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# Basic Energy Sciences

## Roundtable Discussion on *Foundational Research Relevant to SubTER*

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Associate Laboratory Director for Energy Science

Lawrence Berkeley National Laboratory

BESAC July 8, 2015



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# Presentation Overview

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- **What is SubTER?**
  - National Lab working group
  - Four “Pillars” of the initiative
- **BES Roundtable discussion – May 22, 2015**
  - Roundtable results and report overview
- **Grand challenge – imaging stress distributions**
  - What is the problem, and what are the opportunities?
- **Priority Research directions and cross cutting themes**
  - Advancing experimental, theoretical, and computational capabilities suggest new advances are possible
- **Relationship to 2007 Basic Research Needs Report**



# National Laboratory “Big Idea” Summit: March, 2014

- DOE asked the National Lab Chief Research Officers to develop a set of “Big Ideas” to be considered for FY16 investment
- Laboratories developed multi-lab teams for 8 ideas:
  - Advanced Manufacturing
  - Nuclear Energy
  - Climate
  - Energy/Water
  - **Subsurface** → **SubTER\***
  - Grid
  - Energy Systems Integration
  - Transportation
- Summit meeting: **March 12-13, 2014**

Department of Energy  
National Laboratory Ideas Summit  
March 12-13, 2014  
Crystal City Gateway Mall

March 12, 2014		
Time	Topics	Speakers & Location
7:45 am	Registration	
8:30 am	Opening remarks	Mike Knecht Deputy Under Secretary for Science & Energy Plenary room
10:30 am	Break	
10:45 am	Sustainable and secure water management: A sustainable and secure energy/water nexus through superior decision tools and technologies	Speakers TBD Plenary room
11:25 am	Climate change science and adaptation: Enabling regional energy and water resilience to climate change	Speakers TBD Plenary room
12:00 pm	Desk lunch (provided)	Plenary room
1:00 pm	Accelerating materials to manufacture: Beyond Edison: Taking Materials from Lab to Market Twice as Fast	Speakers TBD Plenary room
1:45 pm	Systems Integration: The optimization of energy systems across multiple pathways (electricity, thermal, fuel, water, communications) and time and space scales (campus, city, region)	Speakers TBD Plenary room
2:25 pm	Creating an adaptive and intelligent U.S. electric grid: Evolve the electric grid to be: incorporates clean and distributed energy; adapts to climate and demographic change; eliminates large-scale and long-term backlogs and energy delivery bottlenecks	Speakers TBD Plenary room
3:00 pm	Sustainable transportation: A consumer-driven, carbon-neutral, ground transportation fleet that is fueled by renewable domestic sources	Speakers TBD Plenary room
3:45 pm	Break	
4:00 pm	Subsurface: Control of subsurface fractures and fluid flow	Speakers TBD Plenary room

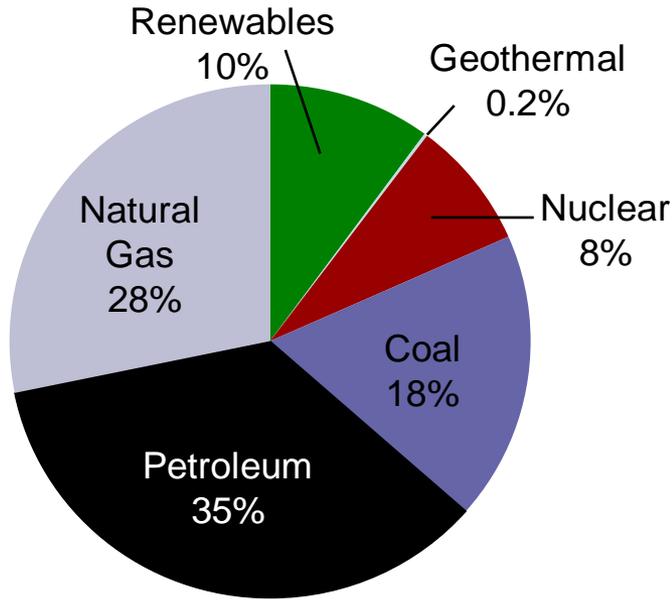
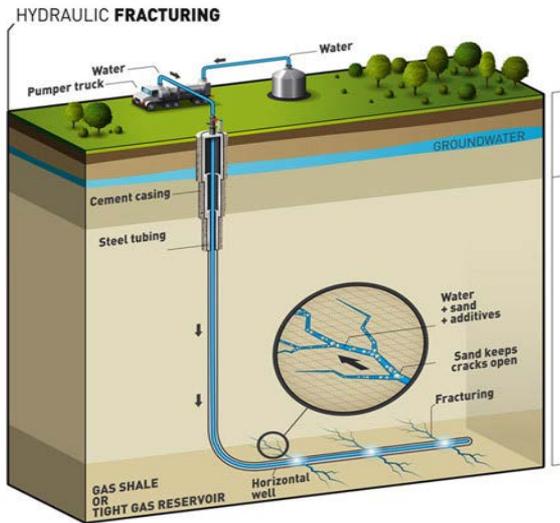
National Laboratory Ideas Summit  
Crystal City Gateway Mall

March 13, 2014	
Topics	Speakers
Opening remarks	Ernest Moniz Secretary of Energy Plenary room
Working group session I	Breakout Rooms
Working group session II	Breakout Rooms
Joint end of working group sessions	Plenary room
Closing remarks	Mike Knecht Deputy Under Secretary for Science & Energy Plenary room

\*SubTER: **S**ubsurface **T**echnology and **E**ngineering **R**D&D **C**rosscutting **T**eam

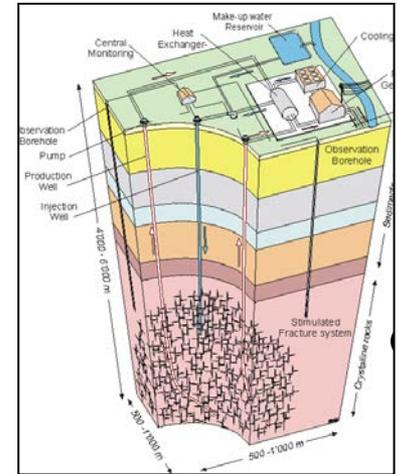
# Subsurface Engineering: Critical for current & future energy systems

## Shale hydrocarbons

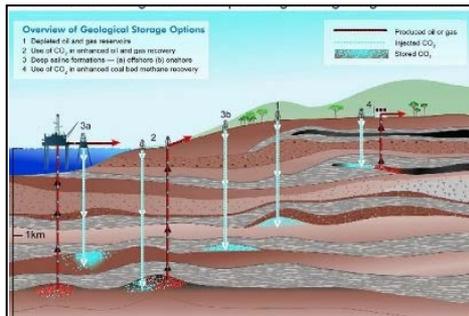


**Primary Energy Use by Source, 2014**

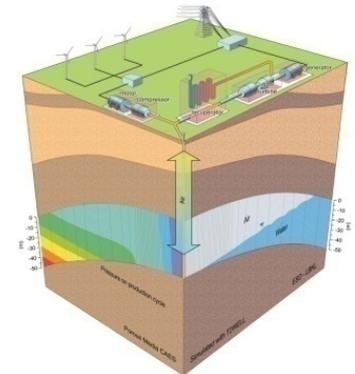
## Enhanced geothermal



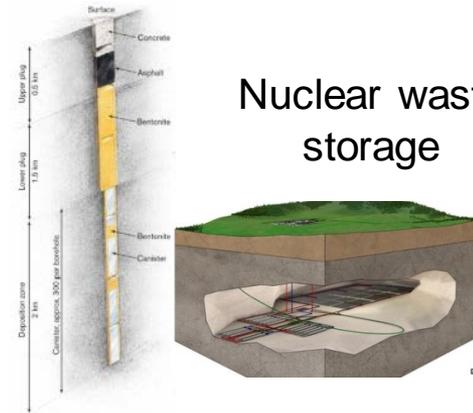
## CO<sub>2</sub> Storage



## Compressed Air Energy Storage

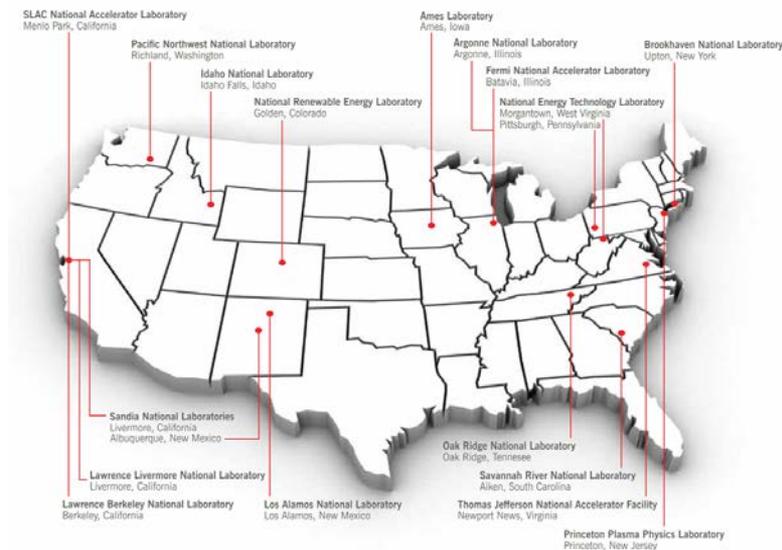


## Nuclear waste storage

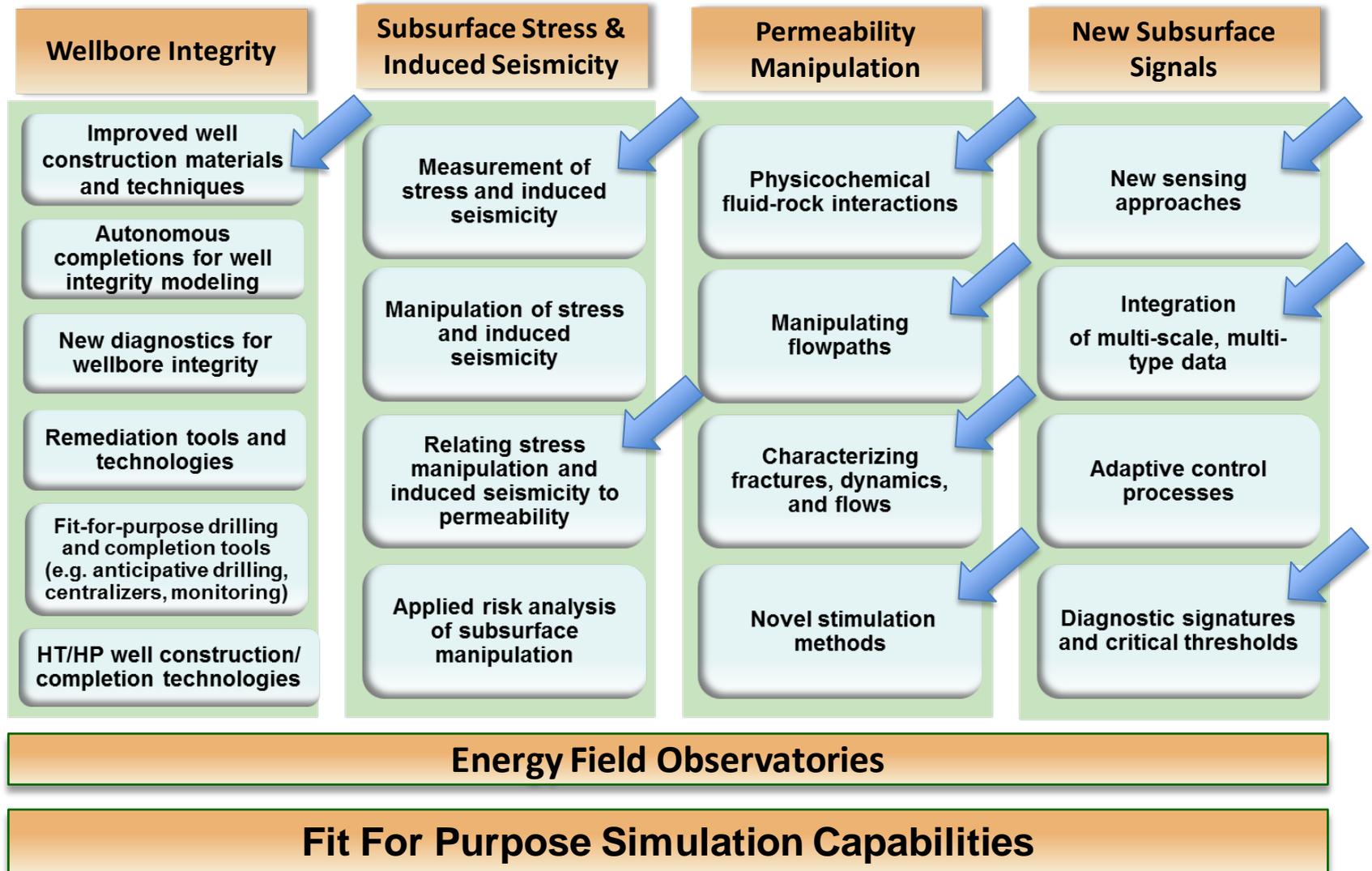


# SubTER Working Team: 13 Laboratories

- ANL:** Randall Gentry
- BNL:** Martin Schoonen
- INL:** Earl Mattson, Hai Huang, Rob Podgorney
- LANL:** Rajesh Pawar, Melissa Fox, Andy Wolfsberg
- LBNL:** **Susan Hubbard (co-lead)**, Curt Oldenburg (deputy), Jens Birkholzer, Tom Daley
- LLNL:** Roger Aines, Jeff Roberts, Rob Mellors, Susan Carroll
- NREL:** Charles Visser
- NETL:** Grant Bromhal, Kelly Rose
- ORNL:** Eric Pierce, Yarom Polsky
- PNNL:** Alain Bonneville, Dawn Wellman, Tom Brouns
- SLAC:** Gordon Brown, Mark Hartney
- SNL:** **Marianne Walck (co-lead)**, Doug Blankenship (deputy), Susan Altman, Moo Lee
- SRNL:** Lisa Oliver, Ralph Nichols



# SubTER Theme: Adaptive Control of Subsurface Fractures and Fluid Flow



# BES Roundtable on Foundational Research / SubTER

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- **Purpose:** Convene national lab, university and industry experts in the geosciences to brainstorm basic research areas that *underpin the goals of the broader SubTER Technology Team efforts*, and are *currently underrepresented* in the BES research portfolio. The output goal is a document with *prioritized research questions* and descriptive narrative that could inform future BES research directions or a potential follow-on workshop.
- **Participants:** By invitation only, approximately **12-15 external scientists (DOE laboratories, university and industry)**. Two co-chairs will help select participants and lead the discussion. Several (3-5) Federal Program Managers from BES, EERE and FE will attend as observers. Total meeting size limited to about 20.
- **Logistics:** DOE Germantown, May 22, 2015 (9:00 – 5:00 pm)
- **Target report completion date:** July, 2015



# BES Roundtable Participants

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## National Laboratory

- Don DePaolo (Co-chair), Associate Laboratory Director for Energy Sciences, LBNL
- Ben Gilbert, Staff Scientist, LBNL
- Joe Morris, Group Leader for Computational Geosciences, LLNL
- Steve Pride, Staff Scientist, LBNL
- Kevin Rosso, Laboratory Fellow and Associate Director for the Chemical and Material Science Division , PNNL
- Andrew Stack, Staff Scientist, ORNL
- Marianne Walck, Vice President California Laboratory and Energy Climate Programs, SNL

## University

- Nicholas Davatzes, Associate Professor, Temple University
- Peter B. Kelemen, Professor and Chair Dept. of Earth & Environmental Sciences, Columbia
- Kate Maher, Assistant Professor of Geological Sciences, Stanford
- Catherine A. Peters, Professor Dept. of Civil and Environmental Engineering, Princeton
- Laura Pyrak-Nolte (Co-chair), Professor of Physics, Purdue
- Wen-lu Zhu, Associate Professor Department of Geology, University of Maryland

## Industry

- Joanne Fredrich, R&D Manager, BP
- James R. Rustad, Scientist, Corning

# Outline - Results of the Roundtable Discussion

## Grand challenge

- Imaging subsurface stress distributions and geochemical processes

## Priority Research Directions

- Nanoporous geomaterials – reactivity, flow and mechanics
- Chemical-mechanical coupling in stressed rocks
- Reactive Multiphase Flow in Fractured Systems

## Crosscutting themes and approaches

- Advanced computational methods for heterogeneous time dependent geologic systems
- Architected geomaterials to address heterogeneity and scaling

# Grand Challenge: Imaging subsurface stress and geochemistry

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- **Problem:**

- The responses of rocks to stresses imposed by fluid injection are determined not only by the rock properties, and the existence of faults and fractures, but by the *ambient state of stress*
- Stress can be inferred from measurements in boreholes, but *cannot be determined in 3D away from boreholes*, and is difficult to monitor *as the system is perturbed*

- **Opportunity**

- *Multi-modal imaging* of the subsurface combined with geologic structure, surface deformation, borehole data and *advanced computing* could lead to new capabilities to “image” stress in 3D and 4D
- Improved knowledge of stress distribution could be major factor in *maximizing yield and minimizing negative impacts*

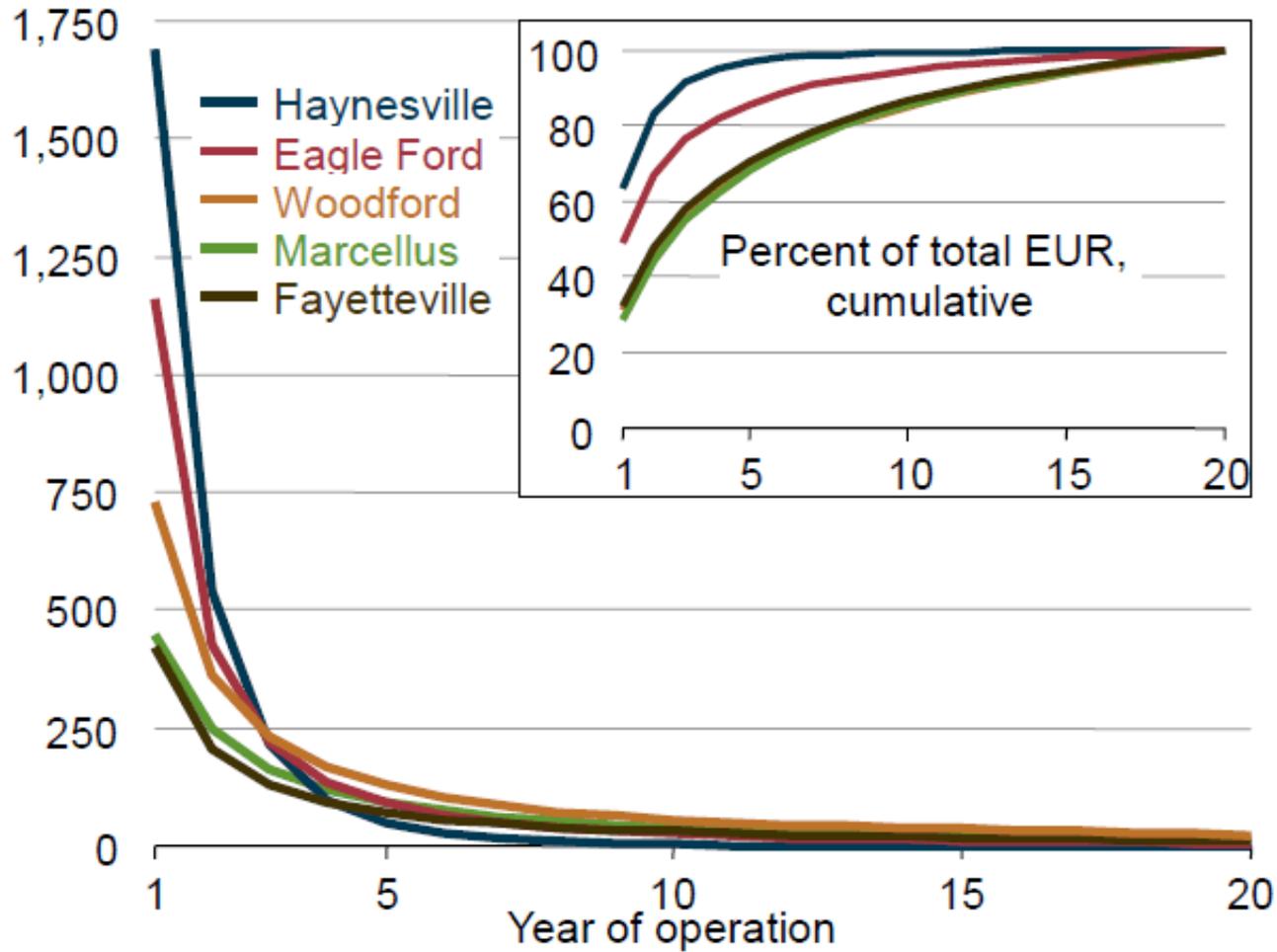
## Fractures and fluid flow in the subsurface are a ubiquitous issue

Conceptualization of hydrofracture for oil and gas extraction from “tight” formations (fine-grained, micro- to nanoporous sedimentary rocks).



What do fracture patterns actually look like? Do fractures stay open? How long? What volume of rock is accessed? How do fluids move into the fractures and into the well?

# Average production curves for shale gas wells from major formations

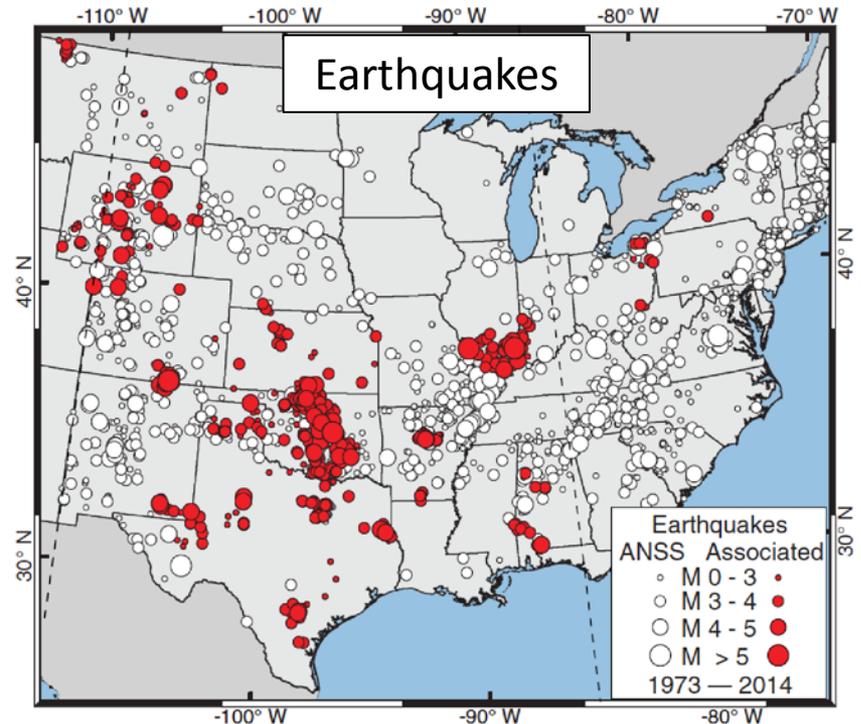
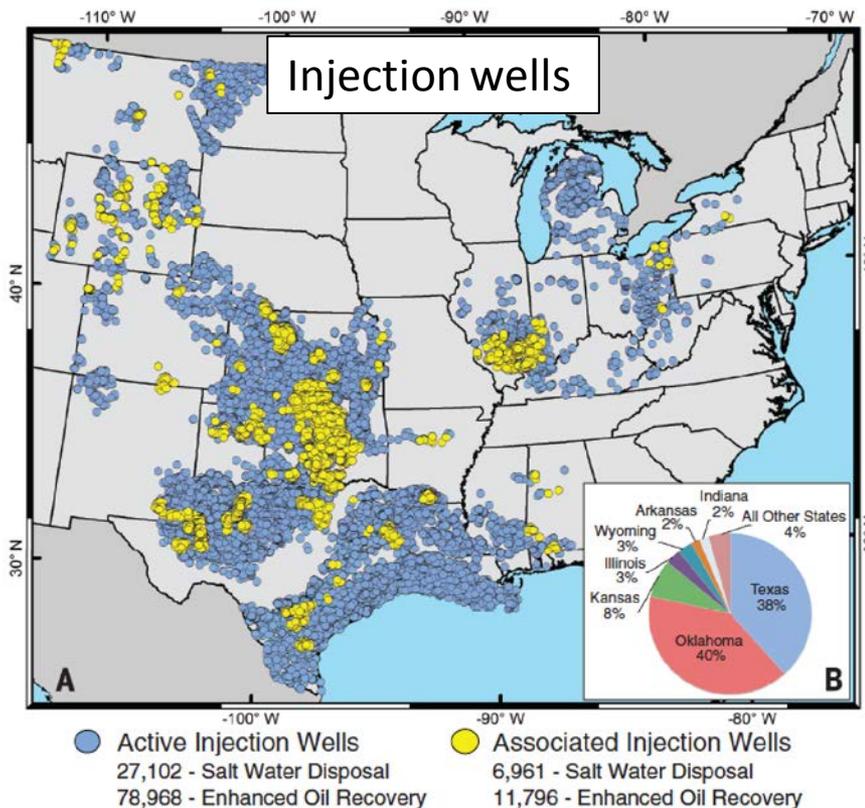
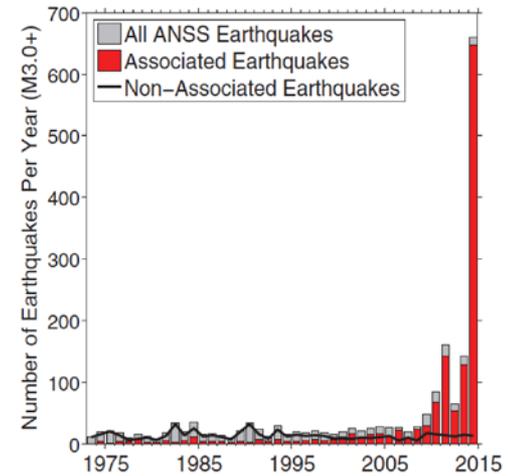


# Induced seismicity in central U.S.

High-rate injection is associated with the increase in U.S. mid-continent seismicity

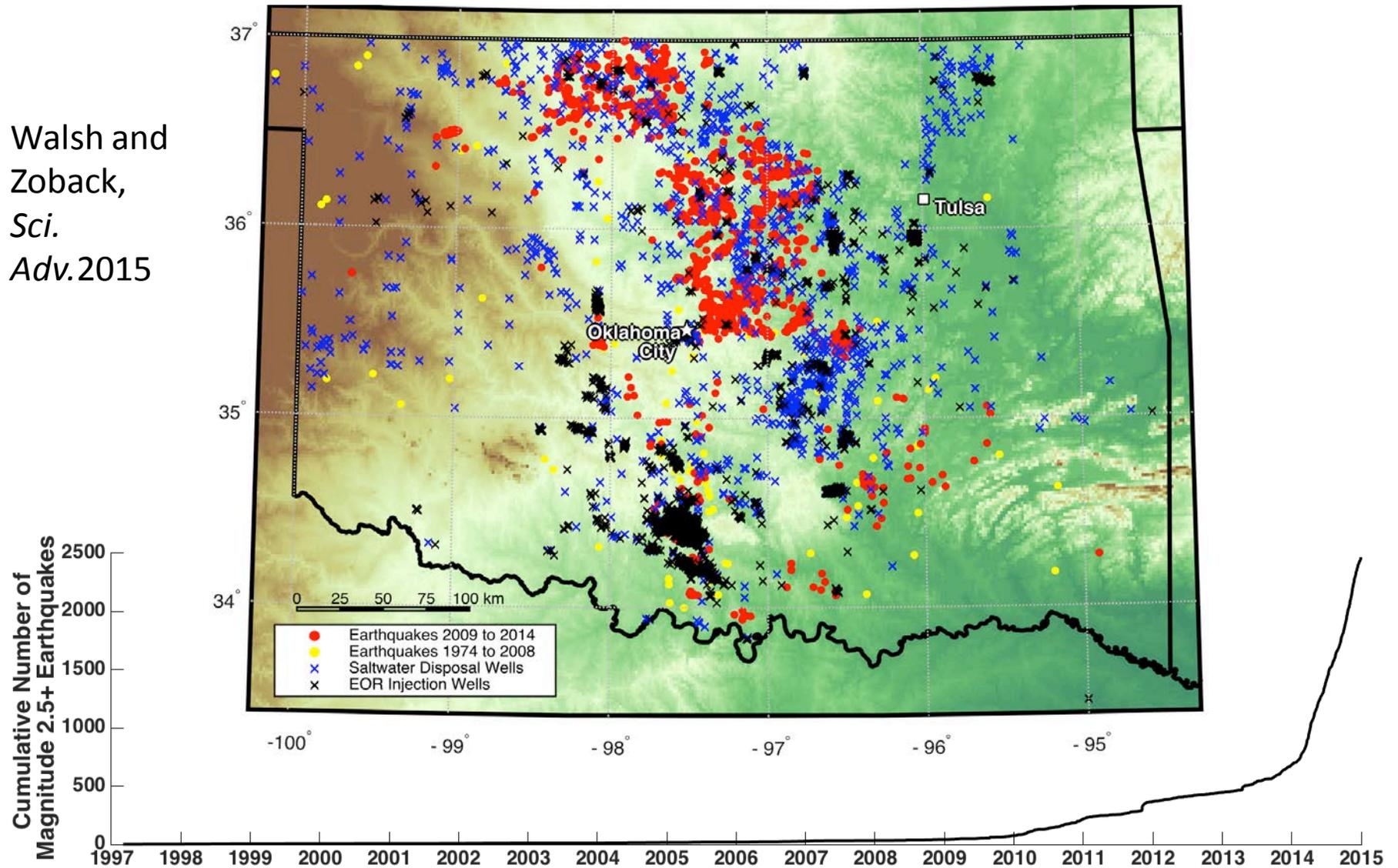
M. Weingarten,<sup>1\*</sup> S. Ge,<sup>1</sup> J. W. Godt,<sup>2</sup> B. A. Bekins,<sup>3</sup> J. L. Rubinstein<sup>3</sup>

Weingarten et al., *Science*, 2015



# Earthquakes (red) and Disposal wells (blue) in Oklahoma

Walsh and  
Zoback,  
*Sci.*  
*Adv.* 2015



# Induced Seismicity – the general idea...

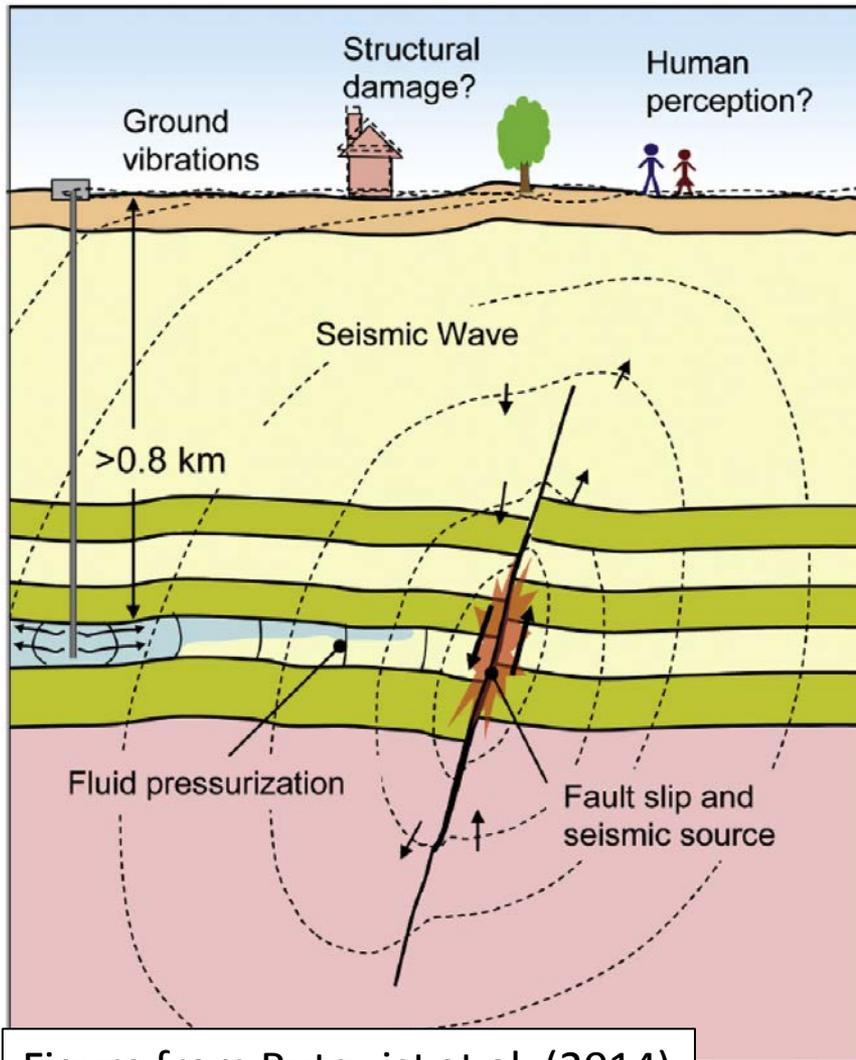
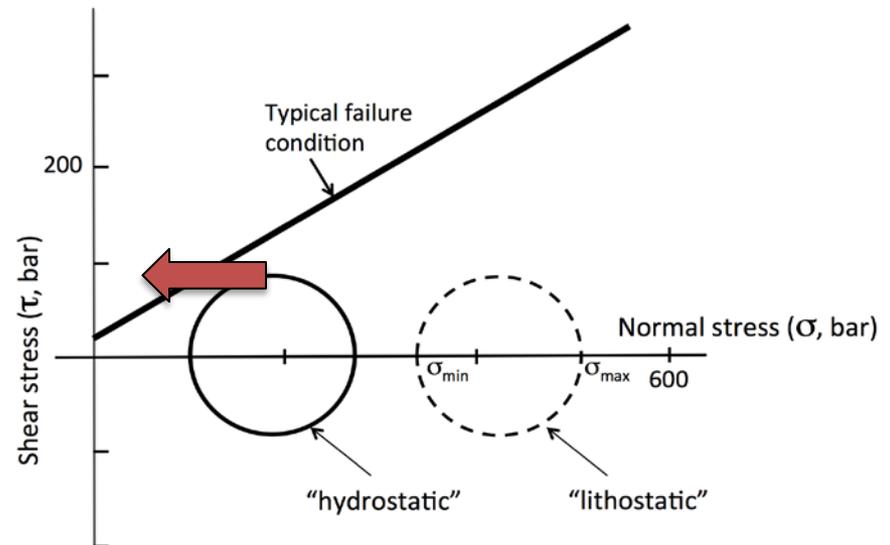


Figure from Rutquist et al. (2014)

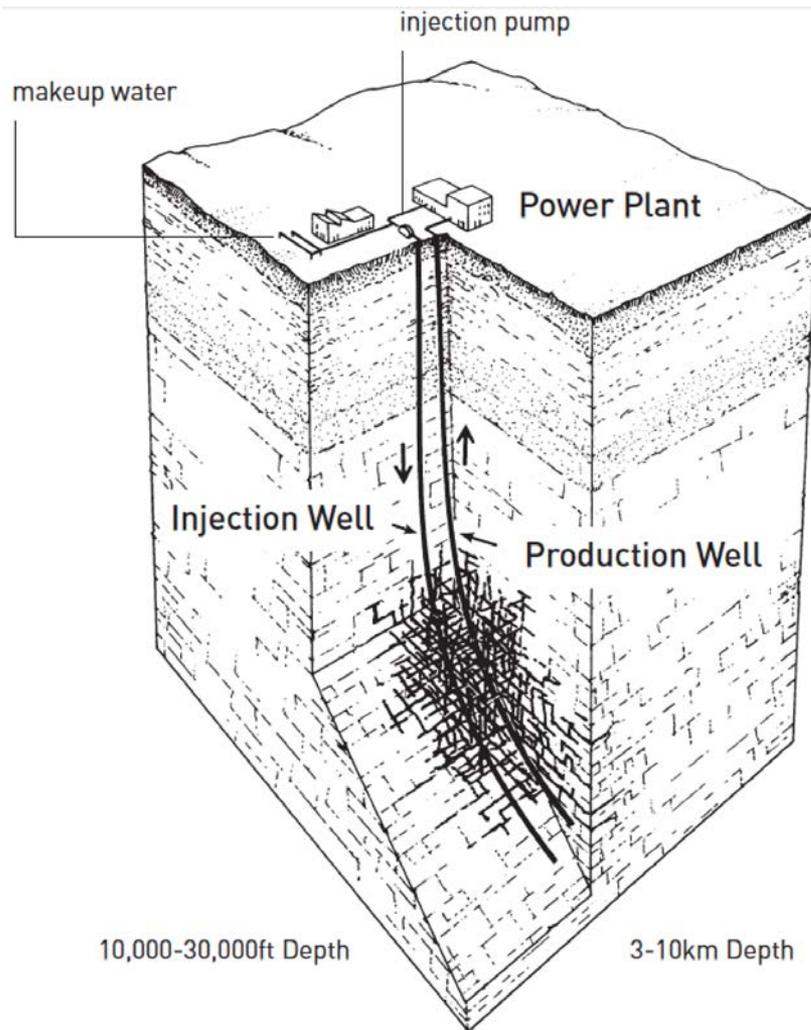
Fluid injection requires “overpressure” to force fluids into porous rocks

*Increased fluid pressure from injection affects a much larger volume of the subsurface than that actually contacted by the new fluids.*

Increased fluid pressure decreases the “normal” stress on faults, allowing them to slip and produce earthquakes



# Enhanced Geothermal Systems require control of fractures and fluid flow

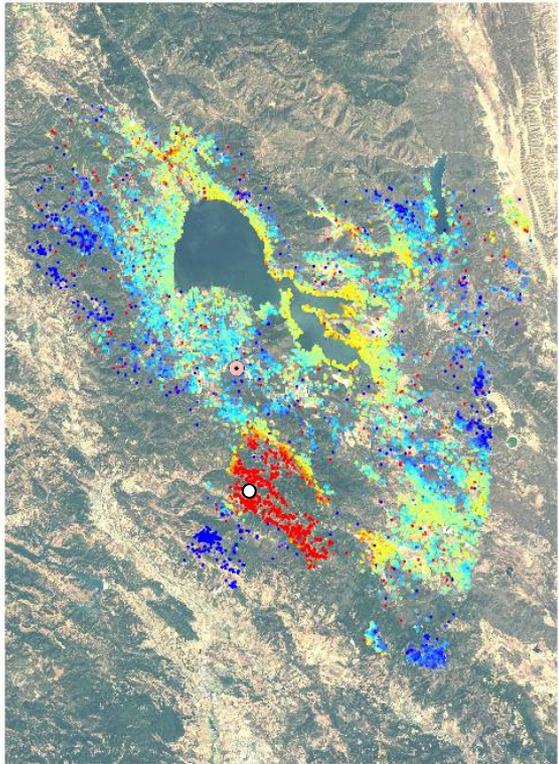


## What is EGS

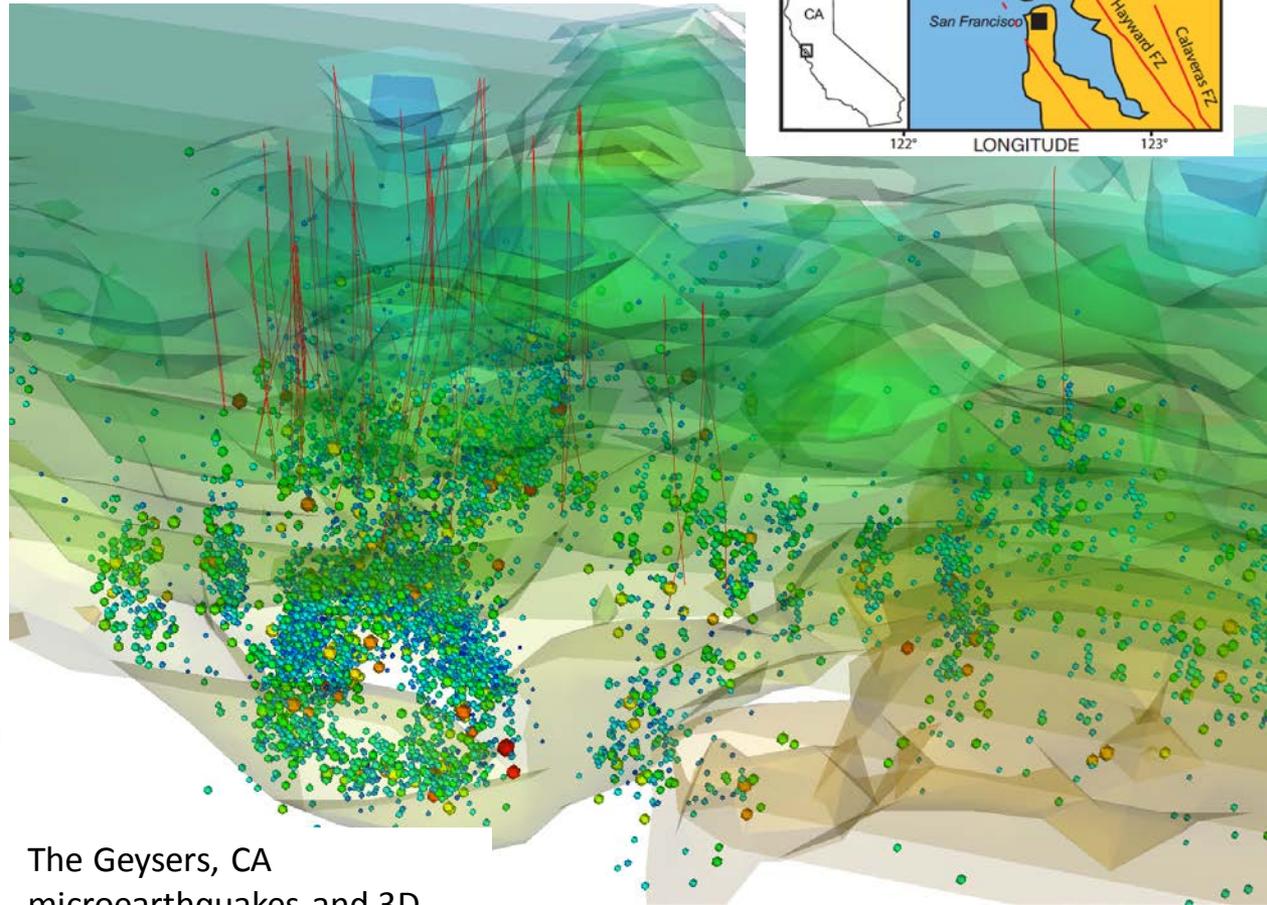
- Artificially create/enhance a fracture network by hydraulic fracturing and/or chemical mechanisms in high temperature, low permeability rock.
- Transfer heat to surface by circulating fluid through the fracture network with injection and production boreholes.

Experimental projects in U.S., U.K., France, Japan, Australia, Sweden, Switzerland, Germany.

# The Geysers geothermal field in Northern California is “enhanced” in that fluid is being added to a natural system



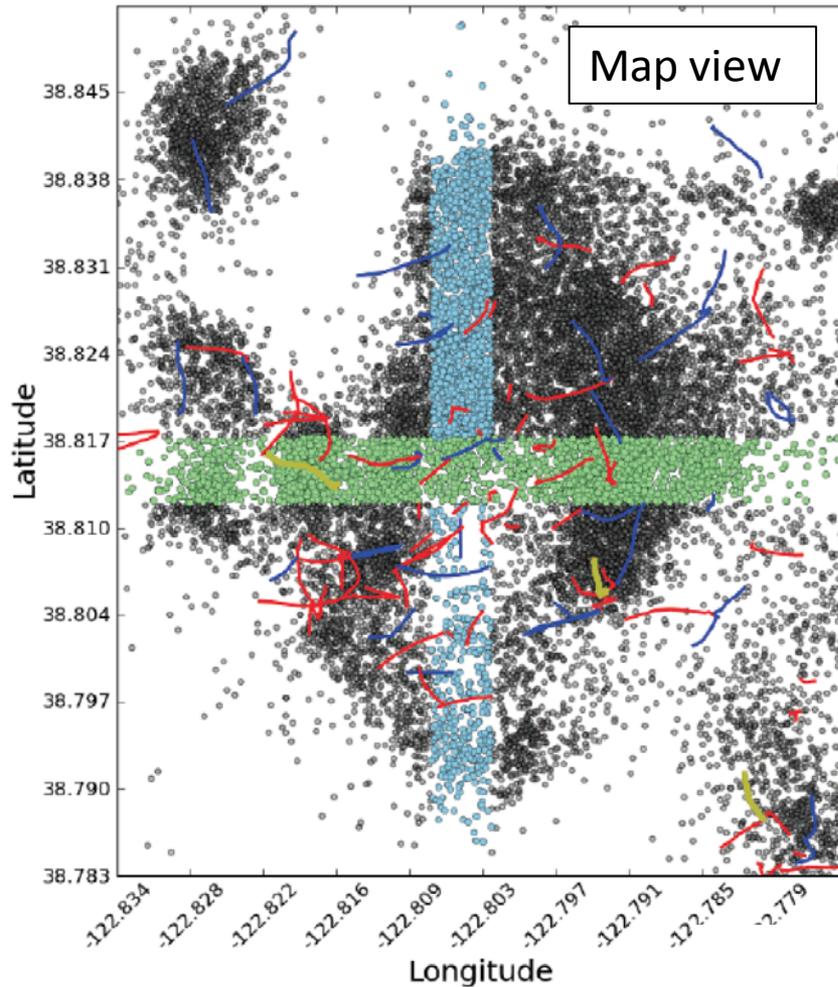
Annual surface deformation  
-5 (red) to +5 (blue) mm/yr



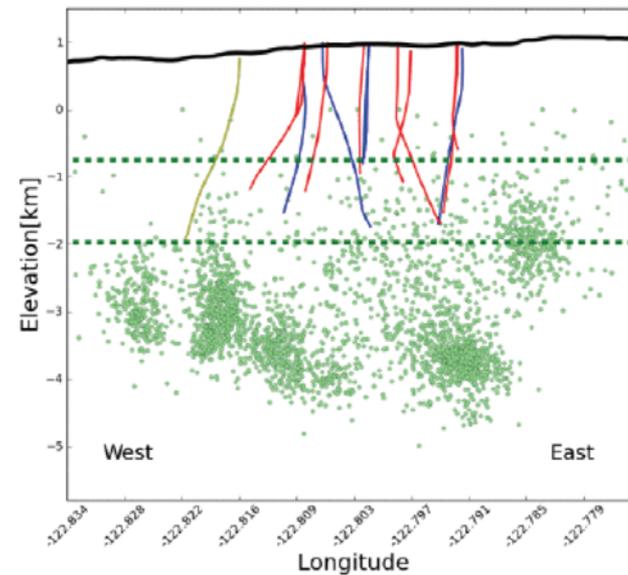
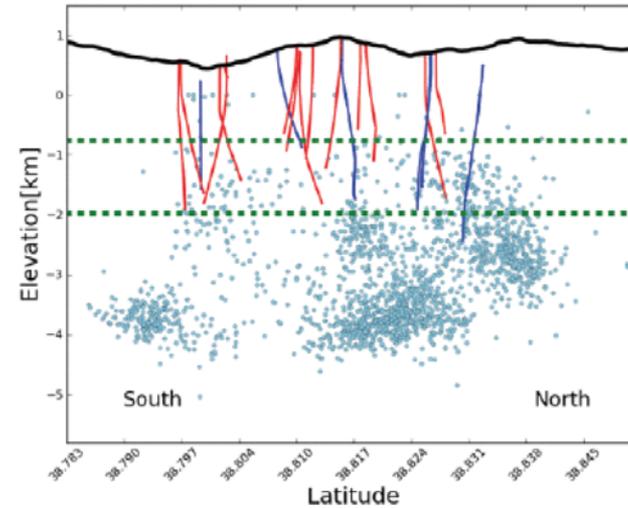
The Geysers, CA  
microearthquakes and 3D  
Velocity Structure

# Geysers earthquakes are not clustered at the points of injection

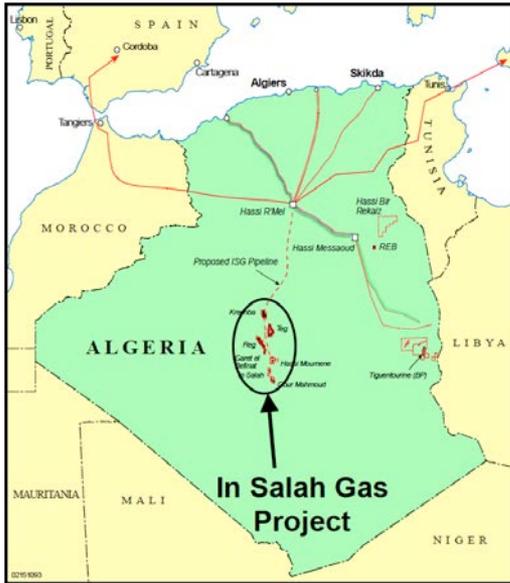
## Microearthquake locations



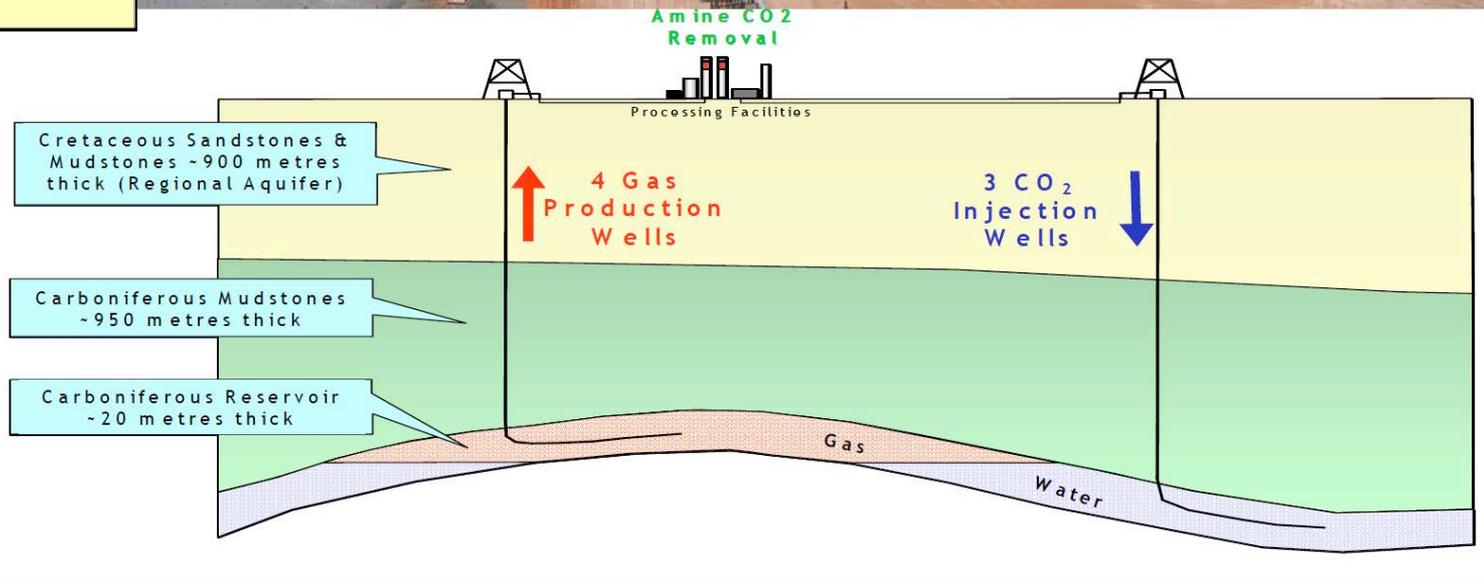
## Cross sections



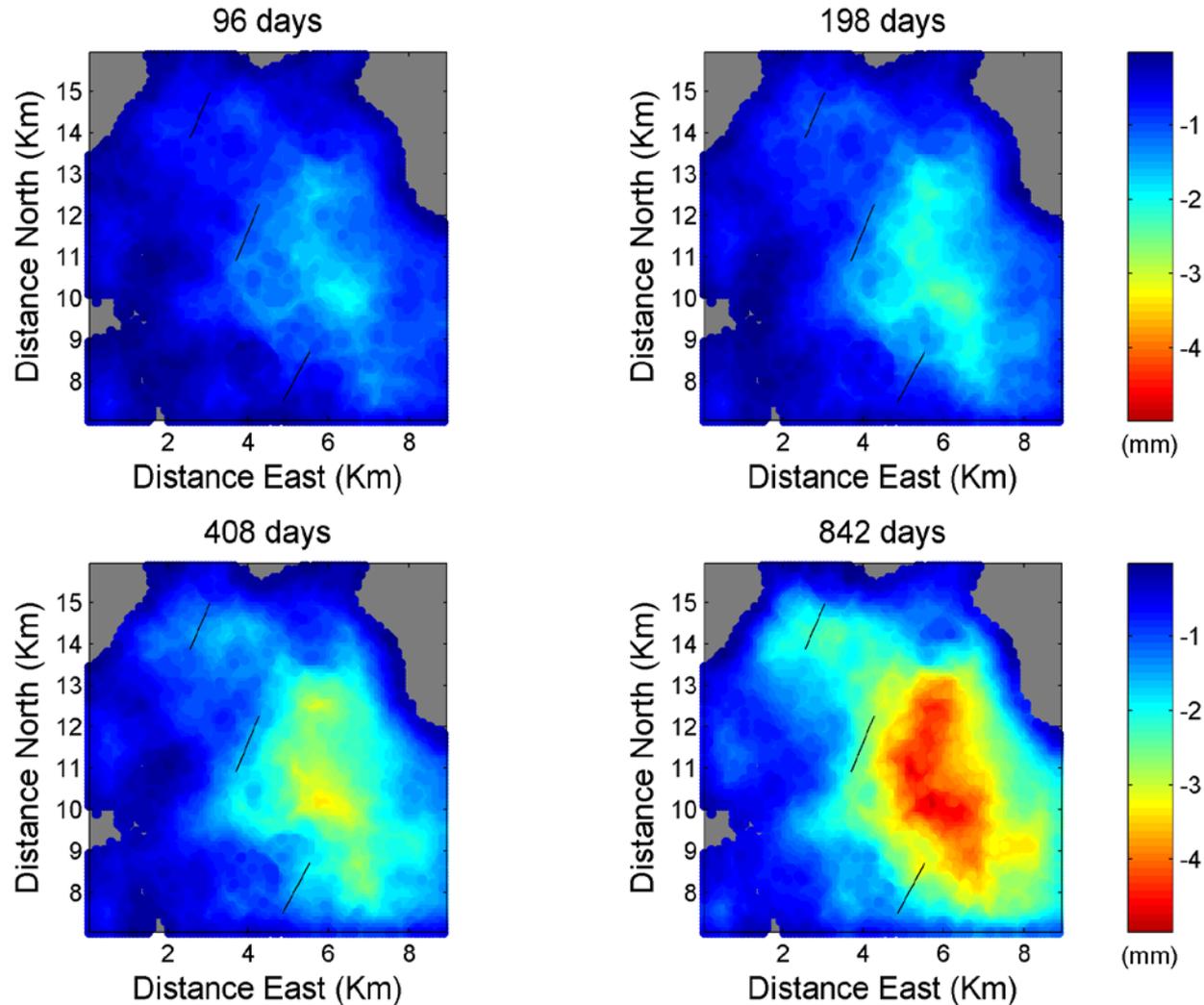
# CO<sub>2</sub> storage experiment at Krechba gas field in Algeria: Another way to observe deformation related to subsurface stress distribution – ground surface uplift



CO<sub>2</sub> separated  
from natural  
gas re-injected  
at 1.9 km  
depth



Ground surface uplift (in mm) following injection of CO<sub>2</sub> at 1.9 km depth at the Krechba gas field, In Salah, Algeria (*Vasco et al.*).



Data obtained using InSAR. Surface-displacement data provides low-resolution but important constraints on how subsurface stress is evolving.

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- Chemical-mechanical coupling in stressed rocks
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## Crosscutting themes and approaches

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- Architected geomaterials to address heterogeneity and scaling

# Nanoporous geomaterials – reactivity, flow and mechanics

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*Shale (s.l.) has become a critical energy material.....*

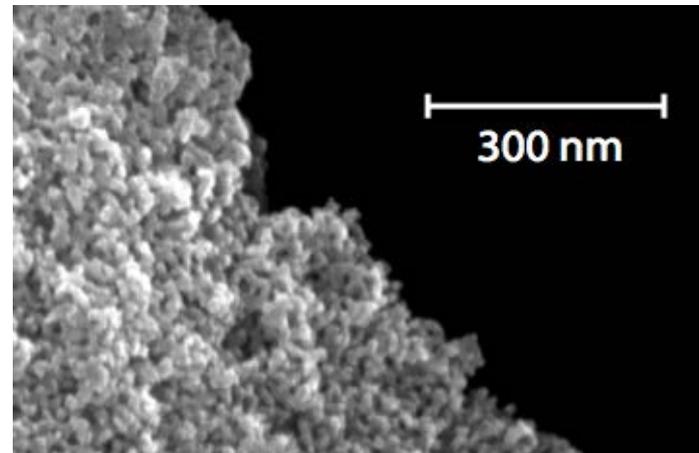
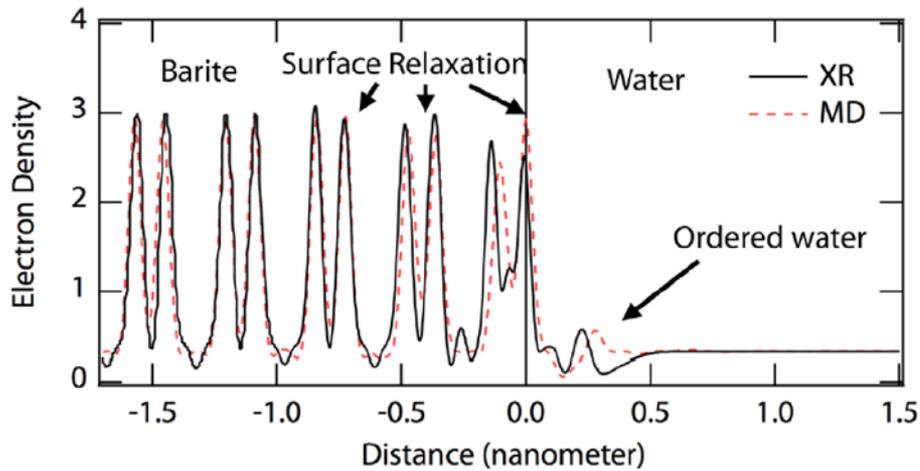
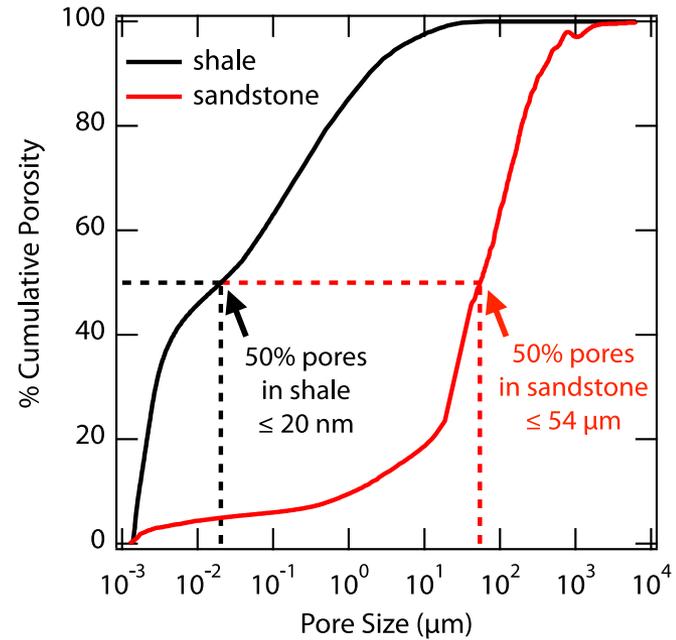
- **Problem:**

- Nanoporous geomaterials (e.g. shale) have properties that are critical for many subsurface engineering issues
- The properties of nanopores, their effects on contained fluids and gases, and the behavior of nanopore networks are poorly known
- The chemical/mechanical response of nanoporous geomaterials to perturbations is a particular challenge

- **Opportunity**

- Advanced molecular models for nanoscale phenomena
- New characterization techniques – Xrays and neutrons – for studying nanoscale features and processes
- New experimental techniques for studying nanoporous materials

# Nanopores can be a large fraction of pore space



# Chemical-mechanical coupling in stressed rocks

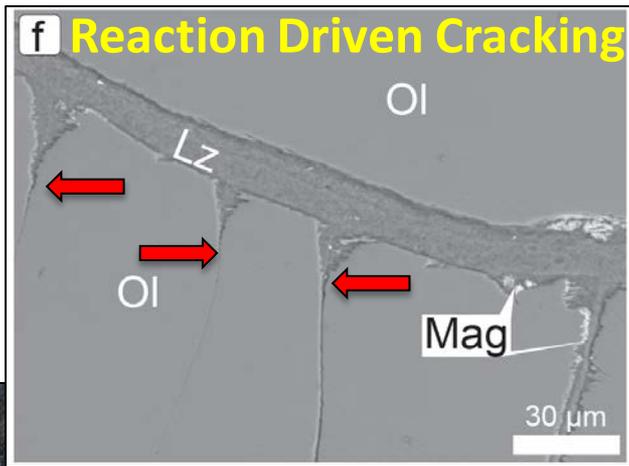
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- **Problem:**

- Response of fluid-saturated rocks to induced stresses can be both physical and chemical.
- Reactive chemistry and deformation can be mutually reinforcing or attenuating
- Models are limited by knowledge of constitutive properties of the rocks (multi-mineralic and heterogeneous on many scales), and by mathematical algorithms that capture the feedbacks

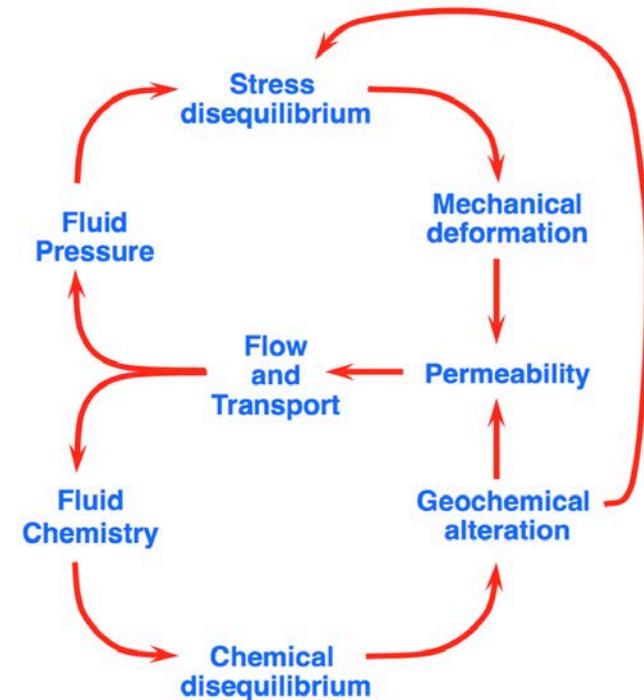
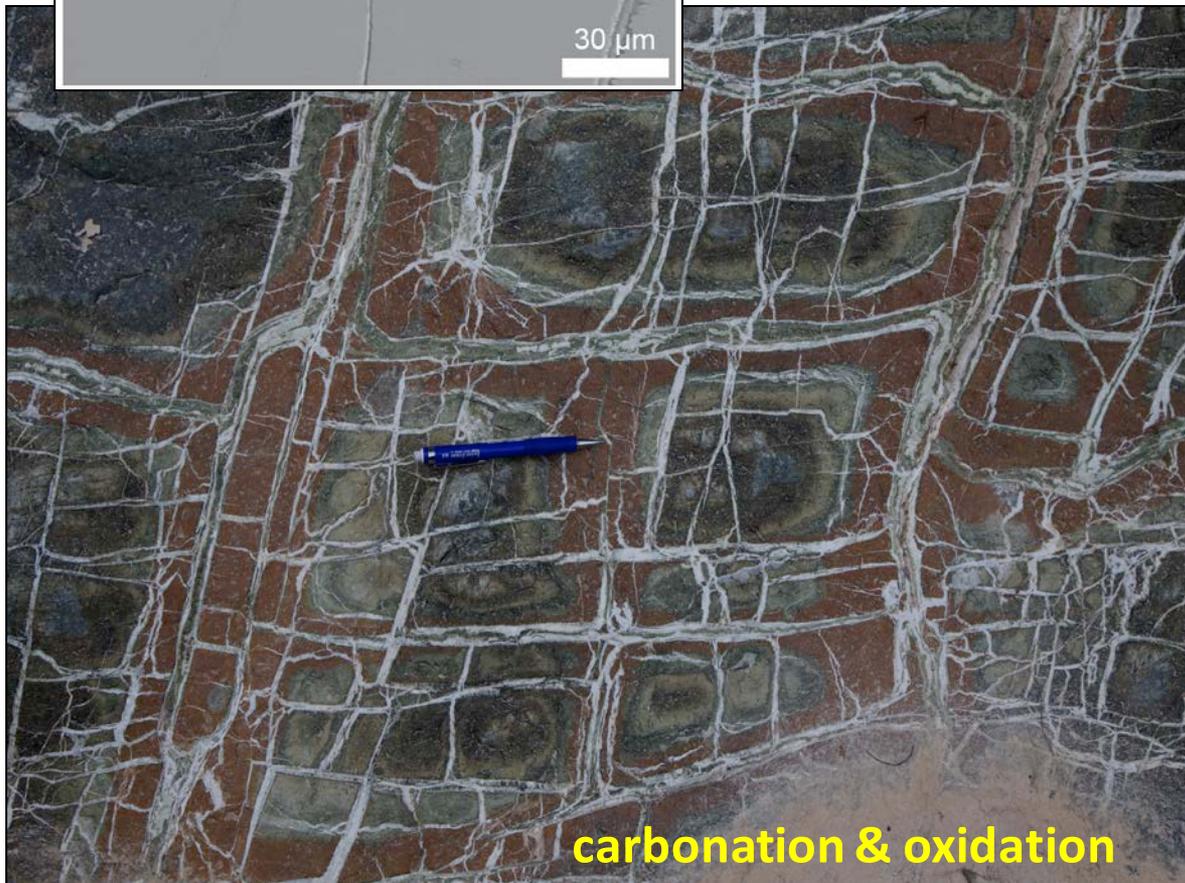
- **Opportunity**

- New capabilities for measuring rates of chemical reactions and 3D imaging of response to applied stresses (Xrays, neutrons)
- Increased computing power combined with algorithm development
- New purpose-built experimental systems designed to be compatible with imaging tools for real time monitoring of experiments



Chemical-mechanical coupling models are needed for measuring and monitoring stress distributions.

*Stress must be inferred from observed material responses*



*Components of a coupled modeling strategy  
Detwiler, 2015*

# Advanced computational methods

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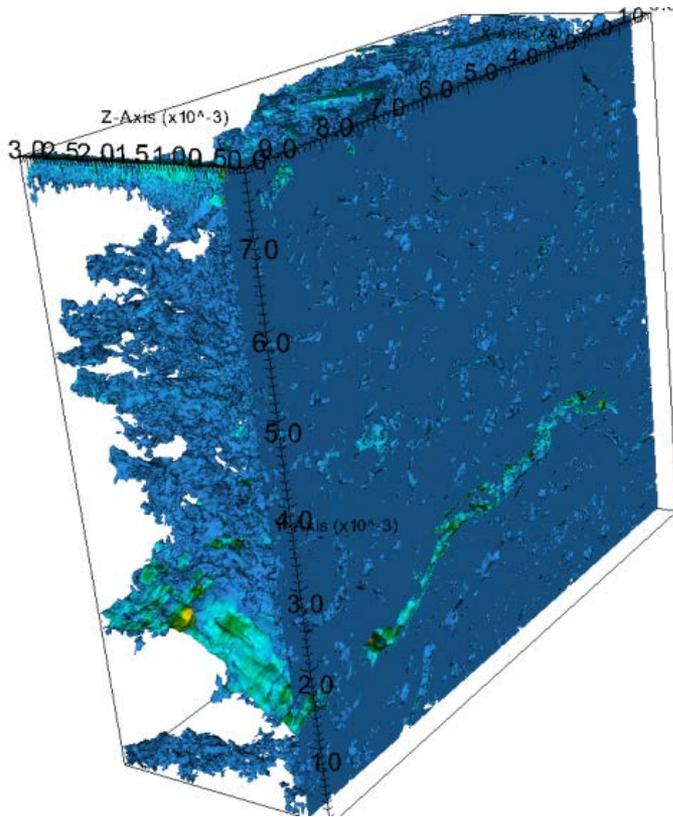
- **Problem:**

- Forecasting the response to stresses caused by fluid injection requires treatment of thermal, hydrological, mechanical and chemical (THMC) effects concurrently
- Formulation of the physics and chemistry, feedbacks, knowledge of constitutive relations and allowance for time-dependent properties (e.g. fracture development & growth) can be done only in a rudimentary, approximate way

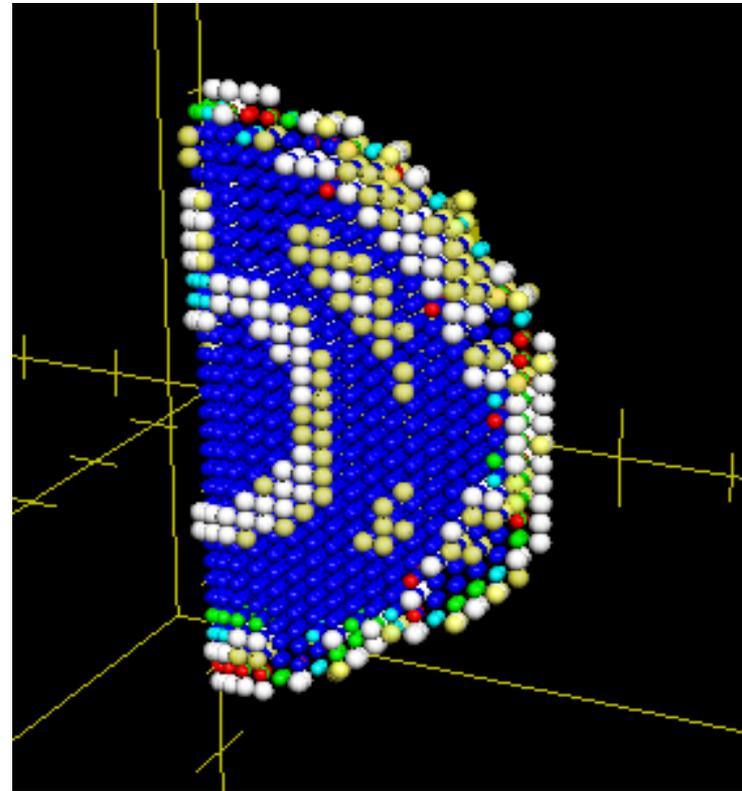
- **Opportunity**

- Recent development of advanced numerical algorithms, discretization techniques, and computation power allow for direct simulation
- Improving database on material properties, chemical-mechanical coupling, mineral-fluid reaction rates

# Advanced computational methods



Simulation of flow in a previously imaged sample of fractured Marcellus shale using 60,000 cores of NERSC Hopper and the software package Chombo-Crunch.



Simulation of permeability in a hydraulic fracture. The permeability variation ranges from over  $10^4$  times the initial permeability (blue) to 1.1 times the initial value (yellow).



# Architected Geomaterials

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## - Systematically addressing heterogeneity and complexity

- **Problem:**

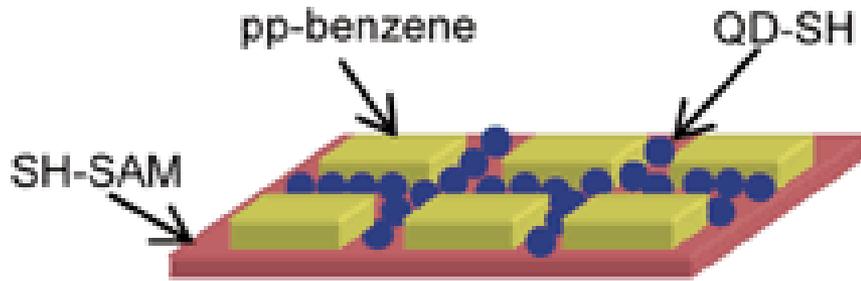
- The step from controlled laboratory experiments to heterogeneous natural materials a giant leap!
- Interactions between mineral and porosity heterogeneity, mesoscale structures, fractures and chemical reactions are difficult to study systematically

- **Opportunity**

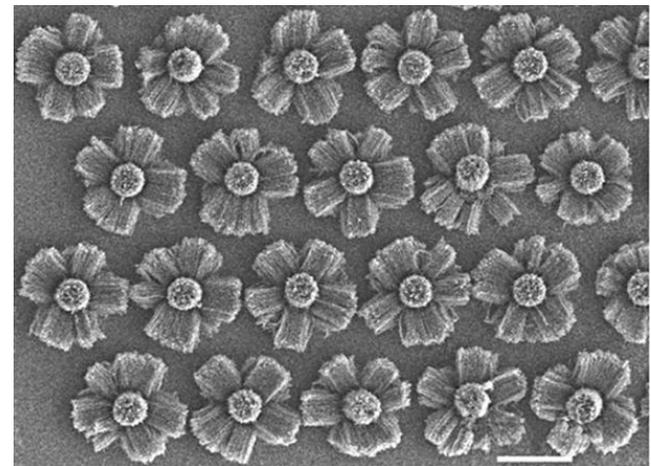
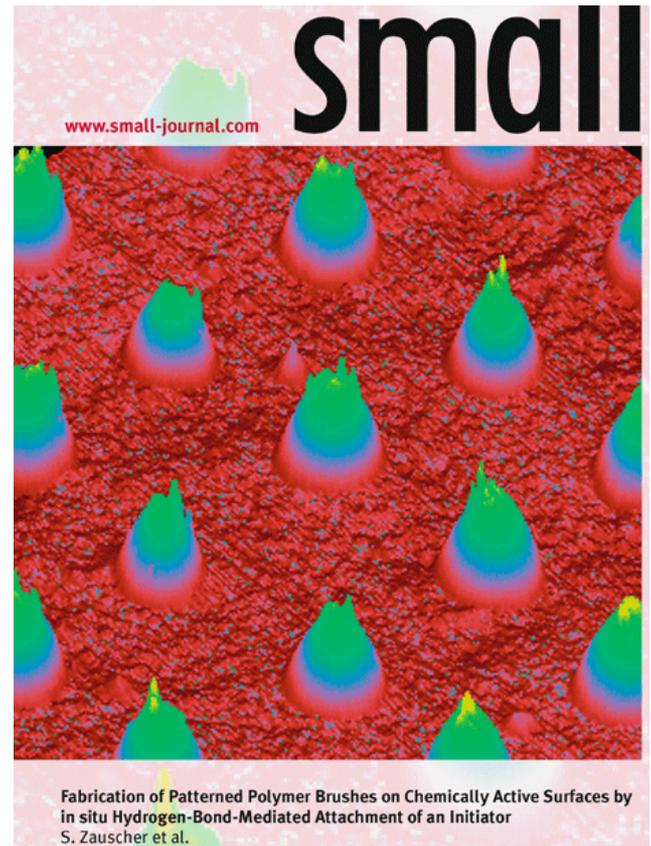
- New capabilities for making artificial materials that approximate natural features, but have limited complexity, may allow coupled processes to be studied more systematically
- Advanced imaging methods can be used to characterize experiments, and provide a computational grid for model development and verification

# Architected Geomaterials:

- controlled complexity



Advances in 3D printing, patterning functionalized surfaces and micro-electronic fabrication provide a new opportunity to make geo-like materials in the laboratory to explore the effects of chemical and structural heterogeneity in a controlled, repeatable manner.



## BES Roundtable – SubTER Matrix

	<b>Wellbore Integrity</b>	<b>Subsurface Stress &amp; Induced Seismicity</b>	<b>Permeability Manipulation</b>	<b>New Subsurface Signals</b>
Advanced computation		X	X	X
Nanoporous geomaterials	X		X	
Reactive multiphase flow	X	X	X	
Chemical-mechanical coupling		X	X	X
Architected geomaterials	X	X	X	X
Imaging Stress and Geochem. features		X	X	X

# Relationship to Basic Research Needs Workshop

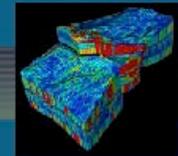
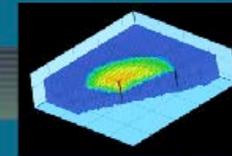
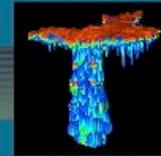


Workshop:  
Feb. 20-24, 2007

Report published:  
July 10, 2007

[http://www.sc.doe.gov/  
bes/reports/list.html](http://www.sc.doe.gov/bes/reports/list.html)

Prepared for the U.S. Department of Energy under Contract Number ??????????  
Available on the web at: <http://www.sc.doe.gov/bes/reports/list.html>



Production support provided by Lawrence Berkeley National Laboratory, Earth Sciences Division.

**Focus was on carbon  
sequestration and  
nuclear waste**



**Basic Research Needs in Geosciences: Facilitating 21st Century Energy Systems**

Sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences

# Basic Research Needs for Geoscience, February 20-24, 2007

## Discovery Research

## Use-inspired Basic Research

## Applied Research

## Technology Maturation & Deployment

- Microscopic basis of macroscopic complexity - scaling
- Highly reactive subsurface materials and environments
- Thermodynamics of the solute-to-solid continuum
- Computational geochemistry of complex moving fluids within porous solids
- Integrated analysis, modeling and monitoring of geologic systems
- Simulation of multi-scale systems for ultra-long times

- Mineral-fluid interface complexity and dynamics
- Nanoparticulate and colloid chemistry and physics
- Dynamic imaging of flow and transport
- Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization
- Fluid-induced rock deformation
- Biogeochemistry in extreme subsurface environments

- Develop and test methods for assessing storage capacity and for monitoring containment of CO<sub>2</sub> storage
- Develop remediation methods to ensure permanent storage
- Demonstrate procedures for characterizing storage reservoirs and seals
- Integrated models for waste performance prediction and confirmation
- Radionuclide partitioning in repository environments.
- Waste form stability and release models.
- Incorporate new conceptual models into uncertainty assessments.

- Develop site selection criteria
- Develop storage and operating engineering approaches
- Storage demonstrations
- Apply assessment protocols and technologies for the lifecycle of projects
- Evaluate release of radionuclide inventory from the repository
- Assess corrosion/alteration of engineered materials
- Long-term safety/risk assessment for emplacement of energy system by-products.

Office of Science

FE, RW, EM, EERE



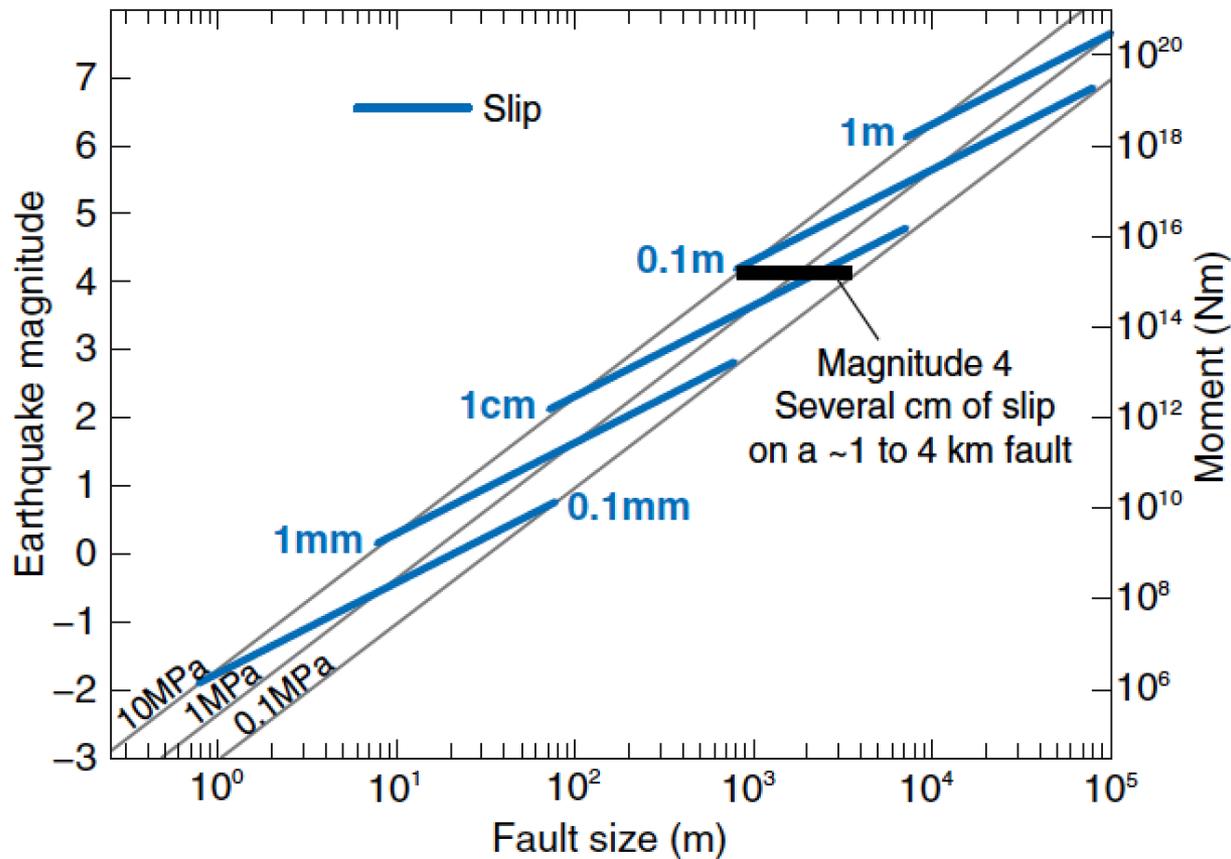
Bedford Canyon Turbidites  
(<http://blogs.agu.org/mountainbeltway>)



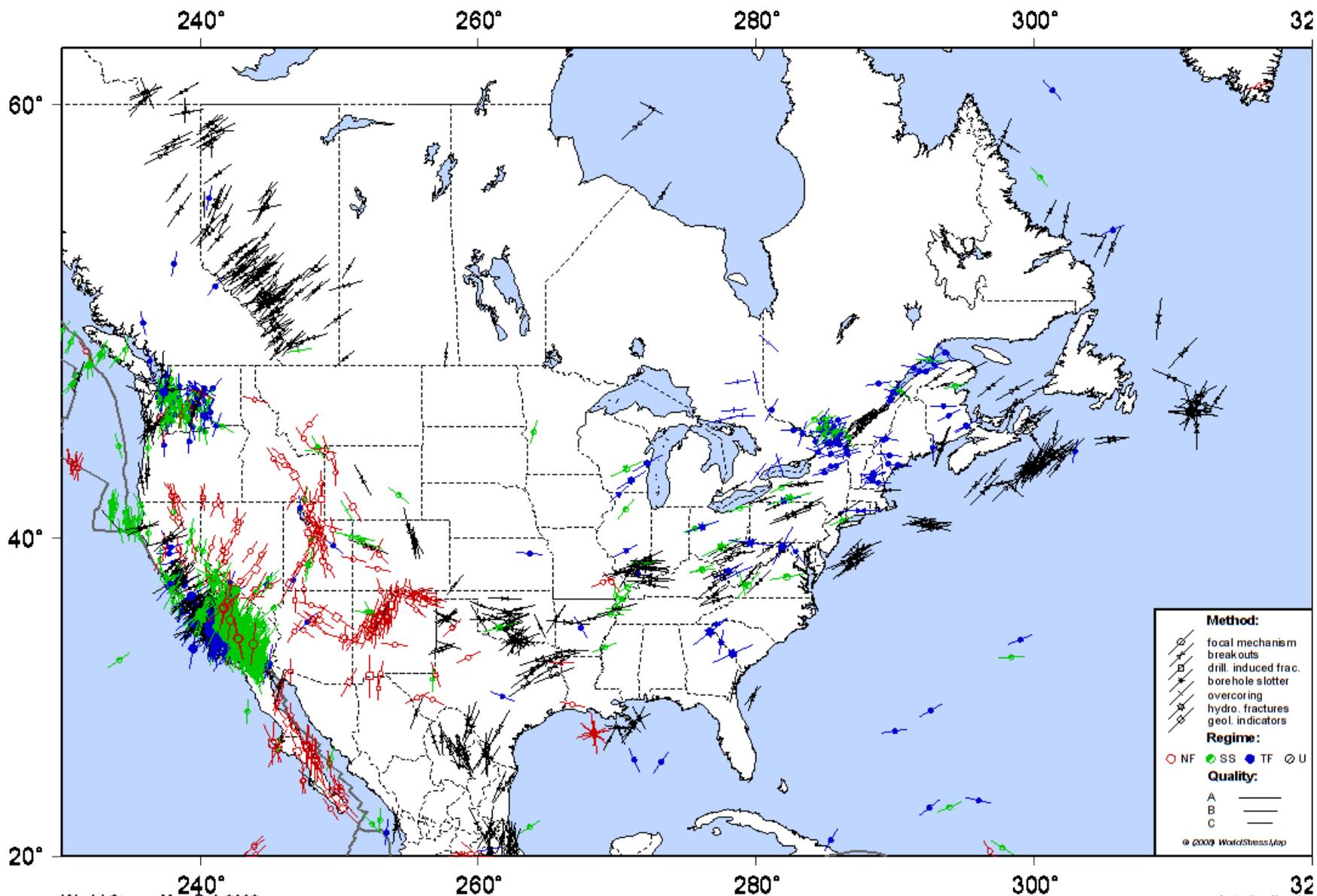
Marcellus Shale

**Thank You**

Additional reference slides



**Fig. 2.** Relationships among various scaling parameters for earthquakes. The larger the earthquake, the larger the fault and amount of slip, depending on the stress drop in a particular earthquake. Observational data indicate that earthquake stress drops range between 0.1 and 10 MPa.



## From Alt and Zoback, 2014

