

USACM Thematic Workshop on Experimental and
Computational Fracture Mechanics:
Validating peridynamics and phase field models for fracture
prediction and experimental design

Venue:
Center of Computation & Technology
Louisiana State University

February 26-28, 2020

This workshop is sponsored by

- Technical Thrust Area on Large Scale Structural Systems and Optimal Design of the US Association for Computational Mechanics
- Louisiana State University Center for Computation & Technology
- Oak Ridge National Laboratory
- Society for Experimental Mechanics
- U.S. National Committee on Theoretical and Applied Mechanics (AmeriMech)

Abstract

Comparison of numerical simulations against experimental data is essential for the validation of fracture models in order to gain confidence in their predictability and reliability. Peridynamics and phase field approaches have recently delivered promising results for modeling complex fracture phenomena and significant efforts have been carried out in the past years to validate the corresponding fracture models using available experimental data. However, on one hand, it is still unclear whether the data obtained from current experiments is informative enough to satisfactorily validate models in fracture mechanics. On the other hand, it would also be interesting to combine simulation tools and experimental design to optimize control parameters in fracture mechanics experiments.

The objectives of this workshop are to bring together experts in experimental fracture mechanics, peridynamics, and phase field methods to discuss the state-of-the-art of experimental measurement and computational modeling with applications in fracture mechanics, to promote a dialogue between these communities, and to identify challenges and pathways for robust validation of phase field and peridynamic models as well as integration of experimental and modeling efforts.

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- Patrick Diehl, Louisiana State University
- Pablo Seleson, Oak Ridge National Laboratory
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- Robert Lipton, Louisiana State University
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- Bethany Roicki and Ruth Hengst, USACM

Welcome Address

Welcome

It is my distinct pleasure to welcome you all to the Workshop on Experimental and Computational Fracture Mechanics (February 26-28, 2020) held at the Center for Computation and Technology (CCT) on the Louisiana State University campus in Baton Rouge, Louisiana.

I am pleased to be able to support and co-sponsor this workshop with a number of others: The Technical Thrust Area on Large Scale Structural Systems and Optimal Design of the US Association for Computational Mechanics, the Oak Ridge National Laboratory, the Society for Experimental Mechanics, and the U.S. National Committee on Theoretical and Applied Mechanics (USNC/TAM). We at CCT greatly appreciate the support of our co-sponsors. In addition, I would like to thank the great work of the organizers of this workshop, Dr. Patrick Diehl, Dr. Serge Prudhomme, and Dr. Pablo Seleson.

This workshop brings together experts in experimental fracture mechanics, peridynamics, and phase field methods to discuss the state-of-the-art of experimental measurement and computational modeling with applications in fracture mechanics. We hope this will promote dialogue between these communities, and help to identify challenges and pathways for robust validation of phase field and peridynamic models as well as the integration of experimental and modeling efforts.

I would like thank the three excellent keynote speakers, Dr. Stewart Silling (Sandia Labs), Prof. Lallit Anand (MIT), and Prof. K. Ravi-Chandar (UT Austin), who are world-class experts in peridynamics, phase field, and experimental fracture mechanics, for sharing their thoughts on the field. In addition, I thank all the participants of the event.

I sincerely hope you enjoy and benefit from this unique workshop and the discussion sessions during the coming two and a half days.

With best wishes,

J. “Ram” Ramanujam

WORKSHOP ON EXPERIMENTAL AND COMPUTATIONAL FRACTURE MECHANICS FEBRUARY 2020

TUESDAY		WEDNESDAY		THURSDAY		FRIDAY	
<i>Arrival</i>	<i>25</i>	<i>Day 1</i>	<i>26</i>	<i>Day 2</i>	<i>27</i>	<i>Day 3</i>	<i>28</i>
Reception The Cook Room, Cook Hotel & Conference Center 7:00 PM-9:00 PM		Registration Coffee and Pastries 8:00 AM-8:45 AM Welcoming Remarks 8:45 AM-9:00 AM <hr/> Silling 9:00 AM-10:00 AM <hr/> Coffee 10:00 AM-10:30 AM <hr/> Madenci 10:30 AM-11:00 AM <hr/> Galvanetto 11:00 AM-11:30 AM <hr/> Bobaru 11:30 AM-12:00 PM <hr/> Foster 12:00 PM-12:30 PM <hr/> Lunch 12:30 PM-2:00 PM <hr/> Seleson 2:00 PM-2:30 PM <hr/> Lipton 2:30 PM-3:00 PM <hr/> Diehl 3:00 PM-3:30 PM <hr/> <i>Discussion (Dolbow)</i> 3:30 PM-4:00 PM <hr/> Coffee 4:00 PM-4:30 PM <hr/> Lin 4:30 PM-5:00 PM <hr/> Guilleminot 5:00 PM-5:30 PM <hr/> Poster session 5:30 PM-6:30 PM		Registration Coffee and Pastries 8:00 AM-9:00 AM <hr/> Ravi-Chandar 9:00 AM-10:00 AM <hr/> Coffee 10:00 AM-10:30 AM <hr/> Tippur 10:30 AM-11:00 AM <hr/> Hild 11:00 AM-11:30 AM <hr/> Lambros 11:30 AM-12:00 PM <hr/> Mesgarnejad 12:00 PM-12:30 PM <hr/> Lunch 12:30 PM-2:00 PM <hr/> Mohr 2:00 PM-2:30 PM <hr/> Fineberg 2:30 PM-3:00 PM <hr/> <i>Discussion (Prudhomme)</i> 3:00 PM-3:30 PM <hr/> Coffee 3:30 PM-4:00 PM <hr/> Anand 4:00 PM-5:00 PM <hr/> Lopez-Pamies 5:00 PM-5:30 PM <hr/> Banquet Industrial talk Danielle Zeng Ford Motor Company The Club at LSU Union Square 7:00 PM-10:00 PM		Registration Coffee and Pastries 8:00 AM-9:00 AM <hr/> Waisman 9:00 AM-9:30 AM <hr/> Weinberg 9:30 AM-10:00 AM <hr/> Coffee 10:00 AM-10:30 AM <hr/> Kamensky 10:30 AM-11:00 AM <hr/> Landis and large structures <hr/> Wick 11:30 AM-12:00 PM <hr/> Final discussion (Fineberg) 12:00 PM-12:30 PM <hr/> Lunch 12:30 PM-2:00 PM	

The venue for all talks is the Louisiana Digital Media Center located at 340 E Parker Blvd, Baton Rouge, LA 70808.

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Industrial talk

Integrated Computational Materials Engineering (ICME) development of carbon fiber composites for lightweight vehicles

27th

Danielle Zeng
Ford Motor Company

Co-Authors: Pablo Seleson, Bo Ren, and C.T. Wu

Automotive manufacturers use lightweight materials to meet the increasing demands of fuel efficiency. The Carbon Fiber Reinforced Polymer (CFRP) composites, with a density of 1.55 g/cm³ and a tensile strength of 2000 MPa in the fiber direction, are among the most promising candidates to replace the metals currently used for structural components. It is important to note that the performance of carbon fiber composites is determined not only by the component design, but also the manufacturing processes. In this talk, the focus is on the application of an Integrated Computational Materials Engineering (ICME) approach to the structural composite design. A suite of predictive models is developed to link materials design, manufacturing process and final performance to enable optimal design and manufacturing of CFRP components for automotive vehicles.

One of the greatest challenges for successfully applying the ICME approach to CF composites is how to accurately simulate the different failure modes during crash scenarios. Especially, the traditional thin shell model in finite element simulation has difficulty in capturing the delamination behavior during complex loading conditions. Recently, a discontinuous Galerkin weak form for bond-based peridynamic models is developed for composite modeling through the collaboration among ORNL, LSTC and Ford. The accuracy and computational efficiency of the developed model for delamination modeling is demonstrated through simulating a dynamic bending test of a laminate structure.

Talks

Nonlocality in peridynamics

Stewart Silling

Sandia National Laboratories

26th
9:00 AM–10:00 AM

Nonlocality is an essential feature of the peridynamic model of solid mechanics, which treats all internal forces as acting through finite distances. This nonlocality, which avoids the need to evaluate partial derivatives of the deformation, helps peridynamics treat singularities such as evolving cracks within its basic field equations.

In this talk I will offer a perspective on the significance and effect of nonlocality in the peridynamic continuum model and other theories. Nonlocality offers a mathematical tool to treat certain physical effects such as wave dispersion and attenuation in more generality than is possible in the local theory. It enables the modeling of interesting phenomena such as solitary waves, as well as fracture and fragmentation. It provides a natural compatibility of peridynamics with nanoscale long-range forces. On the other hand, nonlocality is sometimes inconvenient in macroscale simulations, for example by creating surface effects in material properties.

Is nonlocality real? Is it measurable in experiments or derivable from physical principles? I will consider some actual and hypothetical experiments that help to give insight into the proper role of nonlocality in continuum mechanics and the mechanics of defects

Weak form of bond-associated peridynamics for finite deformation elasticity and rupture in rubber-like materials

Erdogan Madenci
The University of Arizona

Co-Authors: D. Behera and P. Roy

This study considers finite elastic deformation and damage in rubber-like materials under quasi-static loading conditions. The peridynamic equilibrium equation is derived based on the Neo-Hookean hyperelastic model under the assumption of incompressibility. The nonlocal deformation gradient tensor is computed in a bond-associated domain of interaction using the PD differential operator. It is free of oscillations and spurious zero energy modes commonly observed in the PD correspondence models. Also, it permits the direct imposition of natural and essential boundary conditions. The validity of this approach is demonstrated through simulations of experiments concerning progressive damage and rupture in polymers undergoing large elastic deformation.

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Hybrid FEM and peridynamic simulation of hydraulic fracture propagation in saturated porous media

26th
11:00 AM–11:30 AM

Ugo Galvanetto
The University of Padua

Co-Authors: Tao Ni, Francesco Pesavento, Mirco Zaccariotto, Francesco Scabbia, and Bernhard A Schrefler

This paper presents a novel hybrid modeling approach for simulating multi-physics problems involving fracture. The new computational method is applied to hydraulic fracture propagation in saturated porous media: Ordinary State based Peridynamics is used to describe the behavior of the solid phase, including crack propagation, while Classical Continuum Mechanics is used to describe the fluid flow and to evaluate the pore pressure. Classical Biotporoelasticity theory is adopted [1, 2]. The fluid pressure is applied as an internal force to the solid Peridynamic grid, which deforms and may crack under increasing fluid pressure. Crack propagation changes the porosity of the material and the volume in which the fluid is free to move. This information is continuously transferred between the two fields (solid and fluid) to solve the coupled problem. The accuracy of the proposed approach is initially verified by comparing its results with the exact solutions of two examples. Subsequently we will present the solution of several pressure-and fluid-driven crack propagation examples. The phenomenon of fluid pressure oscillation is observed in the fluid-driven crack propagation examples, which is consistent with previously obtained experimental and numerical data [3]. All the presented examples illustrate the capability of the proposed approach to solve problems of hydraulic fracture propagation in saturated porous media. Finally we observe that the solid is completely discretised with a PD based approach, the fluid with a CCM based method and the mentioned ‘coupling’ is a physical coupling involving fluid-structure interaction; that is not to be confused with the numerical coupling [4] often cited in the Peridynamic literature.

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The performance of peridynamic and phase-field models in dynamic brittle fracture

Florin Bobaru
University of Nebraska–Lincoln

Co-Authors: J. Mehrmashhadi and M. Bahadori

We evaluate the performance of three different computational models (an in-house meshfree implementation of peridynamics [1], a discontinuous-Galerkin implementation of peridynamics available in LS-DYNA [2], and a phase-field model implemented in COMSOL, similar to the implementation in [3]) on dynamic brittle fracture in soda-lime glass induced by impact. The evaluation is made against some recent experimental data from [4]. The three models show different crack branching patterns, with the angle of branching being the most significant difference. The fracture pattern predicted by the peridynamic model using the meshfree discretization matches the experimental observations, including some very fine details: small twists in the crack paths as the two crack branches approach the far-right boundary of the sample. The results from the LS-DYNA’s Discontinuous Galerkin implementation of peridynamics show spurious/secondary crack branching events, likely due to the way damage growth is implemented in this model. With the phase-field model, the crack branching angle is significantly smaller than in reality and damage continues to “diffuse” into the body after the crack has passed a certain location. A method to prevent this continuous damage expansion in phase-field models of dynamic fracture might be able to improve the phase-field-based results.

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Peridynamic modeling of large deformation and ductile fracture

26th
12:00 PM–12:30 PM

John T. Foster

The University of Texas at Austin

Co-Author: Masoud Behzadinasab

Prediction of ductile fracture, which is a prevalent failure mode in most engineering structures, is vital to numerous industries. Despite significant advancements in fracture mechanics, ductile fracture modeling has remained a challenging task and a continuing area of research. The peridynamic theory has attracted broad interest in recent years, for its innovative approach for simulating material damage. While peridynamics has been largely utilized to simulate cracking events in brittle materials, its ability in predicting ductile failure remains unclear.

We recently conducted a rigorous investigation into the capabilities of peridynamics in simulating ductile fracture in metallic alloys. The third Sandia Fracture Challenge, as a true blind prediction challenge, was employed in the examination, where the state of the art of peridynamic modeling of ductile fracture was implemented to predict deformations and failure of an additively manufactured metal, with a complex geometry, under the dynamic tensile experiments performed by Sandia National Laboratories. Following the participation in the challenge, while our modeling approach led to qualitatively good results and a correctly predicted crack path, it underpredicted the load-carrying capacity of the structure and simulated an early fracture. Our post-experiment analysis identifies the main sources of discrepancy between the blind simulations and experiments to be (1) material instabilities associated with the finite deformation peridynamic model and (2) unreliability of a Lagrangian peridynamic framework in solving problems involving extremely large deformation and extensive damage.

To address the aforementioned issues, a bond-associated, semi-Lagrangian, constitutive correspondence, peridynamic framework is proposed, in which peridynamic material point interactions depend only on their current properties (e.g. position and stress values) in the deformed configuration, and a rate-based approach is utilized to advance the state of material. A nonlocal version of the velocity gradient is presented to determine the Cauchy stress rate, using local constitutive theories, as an intermediate quantity in computing peridynamic bond forces. A bond-associated, correspondence damage modeling is introduced by using the bond-associated internal properties, e.g. stress and strain values, to incorporate classical failure criteria within the peridynamic framework. The new theory is employed to revisit the Sandia Fracture Challenge problem. Our results indicate that the new approach significantly improves the peridynamic predictions of large deformation and ductile fracture.

Convergence studies in meshfree peridynamic wave and crack propagation

Pablo Seleson
Oak Ridge National Laboratory

Co-Authors: Marco Pasetto and Yohan John

Peridynamics is a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation. Governing equations in peridynamics are based on spatial integration rather than spatial differentiation, allowing natural representation of material discontinuities, such as cracks. A meshfree approach proposed in [1] has been demonstrated to be an effective discretization method for large-scale engineering simulations, particularly those involving large deformation and complex fractures. However, a robust quantitative assessment of the performance of this meshfree method, particularly in fracture scenarios, is lacking. In [2], the convergence of meshfree numerical solutions of static peridynamic problems has been investigated. Related convergence studies for peridynamic wave propagation problems appeared in [3]. In this talk, we will discuss recent convergence studies of wave propagation and extensions to dynamic crack propagation in meshfree peridynamic simulations.

References

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Nonlocal brittle fracture: computational analysis and convergence to LEFM

26th
2:30 PM–3:00 PM

Robert Lipton
Louisiana State University

Co-Author: Prashant K. Jha

We introduce a state based peridynamic model for calculating dynamic fracture. The force interaction is derived from a double well strain energy density function, resulting in a non-monotonic material model. The material properties change in response to evolving internal forces and fracture emerges from the model. The model can be viewed as a regularized fracture model. In the limit of zero nonlocal interaction the model recovers a sharp crack evolution characterized by the classic Griffith free energy of brittle fracture with elastic deformation satisfying the linear elastic wave equation off the crack set, zero traction on crack faces and the kinetic relation between crack tip velocity and crack driving force given in [1], [4], [6], [7], see [3], [5]. We complete the talk with a priori convergence rates for the numerical simulation and several computational examples [2]. This research is funded through ARO Grant W911NF1610456.

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A review of benchmark experiments for the validation of peridynamics models

Patrick Diehl
Louisiana State University

Co-Authors: Serge Prudhomme and Martin Lévesque

Peridynamics (PD), a non-local generalization of classical continuum mechanics (CCM) allowing for discontinuous displacement fields, provides an attractive framework for the modeling and simulation of fracture mechanics applications. However, PD introduces new model parameters, such as the so-called horizon parameter. The length scale of the horizon is a priori unknown and need to be identified. Moreover, the treatment of the boundary conditions is also problematic due to the non-local nature of PD models. It has thus become crucial to calibrate the new PD parameters and assess the model adequacy based on experimental observations. The objective of the present paper is to review and catalog available experimental setups that have been used to date for the calibration and validation of peridynamics. We have identified and analyzed a total of 39 publications that compare PD-based simulation results with experimental data. In particular, we have systematically reported, whenever possible, either the relative error or the R-squared coefficient. The best correlations were obtained in the case of experiments involving aluminum and steel materials. Experiments based on imaging techniques were also considered. However, images provide large amounts of information and their comparison with simulations is in that case far from trivial. A total of six publications have been identified and summarized that introduce numerical techniques for extracting additional attributes from peridynamics simulations in order to facilitate the comparison against image-based data.

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Peri-Net: Analysis of crack patterns using deep neural networks

26th
4:30 PM-5:00 PM

Guang Lin
Purdue University

In this talk, I will introduce convolutional neural networks designed to predict and analyze damage patterns on a disk resulting from molecular dynamic (MD) collision simulations. The simulations under consideration are specifically designed to produce cracks on the disk and, accordingly, numerical methods which require partial derivative information, such as finite element analysis, are not applicable. These simulations can, however, be carried out using peridynamics, a nonlocal extension of classical continuum mechanics based on integral equations which overcome the difficulties in modeling deformation discontinuities. Although this nonlocal extension provides a highly accurate model for the MD simulations, the computational complexity and corresponding run times increase greatly as the simulations grow larger. We propose the use of neural network approximations to complement peridynamic simulations by providing quick estimates which maintain much of the accuracy of the full simulations while reducing simulation times by a factor of 1500. We propose two distinct convolutional neural networks: one trained to perform the forward problem of predicting the damage pattern on a disk provided the location of a colliding object's impact, and another trained to solve the inverse problem of identifying the collision location, angle, velocity, and size given the resulting damage pattern.

Stochastic modeling for uncertainty quantification in fracture mechanics

Johann Guilleminot
Duke University

This talk is focused on stochastic modeling in fracture mechanics for quasi-brittle, heterogeneous materials. The macroscopic behavior of such materials can be strongly affected by subscale variability, including the effects of both microstructural randomness and spatial variations in elastic and fracture properties. In this talk, we present recent advances related to the modeling of spatial, multiscale-informed variability in elastic and fracture properties, and its impact on the macroscopic response [1, 2]. We also discuss how fine scale regularity can be leveraged to achieve dimensionality reduction and augment datasets obtained from simulations or physical experiments [3].

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Experiments in fracture mechanics

Krishnaswa Ravi-Chandar
The University of Texas at Austin

27th
9:00 AM–10:00 AM

One hundred years after Griffith's landmark paper on the theory of rupture, the problem of fracture remains of significant interest. While much success has been achieved in the reliability assessment of structures with cracks, much remains to be done in terms of predictive assessment of failure. In this talk, I will focus on the crucial role played by experiments in all aspects of the development of the theory of rupture, providing physical insight and detailed measurements to challenge and to stimulate modeling and simulation methods. Specifically, I will describe a selection of fracture mechanics experiments, encompassing quasi-static and dynamic fracture as well as nucleation of damage and cracks in brittle and ductile materials. Leveraging on the advances in experimental measurement, I will attempt to pose challenges for proper validation of modeling and simulation methods.

Experimental identification of dynamic crack branching precursors in soda-lime silicate glass

Hareesh Tippur
Auburn University

Co-Author: Sivareddy Dondeti

The dynamic fracture of high-stiffness and low-toughness materials such as soda-lime silicate glass (SLSG) involves crack initiation and growth prior to branching, underlying mechanics of which is not yet understood. Addressing this issue using full-field optical techniques have faced numerous spatio-temporal challenges since crack speeds in this material reach excess of 1500 m/s and are accompanied by highly localized sub-micron scale deformations. Recent work by the authors have shown that transmission-mode Digital Gradient Sensing method [1, 2] is capable of overcoming many of these challenges to visualize crack-tip fields in the whole field and quantify fracture parameters associated with each of the phases of crack growth in SLG plates. In this work, time-resolved stress gradient and stress measurements in SLSG plates of two different geometries subjected to dynamic wedge-loading are performed. The LEFM-based precursors extracted from optical measurements leading up to single or sequential/cascading branch formations in SLSG are reported. The identification of precursors are based on crack velocity, stress intensity factors, higher order coefficients of the asymptotic crack tip fields and non-dimensional parameters based on a combination of these. Fracture surface roughness and its features are also separately quantified using high resolution post-mortem examination and corroboration with optically measured quantities.

References

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On the identification and validation of fracture mechanics models for curved crack in mortar

27th
11:00 AM–11:30 AM

Francois Hild

École Normale Supérieure Paris-Saclay

Co-Authors: R. Vargas, A. Tsitova, F. Bernachy-Barbe, B. Bary, and R.B. Canto

In this presentation, an approach to defining the path of a curved crack in a single edge notched specimen with gray level residuals extracted from digital image correlation [1], is followed by the calibration of the parameters of a cohesive zone model [2, 3]. Only the experimental force is used in the cost function minimized in finite element model updating. The displacement and gray level residual fields allow for the validation of the calibrated parameters. Last, a phase field model is probed with the previously calibrated parameters.

References

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Full-field experimental measurements in extreme loading environments for property extraction and simulation validation

27th

11:30 AM–12:00 PM

John Lambros

University of Illinois at Urbana-Champaign

Numerical simulations, whether based on finite element, boundary element, peridynamics or other methods, have always been intimately linked with companion experiments. Traditionally experiments have been used to provide direct input to numerical simulations for quantities that could not be directly derived from first principles, e.g., elasto-plastic mechanical properties and the like. However, linking simulations with experiments also allowed for indirect extraction of properties that might not have been directly measurable, e.g., strength properties or thermal dependence of properties. In such cases, inverse problem techniques have been used which provide indirect extraction of the desired quantities by minimizing/optimizing some error or objective function. Finally, even for the case of fully-predictive simulations, companion experiments are critical in validating the simulation framework and its assumptions. Early attempts to couple experiments and simulations in these ways were based on the limited data obtained by point measurements (e.g., strain gauges) and were applied to simple or idealized environments (e.g., under slow loading rates and/or at room temperature). However, as full-field optical measurement techniques gained popularity, experimental data of larger portions of a structure/material allowed for much larger amounts of data to be used in these roles (i.e., material input, property extraction, or simulation validation). More recently, with the advent of the optical metrology technique of two-dimensional (2D) Digital Image Correlation (DIC), and now its three-dimensional (3D) extension Digital Volume Correlation (DVC), we can obtain very large data sets of experimental measurements of displacement and strain on the surface or in the interior of an object. In addition, this is increasingly done under extreme conditions involving high loading rate and/or temperature. In this work we will present a series of experimental measurement techniques and approaches both for the inverse numerical extraction of material properties from experiments and the validation of predictive simulations based primarily on the finite element framework. In the first we will present examples on the extraction of cohesive failure laws from both 2D and 3D experimental data. We have employed 2D DIC on materials with complex microstructures, such as Functionally Graded Materials (FGMs) and particulate reinforced composites, and have used gradient-based inverse schemes to extract cohesive failure relations for these materials. We have also employed stereo-vision DIC for the validation of thermomechanical loading simulation results. The validation methodology uses image decomposition techniques together with an error analysis framework to provide confidence levels of the simulations when compared to companion experiments. Examples will be provided for both dynamic loading situations (e.g., dynamic fracture or vibratory loading) and high temperature loading (e.g., thermomechanical fatigue).

Interplay of fracture and plasticity in swelling-driven fracture of phase-transforming battery materials

27th
12:00 PM–12:30 PM

Ata Mesgarnejad
Northeastern University

Co-Author: Alain Karma

Due to their tenfold higher storing capacities, silicon and germanium have emerged as a promising replacement for Carbon-based anodes in Li-ion batteries. However, lithiation of both materials results in large (300%) volume expansion that results in an amorphization of their crystalline structure. The significant volume expansion causes the anode particles to change shape and drives inelastic deformation, plastic flow, and fracture within the particle. Experimental observations show that lithiation in both materials is reaction controlled; thus, an invading lithiation front is created that is atomically sharp. Crucially, the initial lithiation of crystalline Si(c-Si) is highly anisotropic while it remains isotropic for crystalline Ge and amorphous Si, which has been suggested as a source of its inferior performance. Here we exploit the power of the phase-field approach to describe both the motion of phase boundaries and stress-driven fracture within a self-consistent set of equations to shed light on the failure modes of Si battery anode material. We simulate the crystalline to amorphous phase transformation of Si and Ge using a modified Allen-Cahn model with anisotropic mobility to replicate the experimental observations. The mechanical response due to lithiation-driven swelling of the anode is modeled using neo-Hookean elasticity coupled with finite J-2 plasticity. Finally, we model fracture using a variational phase-field formulation that is able to describe both nucleation and propagation of cracks without interpenetration of crack surfaces under compression. We use our framework to probe deformation and fracture of Si nanopillars due to lithiation over a wide range of yield strengths. Using 1D axisymmetric simulations, we show how the stresses generated in the nanopillar attain a maximum at a critical yield strength. Then using full 2D plane stress simulations of a nanopillar cross-section, we highlight the emergence of plastic instabilities, which augment the stresses. Finally, we combine our results of 2D simulation with 1D stability analysis of our phase-field model and experimental observations of the critical size of nanopillars for failure to estimate the lithiation-driven yield strength of Si and Ge. The results highlight the complex interplay between fracture and plasticity in the failure of the silicon anodic components. In addition, we present the results of 2D and 3D simulations that investigate the non-trivial effects of anode geometry on mechanical stability.

Shear fracture of metals during in-plane torsion experiments

Dirk Mohr
ETH Zurich

Co-Authors: C.C. Roth, V. Grolleau

The comparison of different simple shear experiments revealed that the great potential of the in-plane torsion configuration for characterizing the fracture response of sheet metal. Only the in-plane torsion configuration seems to be able to provide perfectly proportional simple shear loading histories for isotropic materials. State-of-the-art torsion tests are machined free of slits, but a circular groove is introduced to reduce the thickness of the material and to ensure defined strain localization away from the clamped boundaries. However, this configuration tends to limit the observability of the entire shear zone. Here, an enhanced in-plane torsion test is developed using a grooved specimen with full optical access to the specimen surface for DIC measurements and enlarged strain rate range up to several 100/s. Its main feature is a new clamping and loading technique from the inner boundary of the specimen. Validation experiments are performed on specimens extracted from an aluminum alloy and steel sheets of various ductility. The experimental campaign includes proportional loading, cyclic loading and strain rate jump tests to demonstrate the ability of the newly-proposed technique. Full optical access to the specimen surface is used to reveal the effect of the material anisotropy on the strain field along the sheared area. The findings are compared to results from numerical simulations and with other in-plane shear tests.

How moving cracks in brittle solids choose their path

27th
2:30 PM–3:00 PM

Jay Fineberg

The Hebrew University of Jerusalem

Co-Authors: L. Rozen-Levy and J. Kolinski

While we have an excellent fundamental understanding of the dynamics of ‘simple’ cracks propagating in brittle solids, we do not fully understand how the path of moving cracks is determined. Here we experimentally study cracks that propagate between 10-95% of their limiting velocity within a brittle material. We deflect these cracks by either allowing them to interact with sparsely implanted defects or driving them to undergo an intrinsic oscillatory instability in defect-free media. Dense, high-speed measurements of the strain fields surrounding the crack tips obtained via imaging reveal that the paths selected by these rapid and strongly perturbed cracks are entirely governed by the direction of maximal strain energy density and not by the oft-assumed principle of local symmetry. This fundamentally important result may potentially be utilized to either direct or guide running cracks.

References

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A gradient-damaged theory for fracture of quasi-brittle materials

Lallit Anand

Massachusetts Institute of Technology

I will present a gradient-damage theory for fracture of “quasi-brittle” materials under tensile dominated stress states. The theory is developed using the method of virtual-power. The macro- and microforce balances, obtained from the virtual power approach, together with a standard free-energy imbalance equation under isothermal conditions, when supplemented with a set of thermodynamically-consistent constitutive equations provide the governing equations for the theory. The general theory has been specialized to formulate a model for fracture of concrete — a quasi-brittle material of vast importance. We have numerically implemented our theory in a finite element program, and we present results from representative numerical calculations which show the ability of our simulation capability to reproduce the macroscopic load-deflection characteristics as well as crack-paths during failure of concrete in several technically relevant geometries reported in the literature.

References

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Revisiting nucleation in the phase-field approach to brittle fracture

27th
5:00 PM–5:30 PM

Oscar Lopez-Pamies

University of Illinois at Urbana-Champaign

Co-Authors: Aditya Kumar, Blaise Bourdin, and Gilles A. Francfort

Twenty years in since their introduction [1], it is now plain that the regularized formulations dubbed as phase-field of the variational theory of brittle fracture of Francfort and Marigo [2] provide a powerful macroscopic theory to describe and predict the propagation of cracks in linearelastic brittle materials under arbitrary quasistatic loading conditions. Over the past ten years, the ability of the phase-field approach to also possibly describe and predict crack nucleation has been under intense investigation. The first of two objectives of this talk is to establish that the existing phase-field approach to fracture at large — irrespectively of its particular version — is fundamentally incomplete to model crack nucleation. This is because the approach is purely energetic and cannot account for one essential ingredient that is not energetic but rather stress-based: the strength of the material. The second objective is to introduce an amendment that renders a phase-field theory capable of modeling crack nucleation in general, be it from large pre-existing cracks, small pre-existing cracks, smooth and non-smooth boundary points, or within the bulk of structures subjected to arbitrary quasistatic loadings. Following Kumar, Francfort, and Lopez-Pamies [3], the central idea is to implicitly account for the presence of the inherent microscopic defects in the material — whose defining macroscopic manifestation is precisely the strength of the material — through the addition of an external driving force in the equation governing the evolution of the phasefield. To illustrate the descriptive and predictive capabilities of the proposed theory, the last part of the talk will be devoted to present sample simulations of experiments spanning the full range of fracture nucleation settings.

References

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Thermal-conductivity degradation across cracks in coupled thermo-mechanical systems modeled by the phase-field fracture method

Haim Waisman
Columbia University

Co-Authors: Lampros Svolos and Curt A. Bronkhorst

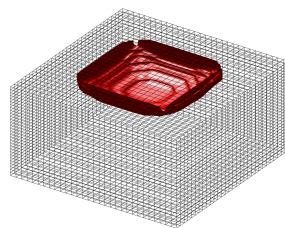
Dynamic loading of polycrystalline metallic materials can lead to brittle or ductile fracture depending on the loading rates, geometry and material type. Cracks develop rapidly with minimal plasticity and minimal heat dissipation when brittle fracture is observed (e.g. Kalthoff problem under low strain rates). At high strain rates for metallic materials which can accommodate plastic deformation, material instabilities known as shear bands, can occur. Shear bands are narrow localization bands which reduce the stress bearing capacity of the material and act as a precursor to ductile fracture (e.g. cracks that develop rapidly on top of a shear band). A unified model, which has been developed in [1,2], accounts for the two aforementioned failure processes simultaneously. In this model, the phase-field method is used to model crack initiation and propagation, and is coupled to a temperature dependent visco-plastic model that captures shear bands. In this work, an improvement to the unified model is presented in order to capture more accurately the heat transfer across the fracture surfaces. Specifically, an isotropic degradation of the thermal conductivity is proposed, which couples the thermal diffusion process with the extent of damage across a crack. The closed form solution is derived analytically based on a micro-mechanics void extension model of Laplace's equation. We investigate the behavior of the aforementioned technique on two benchmark problems and show the necessity of such physics-based degradation function in dynamic fracture problems.

References

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Kerstin Weinberg
University of Siegen

While cracks are actually sharp two-dimensional hypersurfaces the phase-field fracture approach regularizes the sharp material discontinuities with smooth transitions between broken and unbroken regions. The evolution of the phase-field follows an evolution equation where the driving forces of crack growth are derived from an energy minimization principle, typically based on an Ambrosio-Tortorelli type functional. Modifications allow accounting for the no-healing irreversibility constraint of crack evolution and, especially important, for the asymmetry of fracture, i.e., the fact that cracks only grow under tensile loadings but not under compression. Further modifications consider the evolution problem at finite strains using energy densities, which are polyconvex functions of the deformation, [1, 2]. In this contribution different decompositions of the elastic energy and the pros and cons of variational and ad hoc formulations for the crack driving forces will be discussed. The latter may base on positive principal stresses or strains for example. We compare different models in linearized and in finite elasticity and present recent results on the mathematical analysis for a phase-field model at finite strains, where we formulate the phase-field with energy densities in terms of the modified invariants of the right Cauchy-Green strain tensor. To illustrate the capability of a phase-field fracture approach we present finite element simulations of brittle fracture and compare it to our experimental results. The main challenge of such fracture simulations is, that it requires the ability of a numerical method to predict crack nucleation and fracture without stress concentration at a notch or at an initial crack.



References

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Isogeometric and meshfree analysis of hyperbolic phase field fracture

David Kamensky
University of California San Diego

Co-Authors: Georgios Moutsanidis and Yuri Bazilevs

We introduce a phase field fracture formulation that results in a hyperbolic partial differential equation (PDE) for the order parameter distinguishing broken and unbroken phases of the material [1, 2]. This PDE can be formally derived from microforce balance theory by associating a microscopic kinetic energy with the order parameter’s rate of change. An important practical advantage is that hyperbolic PDEs are more amenable to explicit time stepping, which is almost universally favored in simulations of extreme events like explosions, where small time steps are needed to resolve rapid phenomena. Finite element computations of benchmark problems demonstrate that the properties of the new model are similar to elliptic phase field models (relative to typical modeling errors of current methods), although there is a noticeable rate- toughening effect, which becomes more pronounced as the wave speed is reduced. The model is then implemented into a hybrid meshfree–isogeometric hydrocode to simulate more complicated scenarios and perform qualitative comparisons with experimental results from the literature on blast-induced fracture of PMMA. We conclude with some discussion of ongoing and future work on efficient implementation of isogeometric and meshfree technologies, such as using automatic code generation [3] to rapidly test new formulations.

References

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Some recent progress on phase-field modeling: fatigue, r-curves, and large structures

28th
11:00 AM–11:30 AM

Chad Landis

The University of Texas at Austin

Co-Authors: Yu-Sheng Lo, Amin Anvari, K. Ravi-Chandar, Thomas J.R. Hughes, and Michael J. Borden

Over the last few decades, the phase-field approach to fracture has been shown to be a useful tool for modeling complex crack path evolution. Features including the nucleation, turning, branching, and merging of cracks as a result of quasi-static mechanical and dynamic loadings are captured without the need for extra constitutive rules for these phenomena. This presentation will touch on our recent work on the phase-field modeling approach for fatigue crack growth, R-curve behavior for brittle fracture in the presence of plastic flow, and modifications for large-scale structures will be discussed. For fatigue, a modified J-integral will be developed to demonstrate how the phase-field approach can be used to generate Paris-Law type crack growth rates. A steady-state finite element method is then applied to generate fits of the phase-field theory to measured crack growth rate data. Full transient simulations are performed and compared to experimental measurements on samples where crack turning is induced by the presence of a hole in the vicinity of the crack. To model R-curve behavior plasticity is introduced into the formulation and adaptive refinement is used to capture different length scales. Finally, modifications to the damage functions are introduced to allow for the analysis of large scale structures and some issues are identified and discussed.

Attempts to validate phase-field fracture for nearly incompressible solids with experimental data

Thomas Wick
University of Hannover

Co-Authors: Katrin Mang, Nils Kröger, Mirjam Walloth, and Winnifried Wollner

In this presentation, we propose the first steps of validating a phase-field model for nearly incompressible solids. To avoid locking effects therein, we propose a mixed form for the solid displacement equation as formulated in [1]. For the numerical solution, we adopt a fully-coupled approach, which is implemented in DOpElib [2] and currently extended with adaptive mesh refinement and parallelization using the deal.II-github-phase-field framework [3]. To validate this new phase-field model for rubber-like materials, we compare - in collaboration with the Deutsches Institut für Kautschuktechnologie e. V., Hannover, Germany, - experimental data of crack propagation in Carbon Black filled EPDM rubber against our numerical simulations and figure out differences, difficulties and challenges.

References

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Posters

Simulating fractures in rubber – one step further with phase-field modeling

Katrin Mang

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Co-Authors: Andreas Fehse, Nils-Hendrik Kröger, and Thomas Wick

Full field in-situ Digital Image Correlation measurements of Mode I and Mode II crack growth for polymeric materials

Ilyass Tabiai

Polytechnique Montréal (Canada)

Co-Authors: Martin Lévesque, Daniel Therriault, Damien Texier, and Philippe Bocher

Asymptotically compatible reproducing kernel collocation and meshfree integration for Peridynamic Navier equation

Yu Leng

University of Texas at Austin

Co-Authors: Xiaochuan Tian, Nathaniel Trask, and John T. Foster

Fractional Derivatives and Viscoelasticity

Mary Vaughan
Iowa State University

Co-Authors: Pablo Raúl Stinga and Pablo Seleson

Two dimensional reduction of 3D axisymmetric peridynamic models

Debdeep Bhattacharya
George Washington University

Co-Authors: Pablo Seleson and Jeremy Trageser

Peridynamic modeling of large deformation and ductile fracture

Masoud Behzadinasab
Brown University

Co-Authors: John Foster and Yuri Bazilevs

Convergence in peridynamic fracture modeling

Marco Pasetto
Oak Ridge National Laboratory

Co-Author: Pablo Seleson

Fast algorithm for peridynamics and nonlocal models in heterogeneous media

Xiaochuan Tian
The University of Texas at Austin

Co-Author: Bjorn Engquist

Dynamic fracture modeling with peridynamics

Sahir Butt
Ruhr University Bochum (Germany)

Co-Author: Günther Meschke

Additional information

Addresses

Workshop venue

Digital Media Center, Center for Computation & Technology, 340 E Parker Blvd.,
Baton Rouge, LA 70803

Hotel

The Cook Hotel at LSU, 3848 W Lakeshore Dr, Baton Rouge, LA 70808
(225) 383-2665

Banquet

LSU Faculty Club, 101 Tower Dr, Baton Rouge, LA 70803
(225) 578-2356

Restaurants

Walking distance

- The Chimes – Lively campus-area hangout from a local chain featuring a worldwide beer list & hearty bar fare: 3357 Highland Rd, Baton Rouge, LA 70802 (225 383-1754)
- Louie’s Cafe – LSU-area fixture dating to 1941 serves a diner menu 24/7 in a classic lunch-counter setting: 3322 Lake St, Baton Rouge, LA 70802 (225 346-8221)
- Highland Coffees – Charming, airy locale with a laid-back vibe for coffee roasted on-site & a variety of baked goods: 3350 Highland Rd, Baton Rouge, LA 70802 (225 336-9773)

Local cuisine

- Parrain’s Seafood Restaurant – Local seafood specialist cooking up Louisiana recipes in a rustic space with porch seating: 3225 Perkins Rd, Baton Rouge, LA 70808 (225 381-9922)

- Mike Anderson's - Baton Rouge – Area staple for regional seafood in a spacious, wood-lined setting with a sports-friendly vibe: 1031 W Lee Dr, Baton Rouge, LA 70820 (225 766-7823)
- Stroubes Seafood and Steaks – Chophouse presenting local preparations of meat & seafood in comfortable digs with a lounge: 107 3rd St, Baton Rouge, LA 70801 (225 448-2830)

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