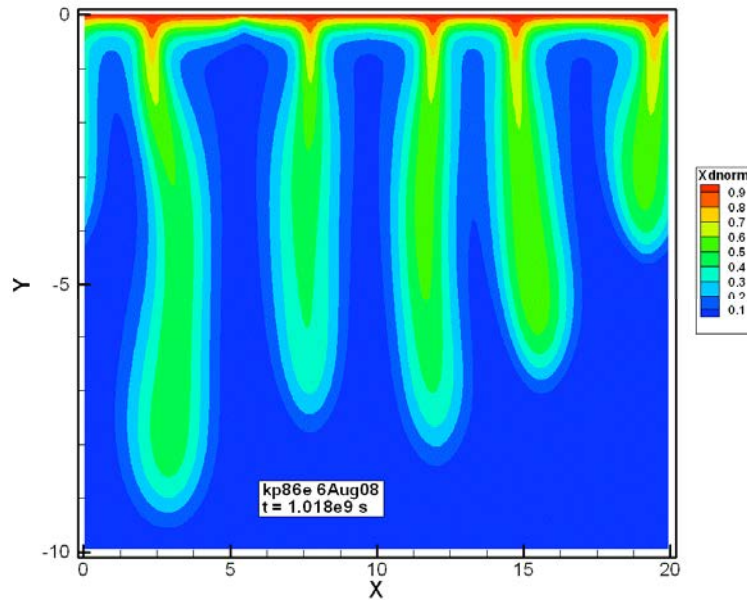
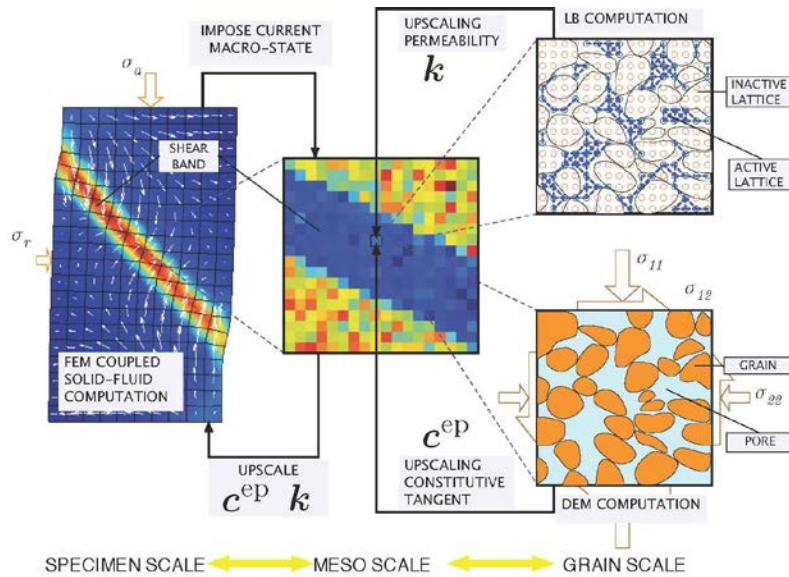


# Office of Basic Energy Sciences Geosciences Research Program, Geophysical Properties and Processes April 5-6, 2012

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## FORWARD

“Geophysical Properties and Processes” is the eighteenth in a series of Geosciences Research Program Symposia dating from 1995. These symposia are topically focused meetings for principal investigators in the program and provide opportunities for our investigators to give presentations on their Office of Basic Energy Sciences’ supported research. We are fortunate to have as guest session co-chairs Prof. Gautam Mitra of the University of Rochester, Prof. Christopher Marone of Pennsylvania State University, Prof. Chester Weiss of Virginia Tech, and Dr. Christopher Neuzil of the U. S. Geological Survey. They join our Principal Investigator co-chairs Dorthe Wildenschild, Seiji Nakagawa, Akhil Datta-Gupta, and William Durham. For their efforts on behalf of the investigators I thank them all. We are looking forward to an outstanding series of presentations. In addition to the recognition the symposium gives to all of the investigators, we traditionally also recognize one outstanding contribution from a National Laboratory Project and one from a University Project. The outstanding contributions are selected by our session chairpersons.

Nicholas B. Woodward  
Geosciences Research Program  
Office of Basic Energy Sciences  
U.S. Department of Energy

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### Cover illustrations:

Figure 1: 2010 Best Paper Award winner – T. Kneafsey and K. Pruess – Lawrence Berkeley National Laboratory - Multi-Scale Coupling: Convectively- Enhanced Dissolution of CO<sub>2</sub>: modeling and theory

Figure 2: 2010 Best Paper Award Winner – Jose Andrade and John Rudnicki, Northwestern University – Multi-Scale Calculation of Permeability inside Compaction Bands

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## **Agenda - Geophysical Properties and Processes, Gaithersburg, Maryland**

**Thursday Morning, April 5, 2012**

**7:30 Registration/Continental Breakfast**

**8:00 Introductions and Greetings** - Nicholas B. Woodward, Department of Energy

### **Session 1: Fracture and Flow**

**Chairs: Gautam Mitra and Seiji Nakagawa**

8:15 Tom Dewers, Sandia National Lab, Coupled mudstone multiphysics

8:40 James P. Evans, Elizabeth Petrie, Leslie Clayton, David Richey, Nathan Giles, Santiago Flores, and Sangeetha Pasala, Utah State University: Impact of micro- to meso-Scale fractures and faults on the sealing behavior of argillaceous caprocks on carbon sequestration: results from field, laboratory, and numerical modeling studies

9:05 Katherine Klise and Sean McKenna, Sandia NL, and Zuleima Karpyn and Josmar Celauro, Penn State: Modified invasion percolation models for multiphase processes

9:30 Stephen J. Bauer, Sandia NL and Kathleen Issen, Clarkson University: Thermo-mechanics based constitutive framework for porous geomaterials

### **9:55 Coffee/refreshments**

10:20 Atilla Aydin, Xiaoxian Zhou, Shang Deng, Lou Durlofsky, Mohammad Karimi-Fard, Stanford University: Distribution of structural heterogeneities in an aeolian sandstone and their impact on fluid flow

10:45 David D. Pollard, Chunfang Meng, and Elizabeth Ritz, Stanford University: Applications of Eshelby's heterogeneity to model deformation bands and complementarity to model faults

11:10 Jon E. Olson<sup>1</sup>, Stephen E. Laubach<sup>2</sup>, Rob H. Lander<sup>3</sup> and Peter Eichhub<sup>2</sup>, <sup>1</sup>University of Texas, <sup>2</sup>University of Texas, BEG and <sup>3</sup>Geocosm, LLC: Geomechanical and diagenetic constraints on how fracture attributes develop in subsurface environments

11:35 Peter Eichhubl<sup>1</sup>, Stephen E. Laubach<sup>1</sup>, Jon E. Olson<sup>2</sup>, A. Fall<sup>1</sup>, T. Weisenberger<sup>1</sup> and J. N. Hooker<sup>1</sup>, <sup>1</sup>University of Texas, Bureau of Economic Geology and <sup>2</sup>University of Texas at Austin: Open natural fractures in low porosity sedimentary rocks: mechanisms, significance to flow, and prediction.

**12:00 – 1:30 Working Lunch** Scott W. Baldrige, John F. Ferguson, Lawrence W. Braie, Los Alamos National Laboratory: SAGE: Structural Basins and Accommodation Zones in the Central Rio Grande Rift, New Mexico: New results from Geophysics

**Thursday Afternoon, April 5, 2012**

**Session 2 – Geophysical Responses to Fluids**

**Chairs: Chet Weiss and Dorte Wildenschild**

- 1:35 Seiji Nakagawa, LBNL: Static and dynamic coupling of fractures and fluid--laboratory investigations
- 2:00 James Berryman, LBNL: Seismically-induced flow in granular media and flow-induced seismicity in fractured networks
- 2:25 Donald Vasco, LBNL: Modeling coupled deformation and fluid flow using an asymptotic approach
- 2:50 Gregory Newman, LBNL: Homogenization of electromagnetic and seismic wavefields for joint inverse modeling

**3:15 Coffee/refreshments**

- 3:35 John Scales, Nathan Greeney, Michael Batzle, Manika Prasad, Colorado School of Mines: Spatial scanning of rocks to achieve high resolution maps of dielectric permittivity and elastic moduli
- 4:00 Akhil Datta-Gupta, Texas A & M University: Multi-scale parameterization for model calibration using time lapse seismic data
- 4:25 David Johnson<sup>1</sup>, Hernan Makse<sup>2</sup> and John J. Valenza<sup>1</sup>, <sup>1</sup>Schlumberger and <sup>2</sup>City College of New York: Elasticity and damping of acoustic modes in granular materials with applications to oil recovery
- 4:50 Amos Nur, Stanford University: Porous rocks with fluids: the emergence of digital rock physics

**5:15 Adjourn, Dinner (On your own)**

**Friday Morning, April 6, 2012**

**7:30 Coffee/Continental Breakfast**

**Session 3 – Material Properties of Rocks**

**Chairs: Chris Marone and Akhil Datta-Gupta**

- 8:00 Paul Johnson, Los Alamos National Laboratory and Tim W. Darling, University of Nevada, Reno: A new probe for rock elasticity - Time-of-Flight Modulation (TOFM)
- 8:25 Timothy W. Darling<sup>1</sup>, Paul A. Johnson<sup>2</sup> and Rachel A. Miller<sup>1</sup>, <sup>1</sup>University of Nevada and <sup>2</sup>Los Alamos National Laboratory: Acoustic studies of the behavior of Berea sandstone in an extremely dry state
- 8:50 Brian Evans, Yves Bernabe and Uli Mok, MIT: Evolution of pore structure and permeability of rocks under hydrothermal conditions
- 9:15 Harrison Lisabeth, Audrey Ougier-Simonin and Wenlu Zhu, University of Maryland: Evolution of permeability and pore structure of porous limestone at elevated temperature
- 9:40 William Durham and N. A. Dixon, MIT and A. Suzuki and S. Mei, UMN: How pressure affects the strength of dry olivine at upper mantle conditions

**10:05 Coffee/refreshments**

- 10:25 Shenghua Mei, A. M. Mei, L. Xu and David Kohlstedt, University of Minnesota and N. A. Dixon and W.B. Durham, MIT: Experimental constraints on the rheology of mantle rocks
- 10:50 Teng-fong Wong<sup>1</sup>, Waichung Sun<sup>2</sup>, Yuntao Ji<sup>1</sup> and Patrick Bau<sup>3</sup>, <sup>1</sup>Stony Brook University, <sup>2</sup>Sandia NL, Livermore, CA and <sup>3</sup>Institut de Physique du Globe de Strasbourg: MicroCT imaging of porous sandstone and limestone: Implications on permeability evolution and mechanical damage
- 11:15 Waruntorn (Jane) Kanitpanyacharoen and Hans-Rudolf Wenk, University of California at Berkeley: Anisotropy in shales: from microstructures to seismic signature
- 11:40 Laura Pyrak-Nolte, Eric Boomsma and Nolan Teasdale, Purdue University: The physics of swarms in fracture networks: integration of seismic characterization and controlled micro-transport

**12:05 – 1:20 Working Lunch –**

**Friday Afternoon, April 6, 2012**

**Session 4 – Modeling Physical Properties and Flow Properties**

**Chairs: Chris Neuzil and Bill Durham**

1:20 John B. Rundle, J.D. Gran and J.R. Holliday, University of California at Davis and William Klein, Boston University: Statistical physics models for damage, fracture, and fracking in rocks: bumps on the road to energy independence

1:45 William Klein, Boston University: The effect of defects on phase kinetics, fracture and Gutenberg-Richter scaling

2:10 Joel Koplik, CUNY: Transport and clogging of particulate flow in fracture systems

2:35 Ruben Juanes, MIT: Fingering and fracturing in granular media

**3:00 Coffee/refreshments**

3:30 Daniel H. Rothman, MIT: Ramification of stream networks

3:55 Dorthe Wildenschild, Oregon State University and Marcel Schaap, University of Arizona: Optimizing capillary trapping of CO<sub>2</sub> during geological carbon sequestration

4:20 Marcel G. Schaap, University of Arizona and Dorthe Wildenschild, Oregon State University: Realistic equations of state in a Lattice Boltzmann model

**4:45 Nick Woodward - *Concluding remarks***

**Working Dinner 6-8 PM**



## **ABSTRACTS:**

## **Coupled Mudstone Multiphysics**

Thomas A. Dewers, *Sandia National Laboratories, Albuquerque*

Shales and other mudstones are an enigmatic rock type with heterogeneity at all scales. Small pore and grain sizes, large specific surface areas, and clay mineral structures lend themselves to rapid reaction rates, high capillary pressures, shrink/swelling, and semi-permeable membrane behavior accompanying changes in stress, pressure, temperature and chemical conditions. Under far from equilibrium conditions, mudrocks display a variety of spatio-temporal self-organized phenomena arising from nonlinear thermo-mechano-chemo-hydro coupling.

Beginning with a detailed examination of nano-scale pore network structures in mudstones, we discuss the dynamics behind such self-organized phenomena as pressure solitons in unconsolidated muds, chemically-induced flow self focusing and permeability transients, localized compaction, time dependent well-bore failure, and oscillatory osmotic fluxes as they occur in clay-bearing sediments. FIB/SEM, TEM, Small Angle Neutron Scattering, and routine porosimetry are used to investigate mudstone pore sizes and pore lining phases down to nm scale. Image analysis techniques combined with pore scale modeling assess sizes and hydrologic properties of REV's and permit an evaluation of the disposition of water in micron-sized samples. Experimental sorption and membrane potential measurements on core-scale samples show behavior directly resulting from the change in water properties as pore sizes decrease through compaction. Novel micro-pillar compression tests address size of REV's applicable to continuum-scale mudstone deformation, anisotropy, and size-scale plasticity effects. These phenomena and observations bear on the ability of these rock types to serve as containment barriers.

This work is funded by the US Department of Energy, Office of Basic Energy Sciences. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

# **Impact of Micro- to Meso-Scale Fractures and Faults on the Sealing Behavior of Argillaceous Caprocks on Carbon Sequestration; Results from Field, Laboratory, and Numerical Modeling Studies**

James P. Evans, Elizabeth Petrie, Leslie Clayton, David Richey, Nathan Giles, Santiago Flores, and Sangeetha Pasala, *University of Utah*

In conjunction with co-workers at Sandia National Laboratories, we investigate the nature of fracture propagation, and fluid flow from reservoir rocks into overlying shale/siltstone at geologic analogs for CO<sub>2</sub> storage and hydrocarbon reservoir-seal pairs. In the field component of this work, our research in SE Utah has characterized fracture distributions and changes in fracture morphologies observed in exhumed seal analogs that show evidence for open mode fractures and fluid flow at depth. These fractures occur at the mm to cm-scale and would be overlooked in seismic data. Fractures significantly change the permeability of a seal and should be incorporated in subsurface fluid flow models. Fracture spacing and morphology changes with changes in lithology and across lithologic boundaries. We use wireline log data to estimate changes in rock strength within sealing lithologies and have tied these changes to the outcrop observations. Both rock strength and fracture distribution data will be used in geomechanical models to better understand the response of changing stress conditions, such as increased pore fluid pressure, on hetero-lithic sealing lithologies. We also have examined the field permeability of deformation band faults with m-scale offsets in sandstone reservoirs, and examine the transition from faulted sandstones to siltstone-rich caprock. Mineralization along the faults indicates that the faults act as barrier-baffle systems, and flow into the “seal” occurs along zones of open mode fractures. The impact of faults with 10’s m of offset is being examined along one fault that cuts three reservoir-seal pairs. We examine the variable nature of the fault zone structure as a function of lithology juxtaposition, and are currently evaluation the permeability of host and fault-related rocks. As an outgrowth of an undergraduate research project, we have designed, built, and are now running CO<sub>2</sub>-water-rock flow experiments at supercritical conditions. Several examples run to date show distinct evidence for fracture development and flow in shale at reservoir pressure, changes in rock texture as a result of CO<sub>2</sub>-rock reactions, and creation of porosity due to dissolution.

We use these field sites as the starting point for numerical flow modes of CO<sub>2</sub> in potential injection systems via simulation of flow of CO<sub>2</sub> in faulted and fractured sandstone. Two end-member fault types are considered: low-permeability faults dominated by deformation-band networks, and high-permeability faults dominated by fracture networks in a damage zone. Simple averaging calculations indicate that equivalent permeability ( $k$ ) values for the fault zones can range from less than  $10^{-14}$  m<sup>2</sup> for deformation-band-dominated faults to greater than  $10^{-12}$  m<sup>2</sup> for fracture-dominated faults regardless of the permeability of the unfaulted sandstone. A set of water-CO<sub>2</sub> fluid-flow simulations model the injection of CO<sub>2</sub> into high- $k$  sandstone with either low- $k$  or high- $k$  fault zones that correspond to deformation-band- or fracture-dominated faults, respectively. After 500 days, the CO<sub>2</sub> rises to produce an inverted cone of free and dissolved CO<sub>2</sub> that spreads laterally away from the injection well. Free CO<sub>2</sub> fills no more than 40% of the pore space behind the advancing CO<sub>2</sub> front, where dissolved CO<sub>2</sub> is also at or near geochemical

saturation. The low- $k$  fault zone exerts the greatest impact on the shape of the advancing  $\text{CO}_2$  front and restricts the bulk of the  $\text{CO}_2$  (both dissolved and free) to the region upstream of the fault barrier. In the high- $k$  aquifer, the high- $k$  fault zone exerts only a small influence on the shape of the advancing  $\text{CO}_2$  front. In lower-permeability aquifers, high-permeability fault zones will become more important as pathways for  $\text{CO}_2$  to bypass unfaulted sandstone. Although high-permeability fault conduits might lead to reduced sequestration efficiency, aquifer compartmentalization by low-permeability fault barriers may lead to improved efficiency because the barriers restrict lateral  $\text{CO}_2$  migration and maximize the volume of  $\text{CO}_2$  that might be emplaced in each fault-bound compartment.

## Modified invasion percolation models for multiphase processes

Katherine Klise<sup>1</sup>, Sean McKenna<sup>1</sup>, Zuleima Karpyn<sup>2</sup>, and Josmar Celauro<sup>2</sup>

<sup>1</sup> Sandia National Laboratories, Albuquerque and <sup>2</sup>The Pennsylvania State University

Our ability to predict the migration of multiphase fluids under capillary flow regimes is central to the design of engineering operations including carbon sequestration, site remediation, and fossil fuel extraction. Invasion percolation (IP) and modified invasion percolation (MIP) algorithms have been used to simulate drainage and imbibition in multiphase systems using pore network models. MIP algorithms have been developed to include additional processes, such as vacating pores, the effects of buoyancy and gravity, and transitions to viscous and stable growth patterns. To a large extent, these modifications are adopted depending on individual research and application needs. In this investigation, we propose to create a unified framework for MIP algorithms with direct validation from experimental observations using 3D micro-computed tomography (CT) imaging. Additionally, we plan to extend the current MIP algorithms to include heterogeneous surface properties and time-based processes such as diffusion.

In this talk, we outline a series of experiments that will improve understanding of capillary driven flow in complex pore structures. Numerical and laboratory experiments have been specifically designed to investigate the effects of mixed wettability and transient diffusion processes on percolation. High-resolution CT imaging experiments are used to investigate structural and surface properties of the media, and how they influence percolation pathways under capillarity dominated flow regimes. Initial core flood experiments have been performed using a mix of hydrophilic and hydrophobic beads (0.6mm mean diameter) to track the influence of variable contact angle on capillary flow. Experimental results are then used to generate three-dimensional maps of fluid distribution relative to local wettability of the solid matrix and pore structure for subsequent validation of MIP algorithms. Numerical analysis uses the MIP algorithm in PERC++ as a starting point for simulation. Upscaling techniques are investigated as part of the validation process. This presentation will cover preliminary results from both the experiments and numerical analysis.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

## **Thermo-mechanics based constitutive framework for porous geomaterials**

Stephen J. Bauer, *Sandia National Laboratory* and Kathleen A. Issen, *Clarkson University*

Porous geomaterials exhibit a range of deformational responses under stress conditions typical of the earth's subsurface. Understanding these responses and quantifying the behavior mathematically is necessary to predict response of porous geomaterials for a variety of sub-surface geo-engineering pursuits for oil and gas production and exploration, as well as carbon sequestration in deep saline sandstone formations and depleted oil and gas reservoirs. Excluding time-dependent effects, porous rocks exhibit elasticity, have cohesion, are dilatant or compactant, fail with pressure dependence, and are frictional. These phenomena are collectively included in elastic-plastic constitutive modeling. This project consists of theoretical and experimental work aimed at improving constitutive descriptions of the elastic-plastic deformation of porous geomaterials in general and sandstone deformation in particular. This talk focuses on aspects of the theoretical work to develop a thermodynamically rigorous constitutive framework that represents known behaviors of geomaterials.

The plastic response of geomaterials is often derived using a classical plasticity approach, originally developed for metals, but adapted for geomaterials by use of non-associated flow (non-normality). The yield surface in stress space separates elastic from plastic response; for metals, the plastic strain increment is perpendicular to the yield surface. However, for geomaterials, a well-known experimental result is that the plastic strain increment is not perpendicular to the yield surface. Thus, the plasticity framework is traditionally modified to include the use of a plastic potential: the surface to which the plastic strain increment is perpendicular. Recently, the use of a plastic potential has been questioned, in part, because it admits the possibility of negative work.

Following the thermo-mechanics approach of Collins, Houlsby and colleagues (e.g., Collins and Houlsby, 1997), elastic strains are determined from Gibbs free energy. Recent experiments on Castlegate sandstone reveal that the elastic moduli evolve with stress and plastic strain; these dependencies are achieved through proper selection of a Gibbs free energy function. The resulting elastic strain consists of three components: 1) strain due to change in stress at a constant moduli, 2) strain due to stress dependence of the moduli, and 3) coupled strain due to plastic strain dependence of the moduli. The fourth component of total strain is the plastic strain, which is determined using a plasticity-like approach; however, the yield surface is represented in dissipative stress space, where the plastic strain increment is perpendicular to the yield surface. Subsequently, the yield surface in traditional stress space is found to be a translation and distortion of the yield surface in dissipative stress space; this distortion causes the plastic strain increment to be non-normal to the yield surface in traditional stress space.

Collins, I., Houlsby, G., 1997. Application of thermo-mechanical principles to the modeling of geotechnical materials. *Proc. R. Soc. Lond. A* 453, 1975-2001.

## **Distribution of structural heterogeneities in an aeolian sandstone and their impact on fluid flow**

Atilla Aydin, Xiaoxian Zhou, Shang Deng, Lou Durllofsky and Mohammad Karimi-Fard,  
*Stanford University*

During the previous award periods, the formation of a wide variety of structural heterogeneities such as compaction bands, joints, and sheared joint-based faults in the Jurassic aeolian Aztec Sandstone exposed at the Valley of Fire State Park (NV), and the influence of each structure arrays on fluid flow were investigated (Taylor et al., 1999; Flodin et al., 2001; Jourde et al., 2002; Eichhubl et al., 2004; Flodin et al., 2005; Sternlof et al., 2006; Ahmadov et al., 2007; Aydin and Ahmadov, 2009). Within the current project period, we documented the orientation and distribution of compaction bands compartmentalizing the medium (Deng and Aydin, 2012, submitted to *Tectonophysics*). In addition, we modeled fluid flow across sandstone with multi-set compaction bands and with compaction band arrays and intersecting joints and faults in primarily 3D (Zhou et al., 2012, submitted to *Geological Society Special Paper on Advances in the Study of Fractured Reservoirs*) using a discrete fracture model developed by Karimi-Fard et al. (2004). The representative cases include (1) single set of compaction bands, (2) two sets of compaction bands along bedding and at high-angle to bedding, (3) a younger set of joints intersecting a set of compaction bands, and (4) younger faults and the associated structures overprinting a set of compaction bands.

The results indicate that:

- The 3D distribution and patterns of compaction bands in the aeolian sandstone are more complex than previously thought.
- The intersection angle of multiple sets of vertical compaction bands and the dip angle of inclined compaction bands have a strong effect on the up-scaled permeability tensor.
- The intersection angle between joint sets and older compaction band sets strongly influences the principal directions and values of the up-scaled permeability tensor.
- For the case of a small fault overprinting a set of compaction bands, the combined effect of fault rock, slip surfaces, splay joints and compaction bands is to reduce equivalent permeability in the fault-normal direction and to increase permeability in the vertical direction.

Future study includes a better characterization of the compartmentalization of various structure networks and their influence on the overall fluid flow in 3D analog reservoirs.

## **Applications of Eshelby's heterogeneity to model deformation bands and complementarity to model faults**

David D. Pollard, Chunfang Meng, and Elizabeth Ritz  
*Stanford University*

We have developed a MATLAB® code to evaluate Eshelby's solution for an arbitrary ellipsoidal inclusion or heterogeneity embedded in an elastic, isotropic and infinite body. The code evaluates the elastic fields (i.e. strain, stress and displacement) inside and outside the ellipsoidal inclusion/heterogeneity. With this code, we review research on localized volumetric deformation in Earth's crust that has used special cases of Eshelby's solution (e.g. heterogeneity modeled as a 2D ellipse or an ellipsoid with two equal axes, a spheroid), and 2D rectangular inclusions. The model compaction band has different isotropic elastic moduli than the surroundings based on measured porosity change, a prescribed eigenstrain to account for the volume reduction, and remote tri-axial stress to drive the compaction. We discuss how the arbitrary ellipsoidal geometry provides new results and insight. One application of the code is to evaluate the stress field about the tip-line of a compaction band to understand the propagation mechanism and path. Unlike numerical methods, e.g. finite element and boundary element methods, the accuracy is not affected by the distance-to-tip at which the stress is evaluated. This feature enables us to accurately evaluate the stress field in an arbitrary near-tip region for a model compaction band that is not restricted to a straight tip-line. With this code, we investigate how the varying tip-line curvature would affect the near-tip stress and further the deformation growth.

We have developed a MATLAB® code for the two-dimensional displacement discontinuity method (DDM) for quasi-static boundary value problems to investigate the mechanical behavior of sinusoidal faults of finite length in an otherwise homogeneous and isotropic elastic material. Although fault mechanics theory has developed from idealizing faults as planar structures, faults in the brittle upper crust are geometrically complex structures and exhibit a variety of surface and tipline shapes. The DDM incorporates a complementarity algorithm to enforce appropriate contact boundary conditions along the model fault. The numerical solution for the model sinusoidal fault does not converge to the analytical solution for an infinite sinusoidal interface as the ratio distance/wavelength goes to zero. We provide stick, slip, and opening distributions along wavy faults with a range of uniform coefficients of friction, amplitude/wavelength ratios, and wave numbers to demonstrate that the displacement discontinuity of wavy faults cannot be prescribed a priori, apparently precluding an analytical solution. We employ the terms lee and stoss instead of releasing and restraining bends because a local minimum in slip may occur along lee sides, as well as stoss sides. In some cases, lee sides stick while stoss sides slip. The occurrence and magnitude of opening observed along lee sides increases with wave number, but has a more complicated dependence on amplitude/wavelength. In general the fault geometry causes slip to deviate significantly from the elliptical distribution of a planar fault. Trends in the slip perturbation can be explained by the angular relationship between the local fault trace and the orientation of the remote principal stresses; however, the displacement discontinuity along a wavy model fault also depends on the magnitude of the remote stress, the frictional properties of the slip surfaces, and the elastic moduli of the material.



## **An integrated approach to assessing natural fracture initiation, spatial arrangement, aperture preservation and flow properties in sandstones versus shales**

Jon E. Olson<sup>1</sup>; Stephen E. Laubach<sup>1</sup>; Rob H. Lander<sup>3</sup>; Peter Eichhubl<sup>1</sup>

<sup>1</sup>*The University of Texas at Austin*, <sup>2</sup>*The University of Texas at Austin, Bureau of Economic Geology*, and <sup>3</sup>*Geocosm, LLC*

Accurate predictions of natural fracture flow attributes in sandstones and shales requires an understanding of the underlying mechanisms responsible for fracture growth and aperture preservation. Poroelastic stress calculations combined with fracture mechanics criteria show that it is possible to sustain opening mode fracture growth with sub-lithostatic pore pressure without associated or pre-emptive shear failure. Crack-seal textures and fracture aperture to length ratios suggest that preserved fracture apertures reflect the loading state that caused propagation. This implies that for quartz-rich sandstones, the synkinematic cement in the fractures and in the rock mass props fracture apertures open and reduces the possibility of aperture loss on unloading and relaxation. Fracture pattern development due to subcritical fracture growth for a limited range of strain histories is demonstrated to result in widely disparate fracture pattern geometries. Substantial opening mode growth can be generated by very small extensional strains (on the order of  $10^{-4}$ ); consequently, fracture arrays are likely to form in the absence of larger scale structures. The effective permeabilities calculated for these low strain fracture patterns can be considerable. To replicate the lower permeabilities that typify tight gas sandstones requires the superimposition of systematic cement filling that preferentially plugs fracture tips and other narrower portions of the fracture pattern.

Natural fractures in shales seem to have some fundamental differences with sandstones. One aspect commonly observed in shales is a very small fracture spacing to mechanical thickness ratio, often much less than 1. To address this problem, we have developed a coupled poroelastic fracture growth model to investigate the influence of host rock permeability during natural fracture growth. The hypothesis is that for a fracture to develop a substantial stress shadow around it, which would promote wider fracture spacing, it needs to grow faster than its neighbors in order to suppress their growth. Given that for opening mode fractures, fracture volume must increase for continued growth (otherwise the driving stress in the fracture drops and fracture growth arrests), then fast fracture growth (promoted by favorable mechanical interaction and fracture size) can be retarded by the lack of fluid replenishment to the fracture in extremely low permeability in mudrocks. This allows slower fractures to catch up, and the result should be very close spacing. Preliminary modeling confirms the growth retardation for low permeability rocks, which can change fracture growth time from thousands of years to millions of years. We are currently working towards multi-fracture modeling to assess opening mode pattern development, for which the challenge is marrying the disparate timescales required for the mechanical versus the fluid flow simulations.

## **Open and sealed natural fractures in sedimentary rocks: mechanisms, significance to flow, and prediction.**

Peter Eichhubl<sup>1</sup>; Stephen E. Laubach<sup>1</sup>; Jon E. Olson<sup>2</sup>; A. Fall<sup>1</sup>; T. Weisenberger<sup>1</sup>; J. N. Hooker<sup>1</sup>

<sup>1</sup>*The University of Texas at Austin, Bureau of Economic Geology, and*

<sup>2</sup>*The University of Texas at Austin*

Natural fractures can significantly influence fluid flow in sedimentary rocks, particularly those that are deeply buried or that have been so in the past. Open and partially cemented natural fractures provide flow pathways connecting matrix pores to hydraulic fractures and the wellbore. Cemented and some partially cemented fractures may inhibit matrix flow in some low porosity rocks, if the fractures are more tightly sealed than the host. Open fractures can also interfere with engineering operations. They may arrest or divert hydraulic fracture propagation through fluid loss and tip blunting and fractures with weak cement may be reactivated in opening or shear during hydraulic fracture stimulation increasing fracture surface and drainage volume. Characterization and prediction of natural fractures and their attributes are thus essential for accurately predicting the movement of natural and introduced fluids in the subsurface. Conventional core and borehole imaging surveys tend to under-sample large and widely spaced natural fractures, so successful characterization needs to encompass fracture-related features over a wide scale range, including that which is readily sampled. And an understanding of how structural and diagenetic features are related is needed to successfully extrapolate from limited samples, to test predictive models, and to calibrate and test indirect geophysical detection methods.

In many rocks, temperature-sensitive geochemical processes and fracturing have interacted resulting in features amenable to integrated structural, geochemical, experimental, and numerical approaches. To understand these features we combine observations from vertical and horizontal core and select outcrop analogs that share relevant fracture parameters with producing reservoirs. This approach includes 1. size scaling analyses of micro- to macro-fracture opening displacement and frequency, 2. fracture diagenetic studies addressing fracture porosity structure, cement distribution, and timing of cementation relative to reactions including hydrocarbon charge, 3. matrix diagenetic studies designed to predict degree of fracture cement precipitation and mechanical property evolution, 4. laboratory tests of rock and fracture mechanics properties and cement strength, and 5. numerical simulations of fracture network evolution and hydraulic-natural fracture interaction.

## **Structural Basins and Accommodation Zones in the Central Rio Grande Rift, New Mexico: New results from Geophysics**

W. Scott Baldrige, J.F. Ferguson, Larry W. Braile, and the faculty and students of SAGE, *Los Alamos National Laboratory*

The active young (<35 Ma) Rio Grande rift of the southwestern U. S. comprises numerous faulted basins separated by complex structural “accommodation” zones. For several years the SAGE (*Summer of Applied Geophysical Experience*) student program has conducted multiple geophysical surveys along the eastern margin of the rift, 10-35 km southwest of Santa Fe, New Mexico. The specific goal has been to investigate structures and history of a complex NE-trending accommodation zone (Santo Domingo), separating the larger Española (to north) and Albuquerque rift basins. Crustal extension is transferred dominantly along north- to northwest-trending *en echelon* faults, creating sub-basins and plunging ramps oblique to the overall strike of the accommodation zone.

SAGE has produced seismic reflection images of two of these faults (“ramp faults”), the La Bajada (LB) and San Francisco (SF) faults, allowing determination of their dips (near 60° down to west). Vertical offset on the basin-bounding LB fault increases from near zero at the south to a maximum of ~3000 m 13 km to the north, where the uplifted footwall comprises the flanking Cerrillos uplift. Time of initiation of the LB fault is not well constrained, but vertical offset since 2.7 Ma is only ~200 m. Uplift of the Sandia Mountains ~20 Ma warped the hanging wall into a northward plunging structural basin. Preliminary gravity data across the intra-rift SF fault are compatible with ~1.3 km of down-to-the west offset. Combining new seismic, gravity, and other geophysical data obtained in the SAGE program, and integrating these with industry seismic reflection, geological, and borehole data allow us to estimate extension and block rotation along these faults.

We are able to discriminate pre-rift (Laramide) from post-middle Miocene (rift) structures beneath rift sediments, and to quantify thickness of basin fill and vertical offsets across faults. We are working to infer kinematic development, linkages among faults, growth history, and possible pre-rift structural controls, which together will better define the segmentation and propagation of the rift. An overall goal is to determine weak and strong zones and lateral variations in crust and lithosphere to understand factors such as heat and strain weakening that control incipient continental breakup.

## Static and dynamic coupling of fractures and fluid—Laboratory investigations

Seiji Nakagawa, *Lawrence Berkeley National Laboratory*

Fluid within a fracture can impact its mechanical properties through both poroelastic and chemical processes. Dynamic poroelastic effects result in fractures having a frequency-dependent compliance, which in turn influences the scattering of seismic waves. Quasi-static changes in applied fluid pressure can destabilize fractures subjected to shear stress resulting in slip. In both cases, precipitation and dissolution of minerals on the fracture alter its behavior by changing the fracture's mechanical and hydraulic properties. Our current laboratory research investigates the coupled behavior of fractures and fluid in rocks. In this presentation, an on-going experiment for measuring frequency-dependent compliance of single fractures will be introduced, including a theoretical model for predicting the scattering of seismic waves as a function of wave frequency and fracture and fluid properties. Unlike conventional measurements, this experiment aims to measure the fracture compliance for a continuous, broad range of frequencies below 1 kHz. An experimental technique of rapidly precipitating calcite on a fracture and within a porous rock will also be presented, which has been developed for the purpose of altering the fracture compliance and flow properties. Next, we will discuss the behavior of fracture waves, which are extremely slow seismic waves trapped on a fracture (also called Klauklis waves). A laboratory experiment for measuring these waves at low frequencies (below 1 kHz) in an analogue fracture model will be presented. Lastly, we will present a new direct shear experiment for studying destabilization of a fracture subjected to increased pore pressure and chemical alternation. This experiment, conducted within a conventional triaxial loading cell, examines coupling between the mechanical behavior (deformation, acoustic emission), hydrological properties (permeability), and pore fluid chemistry during shearing.

## **Seismically-induced flow in granular media and flow-induced seismicity in fractured networks**

James G. Berryman, *Lawrence Berkeley National Laboratory*

The BES-funded geophysics research at LBNL has an important focus on understanding the coupling between fluid flow and deformation/slip processes. Two classes of earth materials for which relatively small changes in fluid pressure can induce significant deformation are (1) unconsolidated sediments and (2) fractured rocks. Both material classes are under active theoretical and experimental investigation as part of this BES-funded research.

It is known from both laboratory and numerical experiments that unconsolidated granular media have some fraction of their grains in the grain-pack that do not contribute to the overall mechanical strength of the granular system. Such loose grains are called “rattlers” and at low confining pressure can represent up to 10% of the grains. Their presence affects both acoustic attenuation and wave speeds. Sound wave speeds tend to be reduced while the wave attenuation tends to be increased. An analytical model of grain packs with rattlers is presented and comparisons to available acoustic data will be discussed. A long-standing question about the validity of Biot theory at higher frequencies (20 kHz and above) in ocean-bottom sediments can be quantitatively resolved by invoking these rattler effects.

As time permits, we will also discuss some of the implications of fluid-stress in fractured systems to induced seismicity, while again taking a general point of view grounded in Biot’s theory. Fractured media are particularly sensitive to changes in fluid pressure, and to the orientations of the fractures themselves. Recent work by the author on effective stress for fractured porous media will be summarized and, in particular, the nature of the effective-stress law for the anisotropic permeability tensor presented. The changing of permeability with fluid pressure results in fluid-pressure diffusion being a non-linear process and this has implications for induced seismicity.

## **Modeling coupled deformation and fluid flow using an asymptotic approach**

Donald Vasco, *Lawrence Berkeley National Laboratory*

The modeling of coupled processes related to deformation and fluid flow within the Earth can quickly lead to complicated governing equations. For example, the physical processes governing fluid flow and solid deformation are very different in character. This can lead to great differences in temporal scales, whereby a fast elastic disturbance can take a fraction of a second to propagate out of a region, while a slow diffusive wave can take minutes or even hours. Furthermore, due to such processes as multiphase flow and inelastic deformation, the governing equations are often nonlinear. Combining such complications with the inherent heterogeneity of the Earth results in difficulties in both the forward and inverse modeling of coupled deformation and flow. In this work I use an asymptotic technique, valid when the medium properties are smoothly-varying, to model coupled processes associated with fluid flow and deformation. I use this approach to attack two types of problems.

First, the coupled modeling of the flow of two or three immiscible fluid phases in a heterogeneous, elastic, porous material is formulated in a manner analogous to that for a single fluid phase. The asymptotic technique is used to derive equations for the phase velocities of the various modes of propagation. A polynomial equation determines the phase velocities of the longitudinal modes. The coefficients of the polynomial are expressed in terms of sums of the determinants of matrices whose elements are the parameters found in the governing equations. In addition to the various longitudinal modes, there is a transverse mode of propagation, a generalization of the elastic shear wave.

Second, the asymptotic approach has been applied to coupled nonlinear processes associated with fluid flow and deformation in a heterogeneous Earth. That is, given a set of coupled nonlinear governing equations, one can derive a semi-analytic expression for the phase of a disturbance traveling within a heterogeneous porous medium. This Hamilton-Jacobi equation is a generalization of the Eikonal equation. The phase, a function related to the propagation time of the coupled disturbance, depends upon the properties of the medium, and upon the amplitude changes across the front. Thus, the propagation velocity of the disturbance depends upon its amplitude, as would be expected for a nonlinear process. Time permitting, examples from two phase flow, coupled heat and fluid flow, and coupled deformation and fluid flow in a medium with pressure dependent properties, will be discussed.

## Homogenization of Electromagnetic and Seismic Wavefields for Joint Inverse Modeling

Gregory A. Newman, *Lawrence Berkeley National Laboratory*

A significant obstacle in developing a robust joint imaging technology exploiting seismic and electromagnetic (EM) wave fields is the resolution at which these different geophysical measurements sense the subsurface. Imaging of seismic reflection data is an order of magnitude finer in resolution and scale compared to images produced with EM data. A consistent joint image of the subsurface geophysical attributes (velocity, electrical conductivity) requires/demands the different geophysical data types be similar in their resolution of the subsurface. The superior resolution of seismic data results from the fact that the energy propagates as a wave, while propagation of EM energy is diffusive and attenuates with distance. On the other hand, the complexity of the seismic wave field can be a significant problem due to high reflectivity of the subsurface and the generation of multiple scattering events. While seismic wave fields have been very useful in mapping the subsurface for energy resources, too much scattering and too many reflections can lead to difficulties in imaging and interpreting seismic data. To overcome these obstacles a formulation for joint imaging of seismic and EM wave fields is introduced, where each data type is better matched in resolution. In order to accomplish this, seismic data are first transformed into the Laplace-Fourier Domain, which changes the modeling of the seismic wave field from wave propagation to diffusion. Though high frequency information (reflectivity) is lost with this transformation, several benefits follow: (1) seismic and EM data can be easily matched in resolution, governed by the same physics of diffusion, (2) standard least squares inversion works well with diffusive type problems including both transformed seismic and EM, (3) joint imaging of seismic and EM data may produce better starting velocity models critical for successful reverse time migration or full waveform imaging of seismic data (non transformed) and (4) possibilities to image across multiple scale lengths, incorporating different types of geophysical data and attributes in the process. Important numerical details of 3D seismic wave field simulation in the Laplace-Fourier domain for both acoustic and elastic cases will also be discussed.

## **Spatial scanning of rocks to achieve high resolution maps of dielectric permittivity and elastic moduli**

John Scales, Nathan Greeney, Michael Batzle, Manika Prasad,

*Colorado School of Mines*

Using techniques that are analogs of near-field optical scanning we will show how electromagnetic waves in the hundreds of GHz can be used to measure the real and imaginary parts of the permittivity of rocks with sub-millimeter spatial resolution. The technique is relatively fast and since oil and kerogen have low (real) permittivity, they show up with high contrast. Time-lapse images (before/after pyrolysis, for example) are especially revealing. Although we will focus on transmission measurements, this technique could readily be adapted to reflection scanning of large area samples such rock cores. We have also developed a technique using time-domain laser ultrasound to extract high-resolution acoustic properties. Unlike acoustic microscopy, we use thermo-elastically generated pulses and record the times of first-arriving pulses propagating through thin samples. So the method is non-contacting and doesn't require the sample to be immersed in water. The dielectric and acoustic properties of samples can thus be spatially mapped and co-located in a relatively short time, even inside an oven or pressure vessel. Having a rapid spatial indicator of the presence of organics is very useful; however, our ultimate goal is to be able to use these data to understand how the electromagnetic and mechanical properties of rocks are fundamentally related.



# Multi-scale Parameterization for Model Calibration Using Time Lapse Seismic Data

Akhil Datta-Gupta, *Texas A&M University*

We introduce a novel parameterization approach to mitigate the challenges associated with field-scale history matching/calibration of geologic models to time-lapse seismic data. In this approach, the reservoir property field is mapped to and updated in a low-dimensional transform domain using a linear transformation basis. The transformation basis vectors are the eigenvectors of a Laplacian matrix that is constructed using grid connectivity information and the main features in a given prior model. Because the grid connectivity information is computed only within a small multi-point stencil, the Laplacian is always sparse and is amenable to efficient decomposition. The resulting basis functions are ordered from large to small scale and include prior-specific spatial features. Therefore, the variability in reservoir property distribution can be effectively represented by projecting the property field onto subspaces spanned by an increasing number of leading basis vectors, each incorporating additional heterogeneity features into the model description. This property lends itself to a multiscale history matching algorithm where basis elements are sequentially included to refine the heterogeneity characterization to a level of complexity supported by the resolution of the data (Fig.1). While the method can benefit from prior information, in the extreme case where reliable prior knowledge is not available the transformation reduces to a discrete Fourier expansion with model-independent parameterization properties.

We present the important properties of the proposed reservoir parameterization including efficient one-time construction of the basis prior to calibration, applicability to any grid geometry and strong compression performance. The multiscale history matching algorithm begins by updating the prior reservoir model using a parameterized multiplier field that is superimposed onto the grid and assigned an initial value of unity at each cell. The multiplier is sequentially refined from the coarse to finer scales during minimization of data misfit. This method permits selective updating of heterogeneity at locations and levels of detail sensitive to the available data, otherwise leaving the prior model unchanged as desired. The efficacy of our proposed approach is demonstrated with synthetic and field applications. The synthetic example is the SPE benchmark Brugge field case. The field example involves a North Sea reservoir with multiple seismic surveys. For both the synthetic and field case, the advantages of incorporating the time-lapse variations are clearly demonstrated through improved estimation of the permeability heterogeneity, fluid saturation evolution, and swept and drained volumes. The value of the seismic data integration is demonstrated in the identification of the continuity of reservoir sands and barriers, and by the preservation of geologic realism in the calibrated model.

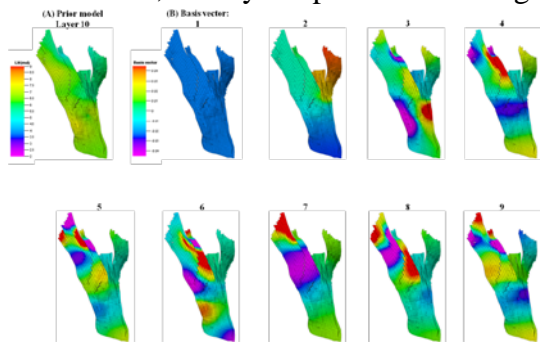


Fig. 1: (A) Layer 10 of the prior permeability model: North Sea Reservoir. (B) The leading basis vectors constructed using the prior together with the grid connectivity information.

**Elasticity and damping of acoustic modes in granular materials with applications to oil recovery.**

David Johnson, *Schlumberger*, Hernan Makse, *City College of New York*, and  
John J. Valenza, *Schlumberger*

The goal of this project is to develop a theoretical and experimental understanding of sound propagation, elasticity and dissipation in granular materials. The topic is relevant for the efficient production of hydrocarbon and for identifying and characterizing the underground formation for storage of either CO<sub>2</sub> or nuclear waste material. We employ a set of experimental and theoretical concepts including the dynamic effective mass of granular media, normal modes analysis, and numerical simulations based on Discrete Element Methods to study acoustics and dissipation in granular media. We have analyzed the acoustic response of a cavity filled with a loose granular material and derived expressions of the effective mass in terms of the complex valued normal modes of the confined granular medium. The theory accurately predicts the frequencies, widths, and relative amplitudes of the various mode resonances. A set of computer simulations has been performed to test the theory and finds agreement with theoretical and experimental results.

## **Porous Rocks with fluids: The Emergence of Digital Rock Physics**

Amos Nur  
*Stanford University*

The need for Rock Physics information is growing exponentially for oil and gas exploration and production as well as a much better understanding of crustal processes in general. However physical measurements of rock properties and pore scale processes in the lab are cumbersome (2 or 3 phase flow), and often impossible to do (shales) or do well (micritic carbonates). Consequently rock property data sets are very sparse: what is needed are properties not for 10's of samples but 1000's or tens of thousands samples.

With the advent of higher resolution 3D imaging technology and faster computing technology it is becoming obvious that the most promising way to obtain massive data sets in the future is through the emerging digital rock physics methodology. At Stanford we have been developing this methodology over the past 15 years. What is involved is very high-resolution 3D (< micron down to nanometers) and very fast imaging of the pore spaces of cores, plugs, or cuttings, followed by using the images to (a) accurately compute bulk properties very fast (minutes) and (b) accurately simulate pore scale processes (relative perm, fine migration, Formation damage, Compaction associated with production; the injection of CO<sub>2</sub>, steam, and water, diagenetic processes and chemical reactions in pore spaces) also very fast (tens of minutes).

The most immediate impact of this emerging technology is to (1) transform routine and special core analysis as practiced today, (2) obtain permeability logs from cuttings at the well head in quasi real time, (3) rigorously link logs and rock properties, (4) link log and rock properties and seismic to look away from the borehole, (5) significantly enhance the interpretations of time-lapse InSar, EM, Gravity and Seismic, including the monitoring of sequestered CO<sub>2</sub> and associated sub surface pore pressure changes.

In the future a much broader range of applications will emerge including such diverse long standing challenges as up-scaling from pore to seismic to reservoir scales, linking pore scale diagenesis to basin analysis, simulate nanobots migration in actual pore spaces, model fault healing, simulate partial melting, or explore such outstanding issues as the physics of rate and state friction and aftershocks.

## A new probe for characterizing rock elasticity: Time of Flight Modulation

Paul A. Johnson<sup>1</sup>, Tim W. Darling<sup>3</sup>,  
Collaborators: P-Y. LeBas<sup>1</sup>, W. Carey<sup>1</sup>, G. Renaud<sup>2</sup>, R. Guyer<sup>1,3</sup>, L. Ostrovsky<sup>4</sup>, K. E.-A. Van Den  
Abeele<sup>5</sup>, J. Riviere<sup>1</sup>

<sup>1</sup>*Los Alamos National Laboratory*, <sup>2</sup>*University of Rotterdam, Netherlands*  
<sup>3</sup>*University of Nevada, Reno*, <sup>4</sup>*NOAA Earth Science Research Laboratory, Boulder CO*  
<sup>5</sup>*Catholic University, Leuven, Belgium*

Unraveling the physics of an earthquake source, reliable sequestration of CO<sub>2</sub>, predicting wellbore breakout in oil and gas reservoirs, monitoring thermal damage to rock in nuclear waste storage, and probing cement integrity require new approaches to material characterization and imaging. The elastic nonlinear response (anelasticity) is highly promising in this regard, as there is no more sensitive measure of material mechanical integrity. The elastic nonlinear response is also highly sensitive to moisture content as well as effective pressure. A persistent problem has been a quantitative relation between elastic nonlinearity and modulating influences including mechanical integrity, because a physics-based theory does not yet exist; however, a recent breakthrough, termed *Time of Flight Modulation* (also termed *Dynamic Acousto-Elasticity*, *DAE*), has significant implications for development of a physics based theory, and thus ultimately to our ability to quantitatively relate nonlinear response to material integrity, moisture content and effective pressure. Previous approaches contained in the toolkit termed Nonlinear Elastic Wave Spectroscopy provide information about the average material elastic response. This is also true of quasi-static approaches. In contrast, DAE captures the full dynamic nonlinear response through a stress wave cycle. We are developing DAE for application to reservoir and non-reservoir materials in order to fully characterize their elastic behaviors in a manner previous not possible. We will describe recent experimental results that illustrate the surprising details of elastic behavior and the power of the new approach. We expect that the outcome of this work will be a major advance in the domain of nonlinear mesoscopic elasticity and will be important for OBES interests in wellbore collapse, near wellbore fracture conduits, CO<sub>2</sub>-induced mechanical changes and cement integrity.

## Acoustic studies of the behavior of Berea sandstone in an extremely dry state

Tim W. Darling<sup>1</sup>, Paul A. Johnson<sup>2</sup>, Rachel A. Miller<sup>1</sup>

<sup>1</sup>*University of Nevada, Reno and* <sup>2</sup>*Los Alamos National Laboratory*

Acoustic linear and nonlinear measurements of the mechanical responses of rock show us a wide range of complex behaviors which are linked, through modeling, to fundamental nonlinear and hysteretic elements. In this sense the behavior is ubiquitous yet many possible known mechanisms may be involved in the list of elemental nonlinear units. A persistent problem has been a quantitative relation between elastic nonlinearity and modulating influences including mechanical integrity, because a physics-based theory does not yet exist. Porous rocks such as sandstones add large surface energy contributions, coupling chemistry and strain. Water, potentially implicated in bulk-fluid anelastic effects may have very large influences at the few to sub-monolayer coating levels. Reducing the amount of water in sandstones of  $\sim$  square meters/g specific area and low gas permeability to these levels is time consuming and has rarely been attempted with large ( $>$  several cm) samples to pressures better than about  $10^{-6}$  Torr. We use a multistage UHV system with a bakeable chamber, RGA analysis of the actual gas evolution and resonance and TOF measurements of the properties of a sandstone sample. The Berea sandstone sample is mechanically dominated by quartz cementation bonded grains. The well documented nonlinear response of this rock at low stresses implicates the cemented links rather than the grains. We observe a rapid change in the elastic and anelastic response upon evacuation supporting a surface effect. The rock reached a state where the room temperature pressure was well in the UHV regime ( $3 \times 10^{-9}$  Torr). While the amount of water evolved increased minimally as the temperature was raised, a dramatic change in the response of the rock at temperatures near 40C appeared. The rock softened dramatically and the nonlinear behaviors (distorted peak, “memory” effects, etc.) diminished. This is a very low temperature for an activated, reversible process. We will discuss the consequences of this surprising result and implications for OBES interests in terms of an improved understanding of the coupling between mechanical integrity and surface chemistry in near-surface porous rocks.

## Evolution of Pore Structure and Permeability of Rocks under Hydrothermal Conditions

Brian Evans, Yves Bernabe, and Uli Mok, *Massachusetts Institute of Technology*

Rock permeability is a dynamic property whose changes occur by diverse mechanisms, including elastic and inelastic deformation, chemical interactions of the rock with pore fluids, and metamorphic reactions between the mineral phases. Thorough understanding of both engineering and scientific applications requires accurate kinetics and constitutive laws for each mechanism and detailed description of the coupling between rate of change of porosity and of other bulk properties. Our current work focuses on the evolution of permeability during cataclasis and pressure solution, on the effective pressure law in tight reservoir sandstones, and on the effect of metamorphic reactions and crack healing on transport.

In initial calculations of pressure solution at a single pair of axi-symmetric asperities, we combined Lehner's theoretical model and contact mechanics to provide a realistic and accurate stress distribution at the contact. The model explicitly coupled diffusion transport and mineral dissolution along the fluid-laden boundary. Results indicated that long-duration transients in strain rate may exist, and that simple interpretations of laboratory tests may be misleading. The long-term behavior approaches an analytical expression by *Lehner and Leroy [2004]*. Subsequent numerical models simulate creep deformation of random packs of mono-disperse or poly-disperse spheres. At each step, the number of grain contacts and the elastic displacements are computed. The LL equation is then applied to each contact and global compaction monitored with time. At regular time intervals we simulate fluid flow in the model pack using a lattice-Boltzmann technique. The volumetric strain rate that results is a complex function involving both transient creep at the contacts and changes in coordination number of the grain contacts. Increases in the latter are sometimes quite large, resulting in decreased mean normal force at grain contacts, and, also, in strong decelerations of compaction rate and lowered permeability; such effects are often not included in constitutive laws. To compare with the numerical calculations, we conducted two suites of experiments.

The first set monitored deformation at the contact region formed when a convex quartz lens was pressed against a flat quartz surface under hydrothermal conditions: at 425°C and 150 MPa fluid pressure for times up to 400 hours. We continuously monitored deformation and the evolution of several different boundary morphologies, including polished flats, etched and roughened flats, and an island-channel structure fabricated by precision plasma etching. The island-channel structure had square pillars of quartz, either 4 or 8  $\mu\text{m}$  on a side, surrounded by an interconnected grid of open channels of comparable width. This geometry introduces stress concentrations within the intergranular contact and dramatically reduces the diffusional path length within the solid-to-solid contact region from that present with polished, flat surfaces. The relative motion between the quartz flat and lens was monitored using optical interferometry. Contact spot radius ranged from 25  $\mu\text{m}$  to 60  $\mu\text{m}$  and mean effective normal stress at the contact ranged from 800 MPa to 150 MPa. For all morphologies, the shapes of the surface structures in both the loaded and unloaded regions evolved, probably owing to capillarity forces. Smooth interfaces never exhibited convergence by pressure solution. When an interconnected island-channel structure was initially imposed, the open, fluid-filled, boundary structure was destroyed in all, but one experiment. Deformation at the interface between the two grains was observed in only two

experiments. In the first case, deformation at the boundary involved significant cataclasis within and adjacent to the pillars and the deformation rate decreased rapidly with time. However, in a single instance, there was clear evidence of pressure solution deformation without cataclasis. Although further work is needed to confirm these results, two variables seem to be important: roughness of the interface between the two grains and details of the chemistry of the pore fluid. In the second suite of experiments, we completed measurements of permeability reduction in cracked Sioux quartzite under isostatic compression. Experiments have been done for periods as long as one week at  $T=100-550^{\circ}\text{C}$ ,  $P_c=30-300\text{ MPa}$ , with water as a pore fluid, and  $P_f=10-250\text{ MPa}$ . In these experiments the Darcy velocity and the quantity of pore fluid moving through the rock were small. In all experiments, permeability decreased at rates that accelerated independently with increases in time, temperature, effective pressure and pore fluid pressure. The accelerating rate of permeability decrease could be attributed to decreasing connectivity of the crack network.

Detailed interpretations of the experimental and numerical results mentioned above require improved knowledge of permeability in elastically deforming rocks. We devised a new method for measuring the (possibly non-linear) effective pressure law for permeability, applied it to tight reservoir sandstones and assessed the validity of various pressure dependence models, with the somewhat negative result that a single, "universal" model cannot be identified. The most frequently validated models were the empirical power law and Walsh's microcrack model. We need now to investigate whether or not these models correspond to unambiguous microstructural characteristics. Lastly, owing to the mounting importance of  $\text{CO}_2$  sequestration projects, there is an increasing need for experimental data on the permeability of rocks saturated with a brine- $\text{CO}_2$  mixture and its evolution with time. As a preliminary step, we performed experiments to investigate changes in relative permeability of a fissured rock produced by temperature variations and associated exsolution of immiscible  $\text{CO}_2$ .

## **Evolution of Permeability and Pore Structure of Porous Limestone at Elevated Temperature**

Harrison Lisabeth, Audrey Ougier-Simonin and Wenlu Zhu,  
*University of Maryland College Park*

With increasing pressure and temperature, rocks undergo a transition in failure mode from localized brittle fracture to non-localized plastic flow. In the brittle regime, localized fracturing is generally accompanied by dilatancy and permeability enhancement, but non-localized cataclastic, shear-enhanced flow could induce significant reduction of void space and permeability. In this study, we deformed porous Indiana limestone samples with initial porosity of ~16% at temperatures of 298, 323 and 348 K under confining pressures ranging from 10 to 120 MPa. In each deformation test, pore fluid (distilled water) pressure and strain rate remained constant at 10MPa and  $1 \times 10^{-5}$ /s. We use both strain gauges and pore pressure intensifier to track pore volume change during deformation. Simultaneous changes in permeability and sonic velocity were measured in a subset of samples. In comparison to dry samples, our data show lower yield strength and enhanced compaction in water-saturated samples, and these effects are exacerbated at elevated temperature. The initial yield envelopes (in the differential versus effective mean stress domain) indicate a strong temperature-dependence of yield strength. Furthermore, the shape of a yield envelope changes considerably with increasing temperature, indicating a transition in dominant deformation micromechanism. Initial microstructural analysis shows that both dilatant microcracking and mechanical twinning play a role in the bulk behavior of the material. We suggest that increased water-weakening at elevated temperatures is the result of the interplay of crystal plasticity, microcracking and pore collapse with chemically active pore fluid. Stress-induced changes in permeability and its anisotropy in carbonate rocks can be significantly different from siliciclastic rocks owing to the interplay between microcracking, crystal plasticity and pore collapse.

Other topics investigated include quantifying the failure process in which accumulation and coalescence of microstructural damage leads to macroscopic fracture. A new deformation loading configuration, the lateral relaxation path, was devised. Under the new loading path, a rock sample is deformed to failure as differential stress increases with decreasing effective mean stresses. Experimental results show that porous rocks subjected to such a lateral relaxation loading exhibit a rather stable post-yielding fault growth, which provides a window of opportunity for studying the correlation between the accumulation of microscopic damage and the formation of macroscopic fracture.

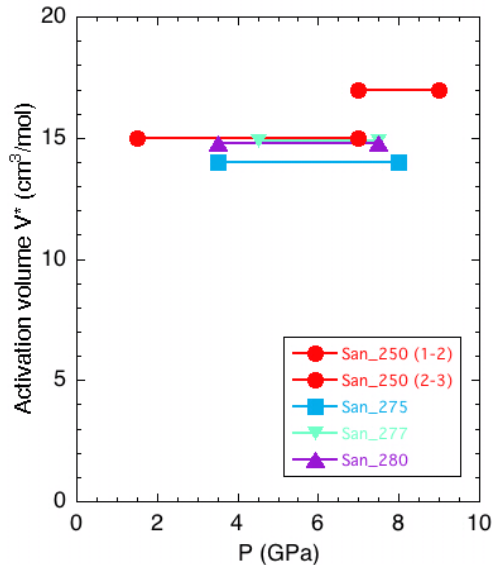


## How pressure affects the strength of dry olivine at upper mantle conditions

W.B. Durham and N. A. Dixon, *Massachusetts Institute of Technology* and D.L. Kohlstedt, A. Suzuki and S. Mei, *University of Minnesota*

We conduct experiments aimed at constraining the effect of pressure on the ductile flow of dry olivine under extremely high pressure. Olivine is the primary constituent of the upper mantle and its rheological behavior is fundamental to upper mantle dynamics. The effect of hydrostatic pressure  $P$  on ductile strength is not as pronounced as at crustal pressures where brittle fracture limits strength, but the pressure change from top to bottom of the upper mantle is large (nearly 15 GPa), so even a small pressure sensitivity can mean a very large viscosity change. Physically, we can expect that compressing the olivine lattice changes the activation energy  $E^*$  of thermally activated creep by an amount  $PV^*$ , where  $V^*$  is called the activation volume. Thus if flow strength  $\dot{\epsilon}$  at fixed temperature  $T$  and fixed other conditions is  $\dot{\epsilon} = A \cdot \exp(E^*/RT)$ ,  $A$  being a constant and  $R$  the gas constant, then at pressure  $P$  the strength will be  $\dot{\epsilon} = A \cdot \exp((E^* + PV^*)/RT)$ . A value of  $V^* = 10 \text{ cm}^3/\text{mol}$ , for example means a viscosity contrast of nearly four orders of magnitude. For  $V^* = 20 \text{ cm}^3/\text{mol}$ , the contrast grows to over eight orders of magnitude. Such a contrast cannot exist, of course, because the mantle is not isothermal. What  $V^*$  ultimately tells us therefore is the thermal structure of the mantle, and the effects on dynamics that follow.

Figure 1 shows  $V^*$  as calculated from the four pressure-stepping tests we have conducted over the past 1.5 years. Our experiments are done in the D-DIA apparatus at the X17B2 beam line at the National Synchrotron Light Source, Brookhaven National Lab. These results are less scattered and individually far better resolved than measurements made earlier, owing to significant improvement to hardware and techniques. These, and related measurements made by us, speak to several effects that will help us provide a full rheological description of the upper mantle, including the putative pressure dependence of  $V^*$  (which appears not to exist within the resolution of Figure 1), and changes in mode of deformation (namely dominant slip system) with changing pressure. Another accomplishment of these experiments beyond constraining mantle dynamics is establishing the maturity of the synchrotron-based strength measurement technique that we have been developing during the course of this work. It has reached a level of accuracy and utility that benefits the study of strength of all materials at extreme conditions.

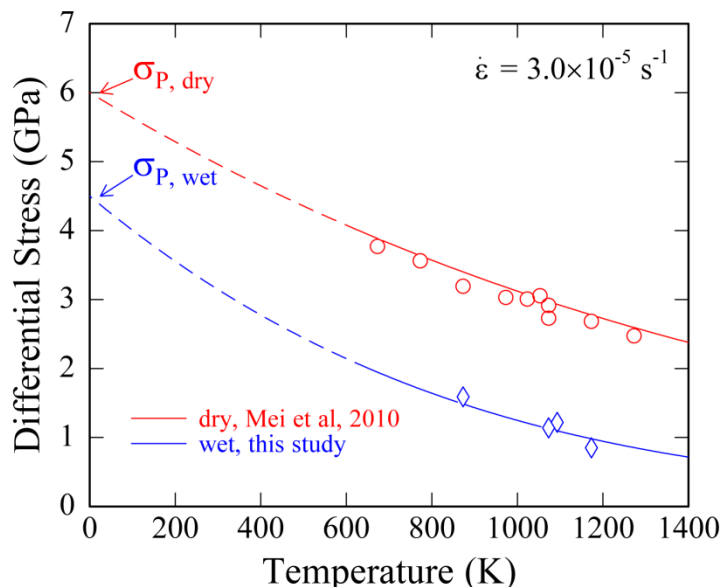


**Figure 1.** Calculated values of  $V^*(P)$  based on strength measurements at 1173-1273 K. Individual measurements of strength are given by the dots. Individual calculations of  $V^*$  are made between pairs of points, indicated by tie lines. Pairs are always from the same run, to minimize the effect of sample variability. The indicated value of  $V^*$  is  $15 \pm 5 \text{ cm}^3/\text{mole}$  including uncertainties not shown, with no detectable pressure dependence. Calculations of  $V^*$  between points where individual flow strengths were measured.

## The influence of water on the Peierls stress of olivine at high pressures

Shenghua Mei, A. M. Suzuki, L. Xu, and D. L. Kohlstedt, *University of Minnesota* and  
N. A. Dixon and W. B. Durham, *Massachusetts Institute of Technology*

To investigate the influence of water on the low-temperature plasticity of olivine under lithospheric conditions, we carried out a series of creep experiments on polycrystalline olivine at high pressures (~6 GPa), relatively low temperatures ( $673 \leq T \leq 1173$  K), and hydrous conditions using a deformation-DIA. Samples were fabricated from fine powdered San Carlos olivine under hydrous conditions. In the experiments, a sample column composed of a sample and alumina pistons was assembled with a talc sleeve and graphite resistance heater into a 6.2-mm edge length cubic pressure medium. Experiments were carried out at the National Synchrotron Light Source at Brookhaven National Laboratory. In a run, differential stress and sample displacement were monitored *in-situ* using synchrotron x-ray diffraction and radiography, respectively. The low-temperature plasticity of olivine under hydrous conditions is constrained by our data with a value for the Peierls stress of  $4.5 \pm 0.3$  GPa. This value is much lower than those reported for olivine under anhydrous conditions (6 – 15 GPa, *Evans and Goetze, 1979; Raterron et al., 2004; Mei et al., 2010*). Comparison of low-temperature plasticity of olivine under both anhydrous and hydrous conditions is given in Figure 1. The figure shows a significant influence of water on the low-temperature plasticity of olivine. The low-temperature flow behavior of olivine under hydrous conditions quantified in this study provides a necessary constraint for modeling the dynamic activity occurring within regions of lithospheric mantle where water might be present, such as beneath mid-ocean ridges and along subducting slabs.



**Figure 1.** Comparison of low-temperature plasticity of olivine under both anhydrous and hydrous conditions at a given strain rate of  $3 \times 10^{-5}$  /s.

## **MicroCT imaging of porous sandstone and limestone: Implications on permeability evolution and mechanical damage**

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MicroCT can be used to characterize the geometry of the pore space of a sedimentary rock, with resolution that may be sufficiently refined for the realistic simulation of permeability based on the 3D image. Previous studies have focused on porous sandstone, and significant advances have been made on the characterization of pore size distribution and connectivity, development of techniques such as lattice Boltzmann method to simulate permeability, and its upscaling. *Sun, Andrade and Rudnicki* (2011) recently proposed a multiscale method that dynamically links these three aspects, which were often treated separately in previous computational schemes. After geometric attributes of the connected pore space had been extracted, a hybrid lattice Boltzmann/finite element scheme was developed to calculate a homogenized effective permeability. When applied to the microCT data of Fontainebleau sandstone acquired by *Lindquist et al.* (2000), this multiscale method has proved to be computationally efficient and our simulations has elucidated the relation among permeability, pore geometry and connectivity. We are currently extending the computational scheme to also include the hybrid modeling of electrical conductivity and formation factor, which would allow one to consistently simulate the hydraulic and electrical transport using the multiscale method.

In comparison to sandstone, the pore geometry of a porous carbonate rock is very complex and its 3D imaging poses significant challenge. Typically the pore space includes micropores well below the microCT resolution, and it is unlikely one can realistically simulate the transport properties on the basis of the images. Nevertheless, microCT imaging has proved to be useful for characterizing the mechanical damage. We studied the pore structure in intact and inelastically compacted Indiana limestone. Guided by detailed microstructural observations and using a global thresholding method, the 3D images acquired at voxel resolution of 4  $\mu\text{m}$  were segmented into three domains: solid grains, macropores and an intermediate zone dominated by microporosity. The macropores were individually identified by morphological processing and their shape quantified by their sphericity and equivalent diameter. Our new data revealed a significant reduction of the number of macropores in hydrostatically and triaxially compressed samples with respect to the intact material, in agreement with previous microstructural analysis and a micromechanical model for cataclastic pore collapse. The intermediate (microporosity) domains remained interconnected in compacted samples. Our data suggest that the inelastic compaction in Indiana limestone is manifested by not only a decrease in the volume fraction of the microporosity backbone, but also a corresponding decrease in its thickness.

## **Anisotropy in shales: from microstructures to seismic signature.**

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Anisotropy in clay-rich sedimentary rocks is receiving increasing attention because of significance for prospecting of petroleum deposits as well as seals in the context of nuclear waste and CO<sub>2</sub> sequestration. The orientation of component minerals is a critical factor but, largely because of small grain size and poor crystallinity, the orientation distribution of clay minerals has been difficult to quantify. A method has been developed that relies on hard synchrotron X-ray to obtain diffraction images. The crystallographic Rietveld method is used to deconvolute diffraction patterns and extract quantitative information about phase fractions and preferred orientation (or fabric) of constituent phases.

Anisotropy also relies on orientation of high aspect ratio pores, including fractures and organic materials. The synchrotron X-ray microtomography can be applied to quantify 3D structures and distribution to a resolution of 1 micron. The information of various components obtained from synchrotron X-ray methods can then be used to model macroscopic physical properties. A self-consistent averaging method is now being developed to calculate elastic properties of shales, based on volume fractions, orientation distribution of phases, and shape distributions of clay minerals and pores, to establish a quantitative relationship between microscopic fabric features and macroscopic properties. Results calculated from the self-consistent model are then compared to the elastic properties obtained by ultrasonic measurements in order to show the similarity and discrepancies. The method has been applied to a wide variety of shales to explore the influence of clay content, burial depth, and maturity. The shales range from hydrocarbon-rich shales from Texas, the North Sea, Nigeria, Germany, and Saudi Arabia, as well as shales from European laboratories that investigate suitability of shales as potential nuclear waste repositories (Meuse / Haute-Marne Underground Research Laboratory near Bure, France, and Benken and Mont Terri Rock Laboratory, Switzerland).

## Imaging Particle Swarms in Fractures with Miscible and Immiscible Fluids

Laura J. Pyrak-Nolte, Eric Boomsma, and Nolan Teasdale  
*Purdue University*

Immiscible fluids occur either naturally (e.g. oil & water) or from anthropogenic processes (e.g. liquid CO<sub>2</sub> & water) in the subsurface and complicate the transport of natural or engineered micro- or nano-scale particles. In this study, we examined, experimentally, the effect of fracture aperture and immiscible fluids on the formation and evolution of particle swarms in a fracture. A particle swarm is a collection of colloidal-size particles in a dilute suspension that exhibits cohesive behavior. Swarms fall under gravity with a velocity that is greater than the settling velocity of a single particle. Thus a particle swarm of colloidal contaminants can potentially travel farther and faster in a fracture than expected for an emulsion of colloidal particles. For uniform aperture fractures saturated with water, there is a range of optimal fracture aperture to swarm diameter ratio,  $B$ , ( $B = 2.5$  to  $10$ ) which suppresses bifurcation or breakdown of a swarm. This suppression is attributed to forces from the walls that keep the swarm from expanding and help maintain the swarm's mass distribution. Below this optimal range, drag forces from the wall dominate and constrain the expansion of the swarm to one direction. An ellipsoidal torus results in a mass distribution that leads to bifurcations. Above the optimal range, the swarm is not confined by the fracture walls and is free to expand uniformly in all directions. This leads to multiple bifurcations after the swarm has fallen only a short distance. For a uniform fracture filled with immiscible fluids, swarms were spherical, remained coherent and decreased in speed until as they came to rest on the oil-water interface. After the interface between a swarm and the oil thinned sufficiently, the swarm was rapidly released into the water. The swarm geometry and velocity in the water layer depended on the aperture of the fracture, the oil viscosity and the hydrophobicity or hydrophilicity of the particles in the swarm. Hydrophobic beads result in multiple mini-swarms after breaking through the interface rather than a single large swarm like that observed for hydrophilic swarms.

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## **Statistical Physics Models for Damage, Fracture, and Fracking in Rocks: Bumps on the Road to Energy Independence**

John B Rundle, JD Gran and JR Holliday, *University of California, Davis and  
William Klein, Boston University*

The processes by which rocks deform and fail under load are of critical interest to a large number of energy and resource recovery and utilization problems. Applications range from the microscale, where we wish to understand laboratory processes of fracture and friction to improve drilling and carbon sequestration technology, to the macroscale, the scale upon which tectonic earthquakes threaten nuclear power plants and other critical energy facilities. In fact, the subject of earthquakes has acquired new importance to the DoE as a result of the process of hydrofracking. Fracking appears to be associated not only with the increased production of natural shale gas, but also of earthquakes, which for the first time represent an environmental concern associated with significant energy production. Recent examples can be found in northeastern Oklahoma, Ohio, and other previously seismically quiescent locations.

The mechanics of rock deformation involve the growth and mobility of damage, defects, dislocations and other modes of fracture and bulk failure in response to applied stress and thermal forcings. These processes can be understood and modeled using the methods of statistical physics. Sudden failure can be understood as a kind of first order phase transition of the bulk structure of the material. Scaling statistics, which are often observed in rock dynamics, are also characteristic signatures seen in many other phase transitions near critical points.

In our research program, we use data, theory, and numerical simulations to develop an understanding of the basic processes. For example, during this period we have focused on new models of sliding friction, in which the clusters of failing asperities on the frictional interface can be identified with percolation clusters. Using a model in which a major sliding event induces a weakening of the failure threshold, we find that the amount of weakening is a scaling field similar to the pressure  $P$  in a thermal phase transition, or the external  $H$ -field in magnetic phase transition. Under certain conditions, we also find that the scaling exponents for the clusters of slipped asperities are the same, within error, to the values for mean field percolation.

We have also focused on tensile fracture, extending a model that was first proposed by us in 1989. Here we find that, depending on the physics of the cohesion or pinning force, a variety of symmetry-breaking transitions can be identified and understood. Several of these transitions were seen previously in studies of Ising models. Finally, we also apply a coarse-grained version of the model to the fracking problem. We find that growth of the frack is similar to the problem of surface growth using either particle deposition or percolation cluster growth, as obtained from the Leath algorithm. We find that the scaling exponent of the correlation function for the surface growth tensile field is similar to values obtained from particle deposition on a surface as described by the Kardar-Parisi-Zhang equation.

## **The Effect of Defects on Phase Kinetics, Fracture and Gutenberg-Richter Scaling**

William Klein, *Boston University*

In materials such as rocks the role of defects in processes such as fracture and phase transitions is very poorly understood. The same statement can be made about other materials such as metals used in nuclear reactor containment vessels and equipment in the toxic environments associated with natural gas and oil wells. In order to better understand the role of defects in these processes we have pursued an integrated theoretical and computational approach to understanding fracture and phase transition kinetics in materials with defects. I will report on our progress in studying two distinct classes of models for these processes. One is a thermodynamic system in which we have introduced defects and studied nucleation and unstable state evolution. The second is a driven system in which stress is applied and fracture is studied. As a byproduct of our fracture studies we have developed a new approach to Gutenberg-Richter scaling which I will also discuss.

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## **Particle jamming in flow through geological fractures**

Joel Koplik - *City College of New York*

Realistic reservoir fluids contain suspended particles which may accumulate and clog the pore space of a fracture, impeding the extraction of water or hydrocarbons. We have begun to study this process at the particle level, using lattice Boltzmann simulations of spherical particles suspended in a Newtonian fluid and driven through a fracture with self-affinely rough walls. Particles are trapped in regions where the aperture narrows, and we study the resulting deposit, in terms of growth rate, flow reduction, force chains, stress exerted on the fracture walls, effects of gravitational sedimentation, and response to perturbations in the driving pressure gradient. A key focus is the correlation between neighboring jamming sites and their relation to flow channeling induced by roughness.



## Fingering and fracturing in granular media

Ruben Juanes

*Massachusetts Institute of Technology*

This talk will cover two recent results.

The first is a *macroscopic phase-field model of partial wetting* that permits describing the statics and dynamics of two-phase flow in a capillary tube. Drops and bubbles are non-spreading, local, compactly supported features. They are also equilibrium configurations in partial wetting phenomena. Yet, current macroscopic theories of capillary-dominated flow are unable to describe these systems. We propose a framework to model multiphase flow in porous media with non-spreading equilibrium configurations. We illustrate our approach with a one-dimensional model of two-phase flow in a capillary tube. Our model allows for the presence of *compactons*: non-spreading steady-state solutions in the absence of external forces. We show that local rate-dependency is not needed to explain globally rate-dependent displacement patterns, and we interpret dynamic wetting transitions as the route from equilibrium, capillary-dominated configurations, towards viscous-dominated flow. Mathematically, these transitions are possible due to non-classical shock solutions and the role of bistability and higher-order terms in our model.

The second is the phenomenon of *capillary fracturing in granular media*. We study the displacement of immiscible fluids in deformable, non-cohesive granular media. Experimentally, we inject air into a thin bed of water-saturated glass beads and observe the invasion morphology. The control parameters are the injection rate, the bead size, and the confining stress. We identify three invasion regimes: capillary fingering, viscous fingering, and “capillary fracturing”, where capillary forces overcome frictional resistance and induce the opening of conduits. We derive two dimensionless numbers that govern the transition among the different regimes: a modified capillary number and a fracturing number. The experiments and analysis predict the emergence of fracturing in fine-grained media under low confining stress, a phenomenon that likely plays a fundamental role in many natural processes such as primary oil migration, methane venting from lake sediments, and the formation of desiccation cracks.

## **Ramification of Stream Networks**

Daniel H. Rothman

*Massachusetts Institute of Technology*

The geometric complexity of dendritic river networks has been a source of fascination for centuries. Yet a comprehensive understanding of ramification---the mechanism of branching by which these networks grow---remains elusive. Progress requires quantitative theory and comparison with unambiguous observations. This talk reports advances made in both realms. Our observational work focuses on thousands of bifurcated streams growing in a 100-km<sup>2</sup> groundwater field. Our theory represents streams as a collection of paths growing and bifurcating in a harmonic field. We predict that streams incised by groundwater seepage branch at a characteristic angle of  $2\pi/5 = 72$  degrees. Our measurements yield a mean angle of 71.8 +/- 0.8 degrees.

This good accord between theory and observation suggests that the network geometry is determined by the external flow field rather than flow within the streams themselves.

## **Optimizing capillary trapping of CO<sub>2</sub> during geological carbon sequestration**

Dorthe Wildenschild, *Oregon State University* and Marcel Schaap, *University of Arizona*

A relatively new mechanism for geologic sequestration of CO<sub>2</sub> is the capillary trapping process, sometimes also referred to as residual trapping or relative permeability hysteresis trapping, which immobilizes CO<sub>2</sub> at the pore-scale, thus preventing large-scale movement of CO<sub>2</sub> within an aquifer. As a sequestration mechanism, capillary trapping has several advantages over structural trapping, including not being affected by potentially compromised reservoir caprock; facilitating enhanced dissolution of gaseous CO<sub>2</sub> into the brine; and allowing gaseous CO<sub>2</sub> to be distributed over a larger reservoir volume, thus enhancing the potential for mineral weathering and carbonate precipitation. To date, relatively few experiments and models have addressed capillary trapping mechanisms in detail and at relevant reservoir conditions. Compared to most current large-scale reservoir studies, the proposed research takes several steps back in scale to observe and model trapping at the pore-scale and to learn how these findings translate into continuum scale properties that can subsequently support improved modeling of sequestration at large spatio-temporal scales.

Our first experiments are conducted at ambient conditions using proxy fluids to explore the effect of varying interfacial tension, viscosity and flow rate on the resulting trapped amount of CO<sub>2</sub>. Simultaneously, we are building an x-ray tomography compatible core holder and experimental setup where we can address similar questions under reservoir conditions, i.e., with CO<sub>2</sub> in its supercritical state. We are using both synchrotron-based and conventional x-ray computed microtomography to quantify trapped CO<sub>2</sub> amount, distribution, and morphology as a function of the three properties (viscosity, interfacial tension, and flow rate).

Supporting pore-scale simulations will be carried out using a multi-phase, multi-component, lattice-Boltzmann (LB) model, modified to handle supercritical CO<sub>2</sub> and consolidated (fine-grained) material (see companion abstract by Marcel Schaap of Univ of Arizona)).

## **Optimizing capillary trapping of CO<sub>2</sub> during geological carbon sequestration: Realistic Equations of State in a Lattice Boltzmann Model**

Marcel G. Schaap, *University of Arizona* and Dorthe Wildenschild, *Oregon State University*

A relatively new mechanism for geologic sequestration of CO<sub>2</sub> is the capillary trapping process, sometimes also referred to as residual trapping or relative permeability hysteresis trapping, which immobilizes CO<sub>2</sub> at the pore-scale, thus preventing large-scale movement of CO<sub>2</sub> within an aquifer. As a sequestration mechanism, capillary trapping has several advantages over structural trapping, including not being affected by potentially compromised reservoir caprock; facilitating enhanced dissolution of gaseous CO<sub>2</sub> into the brine; and allowing gaseous CO<sub>2</sub> to be distributed over a larger reservoir volume, thus enhancing the potential for mineral weathering and carbonate precipitation. To date, relatively few experiments and models have addressed capillary trapping mechanisms in detail and at relevant reservoir conditions. Compared to most current large-scale reservoir studies, the proposed research takes several steps back in scale to observe and model trapping at the pore-scale and to learn how these findings translate into continuum scale properties that can subsequently support improved modeling of sequestration at large spatio-temporal scales.

A companion abstract by Dorthe Wildenschild describes our first experiments regarding the effect of varying interfacial tension, viscosity and flow rate on the resulting trapped amount of super-critical CO<sub>2</sub> or its functional analogs. The current presentation deals with development of functionality into lattice Boltzmann models that to handle the physical conditions found in the experiments as well as relevant pressure and temperatures found in candidate geological reservoirs. The current focus is to test several van der Waals-type Equations of State (EOS, the relation between pressure, density and temperature) for the pure water-vapor and the CO<sub>2</sub> system near their respective critical points. We show that a wide range of conditions can be simulated and demonstrate that liquid and vapor densities and surface tension qualitatively (but not yet quantitatively) agree with published experimental data. Future modifications to the parametrization of the equation of state should lead to a better quantitative match for the water-vapor and CO<sub>2</sub> systems as well as the brine – super critical CO<sub>2</sub> system. After obtaining suitable EOS's the Lattice Boltzmann models will be verified using the tomography results obtained by Wildenschild.

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