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Computer Simulation and Physical Testing of Complex Fracturing Processes

A Symposium in Honor of Professor Emeritus **Anthony R. Ingraffea**

School of Civil and Environmental Engineering, Cornell University
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Abstracts of Lectures

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Session 1: Chair: **John F. Abel**, Professor Emeritus of Civil and Environmental Engineering

Opening Remarks

Welcome by **Phillip L. Liu**, Professor and Director of the School of CEE
Introduction by **John F. Abel**, Session Chair
http://hdl.handle.net/1813/38089

A Concrete Damage Plasticity Model for Ancient Roman Pozzolanic Concrete Vaulted Structures

Renato Perucchio, PhD ‘84

Professor of Mechanical Engineering and of Biomedical Engineering; Director of Program in Archaeology, Technology and Historical Structures; University of Rochester

The invention of pozzolanic concrete (*opus caementicium*) provided ancient Roman engineers with an extraordinarily versatile and durable building material, which made possible the construction of some of the largest and most complex vaulted structures built in antiquity. In 2010, in collaboration with Ingraffea, we conducted an experimental study on Mode-I fracture properties of reproduced Imperial Roman pozzolanic mortar using an *ad-hoc* arc shaped bending test. In the present study we use these data in conjunction with post-critical compressive response data available from the literature to construct a non-linear damage plasticity formulation for *opus caementicium* suitable for 3D implementation in Abaqus Explicit. We use this FE formulation to evaluate how the structural design of the vault supporting system of Diocletian's *Frigidarium* (298-306 AD), consisting of flanking shear walls and monolithic granite columns, affects the development and propagation of fractures and ultimately the static and seismic stability of the vault. Slides: http://hdl.handle.net/1813/38093

State-Based Peridynamic Lattice Modeling of Reinforced Concrete Structures

Walter Gerstle, PhD '86

Professor of Civil Engineering, University of New Mexico

Continuum peridynamics provides an alternative to continuum mechanics. However, peridynamics is more general because it allows cracks to emerge. However, peridynamics requires further discretization to be implemented on a computer. Peridynamics assumes the material space is a continuous Cartesian *real* space. In contrast, in this paper we assume the material space is a discrete Cartesian *integer* space, defining a regular lattice of material particles, and proceed to develop the state-based peridynamic lattice model (SPLM). With the SPLM, the forces between neighboring particles are characterized by the force state, T, and the stretches between particles are characterized by the deformation state, Y. The material model arises from a peridynamic function relating the force state to the deformation state. With the SPLM, continuous deformations, elasticity, damage, plasticity, cracks, and fragments can be simulated in a coherent and simple manner. With the ongoing increase in computational storage capacity and processing power, the SPLM becomes increasingly competitive with more traditional continuum approaches such as the finite element method. Slides: http://hdl.handle.net/1813/38094

Thunderhead Engineering – Continuing the Rand Hall Ethos

Daniel Swenson, PhD '86

Principal, Thunderhead Engineering (www.thunderhead.com)
Professor Emeritus of Mechanical and Nuclear Engineering, Kansas State University

Tony Ingraffea inspired us. In me, he reinforced the love of programming and amazement at the ability of applied mathematics to represent the real world. At some level, we all want people to recognize and appreciate what we are doing. If you are developing fundamental engineering concepts, you write papers and pursue research. If you are writing software, you want people to use and apply your programs. Thunderhead Engineering grew out of that desire. As a result of research we were doing at Kansas State, Brian Hardeman and I decided that we wanted to commercialize some of our work. In 1998, we were fortunate to obtain a Small Business Innovative Research grant that supported development of our first product, PetraSim, a user interface for the TOUGH2 code from Lawrence Berkeley National Laboratory. TOUGH2 solves the problem of multi-phase flow in porous media. The development we did for PetraSim has made it possible for us to develop two more products, PyroSim -- that model fires in buildings, and Pathfinder -- that models emergency evacuation. At this time we are completely self-sustaining from software sales and have six full-time employees. I will discuss how a company can be a long-term approach to ensuring that the work one starts will be continued and how we are facing some of the challenges as we look to the future. Slides: http://hdl.handle.net/1813/38095

Session 2: Chair: **Bruce Carter**, Senior Research Associate, Cornell Fracture Group

Working with Tony Is Everything It’s Cracked Up To Be

Keshav Pingali

Professor, Department of Computer Science, University of Texas at Austin
The W.A. “Tex” Moncrief Chair of Computing, Institute for Computational Engineering and Sciences (ICES), UT Austin
Formerly on the faculty of the Department of Computer Science at Cornell from 1986 to 2006, where he held the India Chair of Computer Science

Back in 2000, NSF awarded a consortium of universities, led by Cornell, one of the first large Information Technology Research (ITR) grants for a project titled “Adaptive Software for Field-driven Simulations.” As the Computer Science PI of this multi-disciplinary, multi-institutional project, I knew nothing about partial differential equations, finite-elements, Delaunay mesh generation, h- and p-refinement, or singularities at crack-tips, and I knew even less about how to inspire and lead large teams of researchers. Over the next 5 years and at the cost of 10 million dollars to US taxpayers, I learned these things (and fly-fishing) from Tony Ingraffea. The experience literally changed my life. I will try to convince you that it was for the better. Slides: http://hdl.handle.net/1813/38096

Non-manifold Geometric Modeling as a Framework for Computational Mechanics Simulations

Luiz Fernando Martha, PhD ‘89

Professor of Civil Engineering, Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Brazil
Member and Manager, Computer Graphics Technology Group (Tecgraf), PUC-Rio

Geometric modeling is an area of computer graphics that deals with creation, manipulation, maintenance, and analysis of representations of geometric forms of two- and three-dimensional objects. It is applied in several fields, such as movie production, design of industrial mechanical parts, scientific visualization, and reproduction of objects for analysis in engineering. Historically, geometric modeling has evolved from wireframe modeling to surface modeling, solid modeling, and non-manifold modeling. Non-manifold geometric modeling allows the representation of multi-region objects, of internal or dangling structures, and of lower-dimensional degenerated parts. Many application areas of geometric modeling take advantage of the additional features of non-manifold representation. In computational mechanics, for example, it is common to analyze idealized structures such as shells combined with solids and beams. Another application is the representation of heterogeneous objects with regions with common volumes, coincident faces, internal structures, and solids consisting of different materials. This lecture illustrates the use of topological data structures for non-manifold representations as a framework for numerical simulations in computational mechanics. The main focus here is on the development of strategies for mesh generation for modeling heterogeneous objects such as subsurface geological models. Slides: http://hdl.handle.net/1813/38098

A Short History of Crack Growth Simulation Software Developed at Cornell University

Paul Wawrzynek, PhD ‘91

Senior Research Associate, Cornell Fracture Group
Chief Technology Officer, Fracture Analysis Consultants, Inc.

During his 37 years at Cornell University, Dr. Anthony Ingraffea has inspired his graduate students to create a series of computer programs for simulating fracture propagation for a wide variety of engineering materials and applications. Each of these programs represented the most advanced and capable fracture simulation programs of their time. On the occasion of his retirement, this talk will review this sequence of programs and highlight their features and the insights they brought to the small, yet important, area of computational mechanics. Slides: http://hdl.handle.net/1813/38099

Session 3: Chair: **Paul Wawrzynek**, Senior Research Associate, Cornell Fracture Group

3D Characterization and Modeling of Fatigue Cracks

Anthony D. Rollett

Professor of Material Science and Engineering, Carnegie Mellon University

Enormous strides have been made in quantifying the growth of fatigue cracks over the years and incorporating that understanding into predictions of component lifetime. Nevertheless, it is clear that the behavior of short cracks is less well quantified, where short is relative to the length scale(s) found in materials' microstructure, e.g. grain size. Ultimately, materials science seeks to predict the location and growth of fatigue cracks in order to design materials' microstructure to maximize fatigue lifetime. Towards that end, it is interesting to study the relationship between cracks and microstructure near the initiation point. Short fatigue cracks in nickel-based superalloys have been characterized by using conventional SEM and orientation mapping. 3D characterization used High Energy Diffraction Microscopy (HEDM), and computed tomography (CT) to map out the crack positions within their embedding grain structure. The main finding is that cracks develop most readily along long twin boundaries with high resolved shear stress on the slip systems parallel to the twin plane. Also, both halves of a different superalloy, fully fractured sample have been fully characterized in 3D using the same tools. The HEDM and CT were performed with high-energy x-rays on beamline 1ID at the Advanced Photon Source (APS). The 3D orientation maps are used as input to computations of the full field stress-strain response. The fracture surface is analyzed with respect to local orientation and inter- versus trans-granular character. The likely origins of fatigue crack initiation in these cases are discussed. Slides: http://hdl.handle.net/1813/38100

Multiscale Materials Modeling

Chuin-Shan David Chen, PhD '99

Professor of Computer-Aided Engineering, Department of Civil Engineering, National Taiwan University

Fracturing processes occur at different materials' length scales and naturally call for multiscale modeling. In this lecture, I present my journey on multiscale materials modeling, descended from my Ph.D. and Postdoc research association with Professor Anthony R. Ingraffea. Two critical length scales and modeling techniques are addressed: one at the dislocation level and the other at the materials grain level. At the dislocation level, I place emphasis on the large-scale atomistic simulation: a new paradigm to study mechanics of materials in which mechanisms and properties emerge directly from the fundamental evolution of atoms. At the grain level, a micromechanics model to simulate inter-granular fracture is addressed. Slides: http://hdl.handle.net/1813/38101

On the Virtual Crack Extension for Calculating the Energy Release Rate and Its Derivatives

Changyu Hwang, PhD '99

Professor/Dean for Research Affairs/President of University-Industry Foundation, Seoul Venture University, South Korea

This presentation introduces a numerical method for calculating the energy release rates and their higher-order derivatives for a multiply cracked body under general mixed-node conditions in two and three dimensions. This work generalizes the analytical virtual crack extension method for linear elastic fracture mechanics presented by Lin and Abel, who introduced the direct integral forms of the energy release rate and its derivatives for a structure containing a two-dimensional single crack. Here Lin and Abel's method is generalized, and derivations are provided for verification of the following: extension to the general case of a system of interacting cracks in two dimensions, extension to the axisymmetric case, extension to three-dimensional crack with an arbitrarily curved front under general mixed-mode loading conditions, inclusion of non-uniform crack-face pressure and thermal loading, and an evaluation of the second-order derivative of the energy release rate. The method provides the direct integral forms of stiffness derivatives, and thus there is no need for the analyst to specify a finite length of virtual crack extension. The salient feature of this method is that the energy release rates and their higher derivatives for multiple cracks in two and three dimensions can be computed in a single analysis. It is shown that the number of rings of elements surrounding the crack tip that are involved in the mesh perturbation due to the virtual crack extension has an effect on the solution accuracy. Slides: http://hdl.handle.net/1813/38102

Session 4: Chair: **Derek Warner**, Associate Professor of CEE, New Director of the Cornell Fracture Group

Methane Emissions Make Shale Gas a Bridge to Nowhere

Robert Howarth

The David R. Atkinson Professor of Ecology and Environmental Biology, Department of Ecology and Evolutionary Biology, Cornell University

Only in the past decade or so have two technologies (high-volume hydraulic fracturing and precision directional drilling) combined to allow extracting natural gas from shale, and half of all shale gas ever developed has been produced only in the past 3-4 years. Consequently, the scientific study of the environmental consequences is also quite new. Nonetheless, these consequences are large and diverse, including contaminating groundwater and surface waters and polluting the air. One of the greatest concerns is with the climatic effects: shale gas is widely promoted as a bridge fuel that allows society to continue to rely on fossil fuels while reducing greenhouse gas emissions. However, my research with Prof. Ingraffea indicates that when emissions of methane as well as carbon dioxide are considered, shale gas has perhaps the largest greenhouse gas footprint of any fossil fuel. Even before the shale gas boom, the natural gas industry was the largest source of methane pollution in the US and one of the two largest sources globally (together with animal agriculture). Without large reductions in emissions of both methane and carbon dioxide, the average temperature of the Earth will reach 1.5°C to 2°C above the 20th Century baseline within the next few decades, creating a risk of runaway feedbacks in the climate system leading to even more rapid warming and climate disruption. To reduce this risk, society should move away from all fossil fuels – but particularly shale gas – as rapidly as possible. Slides: http://hdl.handle.net/1813/38103

X-Ray Micro Computed Tomography Based Study of the Effects of Copper-Rich Segregation Structures on Microstructurally-Small Fatigue-Crack Propagation in Al-Cu Alloys

Jacob Hochhalter, PhD '10

Materials Research Engineer, Durability and Damage Tolerance Branch, NASA Langley Research Center

Microstructural features significantly influence fatigue crack growth, particularly during the early stages of initiation and growth, which can account for the majority of the crack's life. In the present study, high-resolution X-Ray micro computed tomography (uCT) is used to study the influence that individual copper-rich segregation (CRS) structures have on microstructurally-small fatigue-crack (MSFC) propagation. Several single-crystal specimens of Al-Cu are fabricated and heat-treated to produce specific CRS structures, where their density and distribution are varied. By observing the crack propagation path and interaction with the CRS structures periodically using X-Ray uCT, the mechanisms governing how such features influence the early stages of crack growth are examined. With the capability to control the density and distribution of the copper segregation structures relative to loading direction, design of optimal copper segregation structures is proposed to decelerate MSFC growth rates by producing tortuous crack paths to maximize closure. Slides: http://hdl.handle.net/1813/38104

Toward High-Fidelity Multi-Scale Modeling of 3D Crack Evolution

Ashley Spear, PhD '14

Assistant Professor of Mechanical Engineering, Multiscale Mechanics and Materials Laboratory, University of Utah

In the ultimate quest to achieve predictive capabilities for crack evolution across multiple length scales, the final generation of Prof. Ingraffea's graduate students stood on the shoulders of their predecessors, leveraging some of the most advanced materials-characterization and modeling techniques to capture crack geometries and environments with utmost fidelity. The first part of this talk highlights two novel, numerical toolsets that were developed to enable the prediction of 3D crack propagation at the structural or component length scale. The first toolset is one that uses material-state mapping along with FRANC3D-inspired adaptive remeshing to predict propagation of 3D cracks in ductile materials. The second toolset was developed to predict 3D crack-shape evolution by calculating local increments of crack extension, Δa_i, using energy-release-rate principles. The second part of the talk highlights novel characterization and modeling efforts that were carried out to understand (and eventually to predict) the formation and early propagation of 3D cracks at the microstructural length scale. In one effort, 3D characterization of fatigue-crack nucleation in a Ni-base superalloy microstructure was reconstructed using 3D crystal-plastic finite-element (CPFE) modeling. "Big data" concepts were utilized to discover quantitative correlations between the underlying microstructure and fatigue indicator parameters computed from the CPFE results. In another effort, the propagation of a microstructurally small fatigue crack in an aluminum alloy was characterized in 3D for the first time. The 3D measurements were converted to a 3D CPFE model that explicitly represented the history-dependent shape of the 3D fatigue crack as well as the surrounding grain structure. The talk concludes with important lessons learned in the Cornell Fracture Group and a look to the future. Slides: http://hdl.handle.net/1813/38105

Closing Remarks

John F. Abel, Professor Emeritus of CEE
http://hdl.handle.net/1813/38090