fracture of polymer gels is time dependent and rate dependent. Subject to a constant load, a gel specimen may fracture immediately or after a delay (time-dependent, delayed fracture). When a crack grows in a gel, the fracture energy depends on the crack speed (rate-dependent, velocity toughening). The underlying mechanisms for the time and rate dependent fracture of gels may include local molecular processes, polymer viscoelasticity and solvent diffusion coupled with deformation (poroelasticity). This work focuses on the effects of poroelasticity on fracture of polymer gels. For a stationary crack, the time-dependent crack-tip fields and energy release rate are determined numerically along with an asymptotic analysis, with which delayed fracture is predicted under various chemo-mechanical conditions. For steady-state crack growth in a long-strip specimen, the energy release rate is obtained as a function of the crack speed, with which rate-dependent fracture is discussed in comparison with experiments.

CHARACTERIZATION OF THE FRACTURE BEHAVIOR OF POROELASTIC HYDROGELS

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Keywords: fracture, gels

Abstract: Hydrogel-like soft materials are abundant in nature including soft tissues such as cartilage, tendons and ligaments. With similar mechanical properties and biocompatibility, synthetic hydrogels have been used extensively for a wide range of applications such as artificial soft tissues, extra-cellular matrix, drug delivery, for soft machines and soft robotics as well as in the food industry as desserts, candies and jellies. Mechanical properties of the hydrogel-like soft materials are important for many of these applications. Of particular interest is the coupling of the swelling/drying and (viscoelastic) mechanical properties of hydrogel-like soft materials. In this work, we use a hydrogel formed by mixing gelatin, glycerin, and water to alter the mechanical properties over a significant range. We develop both experimental and modeling methodologies for characterizing the swelling/drying and viscoelastic properties. A large range of loading conditions spanning timescales from a few seconds to a few days is used. Parallelepipedic specimens are placed in controlled hydration conditions; the evolution of deformation resulting from swelling and drying is monitored using digital image correlation. The results are used together with a fully coupled three-dimensional poro-elastic simulation, including nonlinear effects, to extract the material properties by matching the experimentally measured deformation evolution to the simulations. The uniaxial stress-stretch response, and subcritical crack growth under controlled humidity and temperature are also characterized to identify appropriate constitutive and failure models. Fracture experiments are performed under controlled humidity and temperature, but with varying loading conditions; attempts to decouple viscoelastic and poroelastic contributions to fracture will be presented.

Self-healing Mechanics of Polymers

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Keywords: Mechanics of Fracture and Failure in Solids

Abstract: Dynamic polymer networks (DPNs) crosslinked by dynamic bonds have received intensive attention because of their special crack-healing capability. Diverse DPNs have been synthesized using a number of dynamic bonds, including dynamic covalent bond, hydrogen bond, ionic bond, metal-ligand coordination, hydrophobic interaction, and others. Despite the promising success in the polymer synthesis, the fundamental understanding of their self-healing mechanics is still at the very beginning. Especially, mechanics models to understand the interfacial self-healing behaviors of DPNs remain largely unexplored. Here, we develop polymer-network based analytical theories that can mechanistically model the constitutive behaviors and interfacial self-healing behaviors of DPNs. We consider that the DPN is composed of interpenetrating networks crosslinked by dynamic bonds. The network chains follow inhomogeneous chain-length distributions, and the dynamic bonds obey force-dependent chemical kinetics. During the self-healing process, we consider the polymer chains diffuse across the interface to reform the dynamic bonds, being modeled by a diffusion-reaction theory. The theories can predict the stress-stretch behaviors of original and self-healed DPNs, as well as the healing strength in a function of healing time. We show that the theoretically predicted healing behaviors can consistently match the documented experimental results of DPNs with various dynamic bonds, including dynamic covalent bonds, hydrogen bonds, and ionic bonds. We also elucidate how lights and electric fields affect the healing performance of DPNs. We expect our models to be powerful tools for the self-healing community to invent, design, understand, and optimize self-healing DPNs with various dynamic bonds.

Submit to Symposium "Mechanics of Fracture and Failure in Solids" organized by Ahmed Elbanna and Krishnaswamy Ravi-Chandar

Transverse Failure of Fiber-Reinforced Composites: Sensitivity on Microstructural Properties and Geometry

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Keywords: Composites, Transverse failure, Sensitivity, IGFEM

Abstract: Transverse failure has long been considered as a key failure mode in fiber-reinforced composite laminates, as it is often a precursor to inter-ply delamination and fiber breakage. The initiation and propagation of transverse cracks are affected by a variety of random microstructural quantities including fiber placement, fiber radii, constitutive properties of the fibers and the matrix, and failure properties of the fiber/matrix interfaces.

We present a gradient-based method to calculate the sensitivity of the transverse failure response with respect to the distribution characteristics (mean and standard deviation) of (i) the cohesive failure properties of the fiber/matrix interface and (ii) the geometrical features (placement and radius) of the fibers. The computational model of the transverse failure event combines a nonlinear Interface-enriched Generalized Finite Element Method (IGFEM) solver specially developed for this application, and a cohesive model of interfacial debonding, which has been shown in experiments to be the primary mode of transverse crack propagation in high-volume-fraction carbon-epoxy composites. The sensitivity analysis relies on an analytic computation (using the direct method) of the sensitivities of the failure response with respect to the cohesive properties of each interface and the geometrical parameters defining every fiber present in the virtual model of the composite.

Strain induced crystallization and fracture of rubber-like materials

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Keywords: Strain-induced crystallization, fracture, maximal advance path constraint

Abstract: A multi-scale polymer network model is proposed for strain-induced crystallization phenomena in rubber-like materials [1] and extended to account for phase field fracture. At the microscopic scale, the thermodynamic behavior of a polymer chain inside a stretching polymer network and its crystallization is studied and a new polymer chain model is presented. The chain model accounts for the thermodynamics of crystallization and presents a rate-dependent evolution law for crystallization based on the gradient of the free energy with respect to the crystallinity variable to ensure the dissipation is always non-negative. The multiscale framework allows anisotropic crystallization of rubber which has been observed experimentally. Two different approaches for formulating the orientational distribution of crystallinity are studied. For the discrete distribution, crystallization is tracked at a finite number of orientations. On the other hand, the continuous distribution captures the anisotropic behavior with only a few distribution parameters. To connect the deformation of the micro with the macro scale, the recently developed maximal advance path constraint is combined with the principle of minimum free energy, resulting in a non-affine deformation model for polymer chains. The model is then combined with a phase field approach to fracture. Various aspects of the proposed model are validated by existing experimental results, including the stress response, crystallinity evolution, crystallinity distribution, the rotation of the principle crystallization direction, and the effect on the fracture behavior of rubber-like materials.

Wednesday, May 22nd

Session 1: Modeling and Computation

Michigan Room, League 10:30 AM – 12:10 PM

Chair: Nhung Nguyen

Homogenization of elastic dielectric composites with rapidly oscillating passive and active source terms

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Keywords: electrets, dielectric elastomer composites, metamaterials, multiscale asymptotic expansions

Abstract: This talk will present the derivation of the homogenized equations for the macroscopic response of elastic dielectric composites containing space charges (i.e., electric source terms) that oscillate rapidly at the length scale of the microstructure. The derivation is carried out in the setting of small deformations and moderate electric fields by means of a two-scale asymptotic analysis. Two types of rapidly oscillating space charges are considered: passive and active. The latter type corresponds to space charges that appear within the composite in response to externally applied electrical stimuli, while the former corresponds to space charges that are present within the composite from the outset. The obtained homogenized equations reveal that the presence of (passive or active) space charges within elastic dielectric composites can have a significant and even dominant effect on their macroscopic response, possibly leading to extreme behaviors ranging from unusually large permittivities and electrostriction coefficients to metamaterial-type properties featuring negative permittivities. These results suggest a promising strategy to design deformable dielectric composites – such as electrets and dielectric elastomer composites – with exceptional electromechanical properties.

A simple explicit homogenization solution for the macroscopic elastic response of isotropic porous elastomers

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Keywords: elastomers, microstructures, porosity, constitutive modeling, Hamilton-Jacobi equations

Abstract: An approximate homogenization solution is put forth for the effective stored-energy function describing the macroscopic elastic response of isotropic porous elastomers comprised of incompressible non-Gaussian elastomers embedding equiaxed closed-cell vacuous pores. In spite of its generality, the solution --- which is constructed in two successive steps by making use first of an iterative technique and then of a nonlinear comparison medium method --- is fully explicit and remarkably simple. Its key theoretical and practical features are discussed in detail and its accuracy is demonstrated by means of direct comparisons with novel computational solutions for porous elastomers with four classes of physically relevant isotropic microstructures wherein the underlying pores are: (i) infinitely polydisperse in size and of abstract shape, (ii) finitely polydisperse in size and spherical in shape, (iii) monodisperse in size and spherical in shape, and (iv) monodisperse in size and of oblate spheroidal shape.

Application of a poromechanical model to the interpretation of field vane test

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Keywords: Field vane test, nonlinear poroelasticity, transient flow, partial drainage, mine tailings, silt behavior

Abstract: The field vane test has been the most commonly used apparatus for in situ measurements of undrained shear strength of clays. Due to its simplicity and low cost, vane-like tests can also be widely found in silty soils investigation. However, attention must be paid to drainage conditions that can take place due to the relatively high permeability of silts, introducing errors on the classical interpretation. Of particular interest, falling in the range of silty behavior, mine tailings has been subject of recent studies due to its distinct behavior and environmental risks tied to its disposal. These materials usually present a silty-grained particle distribution and hence a correct assessment of the consolidation characteristics of this material should be conducted prior to the vane application in this material. In this context, theoretical solutions can be an essential tool helping understand what controls the drainage behavior that occurs during tests executed in silty materials. The present paper describes the application of a nonlinear poroelastic model conceived to capture the transient flow effects of the soil surrounding a rotating cylinder, in order to interpret the drainage conditions in which vane test is conducted for different materials and rates of shearing. The model is based on the local equivalence between the response of a perfectly plastic behavior to monotonic loading and an appropriate fictitious non-linear poroelastic behavior. Closed-form expressions for porepressure distribution were derived according to a simplified framework, while stress and displacement are computed numerically. The theoretical features of the model are briefly described and applied herein to the interpretation of drainage conditions during vane tests executed in clay and silty materials (tailings). Initially, a parametrical analysis is conducted to evaluate the response of theoretical materials varying permeability, strength and stiffness, as well as different influence radius size. Then, the numerical model is applied to experimental data. It has been shown that the proposed model allows the identification of test patterns that ensures the desired drainage behavior, a useful support for interpretation of in situ measured properties and foundation design purposes.

Effects of residual stresses on bored cast in situ piles capacity - computational approach

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Keywords: Bored pile, cast in situ, concrete curing, residual stresses, shaft friction

Abstract: It is already of common sense, considering it explicit or not in design, that piled foundations with driven and jacked-in piles are influenced by locked-in stresses, usually called residual stresses; it was found that the consideration of these stresses may be significant in the interpretation of load test results and load capacity of these piles. For bored cast in situ piles, however, this is not the case. Although several experimental evidences reported in literature have sought to develop the subject, there are still discrepancies regarding the results and interpretation methods used and there is not an established way of how to deal with pre load test data of instrumented bored piles.

In order to evaluate the influence of pre load test stresses in the piles and their influence in design parameters, induced specially due to concrete curing and its effect in soil-structure interaction, a computational approach using finite element method is applied, incorporating established models for concrete and soil behavior besides with experimental data from bored piles from an experimental testing site located in Araquari-Brazil of well-known subsoil conditions. This research is focused particularly in the consequence of taking or not into account the concrete curing induced thermal strains on the evaluation of shaft resistance of bored piles, where a potentially load reversal can take place in the soil-structure interface due the pre load test thermal induced strains, changing the available resistance of the soil.

Alternate Exact Analysis for Vibration of Beams Using Novel Boundary Characteristic Orthogonal Polynomials Satisfying All Boundary Conditions

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Keywords: Mechanical vibrations, Boundary conditions, Orthogonal Polynomials, Natural frequencies

Abstract: Alternate Exact Analysis for Vibration of Beams Using Novel Boundary Characteristic Orthogonal Polynomials Satisfying All Boundary Conditions

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Abstract

Novel Boundary Characteristic Orthogonal Polynomials (BCOP) constructed satisfying all the beam boundary conditions have been used in an alternative exact analysis of the beam vibration problem to obtain natural frequencies of vibrating beams with different boundary conditions. The beam vibration solution is formulated as a generalized Fourier series in terms of the novel BCOP which are orthogonal to each other and at the same time satisfy all the beam boundary conditions. The alternate exact solution described here expresses the exact solution in terms of the linear combination of the BCOP which satisfy all the boundary conditions a priori [2]. Substitution of this solution into the differential equation results in an eigenvalue problem whose solution provides the natural frequencies and the corresponding the natural modes. The first member of the orthogonal BCOP set satisfies all the boundary conditions of the vibrating beam, including the natural conditions. A modified Gram-Schmidt orthogonalization process is used where all the members of the orthogonal set of polynomials satisfy all the boundary conditions including the natural boundary conditions.

Since the beam characteristic orthogonal polynomials form a complete set, and are also linearly independent in view of Eq. (4), the solution can be expressed as a generalized Fourier series in terms of the BCOP. When the beam boundary conditions are applied, solution to the resulting eigenvalue problem provides an “exact” solution to the beam differential equation. The present method provides “exact” solutions in terms of the BCOP whose order steadily changes monotonically.

Natural frequency coefficients, $W=mlw^2/EI$, for different boundary conditions have been computed following the present method.

References

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Wednesday, May 22nd

Session 2: Biomechanics

Henderson Room, League 2:00 PM – 3:40 PM

Chair: Amy Wagoner Johnson

Study the effect of bone microstructure on bone remodeling

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Keywords: Bone microstructure; Statistical reconstruction; Finite element model; Mechanical behavior

Abstract: The development of predictive model for bone remodeling is becoming increasingly important for medical applications such as bone surgery or bone substitutes like prosthesis. However, as the bone remodeling is a complex multiphysics phenomenon and difficult to quantify experimentally, predictive numerical models remain at best, phenomenologically driven. Patient dependency is often ignored as its influence is usually considered secondary compared to other factors. However it is known that this plays an important role over long periods of time. Availability of experimental samples to carry out extensive analysis is another challenge to study the patient dependency in bone analysis.

Using our recently developed statistical reconstruction framework, a set of “bone like” microstructures with variety of distributions has been created to study pseudo “patient variabilities”. The method provides similar effective stiffness tensor, equivalent stresses and strain energy distributions for the original and the statistically reconstructed samples. The main outcome of this study is the correlation of similar effective mechanical properties between samples when bone remodeling will depend on the local strain energy distribution as a function of each bone microstructure. It is expected that two different microstructures with equivalent bone volume fraction will lead to identical bone remodeling in the short period of time, whereas this needs to be proven for long term evolution.

This work could be used to develop precise predictive numerical models while developing parametric studies on an infinite number of virtual samples and correlating patient dependency with more precise mechanobiological numerical models.

Effect of Fatigue on the Impact Response of Rat Ulna

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Keywords: Fatigue; Impact; Bone; Recover ; Woven Bone

Abstract: Fatigue behavior is one of the important properties of bones and impact is also another common loading condition. Combining fatigue and impact loading we may understand the effect of fatigue loading on the impact response given different recovery time of bones. Using rats as animal model, we investigated (1) whether the non-destructive cyclic loading can induce woven bone formation, a repairing response to damage, and (2) how would the impact response change given different rest time after cyclic loading. Cyclic fatigue loading was performed on 12 healthy male Sprague-Dawley rats, at 18 weeks of age, after IACUC approval. Under anesthesia, forelimb of each rat was positioned between the actuator and the load cell and the left ulnae served as control. The ulna was loaded axially in compression with a prescribed haversine waveform pattern at 2Hz. Pain relief was given after the loading. 8 rats were sacrificed within 24 hours after loading. The rest were sacrificed 7 days later. All ulnae were harvested and potted in fixtures with epoxy. Micro-CT scans were acquired for each specimen. Every scan acquired 996 slices of the diaphysis with each image containing 996x1016 voxels. A drop tower was designed for the impact test. The specimen was secured in place and the total energy from the impact was equal to 17.5% of the potential energy of the rat landing from a height of 0.2m. The peak force was recorded for each specimen. The fracture rate of the loaded ulnae was 5-times greater in the 1-day rest group than 7-day, but the fracture rate between the controls was similar. Overall, the peak impact force was 34.23% higher in the control than the loaded. The loaded ulnae with 7-day rest showed woven bone formation on the periosteal surface and increase in vascularity. The normalized bone volume with respect to body weight indicated that the difference between the control and loaded ulnae in 1-day rest group was not significant, but it was in the other group. The controls from both groups were not significantly different. Even with 7-day rest, the peak forces of loaded ulnae were still significantly lower than the control. Woven bone formation on the periosteal side might be resulted from the higher strain in cyclic loading. The partial recovery was attributed to the rapid formation of woven bone. Rest time was crucial in preventing fracture when bones were fatigued. However, woven bone didn't provide as robust support as healthy bone.

Equine proximal phalanx bone properties during growth

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Keywords: equine, bone, growth, fracture, density

Abstract: Introduction: Bone is most responsive to mechanical loads during growth, when the skeletal system continually reorganizes (remodels) its structure and composition to increase in size and mass without compromising strength. The proximal phalanx (P1), a bone in the fetlock joint of horses, accounts for ~25% of all distal forelimb fractures for racehorses. The goal of this study is to identify a period during growth where the P1 is (re)modeling the most and may respond to exercise manipulation, by first characterizing normal morphology and density during growth.

Methods: Three male Standardbred foals were subjected to longitudinal CT scans of the left forelimb during their first year, under IACUC approval. Hydroxyapatite phantoms were included during scans to relate Hounsfield unit and density. The left P1 was segmented and bone properties (area, density, etc.) were calculated using custom Matlab code. Kinematic and force data were collected after each scan at the walk, trot, and extended trot gaits. Area moment of inertia was calculated in BoneJ. Log-transformed data was used to assess scaling exponents of cortical area, indicative of compressive strength, and maximum area moment of inertia, indicative of bending strength, relative to body mass.

Results: Maximum bone length cross-sectional area are achieved by 36 and 47 weeks, respectively. The proximal growth plate closes between 28 and 36 weeks of age. Cortical area, cortical volume fraction, and area moment of inertia in the diaphysis all follow tight relationships with high R² values. Bone properties for the proximal and distal ends do not follow clear trends, but appear to even out after 28 weeks. Cortical area in the diaphysis, proximal, and distal peaks scale with positive allometry, while area moment of inertia at the same locations scales with negative allometry. Between 2-5 months of age, foals spent approximately 8.4% of their time walking, versus 1.4% of time moving at increased speeds. Increased speed of locomotion resulted in a more flexed fetlock joint angle at mid-stance for all ages.

Discussion: Scaling of cortical area and area moment of inertia suggests that the P1 bone does not normally experience significant bending loads and grows to maintain compressive strength. An exercise intervention may have the most impact between birth and 28 weeks of age. Increased speed of locomotion loads the P1 more in bending, and may strengthen the bone in desired regions.

Changes in murine bone morphology, apparent density, and gait during growth

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Keywords: bone, ontogenetic growth, scaling, gait, finite-element analysis, biomechanics

Abstract: Allometric relationships have been queried over many orders of mammals to understand how bone accommodates the mechanical demands associated with increasing mass. However, less attention has been given to the scaling of bone within a single lifetime. Using rats as a model system for development, we aimed to determine if bone morphology and apparent density is related to (1) bending and compressive strength, and (2) gait dynamics. Longitudinal in vivo computed tomography and gait data were collected from female Sprague-Dawley rats (n=5, age 8 - 20 weeks). All protocols were approved by the Institutional Animal Care and Use Committee (IACUC) at UIUC. Cross sectional properties and apparent density were measured at diaphysis, distal, and proximal regions of the tibia, and scaling exponents with respect to body mass were calculated. Each segmented tibia of a representative rat was converted into finite-element model with subject and time specific material properties. For each model, four-point bending and axial compression were simulated using time-specific ground reaction forces to calculate the mean strain energy density (SED) at the midshaft. Area moment of inertia at the diaphysis followed strain similarity based allometry, while bone area was positively allometric. The average SED at the diaphysis decreased, especially after the age of 10 weeks ($R^2=0.99$). However, in compression, the average SED increased after 10 weeks of age ($R^2=0.96$). The peak GRF increased throughout growth, while joint angles decreased until ten weeks and then converged ($p<0.05$). The apparent density in all regions increased and converged and this trend was correlated with joint angle changes. The scaling analysis implies that rodent tibia is (re)modeled in order to sustain bending at the midshaft during growth. The finite element results indicate that SED is not constant in the diaphysis, but rather decreasing suggesting that the tibia is actively adapting to become stronger under bending but not in compression. Interestingly, only when the joint angles reached a plateau did the strain energy density show this clear relationship. The correlations between bone properties and joint angles imply that the changes in posture may affect bone growth in specific regions. The fact that beyond 10 weeks of age density was relatively constant indicates that structural parameters may be the primary determinant of bone strength in the growing rodent tibia.

Mechanics of Skull Fixation in Pediatric Neurosurgery: Modeling Age Dependent Properties and Geometry

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Keywords: bone mechanics, finite element modeling, bone growth models, remeshing

Abstract: Head immobilization devices (HIDs) used in neurosurgery typically utilize a number of sharp pins that are tightened individually against the cranium for rigid fixation. However, numerous complications have been reported in literature, especially for young children, whose skulls are most susceptible to injuries. A major problem is the lack of standard procedure or detailed guidelines due to the lack of understanding of age dependent pin-skull indentation mechanics. Here, we elucidate the effect of age on HID application by developing a data driven model for the evolution of skull thickness and material properties, covering the range from birth to adulthood based on a monomolecular tissue growth model. To understand the biomechanics of the pin penetration process and the effects of age, we develop a non-linear continuum based finite element mechanical model of a single pin in contact with a multi-layer cranial skull disc under both axial and lateral loads with geometrical and material properties corresponding to age. Bone is a naturally anisotropic material due to the directionality of bone osteons and the geometrical nonuniformity in trabecular structures. Subsequently, we assume that cortical tissue behaves according to the Hill anisotropic yield criterion, commonly used to describe cortical bone yielding. In this model we consider the direction of highest compressive strength to be in the osteonal direction. Additionally, we assume the post-yield behavior to be elastic-plastic. To resolve the large element distortions, we implement automatic remeshing of the highly distorted elements during the solution according to an element quality criterion. We validate this approach through comparing simulations with experimental results of wedge penetration of bovine cortical bone. In the validation case, we study the effect of friction between the bone and the pin, which we show to be critical. For the case with an age of 1.54 year, with an axial load under 40 lbf, the pin fully penetrates the outer cortical layer and distorts the diploic layer while for the case with age 21 years, the pin penetrates less than 50% of the outer cortical layer when subjected to axial loads of 80lbf, the recommended load for adults. Our results provide a foundation for quantifying the risk of injury based on age, and hence this model can become instrumental for reducing risk of complications by both enabling redesign of HIDs and providing recommendations for current practices.

Wednesday, May 22nd

Session 2: Fracture Mechanics

Koessler Room, League 2:00 PM – 3:40 PM

Chair: Michael Thouless

**RATE-DEPENDENT TRACTION-SEPARATION RELATIONS FOR A SILICON/EPOXY
INTERFACE INFORMED BY EXPERIMENTS AND BOND RUPTURE KINETICS**

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Keywords: Interfacial fracture; Rate dependence; Cohesive zone model; Bond rupture kinetics; Traction-separation relations

Abstract: Rate dependent separation has been used to effect selective delamination in transfer printing and transfer of 2D materials to target substrates. To date, most of the emphasis has been on the rate dependence of the decohesion energy. However, as traction-separation relations are being increasingly used to represent the interactions between two surfaces during separation, characterizing their rate dependence must be addressed for such applications. In this work, double cantilever beam specimens were used to investigate the rate-dependent fracture of a silicon/epoxy interface. Fracture experiments were conducted at 5 different separation rates, ranging from 0.042 mm/s to 8.5 mm/s. For each separation rate, the interfacial properties were extracted by a beam on elastic foundation model and an iterative method, assuming a bi-linear traction-separation relation. Rate dependence was observed for the silicon/epoxy interface as both the interfacial toughness and strength increased with the separation rates.

Motivated by this observation, a rate-dependent cohesive zone model was proposed based on a thermally activated bond rupture mechanism. This model relates the interfacial fracture to the breakage of molecular bonds at the interface, and the rate effect develops naturally from the kinetics of damage evolution via the statistical concept of bond survival probability. The double cantilever beam problem with the interfacial bond rupture kinetics was then solved numerically, and the model parameters were extracted by fitting the numerical results to the experimental data. Ideally, this model should be able to explain and predict the rate-dependent fracture of a specific interface (e.g., silicon/epoxy interface) with four parameters, including the bond energy, the critical strength, the initial stiffness and a time scale. However, in order to fit the experimental data, the critical strength had to be adjusted. Nevertheless, this mechanism-based cohesive zone model offers a promising approach for modeling the rate-dependent fracture, which may also incorporate other mechanisms in future studies.

A DUAL ACTUATOR MIXED-MODE INTERACTION TESTER

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Keywords: Interfacial fracture, interactions, traction-separation relations

Abstract: Traction-separation relations are being increasingly used to characterize the interactions between surfaces. They provide a functional form for such interactions, whose salient features are the energy, strength and range. This takes the community beyond simply using energy, which is the hallmark the linearly elastic fracture mechanics approach to differentiate between interactions. Accordingly, the richer data set promises to provide further insights into the force fields that result in the measured traction-separation relations and spur theoretical developments. However, because interactions between surfaces usually involve both tensile and shear tractions, it has been challenging to characterize both components at any mode-mix or combination of tension and shear.

The paper describes the development of a dual-actuator loading device for separating laminated beams and extracting the tensile and shear components of the traction-separation relations for the interactions between the contacting surfaces of the beams at any mode-mix. The approach is based on the use of the balanced beam concept that decouples the differential equations for the normal and tangential separation in terms of the corresponding tractions. The use of a dual actuator system allows for non-proportional loading paths in mode-mix space.

As an example of its capabilities, the device has been used to determine the mixed-mode, rate-dependent, normal and shear components traction-separation relations of the interface between silicon and epoxy.

Exploration of non-crack singularities on the single lap-shear joint

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Keywords: lap-shear joint, fillet angle, cohesive-zone model, cohesive-length scale

Abstract: The single lap-shear joint is a commonly used to characterize adhesives; however, to be rigorously valid for linear-elastic fracture mechanics (LEFM) one must have a sharp crack all the way down to the adhesive. In reality, this small-scale sharp crack may not always be present. Indeed, there are many examples in the literature that do not even bother placing a crack in the specimen and use a corner instead. This paper will present results from a cohesive-zone model embedded into a single lap-shear joint with increasing cohesive-length scale and a varying fillet angle, including 90 degrees (a corner) and 180 degrees (a crack). The findings will be compared to LEFM predictions and their implications will be discussed.

Fracture and Healing of Elastomers: A Phase-Transition Theory & Numerical Implementation

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Keywords: Cavitation; Self-Healing Materials; Finite Deformations; Non-Conforming FE

Abstract: Recent experiments, analogous to the classical experiments by Gent and collaborators but carried out at higher spatiotemporal resolution (of 1 micron in space and 60 ms in time), have provided a complete qualitative picture of the nucleation and the ensuing growth and interaction of internal cavities/cracks in elastomers subjected to externally applied quasi-static mechanical loads. Remarkably, the experiments have also revealed that internally nucleated cracks in elastomers can completely heal, even when they have grown to be several tens of micrometers in length scale.

In this talk, I will begin by presenting a continuum field theory seemingly capable to explain, describe, and predict all of the classical and recent experimental observations: from the nucleation of cavities/cracks, to their growth to micro-cracks, to their continued growth to macro-cracks, to the remarkable healing of some of the cracks. The theory rests on two central ideas. The first one is to view elastomers as solids capable to undergo finite deformations and capable also to phase transition to another solid of vanishingly small stiffness: whereas the forward phase transition serves to characterize the nucleation and propagation of fracture, the reverse phase transition characterizes the healing. The second central idea is to take the phase transition to be driven by the competition between a combination of strain energy and hydrostatic stress concentration in the bulk and surface energy on the created/healed new surfaces in the elastomer.

In the second part of the talk, I will present a numerical implementation of the theory capable of efficiently dealing with large deformations, the typical near incompressibility of elastomers, and the large changes in the deformation field that can ensue locally in space and time from the nucleation of fracture.

Rate-Dependent Scaling in Quasibrittle Fracture

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Keywords: Quasibrittle structures, strain rate effect, strength statistics, size effect, fracture

Abstract: It has been well accepted that the failure behavior of quasibrittle structures exhibits a strong size effect. Such a size effect can be characterized by the transitioning from a quasi-plastic failure behavior to a perfectly brittle behavior with an increasing structure size. Recent studies have focused on the implication of this size-dependent failure behavior for the strength distribution of structures that fail at macrocrack initiation. It has been shown that, under quasi-static loading, the strength distribution of quasibrittle structures varies from a predominantly Gaussian distribution to a Weibull distribution as the structure size increases. This study investigates the effect of applied strain rate on the size dependence of strength distribution through stochastic computations of dynamic failure of aluminum nitride (AlN) specimens. The numerical simulation uses a stochastic discrete element model (DEM), which explicitly takes into account both random microstructures and random fracture properties. The model is applied to simulate the nominal tensile strengths of geometrically similar AlN square plates of different sizes under various applied strain rates. The simulation results indicate that, as the applied strain rate increases, the size dependence of the mean structural strength diminishes while the coefficient of variation (CoV) of the strength exhibits a stronger size effect. The simulated rate dependence is explained by a rate-dependent finite weakest-link model, which incorporates the rate effect on the size of the damage localization band. For the range of specimen sizes chosen in this study, the model predicts that, at high strain rates, the size effect on the strength distribution can be described by the Central Limit Theorem. The simulated rate and size effects on strength distribution have some important implications for stochastic simulations of quasibrittle fracture.

Wednesday, May 22nd

Session 2: Modeling and Computation

Michigan Room, League 2:00 PM – 3:40 PM

Chair:

Optimization of a Spherical Geometry for Vacuum Lighter than Air Applications

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Keywords: Lighter than Air, Finite Element Analysis, Non-parametric Optimization, Heterogeneous Media

Abstract: Parametric and non-parametric optimization, as well as meta-models (i.e. surrogate models representing desired responses based on a limited number of variables), are valuable and increasingly used tools in the pursuit of light, stiff, and strong structures that comply with a set of constraints. Of these, non-parametric optimization provides a framework to study a design space based on an initially suboptimal geometry and a set of constraints, without explicitly defining design variables. In this study, we use non-parametric optimization to find an optimal geometry for lighter than air applications that contain a vacuum, rather than a lifting gas, considering the effects of geometric nonlinearities and material stiffness on optimality, and ensuring continuity of the outermost surface for permeability. The resulting geometry is then refined, and evaluated for manufacturing feasibility. Abaqus Finite Element Analysis software and its embedded optimization module, Tosca, are used to conduct topology optimization and structural analysis.

Multi-length Scale Modeling of Dry/ Wet Traction

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Keywords: Tire Contact Mechanics, Multi-scale

Abstract: Because of its influence on vehicle mobility, handling, safety, and stability, tire is an important component of the vehicle. As such, understanding and developing models of the tire-road contact friction on dry and wet surfaces has been an important topic of research for decades. Although the dry surface contact friction has been studied and is relatively understood, wet friction is still not understood very well. Friction coefficient occurring at the contact interface is an important parameter required for the estimation of tire traction.

The present work focuses on estimating the tractive effort at the tire – road contact interface, under dry and wet conditions by considering friction physics at lower scales. Two approaches have been considered, (1) an analytical approach using Hierarchical multiscale modeling, where the approach is broken down into three scales: macro (full tire), meso (tread block element) and micro (Surface roughness scale) and (2) FE (Finite Element) model. For the analytical approach, the frictional losses based on the different mechanism occurring at the micro scale is transferred to the meso scale where the frictional stresses are combined over all roughness length scale to obtain an effective friction coefficient. The friction coefficient thus obtained, for the specific boundary condition can be used in the macro scale to estimate the tractive effort. In case of the finite element approach, a multi-length scale thermo-mechanical tire pavement model is developed to estimate the wet/ dry traction of the tire. The hysteresis frictional losses at the contact interface is obtained considering a rubber block sliding over a rough pavement. The friction coefficient obtained from the rubber block simulation will then be used as an input for the full tire model to estimate the tractive effort. In addition, for the case of wet traction, fluid has been modeled at the contact interface using the ABAQUS CEL approach.

To validate the models, the dynamic friction/wear tester and the ground robot sliding friction mechanism, developed by CenTiRe, will be used with a rotating rubber sample and a sliding rubber block, respectively. The traction forces obtained from the macro scale is validated using tire traction data that will be obtained using the tire-testing trailer developed by CenTiRe.

Theoretical and experimental analysis of nonlinear geometric stiffness effects on machine support structures

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Keywords:

nonlinear dynamics; geometric non-linearity; machine foundations; experimental analysis.

Abstract: We present a study of the effects of geometric nonlinearities on vibrations of rotating machines support structures. Dynamic characteristics of structures depend on their stiffness and mass. The initial stiffness of a structure, computed in its unloaded state, is affected by the applied forces, the so-called geometric stiffness. Compressive forces reduce the stiffness and the frequencies and may lead to buckling, for zero frequencies. Traction loads tends to increase stiffness and frequencies, as in tensostructures.

In bases of machines excited by the supported equipment, vibrations may affect the structures but, in general, may generate damage to the suspended equipment and the quality of the production.

Although machine support structures are, as a rule, very bulky, little affected by geometric stiffness considerations, the tendency of modern structural engineering is towards slender members, due to efficient materials and powerful analysis tools. Here we study these effects via theoretical, numerical and experimental methods. Laboratory essays and Finite Element larger models are developed. A first model is a metal beam under pretension supporting a rotational machine. We suppose the original design provided for natural frequencies away from the excitation frequency. Nevertheless, the presence of large axial compressive force will reduce the beam stiffness and natural frequencies leading to unexpected potentially dangerous resonance states.

A second model is a portal frame, formed by two vertical columns and a horizontal beam. Geometric nonlinearity is introduced by pretension forces. We calibrate the model to have 2:1 internal resonance between the second mode (the first symmetric mode) and the first mode (the sway mode). Further, we impose external resonance between the machine rotation speed and the second mode frequency. We demonstrate that this model may experience large amplitude oscillations, potentially dangerous, not predicted in linear theory that doesn't consider geometric stiffness effects.

Viscoelastic Eshelby analysis of single cardiac myocyte contraction in the cell-in-gel system

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Abstract: During every heartbeat, cardiac muscle cells in the heart experience mechanical stresses that continuously vary with posture, emotion, and physical activity. The healthy heart is an impressive adaptive structure, capable of upregulating its contraction and force in response to cardiac demands by the Frank Starling and Anrep mechano-chemo-transduction (MCT) mechanisms. Under pathological conditions, however, hemodynamic overload can trigger growth and remodeling that lead to arrhythmias, hypertrophy, dilation, or heart failure. A novel Cell-in-Gel system is being used to study MCT mechanisms at the single-cell level under normal and overload conditions in healthy and diseased states. The system consists of isolated live cardiac myocytes that are embedded in a constraining PVA-boronate hydrogel to mimic the in vivo mechanical environment during myocyte contraction. While cell contractions and strains can be measured directly by confocal microscopy and Ca^{2+} transients can be measured by fluorescence measurements, mechanical stress must be inferred by analysis. Here, we demonstrate a mathematical model to quantify the stress and to help interpret ongoing Cell-in-Gel experiments.

The proposed model is based on the classical Eshelby problem with an ellipsoidal inclusion, here extended to account for the viscoelasticity of the inclusion (cell) and the matrix (gel) to provide accurate calculations of time-dependent 3D stress and strain fields present during Cell-in-Gel experiments. Hydrogels of different cross-link densities are used in the experiments to systematically vary the mechanical constraints on the cell. Gel viscoelastic properties are calibrated by torsional rheometry measurements and its relaxation shear modulus is modeled using a Prony series. The Correspondence Principle of Viscoelasticity is exploited to extend the classical elastic Eshelby boundary value problem to solve the corresponding viscoelastic problem. Taking advantage of periodic cell contractions, a Discrete Fourier Transform analysis enables fast computation of time-dependent histories of all mechanical fields.

Using the established model, quantitative comparisons to experimental results are made and parametric studies are performed to establish trends with Gel stiffness and viscosity. The results show that for a purely elastic matrix, the stress within the cell is multi-axial and uniform, yet surface tractions are non-uniform. The presence of Gel viscosity, however, adds a time shift between strains and stresses and causes an increase in mechanical power requirements for cell contraction. With fixed Ca^{2+} transients, a typical cardiomyocyte in a Gel of similar stiffness can only contract 20% of its load-free fractional shortening. A healthy cardiac myocyte, however, up-regulates its Ca^{2+} transients in response to increased mechanical resistance (related to the Anrep effect), and a simple adaptive model is proposed to capture the up-regulated in-gel myocyte response.

Wednesday, May 22nd

Session 3: Biomechanics

Henderson Room, League 4:10 PM – 5:50 PM

Chair: Anastasia Muliana

Characterization of the elastic constants of soft anisotropic tissues using a novel indentation-based approach

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Keywords: Indentation, Soft materials, Anisotropy, Tissue characterization

Abstract: Characterization of tissue mechanical properties can help to understand and diagnose disease and disease progression. Indentation is increasingly used to characterize soft tissue and indentation modulus can be obtained in multiple directions; however, there is no simple method to use indentation to obtain the elastic moduli of anisotropic tissue without additional mechanical tests. The goal in this work is to introduce an indentation-based approach to determine elastic constants of soft anisotropic tissues without additional mechanical tests. The approach uses the indentation modulus, E^* , and the aspect ratio (AR) of the elliptical contact introduced by elastic anisotropy of the tissue and combines that with finite element (FE) analysis to achieve this goal. To quantify the AR of contact, the substrate was indented with a fluorescent bead-coated spherical indenter and the imprinted area was imaged. The AR was independent of indentation load and depth and could be measured simply by using a steel ball as an “indenter” without additional equipment. E^* was determined from instrumented indentation using an anisotropic contact model. A parametric finite element simulation of the indentation tests was performed to find the relationship between the aspect ratio of contact and the non-dimensional bulk ratios, E_x/E_y and G_{xy}/E_y ; here, E_x and E_y are the Young’s moduli ($E_x > E_y$) and G_{xy} is the shear modulus in the xy plane. The simulation highlighted two distinct regimes that depended on E_x/E_y : strongly anisotropic ($E_x/E_y > 150$) and weakly anisotropic ($E_x/E_y < 150$). For strongly anisotropic materials, AR and E^* are sufficient to determine G_{xy} and E_y . For weakly anisotropic materials, indentation modulus in transverse direction, E_y , and the AR of contact in the anisotropic plane can be used to determine the elastic constants. E_x and E_y were independently measured using tensile tests and the measured moduli agreed with those obtained from the proposed method. This approach is exciting because it can help to characterize the elastic properties of anisotropic and heterogeneous tissues by combining the simple stamp method with indentation, and the results from the FE simulations, without the need for a series of bulk mechanical tests.

Known microstructural difference in ACL bundles detected with full-field mechanics methods

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Keywords: biomechanics, full-field methods, anisotropy, constitutive modeling

Abstract: The anterior cruciate ligament (ACL) serves a mechanical function; it stabilizes the knee by restricting motion between the femur and tibia and it becomes injured when it is overstrained. ACL injuries typically lead to knee osteoarthritis, usually within 10 years of the injurious event, and those with complete ACL tears require surgical reconstruction in order to resume normal activity. Thus, there is substantial interest in determining its risk factors – the anatomical features and movement strategies that make an individual more prone to ACL injury. Whole-knee finite element models can be used to systematically examine the effects of possible risk factors on ACL strain. However, current material models for the ACL are unable to accurately predict tissue-level deformation. Ligaments are anisotropic due to their highly aligned collagen fibers. This anisotropy results in unavoidable inhomogeneous deformation – a non-starter for traditional modeling methods. Therefore, the aim of this work is to build accurate material models for the ACL using full-field methods, which capitalize on the deformation inhomogeneity that has made this problem historically difficult to solve.

Displacement-encoded MRI was used to measure the first full-volume, 3D displacement fields of the ACL bundles under tension. The virtual fields method (VFM) was adapted to extract material parameters from this displacement data. This method accounted for structural features like the curved bone boundaries and position-dependent fiber direction, while using the entire measured displacement field to inform the material model fit. Based solely on this mechanical data, the material parameters found for the Holzapfel material model predict that the two ACL bundles have significantly different degrees of collagen alignment ($p < 0.01$). This is a known microstructural difference between the bundles which has not been predicted by previous modeling efforts.

This work advanced the forefront of knowledge on ligament mechanics by demonstrating that full-field methods can be used to decouple material from structural properties, a previously unattainable task with traditional methods. These accurate material models will be used in whole-knee finite element models to identify ACL injury risk factors as well as serve as a benchmark for the mechanics of tissue-engineered ACL replacement grafts.

Monitoring of Skin using a Non-Invasive Skin Diagnosis Methodology

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Keywords: Basal cell carcinoma; Digital image correlation; Eigensolution; Finite element analysis; Healthy skin; Image processing; Malignant melanoma; Non-invasive diagnosis; Non-melanoma skin cancer; Skin; Speckle analysis; Treatment effects; Vibration

Abstract: Several non-invasive imaging techniques have been developed to monitor the health of skin and enhance the diagnosis of skin diseases. Among them, skin elastography is a popular technique used to measure the elasticity of the skin. A change in the elasticity of the skin can influence its natural frequencies and mode shapes. Here, we propose a novel technique to use the resonant frequencies and mode shapes of the skin to monitor its health. This study demonstrates how the resonant frequencies and mode shapes of skin can be obtained using numerical and experimental analysis. In the study, natural frequencies and mode shapes are obtained via two methods: (1) Finite Element Analysis: an eigensolution is performed on a finite element (FE) model of normal skin including stratum corneum, epidermis, dermis, and subcutaneous layers (2) Digital Image Correlation (DIC): several in-vivo measurements have been performed using digital image correlation. The experimental results show a strong correlation between the DIC and FE results suggesting a novel non-invasive method to differentiate healthy skin from diseased skin, particularly skin cancer. Prevention, early diagnosis, and treatment are critical in helping to reduce the incidence, morbidity, and mortality associated with skin cancer; thus, making the current study significant and important in the field of skin biomechanics.

Materials Properties of the Thigh in the Seated and Prone Positions

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Keywords: soft tissue, Ogden model

Abstract: Human body modeling is necessary to describe the interactions between people and the objects they use every day. The implications for modeling the interaction between a person and their chair affect the medical seating industry. Generating a finite element model, which is used to determine internal tissue stresses while seated, requires accurate values for the mechanical properties of the tissues. Because the thigh and buttocks are continuously in contact with the seat, the material properties of these regions are of particular importance. Previous models have used soft tissue material properties obtained from animal studies. Limited human data are available; those that are come from individuals lying face down (prone). Although thigh properties while prone can be used to evaluate stresses in that position, the goal of this work was to determine whether or not thigh soft tissue properties in the prone position differ from those in the seated position in order to ensure that internal stresses can be accurately predicted while seated.

Force deflection curves of twenty individuals' thighs were collected using a custom indenter while in a seated and prone position. The indenter used a six axis load cell and linear potentiometer to measure the force and tissue deflection, respectively. Three thigh regions were tested and the data converted to stress and stretch values, using the contact surface of the indenter and thigh geometry. Finally, the stress and stretch values were modeled using an incompressible Ogden material model under uniaxial compression.

The resulting models for each position showed that while the low stress behaviors of thigh tissue in the seated and prone postures were similar, their behaviors deviated significantly when experiencing seated stress. At these load magnitudes, thigh tissues in the seated position were softer than those in the prone position. This means that prediction of internal stresses while seated can be more accurately represented by using thigh soft tissue properties specific to the seated position. This information will better inform seated models that predict tissue stresses in the office, automotive, and medical seating industries. In turn those models can be used to improve seat designs and for medical seats such as wheelchairs, reducing the chance of pressure related injury.

Wednesday, May 22nd

Session 3: Modeling and Computation

Michigan Room, League 4:10 PM – 5:50 PM

Chair: Alan Wineman

Swelling induced shearing and twisting in fiber reinforced hyperelastic cylinders

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Keywords: hyperelasticity, swelling, fibers, twisting

Abstract: Externally induced volumetric change, such as that associated with swelling, can lead to complicated states of deformation, especially when anisotropy is present in the original material. In particular, specialized patterns of fiber reinforcement can guide the volumetric change into potentially useful shearing and twisting modes of deformation. We consider this effect in hyperelastic tubes that are reinforced with spirally wound non-swelling fibers that proceed from the inner radius to the outer radius. By incorporating swelling into the continuum mechanics description we quantify these deformation modes and gauge their ability to generate controllable twisting. As would be expected, the relative fiber stiffness and the precise nature of the spiral patterning have a pronounced influence on the details of the twisting response as the swelling proceeds. To accommodate the swelling requires that at least one of the boundaries is able to freely expand. The fixation conditions on the remaining boundary has a strong effect on the nature of the overall twisting that can be achieved. Alternative fixation conditions are examined.

In this treatment both the fibers and the matrix are treated as hyperelastic, even though it is only the matrix that exhibits swelling. Of particular interest is the limiting case where the fibers become inextensible due to an increasing relative stiffness with respect to the matrix constituent. We examine the sense in which the extensible fiber theory approaches an inextensible theory as this relative stiffness becomes large. A subtle aspect to the ensuing limit is that one may identify a specific regime of sufficiently large swelling that causes the cross-section of the cylinder to partition itself into a fully twisted inner region and an outer region that still retains some residual twisting capacity. There is a radial interface that separates the two domains, and changes to the overall amount of swelling result in quasi-static movement of this interface.

H. Demirkoparan, T. J. Pence (2017) Swelling-Twist Interaction in Fiber Reinforced Hyperelastic Materials: The Example of Azimuthal Shear. *Journal of Engineering Mathematics*, <https://doi.org/10.1007/s10665-017-9906-x>

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Axisymmetric and Asymmetric Inflation of Circular Membranes with Nonuniform Properties

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Keywords: Hyperelastic membranes, Nonuniform properties, Asymmetric Inflation, Inflatable structures

Abstract: Membranes and inflatable structures have gained a considerable attention recently due to the growing demand for lightweight and low-cost structures. These structures possess an exceptionally high mechanical packaging efficiency and very small stowage volume, which gives them a wide range of applicability ranging from space deployable structures, such as antenna reflectors, solar arrays, inflatable rovers, and human habitats, to implementations in automotive and civil engineering industries. Of particular interest, is to achieve a desired shape upon inflation in order to meet certain criteria or perform a specific task.

In this study, the inflation of circular hyperelastic membranes with nonuniform properties has been investigated. While a membrane with uniform material properties and constant thickness can only achieve a certain deformed configuration upon bulging, changing the distribution of membrane's stiffness and thickness over its surface would result in some irregular axisymmetric and asymmetric configurations that can never be achieved if the properties are deemed constant. A hyperelastic mathematical formulation based on solving equilibrium equations using Ritz method has been proposed and the findings are verified by experimental measurements.

Strong Ellipticity Conditions for Orthotropic Nonlinear Elastic Materials in Plane Strain

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Keywords: Ellipticity Condition, Nonlinear Elasticity, Orthotropy, Plane Strain

Abstract: The equations of nonlinear elastostatics may lose ellipticity at a sufficiently high level of deformation, leading to the possible emergence of material instabilities, such as shear bands. Even though considerable attention has been devoted in the literature to the determination of explicit conditions for strong ellipticity, little is known in the case of nonlinear and anisotropic elastic materials. In this work, necessary and sufficient explicit conditions for strong ellipticity of the equilibrium equations governing finite plane deformations are established for a class of compressible, orthotropic, and hyperelastic materials. The conditions are then specialized to the case of a material having the symmetry axis parallel to a principal direction of deformation. This case is relevant in experimental protocols employed in the characterization of constitutive relations of rubberlike materials and biological tissues. The classical conditions for infinitesimal linear elasticity and isotropic finite elasticity are recovered as particular cases.

Thursday, May 23rd

Session 1: Biomechanics

Henderson Room, League 9:00 AM – 10:40 AM

Chair: Callan Luetemeyer

Soft tissue mechanics during self-healing

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Keywords: microtissue, self-healing, contractility, surface energy, elastocapilarity

Abstract: When tissues are injured, embryonic processes are partially recapitulated, which leads to a reconstruction process. Whereas much research has focused on understanding the chemicals and signaling pathways involved in wound closure, little is known about the mesoscale physical principles of multicellular organization required to re-establish the architecture of three-dimensional (3D) tissues during repair. In adult fibrous soft tissues, fibroblasts physically interact with the surrounding nonlinear extracellular matrix (ECM) with visco-elastic and plastic attributes. These interactions are studied in vitro by encapsulating cells within 3D biopolymer hydrogels, such as collagen and fibrin. With the invent of microengineered in vitro wound healing models, it was experimentally confirmed that tissue repair is regulated by cellular forces. Here, we present a computational model to study the damage response of engineered 3D constrained contractile microtissues. We postulate that active surface energy stemming from the cellular contractility on the surface is critical for the evolution of tissue shape at small scales. A computational framework based on an energetically motivated equilibrium theory is introduced, which consists of a novel constitutive model that couples active and passive elasticity with bulk and surface energy components. A finite element scheme is developed to simulate the response of tissues to injuries and verify our model. Tuning model parameters by comparison with experimental measurements, our framework provides a quantitative description of the shape during self-repair and elucidate the physical mechanisms behind boundary restoration.

Shear and Transverse Characterization of the Patellar Tendon

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Keywords: characterization, biomaterials, nonlinear elasticity

Abstract: Ligaments and tendons are tissues comprised mainly of collagen fibers and of an elastic matrix that connects bony surfaces. They are commonly modeled as nonlinear elastic and transversely isotropic. Mechanical tensile testing along the fiber direction has been conducted for the patellar tendon. Patellar tendon shear and transverse responses have not been quantified. The goal of this study is to quantify shear and transverse properties of ovine patellar tendon to identify which material models best describe these deformation modes.

Ovine patellar tendon samples were dissected from fresh sheep knees and used for either shear or transverse testing. Local displacements were quantified using digital image correlation. Homogenized shear strain was extracted from a central portion of the samples. Experimental data and published tension data along the fiber direction were fit to transversely isotropic material models.

Preliminary data show (1) that transverse and shear behavior of patellar tendon is nonlinear and (2) that the patellar tendon is stiffer in the transverse tension direction than in shear. The Holzapfel-Gasser-Ogden (HGO) model, which is commonly used for ligaments, is unable to capture this nonlinearity. A modified version of the HGO model, which used a modified Mooney-Rivlin or MacKintosh 8-chain isotropic phase, incorporates nonlinearity but is unable to capture the difference in stiffness between the transverse and shear responses. This suggests that an alternative material model is needed that permits greater differences in stiffness between the transverse and shear response.

Mechanical Homogenization of the Liver Tissue with a Combined Method of FE-Optimization

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Keywords: Mechanical Homogenization, Anisotropic Hyperelastic, Finite Element (FE), Optimization, Neural Network

Abstract: The liver is a crucial organ in vertebrates for performing various biochemical reactions in their bodies. Currently, there is no replacing choice for patients suffering from a long-term failure of the liver. Minimum-Invasive Surgery is a breakthrough in patients surgery comfort, increasing the success rate of surgery, and decreasing the surgery complexity. The final purpose is the reconstruction of 3D images of the liver with augmented reality in real-time such that the organ would be displayed in 2D. Therefore, the surgeon(s) can design and eventually perform minimum-invasive surgeries with better working conditions; and increased comfort and security for patients. The developed numerical FE tool for surgery simulation needs coordinate errors below 1 mm and response time below 0.1 s. Having the geometries of patient's Liver with medical imaging and determining the mechanical properties of each section with non-invasive tests, a multi-layer macroscopic homogenization technique should be delivered to account for the effects of major-size vessels in Liver. It must have the ability to differentiate between sections of Liver and patients. The purpose of this study is the mechanical homogenization of Liver tissue with an inventive and combined method of FE-Optimization. Due to the existence of major-size vessels, the surrounding tissue is anisotropic, and the hyperelastic model with the two different sections are costly both in time and processing expenditure. Thus, a homogenized, anisotropic, and hyperelastic model with the nearest response to the real heterogeneous model was designed and presented. Because of various possibilities of the vessel orientation, position, and size, homogenization has been done for enough samples of heterogeneous models to train neural networks as a machine learning method. Then, an unknown sample of heterogeneous material was categorized and mapped to its homogenized material parameters with the trained network for the fast and low-cost generalization of combined FE-Optimization method. The results showed about one percent error with respect to heterogeneous model for the combined method and the efficiency of the neural network for the prediction of effective material properties of unknown heterogeneous samples. This inventive method of homogenization is also presented in an interactive and user-friendly graphical user interface (GUI) to be used for future practical usage and have economic value added.

Dynamics and locomotion of flexible foils in a frictional environment

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Keywords: Friction, locomotion, snakes

Abstract: Flexible foils have long been used as a generic model for the bodies and appendages of organisms (e.g. fish and snakes) in locomotion. To understand the range of possible dynamics including efficient locomotion, we have used analysis and computations together with experiments to study flexible foils in a frictional environment. Resonances can occur at certain flapping frequencies, scaled by elastic parameters. Resonances correspond to peaks in propulsive force, but also input power supplied to the foil, and are often states of low efficiency. Other generic phenomena are the transition from periodic to non-periodic and chaotic dynamics as the heaving amplitude increases or the bending rigidity decreases, and the spontaneous emergence of traveling wave motions. We have determined more generally which planar snake motions are optimal for efficiency. The optimal motions help to explain the widespread observations of traveling wave motions in biological snakes.

Thursday, May 23rd

Session 1: Plasticity

Koessler Room, League 9:00 AM – 10:30 AM

Chair: Oscar Lopez-Pamies

Dynamic recrystallization in adiabatic shear banding: an entropic, effective-temperature model

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Keywords: Dynamic recrystallization, shear banding, plasticity, dislocations, thermodynamics, polycrystal plasticity

Abstract: Dynamic recrystallization (DRX) is often observed in conjunction with adiabatic shear banding (ASB) in polycrystalline materials. The recrystallized nanograins in the shear band have few dislocations compared to the material outside of the shear band. We reformulate the recently developed Langer-Bouchbinder-Lookman (LBL) continuum theory of polycrystalline plasticity and include the creation of grain boundaries. While the shear-banding instability emerges because thermal heating is faster than heat dissipation, recrystallization is interpreted as an entropic effect arising from the competition between dislocation creation and grain boundary formation. We show that our theory closely matches recent results in sheared ultrafine-grained titanium, and in a top-hat 316L stainless steel sample undergoing uniaxial compression. The theory thus provides a thermodynamically consistent way to systematically describe the formation of shear bands and recrystallized grains therein.

Incorporation of deformation twinning in single-crystal elasto-viscoplasticity model with embedded weak discontinuity

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Irene J. Beyerlein, undefined, undefined, undefined

Keywords: Deformation twinning, embedded weak discontinuity, crystal plasticity

Abstract: Deformation twinning is an important plastic deformation mechanism in polycrystalline metals such as titanium. In this talk, we present a new computational framework to explicitly incorporate deformation twinning, in addition to crystallographic slip, into the finite element formulation. Within this computational framework, the deformation twins are treated as embedded weak discontinuities inside individual finite elements, where the jump of the strain field between the untwinned and twinned regions is introduced in the discretized gradient operator. Different deformation gradients are adopted to describe the kinematics associated with the untwinned and twinned crystal regions, respectively. Specifically, for the untwinned crystal region, the plastic deformation is predominated by the plastic slips, and the associated deformation gradient is multiplicatively decomposed into the elastic and the plastic parts. This is consistent with large deformation crystal plasticity formulations. On the other hand, for the twinned crystal region, deformation twinning is included as an additional mode of plastic deformation, and the associated deformation gradient is multiplicatively decomposed into the elastic, the plastic and the twinning parts. The deformation gradients associated with the untwinned and twinned crystal regions are related through the compatibility condition and the traction continuity condition at the interface formed between the two regions. A probability-based twin nucleation model is applied to detect the twin initiation at grain boundaries. And the evolution of the twin length and thickness are considered in the subsequent deformation process. The linearization of the single-crystal viscoplasticity model and the Newton scheme to solve the traction continuity equation are presented. Simulations of the initiation and propagation of the $\{10\bar{1}2\}$ tensile twin system in hexagonal close packed (HCP) titanium are provided to demonstrate the capability of the proposed computational approach. Detailed mesh-sensitivity analyses are also presented.

Multi-Fidelity Crystal Plasticity Modeling for Titanium-Aluminum Alloys

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Keywords: Multi-Fidelity; Crystal Plasticity; Gaussian Process; Optimization; Microstructure

Abstract: A multi-fidelity computational scheme is addressed for the crystal plasticity modeling of Ti-7Al alloy. The crystal plasticity simulations are performed using low and high-fidelity solution techniques. The low-fidelity solution involves the use of a one-point probability descriptor, Orientation Distribution Function (ODF). The ODF is considered as the low-fidelity technique since it cannot capture the effects of microstructural correlations and grain shapes to macro-scale stress-strain responses. The high-fidelity model is the crystal plasticity finite element method (CPFEM), which provides higher resolution in grain-level microstructural features. However, the CPFEM is a computationally expensive technique and it is not feasible to be utilized for computationally costly problems. Therefore, in this work, we present a Gaussian process based multi-fidelity modeling scheme that improves the low-fidelity ODF simulation data with the high-fidelity CPFEM simulations. The multi-fidelity approach uses more samples from the computationally less expensive low-fidelity model and less samples from the computationally expensive high-fidelity model to satisfy both accuracy and computational time objectives. The results of the multi-fidelity framework show a significant improvement on the accuracy of the crystal plasticity modeling of Ti-7Al compared to the low-fidelity solution.

Mechanics of Oxidation of Zirconium Alloys in Pressurized-Water Reactors

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Keywords: Zirconium alloys, Oxidation, Stress relaxation, Phase transformation, Finite Element Analysis

Abstract: Zirconium alloys are used as the cladding material for fuel rods in Pressurized-Water Reactors (PWR). Corrosion of this cladding results in the formation of oxide films that are inherently protective in nature, as they are subjected to in-plane compressive stresses. However, despite this compressive stress, sudden acceleration in the oxidation rate is observed as the oxide layer attains a critical thickness. This phenomenon, called the breakaway, limits the fuel burn-up in reactors. Therefore, this research work is focused on developing an understanding of mechanisms that trigger breakaway.

A plausible cause of breakaway is the relaxation of compressive stresses in the oxide. To elaborate, high compressive stresses within the oxide have been proposed as a major contributing factor that leads to the meta-stability of the tetragonal phase of the oxide (zirconia). As oxidation proceeds, tetragonal zirconia is observed to transform to the thermodynamically stable phase of zirconia, the monoclinic phase, possibly due to stress relaxation. This phase transformation has been postulated as a possible trigger for breakaway, since it may cause micro-cracks. Consequently, a study of how stresses evolve within the oxide and how they effect the energetics of this phase transformation can provide an insight into the breakaway phenomenon.

To this end, we developed a continuum-based mechanistic model for the stress relaxation in an oxide formed on a zirconium alloy through identification of particular creep mechanisms that are active either in the oxide or the zirconium alloy substrate. We also developed a free-energy-based framework to investigate the energetics of tetragonal-to-monoclinic phase transformations in the temperature range of 600 to 1000 K. The finite-element program ABAQUS was used to model 3-D twinning-based phase transformations, and to obtain the strain-energy barriers against transformation. We conclude that loss in coherency is necessary for columnar tetragonal grains to transform to monoclinic grains. Significantly higher energy barrier for the transformation of equiaxed tetragonal grains indicate that ions or dopants present in the oxide layer may have an effect on the thermodynamic driving force for the transformation.

Mixed-mode cohesive law with a physical crack propagation consideration

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Keywords:

Abstract: Mixed-mode fracture is often modelled with cohesive laws which describe the relationship between the normal and shear components of the interfacial tractions and crack face separations. A condition in these laws is required for propagating a crack. Most current approaches, which employ potential-based or non-potential-based formulations for mixed-mode fracture modelling, often use an enforcement criterion to achieve this purpose with negligible consideration of physical crack propagation. Physically, simultaneous vanishing of normal and tangential interfacial tractions must occur for a crack to advance. In this study, this physical requirement is embedded into a general formulation for mixed-mode cohesive law. The model only requires normal and tangential traction separation laws for pure normal and tangential modes, which are typically measured in experiment. The traction-separation law under mixed-mode loading is constructed from these basic measurements. It allows all traction components to disappear simultaneously and naturally as an effective separation is reached. Therefore, no additional criterion for crack propagation is needed. Verification of the proposed formulation is performed using bench-mark tests such as double cantilever beam (DCB), end-notch flexure (ENF), and mixed-mode bending (MMB). Its predictions are also compared against other selected mixed-mode laws and experimental data for further validation.

Thursday, May 23rd

Session 1: Modeling and Computation

Michigan Room, League 9:00 AM – 10:30 AM

Chair: Reyolando Brasil

Solving differential equations on quantum computer

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Keywords: Quantum computing, Differential equation, Axial Bar, Energy methods

Abstract: Recent advances in Quantum computing has accelerated development of discrete algorithms. Particularly, Quantum annealers have shown a great progress in their computation power with D'Wave recently launching a 2048 qubit architecture. This urges effort towards understanding and developing methodologies to solve scientific computation problems on quantum computers. In this work, an iterative numerical procedure to solve 1D Sturm-Louville problems is presented. As a test case, numerical simulations of the equation for an axially loaded bar are exhibited and examined. Results for convergence analysis are provided and it is proved that the procedure can find a solution arbitrarily close to the best approximated solution of the discretized problem.

Numerical methods often rely on functional minimization (e.g. energy minimization). A similar approach is taken by reformulating functional as a Hamiltonian of spin models and minimizing the equivalent Hamiltonian. Quantum annealers provide a distinct advantage of efficiently solving spin models but are limited to the graphs which can be represented on their physical hardware. To alleviate this problem, the spin model needs to be embedded/mapped onto the physical architecture of a quantum processor. Thus, there are two major tasks involved in solving functional minimization on these computers, namely, (1) formulation of the spin model Hamiltonian, and (2) finding an appropriate embedding of the model onto the physical processor. It is shown that these procedures can be efficiently done on a D-Wave processor and that the size of the required quantum bits grows linearly with the number of nodes on the bar.

Quantum computers, unfortunately, often tend to spur out erroneous and sub-optimal results. Therefore the quantum algorithms need to take active measures for correcting these errors. It is shown that this can be efficiently done by scaling the Hamiltonian. In conclusion, this work provides a novel approach for solving differential equations on quantum computers.

Optimization of a Predefined Natural Frequency for Fluid-Structure Systems with Unstructured Mesh

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Keywords: Coupled System, Eigenvalue, BESO, FEM

Abstract: The optimization of fluid-structure coupled systems has been broadly studied in recent years. However, evolutionary optimization methods have not been extensively explored in this class of problems.

Thus, the objective of the present study is the topological optimization of fluid-structure systems in order to improve their dynamic behavior by maximizing or minimizing a predefined natural frequency, far away from the excitation resonance frequency, while the structural part is gradually removed until a prescribed volume.

The addressed problems were discretized by an unstructured mesh, which is not usual in works published in the pertinent scientific literature. The optimization is done with the BEFSO method, which is based on the BESO - Bidirectional Evolutionary Structural Optimization soft-kill method, applying the material interpolation scheme with penalization.

The objective function of the optimization problem quantifies a dynamic characteristic to be optimized and depends on the configuration of the structure in each iteration. In addition, this function is used as the basis for determining the sensitivity function and the iterative stopping criteria. Some obtained results of this work could be validated with relevant benchmark cases of the literature for the topological optimization of fluid-structure systems, in order to verify the applicability of the developed codes.

Model-free forecasting of the flutter speed and post-flutter dynamics

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Keywords: Bifurcation forecasting, Fluid-structural systems, Flutter, Hopf bifurcations, Critical slowing down

Abstract: Subcritical and supercritical Hopf bifurcations (flutters) have been observed in a variety of fluid-structural systems. These phenomena can cause dramatic changes in the system dynamics typically resulting in loss of performance or total failure. Hence, one of the most demanding topics of research in aeroelasticity is determining the speed above which nonlinear aeroelastic systems become dynamically unstable, i.e. determining the flutter speed. Furthermore, identifying the flutter type (supercritical and subcritical) and the limit cycle amplitude beyond the flutter speed are also important especially when operating close to the linear flutter boundary.

Existing analytical and computational methods to analyze the stability of the systems are model-based. Creating accurate models can be infeasible or impractical especially when systems are exceedingly complex. Alternative approaches include experimental methods to determine the stability and bifurcation diagram. Such methods place the system in the post-bifurcation regime, which can result in the collapse of the system.

In this work, we introduce a novel model-free method to forecast the flutter speed and post-flutter dynamics of fluid-structural systems, exemplified by a very flexible high-aspect-ratio wing. The forecasting method uses the fact that in Hopf bifurcations, the rate of the system's recovery from perturbations decreases as the system approaches the bifurcations, known as the critical slowing down phenomenon. Wing response to gust perturbations in the pre-flutter regime are the only required measurements for forecasting. Surrogate data are used instead of experimental data, obtained from numerical simulation using an efficient geometrically nonlinear aeroelastic solver. Using the forecasting method, bifurcation diagrams for displacements and velocities of points along the wingspan are forecasted. Results show that the method successfully forecasts the flutter speed and the post-flutter limit cycle oscillations amplitudes of the fluid-structural system despite the fact that the approach uses only pre-bifurcation regime data and it does not use a model of the system. This type of forecasting opens the door to dynamical analysis of complex systems, in both theoretical and experimental problems, and is important in safety analysis of complex systems.

Thursday, May 23rd

Session 2: Biomechanics

Henderson Room, League 11:00 AM – 12:40 PM

Chair: Nikolaos Bouklas

Biomechanical properties of bioenergy sorghum stems and their constituents

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Keywords: biomechanics, plant tissue, viscoelasticity

Abstract: Sorghum [*Sorghum bicolor* (L.) Moench] is a tropical C4 grass that has emerged as a bioenergy crop, owing to its high productivity, established production systems, widespread adaptability, phenotypic diversity, and relative ease of genomic analysis. Bioenergy sorghum grows tall and has a high content of biomass, but often suffers from stem lodging. Stem lodging was observed in both healthy and disease stems, which was associated with mechanical loading, e.g., wind pressure, imposed to the stem. In order to mitigate stem lodging and breed lodging resistant sorghum, it is important to understand the biomechanical properties of sorghum stems. Sorghum stems like typical plants are composite materials, consisting of various microstructural complexities at multiple length scales. At larger scale sorghum stalks can be distinguished by their sclerenchymatous tissue (outer skin or epidermis and rind comprised of several sub-epidermal cell layers) and parenchymatous tissue (pith, consisting of vascular bundles and soft tissues). These complex microstructures lead to nonlinear inelastic responses when subjected to mechanical stimulus. In this study, we investigate the mechanical properties of sorghum stems and their constituents, i.e., rind and pith. The sorghum specimens were tested under uniaxial loading (tension and compression) at different loading histories. The experimental tests reveal pronounced time-dependent responses of the pith and rind, and therefore the stems exhibit significant time-dependent responses. In order to describe the time-dependent inelastic responses of the sorghum stem and its constituents, a nonlinear time-dependent constitutive model is considered for the pith and rind. The constitutive model is integrated to a simple micromechanics model in order to predict the mechanical responses of the stems.

Exposing the Injection Machinery Dynamics of T-even Bacteriophages through Multi-Scale Modeling

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Keywords: T-even bacteriophages ; Injection machinery; Dynamic model; MD simulation.

Abstract: T-even bacteriophages (T2, T4, T6) are one of the most common and complex tailed viruses, from family Myoviridae, which infect the E.coli bacterium using an intriguing nanoscale injection machine including an elastic contractile tail sheath which powers the injection process. The sheath is composed of helical strands of protein that attaches to a large multi-protein capsid by neck at one end and connects to a baseplate at the other end. During the injection, the sheath simultaneously rotates about and translate along the tail assembly axis and creates a sudden collapse from an energetic, extended conformation prior to infection to a relaxed, contracted conformation. This coupled translation and rotation of injection machinery creates a combination of thrust force and torque that pierces the host membrane. Finally, the genomic DNA is transferred from capsid into the host cell.

Despite extensive progress in resolving the structure of T-even phages, the dynamics of the genome-delivery machine remains largely unknown, including the process time scale and energetics. To fill that gap, we propose a multi-scale dynamic model to approximate the three-dimensional nonlinear dynamics of the injection machinery. The model employs a two-stage, multi-scale approach. First, molecular dynamic (MD) simulations are employed to estimate the elastic stiffness and internal dissipation properties of the protein strands that form the elastic sheath. Second, those material properties are employed in continuum (rod) models for each of the six sheath strands that also couple to rigid body models of the capsid, tail tube and baseplate. Doing so yields a dynamic, multi-body model of the entire assembled virus. The formulation also accounts for likely energy dissipation deriving from 1) hydrodynamic drag acting on the capsid, sheath and tail tube, 2) interaction forces from the tip of the tail tube on the host cell membrane, and 3) internal (material) dissipation of the sheath strands.

The resulting multi-body model reveals the fundamental behavior of the injection machinery including the time scale and energetics of the injection process, the nonlinear conformational changes experienced by the sheath, the contribution of different sources of energy dissipation during injection process, and the required cell rupture force. These research findings may impact on advancing phage therapy and developing nano injection machines that mimic the characteristics of nature's viral machines.

Collective cargo transport on multiple tracks

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Keywords: Coupled-field phenomena, biomechanics, biophysics, intracellular transport

Abstract: The transport of intracellular organelles is accomplished by groups of molecular motors. Previous studies have demonstrated that the cooperative activity of motors on a track helps long transport. However, inside crowded cytoskeletal networks, surplus motors could impair transport and lead to traffic jams of cargos. To understand the effects of the presence of multiple available tracks on the motor cooperation, we developed a stochastic model to calibrate the transient forces in the motors and the transient binding and unbinding of the motors. We found that multiple tracks influence the number of engaged motors (motors bound to the tracks) by changing the binding and unbinding probabilities and the distribution of the stall force. In addition, we observed three types of collective transport (independent, cooperative and tug-of-war) based on the forces generated by motors. The cooperative transport by multiple kinesins is less influenced by the topology of the intersection of two tracks compared with the transport by a single kinesin. However, the availability of many motors to pull a cargo does not always lead to the best transport because the independent dynamics of each motor can lead to a tug-of-war among motors. When an intermediate number of motors (i.e., 16 motors) are uniformly attached to the surface of an 800 nm cargo, we found that the motility of the cargo is the largest for several different track topologies, including a 90° intersection, parallel and anti-parallel tracks.

Thursday, May 23rd

Session 2: Plasticity

Koessler Room, League 11:00 AM – 12:40 PM

Chair: Isha Gupta

Component-Scale Microstructure Reconstruction Using Markov Random Fields: Validation of Microstructural Features

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Keywords: Spatial Microstructure Synthesis, Markov Random Fields, Data-Driven Inference

Abstract: Measurement and analysis of microstructures is an important aspect of materials design and structural performance. Grain sizes, cell structures, and precipitate distributions affect the engineering properties as well as the performance of advanced materials. In this work, we present our progress on data-driven methods for 3D microstructure reconstruction. To enable numerical synthesis of microstructural features of materials, microstructures are represented in the form of undirected graphical models (a.k.a. Markov Random Fields). This algorithm uses novel sampling and reconstruction strategies that can seamlessly synthesize validated 3D microstructural models from representative 2D images. The code incorporates an optimization technique that ensures the patches from the 2D micrographs are meshed seamlessly together in the 3D reconstruction. The efficacy of this approach is demonstrated using the following three cases: (i) disperse spherical inclusions, (ii) anisotropic lamellar microstructures, and (iii) polycrystalline microstructures. The method is validated by comparing the joint-probability function, orientation distribution function, and 3D shape-moment-invariants of the synthesized model to that of original 2D images. Additionally, the mechanical properties of the synthesized microstructures are computed using crystal plasticity finite element method and are found to closely match the experimental results.

Dislocation patterning and pattern transition in fatigue using reaction-advection-diffusion equations

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Keywords: Dislocation patterning, reaction-diffusion, fatigue

Abstract: A number of macroscale and mesoscale plastic localization phenomena are a direct consequence of the collective behavior of interacting dislocation populations forming characteristic patterns under varying regimes. Also, different stages of deformation and the transitions between them can be directly correlated with rearrangements in the dislocation microstructure. This justifies the need to develop a physics-based modeling approach to capture different dislocations patterns intricately coupled with the mechanics of the underlying material.

Reaction-Advection-Diffusion(RAD) systems form an attractive approach to model dislocation density dynamics and are motivated by drawing analogies between interacting dislocation populations and similar phenomena in chemical and biological processes, where reaction-diffusion models have played a vital role. The problem of dislocation pattern formation in the fatigue of copper single crystals is considered with different kinds of patterns appearing for different crystal orientations and strain amplitudes like dislocation veins, ladder structures and labyrinths. Specifically, an attempt is made to model the formation of dislocations veins under low strain amplitudes and subsequent appearance of PSBs with the ladder structure for increased strain amplitudes. A three-dimensional generalized version of the Walgraef-Aifantis model is taken as the starting point for describing the evolution of dislocation densities. The general features of the model involve: (i) Nonlinear gradient terms appearing from a stress-velocity constitutive law for dislocations encompassing their mobility, (ii) Nonlinear reaction terms describing local dislocation production and reaction rates and (ii) Separating the dislocations into immobile, mobile edge and mobile screw dislocations resulting in a three-species RAD system. The system of partial differential equations subject to homogeneous Neumann boundary conditions is discretized and solved using a semi-implicit finite element scheme to obtain steady state spatial patterns. Parametric studies are conducted to explore their effect on the nature of patterns and transitions from one pattern to another, justify their appearance based on changes in the experimental conditions and operating physical mechanisms. Attempts are also made to integrate this approach of continuum dislocation dynamics with elements of elastoplasticity theory for solids.

Classification and data mining approach for deformation process sequence selection to achieve optimal material structure

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Keywords: Texture library, Materials Informatics , Data-mining, unsupervised clustering

Abstract: Considering the computational complexity involved in multi-length scale formulations involving polycrystal plasticity, innovative algorithms need to be incorporated in techniques for designing processes to realize materials with optimized properties. This paper demonstrates the use of a large library (2 million processing sequences) for classification of F.C.C. polycrystal texture for achieving desired properties. The inverse problem of designing processing stages that lead to a desired texture or texture-dependant property is addressed by mining over a database of orientation distribution functions (ODFs). Given a desired ODF, the hierarchical classifier based on X-means algorithm matches its ODF features to a class of textures in the database. Texture classes are affiliated with processing information, hence, enabling identification of multiple process paths that lead to a desired texture.

Theoretical and numerical nonlinear dynamic study of the von Mises structure

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Keywords: Nonlinear Dynamic Analysis; HHT-alpha method; Arc-length method; Nonlinear truss; von Mises truss.

Abstract: A nonlinear numerical study of the von Mises structure was carried out to describe its dynamic behavior under a set of harmonic and non-harmonic load profiles. In addition, a pseudo-static analysis using different cross-section, material and load conditions is developed to obtain the characteristic dynamic snap-through behavior present in literature. The numerical algorithm is written in MATLAB® language and based on the HHT-alpha method (a generalization of the classical Newmark's method used to solve the time domain differential equation). The dynamic equilibrium at each load step is achieved through a modified version of the Crisfield Arch-length method - a path following methodology to solve nonlinear systems of equations. These combinations of numerical procedures seek to describe the exact structural dynamic behaviour at every load step, as well as, ensuring the convergence of the method for nonlinear problems. It is well known that this problem may lead, for certain parameters and initial conditions, to chaotic solutions, among other rich dynamic behaviours, thus justifying this nonlinear analysis in the dynamic context.

Magnitude Frequency Distribution of Simulated Earthquake Sequences in Damaged Fault Zones

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Keywords: Multiscale modeling, Material Heterogeneities, Rate and State Friction, Long-term Fault Slip

Abstract: Mechanical modeling of fault-slip over long timescales is of fundamental importance for understanding earthquake physics and assessing seismic hazard. Observations show that the relationship between the magnitude of earthquakes and the total number of earthquakes in a given region follow a power law distribution, known as the Gutenberg-Richter (GR) law. Earlier numerical and laboratory experiments conclude that the power-law behavior of magnitude-frequency distribution depends either on the material properties of the fault rock or on fault stress heterogeneities.

Seismological and geological observations from mature faults like San Andreas, San Jacinto, and Northern Anatolian faults show that most of the seismicity in the region is constrained by the material properties and the spatial extent of the damaged fault zones. We simulate earthquake cycles in a strike-slip fault system in 2-D elastic halfspace with rate and state dependent friction laws, using a spectral element method. We use a layered medium with low rigidity surrounding the active fault to simulate the damaged fault zone. In this model, the presence of the damaged fault zone causes stress heterogeneity that persists over multiple earthquake cycles.

Our simulations produce a large number of earthquakes with a wide range of magnitudes. The largest earthquakes repeat with an average recurrence interval of ~ 100 years. We analyze the magnitude-frequency distribution of these earthquakes over multiple earthquake cycles and explore the relationship between the spatial extent of damaged zone and the corresponding magnitude-frequency distributions. Our simulated earthquake catalogue implies that the presence of a damaged fault zone induces a power-law magnitude-frequency distribution. Such earthquake cycle models can provide a more realistic description of the physics and statistics of earthquakes in mature strike-slip fault systems.

Thursday, May 23rd

Session 2: Battery Materials

Michigan Room, League 11:00 AM – 12:40 PM

Chair: Neil Dasgupta

Coupling Mechanics and Electrochemistry for Modeling of Li-ion Batteries

KEYNOTE: Wei Lu, University of Michigan, USA, weilu@umich.edu

Keywords: Model, Battery, Multiphysics, Simulation

Abstract: Integrated mechanical-electrochemical modeling and prediction of capacity fade and lifetime of batteries is important for cell design, determination of the optimal operation condition and control, and cell maintenance. In this talk I will present some of our recent work in these areas, including a comprehensive capacity fade model and its experimental validation and application for battery optimization; a multiscale approach that couples mechanics and electrochemistry consistently at both particle and electrode scales which enables simulating various electrode phenomena, and its validation against explicit simulation of particle networks; evaluation of the impact of fracture on battery performance by consideration of realistic anisotropic environment surrounding an active material particle; and simulation of debonding at the interface between active particles and binder. The materials strategy for improving the battery performance and application of machine learning for battery design will also be discussed.

Lithium mechanics: creep as dominant deformation mechanism for battery-relevant temperatures and strain rates

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Keywords: creep; plasticity; lithium; batteries

Abstract: This work presents insights on the mechanical deformation of lithium (Li) from measurements that spanned a wide range of temperatures and strain rates. As Li-ion battery technologies with graphite anodes are approaching their theoretical performance limits, switching to Li-metal anodes could provide up to an order of magnitude higher mass energy-density. However, in order to realize this technology, especially for stable cycling, major challenges with Li-metal anodes must be resolved. There is an increasing consensus that mechanical deformation plays an important role in the performance of Li-metal anodes. However, studies of the mechanical properties of Li are scarce, and none have captured the deformation of Li with enough detail to model accurately its temperature- and rate-dependent viscoplastic response. To address this knowledge gap, measurements were conducted in inert-gas environments, using a new in-glovebox mechanical testing capability with 3D digital-image correlation. This system enabled the deformation of Li to be measured out to true strains of 25%, without chemically perturbing the samples. Power-law creep was determined to be the dominant deformation mechanism under battery-relevant conditions, and a classic power-law creep model was calibrated. These observations were connected to important issues in battery technology, including current-density and rate effects, solid-electrolyte stability, "dead Li," and anode protective coatings.

Delamination study at electrode-binder interface in Lithium Ion Battery

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Keywords: Lithium Ion battery, Viscoelasticity, Michell solution, Delamination

Abstract: Binder, a soft polymeric material encompassing electrode particle has emerged as a promising strategy to counter the huge stresses and related failure in Lithium ion batteries (LIBs) with high capacity electrodes. But despite the reduction in stresses, there have been instances of delamination of the electrode-binder interface which in turn has been correlated to the capacity fade in LIBs. Present work explores the stress in electrode and binder with delaminated electrode-binder interface while being subjected to constant flux charging under plane strain deformation. The former is modeled as an isolated linear elastic isotropic cylindrical particle completely encapsulated by linear viscoelastic isotropic cylindrical binder and the delaminated electrode-binder interface is represented through a circumferential crack of arc length " $2l$ ". The recently proposed methodology wherein mixed boundary conditions are consistently expressed all along the boundary in terms of displacement and/or its gradient, the generalized Michell solution is used to represent stress and displacement field in the electrode and binder and its coefficient found using orthogonality of trigonometric sine/cosine functions. The obtained stress-displacement field is used to compute Griffith energy release rate which is then applied to identify critical conditions for progression of delamination.

Morphology-dependent mass transport model for mechanoelectrochemistry of polypyrrole

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Keywords: conducting polymer, mechanoelectrochemistry, morphology

Abstract: Conducting polymers undergo volumetric deformations due to ingress/egress of counter-ions and solvent molecules during electrochemical reduction/oxidation. A precise measurement of volumetric deformations has been elusive due to lack of experimental methods and hence, different mathematical models make simplifying assumptions in attributing the strain to various transported species. Recently, an investigation into static and dynamic mechanoelectrochemistry of polypyrrole doped with dodecylbenzenesulfonate (PPy(DBS)) has provided morphology-dependent strain data and can be used to precisely attribute volumetric strain of PPy(DBS) to various components. To address the longstanding need for a mass transport-based mechanics model, we introduce porosity as an additional metric to characterize morphological influence on cation and solvent ingress through physical properties of a film during electrochemical reduction. The model is applied to analyze extensional strains in PPy(DBS) films of various charge densities. The major findings are summarized as follows –

1. There exists an inverse relationship between electrochemical deposition charge density and porosity of the PPy(DBS) film. The porosity of a film in the oxidized state appears to be reflective of structural morphology of the polymer, with thin films demonstrating higher porosity.
2. The influx of water molecules into a film is strongly influenced by porosity of the polymer in the oxidized state. Highly porous films are observed to accommodate larger number of water molecules per ingressing cation in their pore space during electrochemical reduction.
3. The number of water molecules that accompany an ingressing cation during electrochemical reduction of a film appear to be governed by the interplay between osmotic pressure and structural deformability of the film. Highly porous films appear to accommodate more water molecules in their pore space per ingressing cation during electrochemical reduction despite developing lower osmotic pressure due to greater deformability.

Although this work characterizes volumetric strain of PPy(DBS) films in aqueous electrolytes during electrochemical reduction, the mathematical model presented in this work can be extended to characterize mechanoelectrochemistry of any conducting polymer in aqueous/organic solvents. The results presented in this discussion are anticipated to serve as guidelines in the design of robust biomedical devices and energy storage materials.