

Basic Energy Sciences

Roundtable Discussion on
Foundational Research Relevant to SubTER

Don DePaolo
Associate Laboratory Director for Energy Science
Lawrence Berkeley National Laboratory
BESAC July 8, 2015

Presentation Overview

- **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**

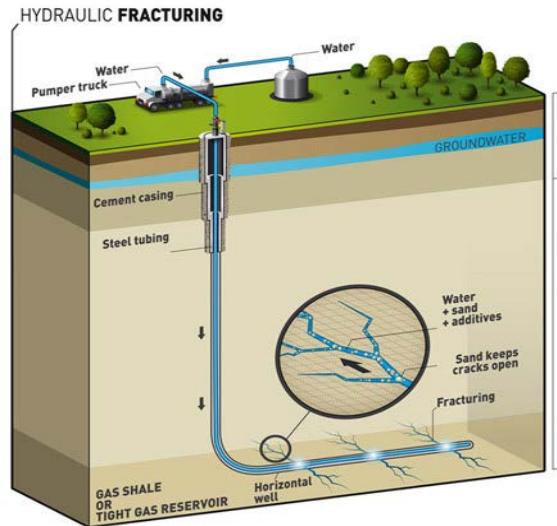
Department of Energy National Laboratory Ideas Summit March 12-13, 2014 Crystal City Gateway Marriott		
March 12, 2014		
Time	Topics	Speakers & Location
7:45 am	Registration	
8:30 am	Opening remarks	Mike Kostek Deputy Under Secretary for Science & Energy Plenary room
9:30 am	Break	
10:45 am	“Transformable and secure water management: A sustainable and secure environment nexus through superior decision tools and technologies”	Speakers TBD Plenary room
11:25 am	“Climate change science and adaptation: Ensuring regional energy and water resilience to climate change”	Speakers TBD Plenary room
12:05 pm	“Debt lunch (Provided)”	Plenary room
1:05 pm	“Accelerating materials to manufacture: Beyond Status: Taking Materials From Lab to Market Faster as Fast”	Speakers TBD Plenary room
1:45 pm	“Systems integration: The optimization of energy systems across multiple pathways (transportation, 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: distributed generation, microgrids, distributed load, and distributed energy, adapted to climate and energy system change, eliminates large-scale and long-term blackouts and keeps electricity bills affordable”	Speakers TBD Plenary room
3:05 pm	“Sustainable transportation: A sustainable, 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

March 13, 2014		
Time	Topics	Speakers
Check-in for Day 2		
Opening remarks		Ernest Moniz Secretary of Energy Plenary room
Working group session I		Breakout Rooms
End lunch (Provided)		Breakout Rooms
Working group session II		Breakout Rooms
Port out of working group sessions		Plenary room
Including remarks		Mike Kostek Deputy Under Secretary for Science & Energy Plenary room

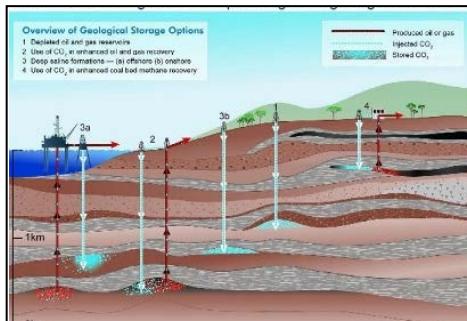
*SubTER: **S**ubsurface **T**echnology and **E**ngineering **R&D** **D**crosscutting Team

Subsurface Engineering: Critical for current & future energy systems

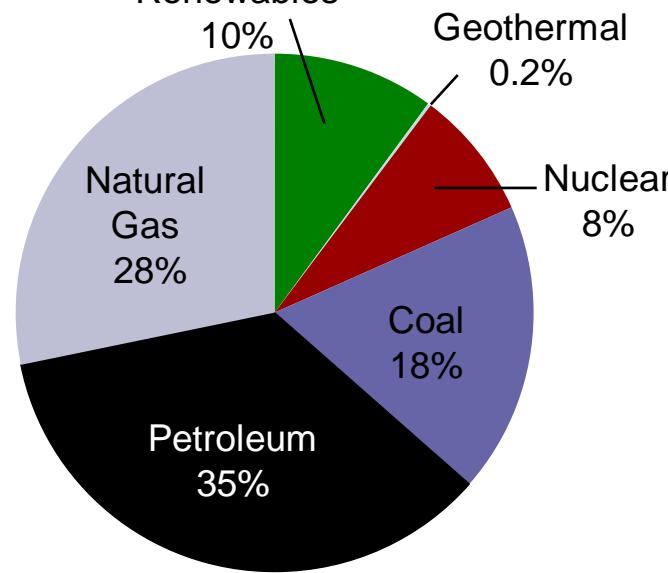
Shale hydrocarbons



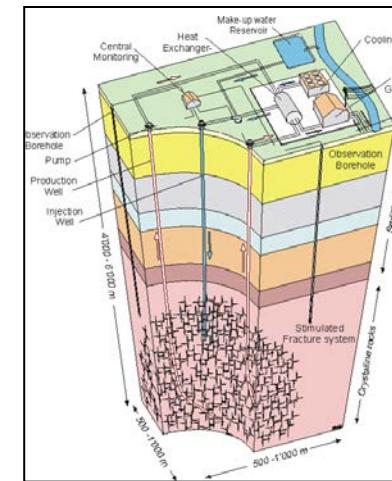
CO₂ Storage



Renewables

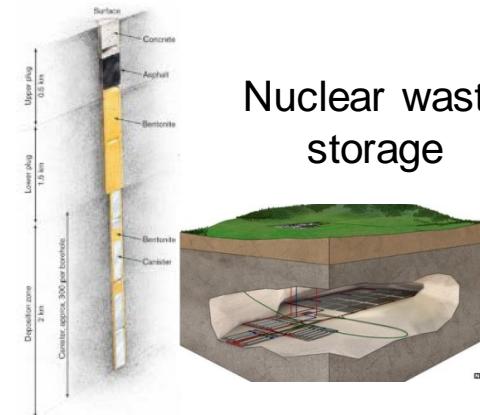


Enhanced geothermal

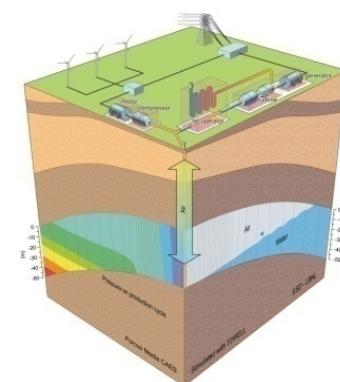


Primary Energy Use by Source, 2014

Nuclear waste storage



Compressed Air Energy 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

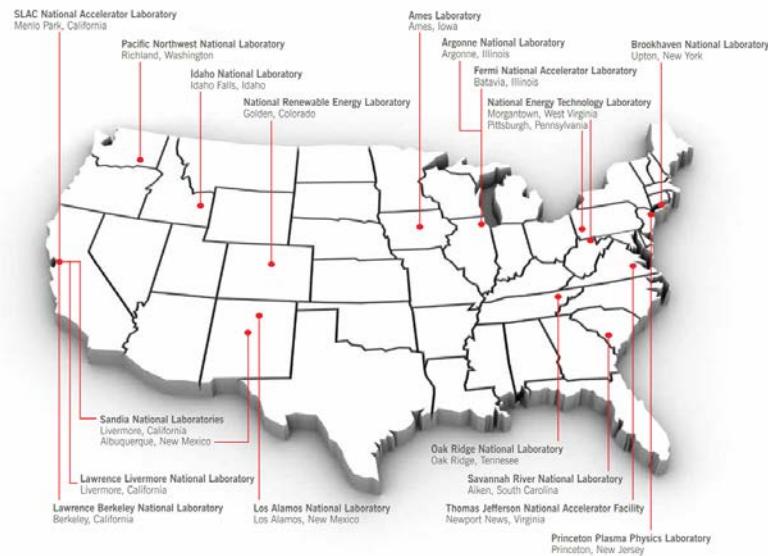
ORNL: Eric Pierce, Yarom Polksky

PNNL: Alain Bonneville, Dawn Wellman, Tom Brouns

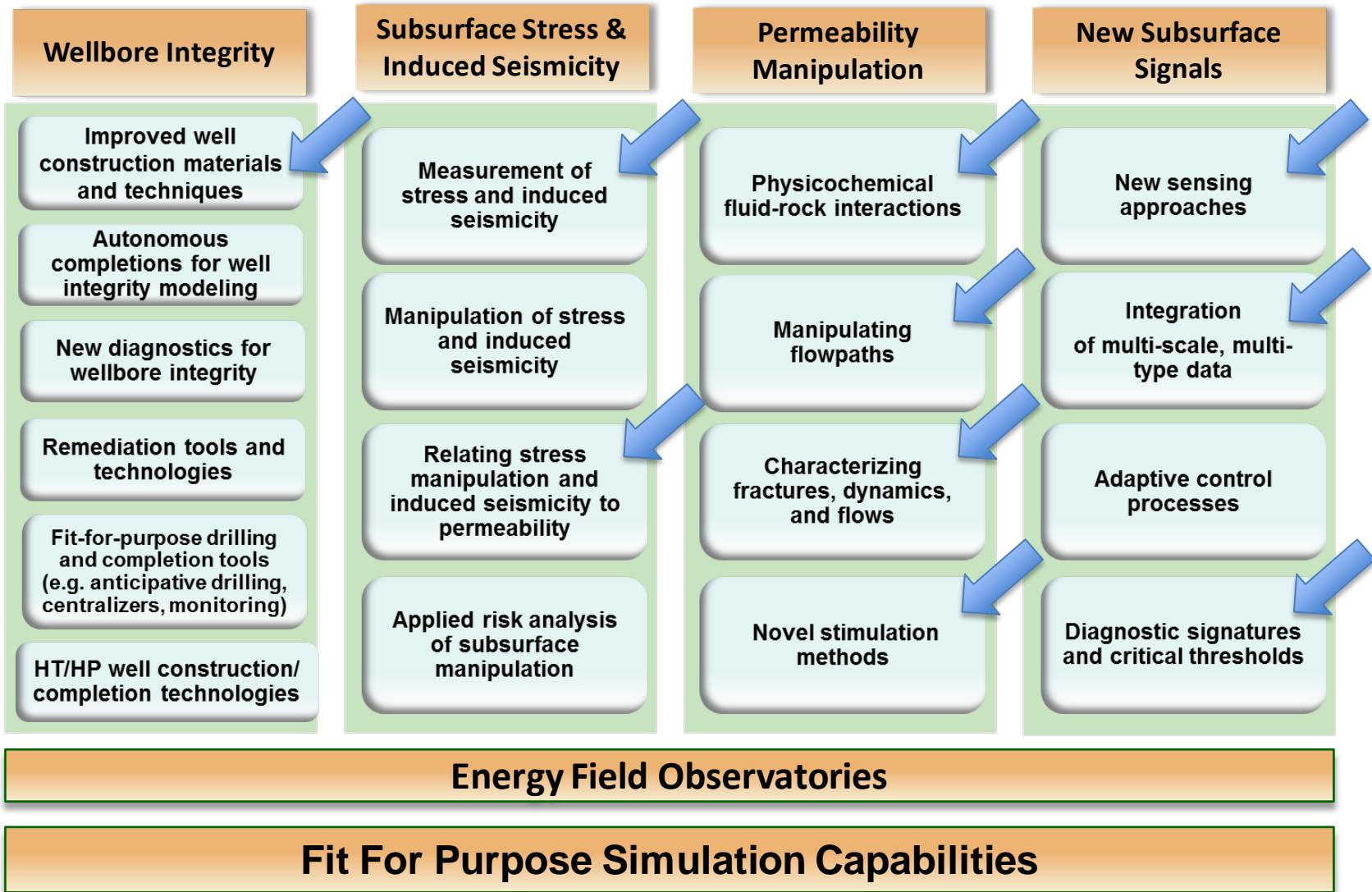
SLAC: Gordon Brown, Mark Hartney

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

- **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

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-Iu 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

- **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*

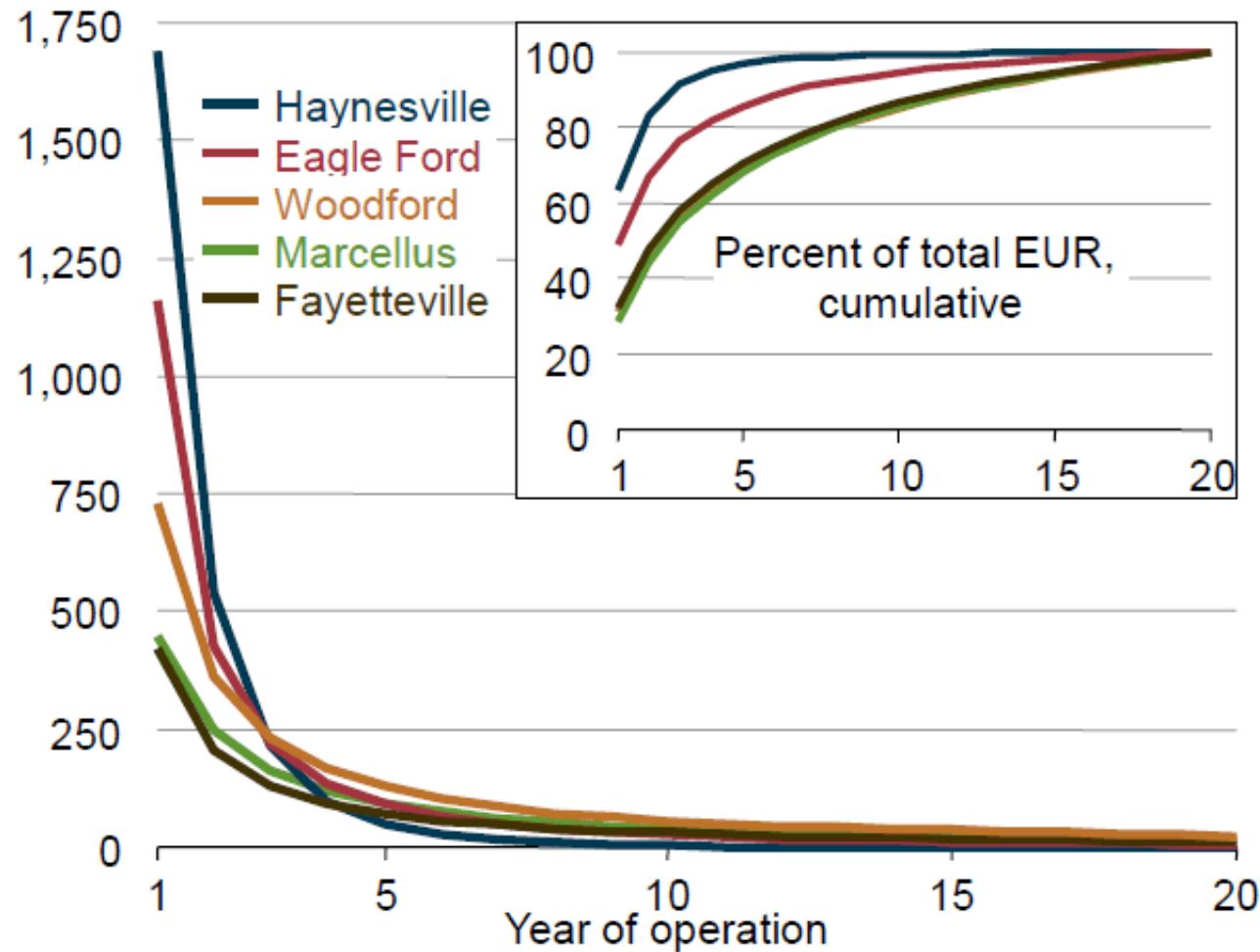
Fractures and fluid flow in the subsurface are a ubiquitous issue

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

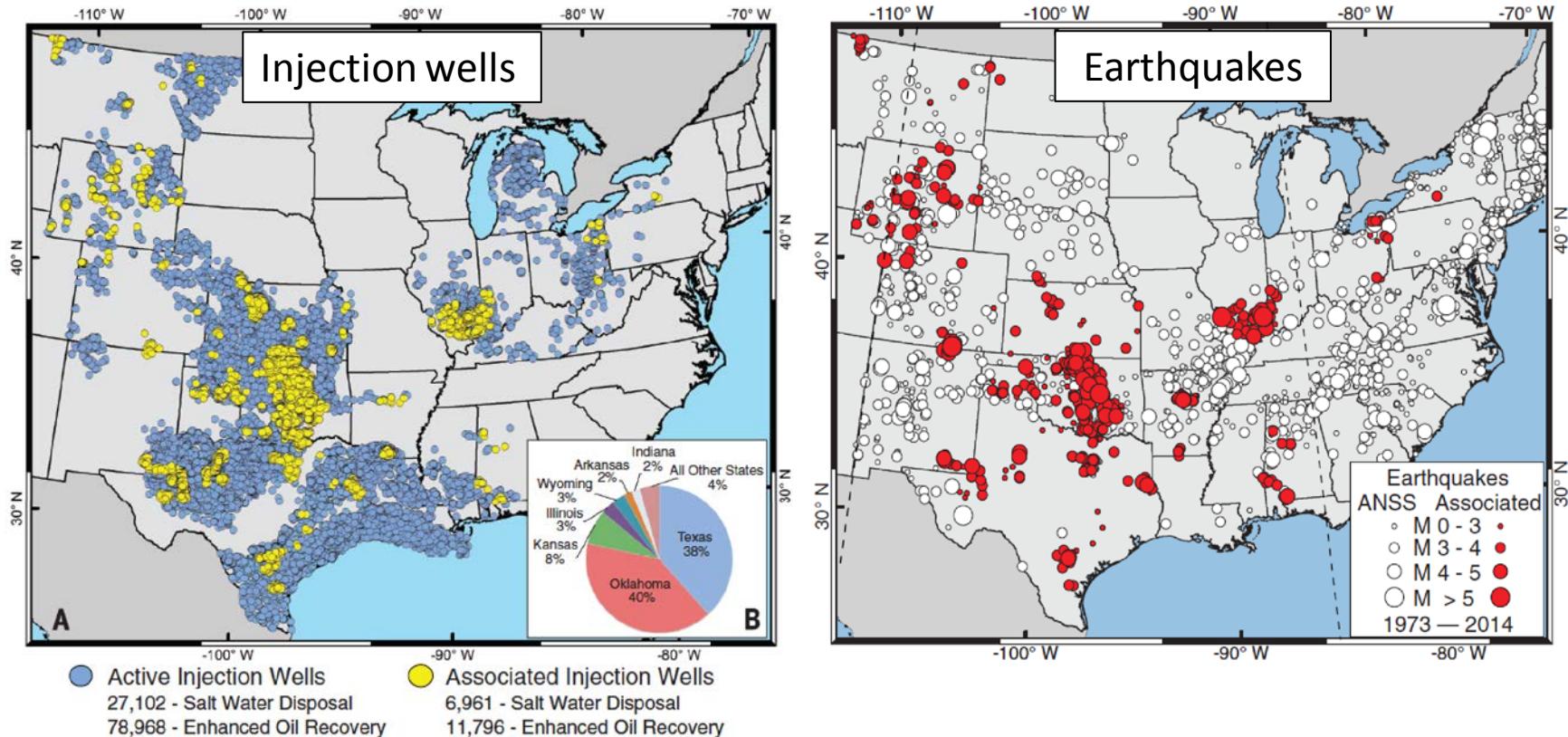
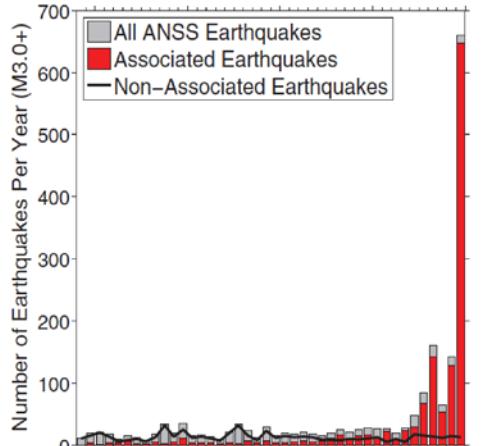


Induced seismicity in central U.S.

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

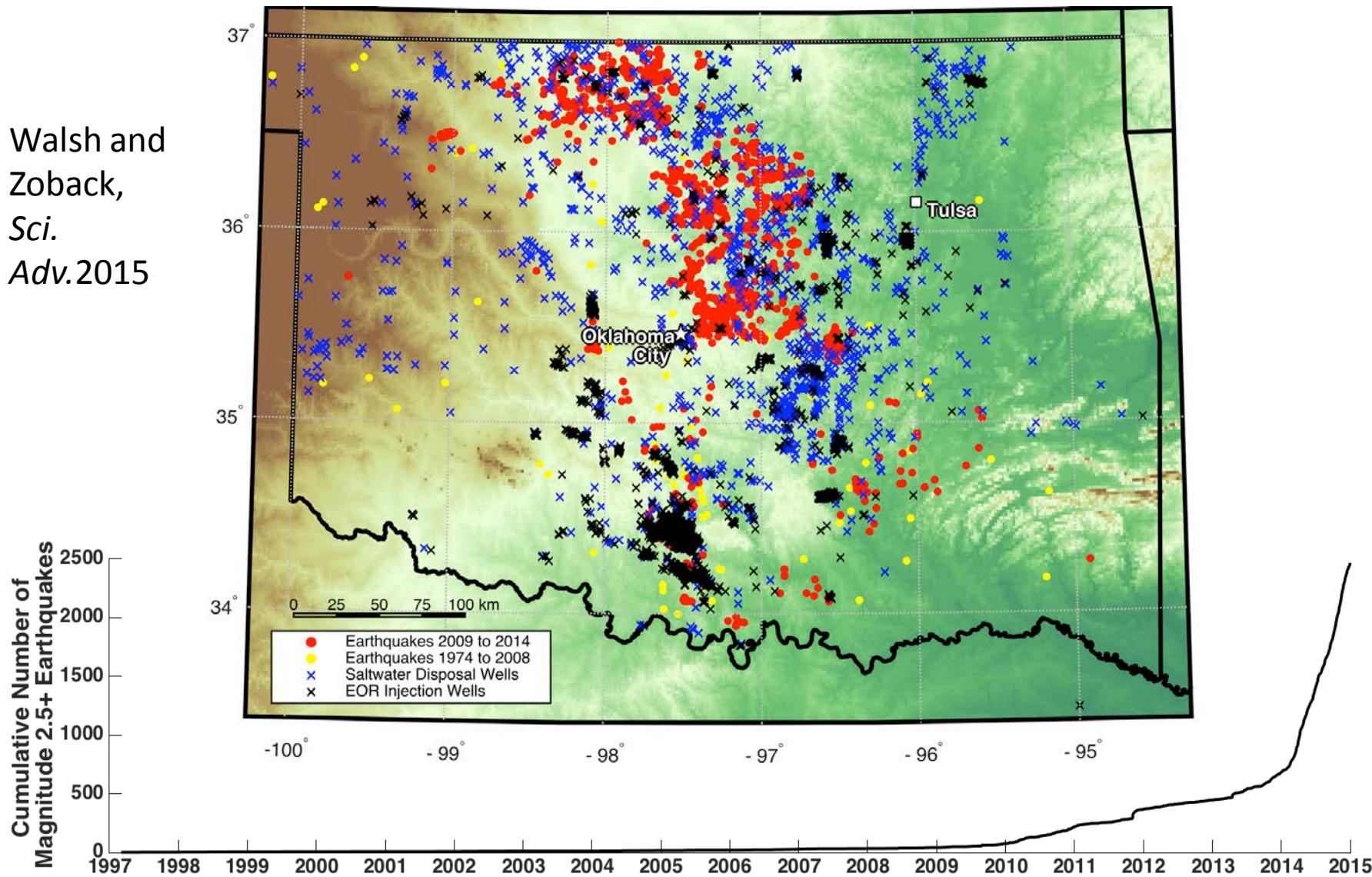
M. Weingarten,^{1*} S. Ge,¹ J. W. Godt,² B. A. Bekins,³ J. L. Rubinstein³

Weingarten et al., *Science*, 2015

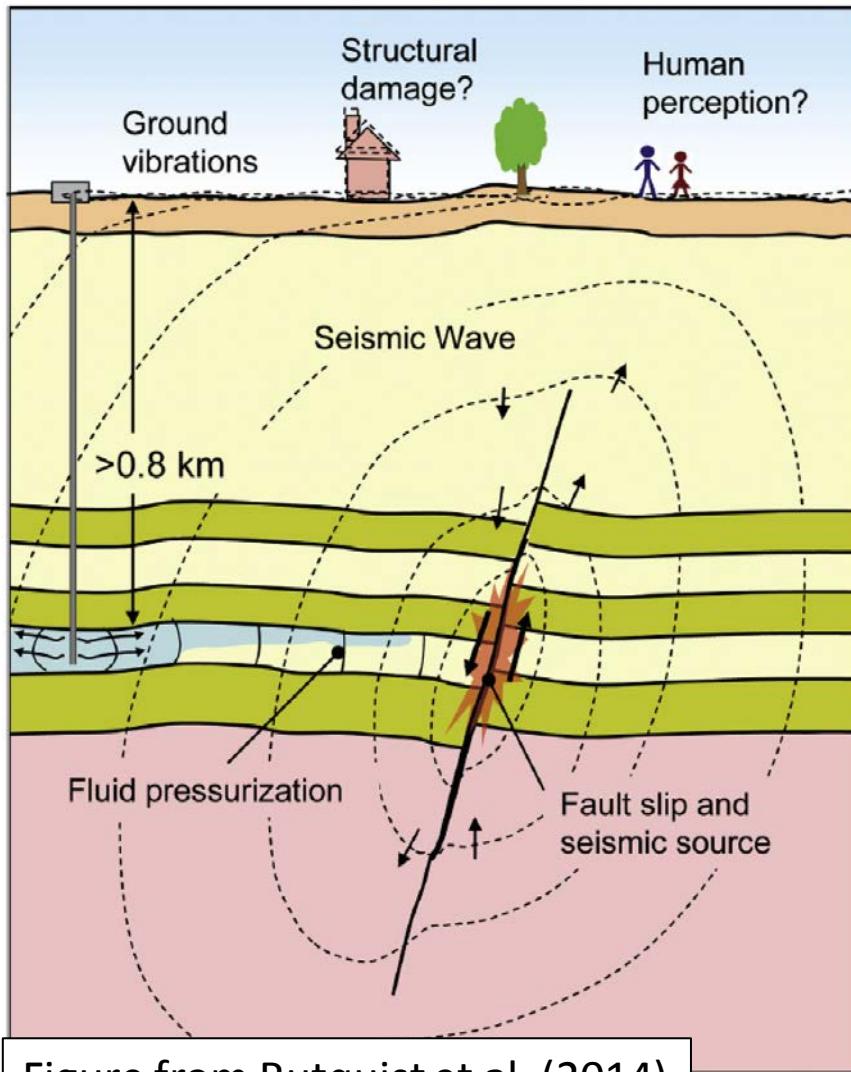


Earthquakes (red) and Disposal wells (blue) in Oklahoma

Walsh and
Zoback,
Sci.
Adv. 2015



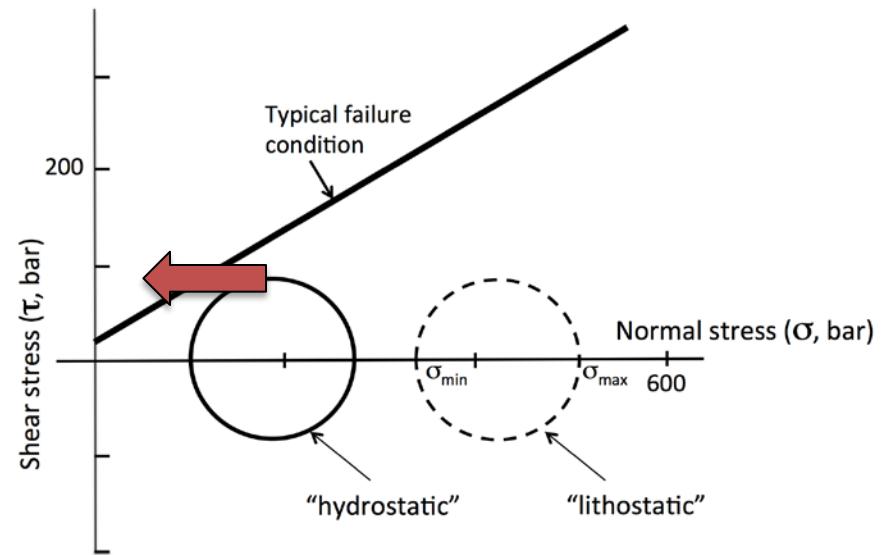
Induced Seismicity – the general idea...



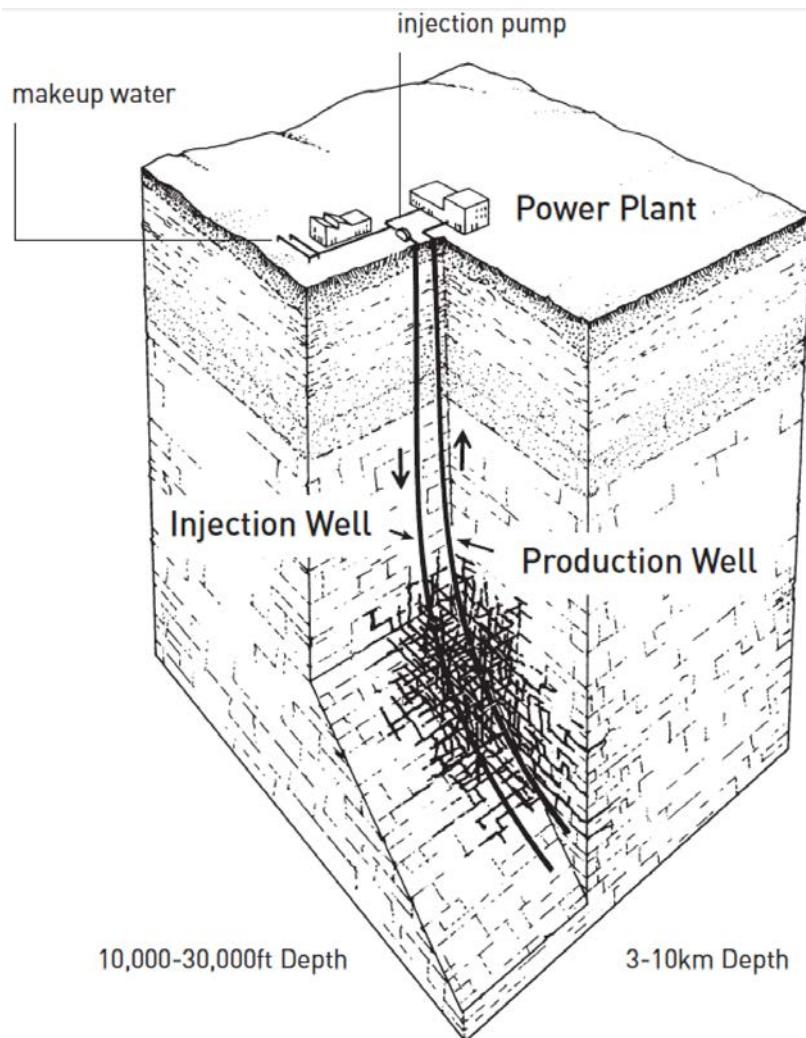
Fluid injection requires “overpressure” to force fluids into porous rocks

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

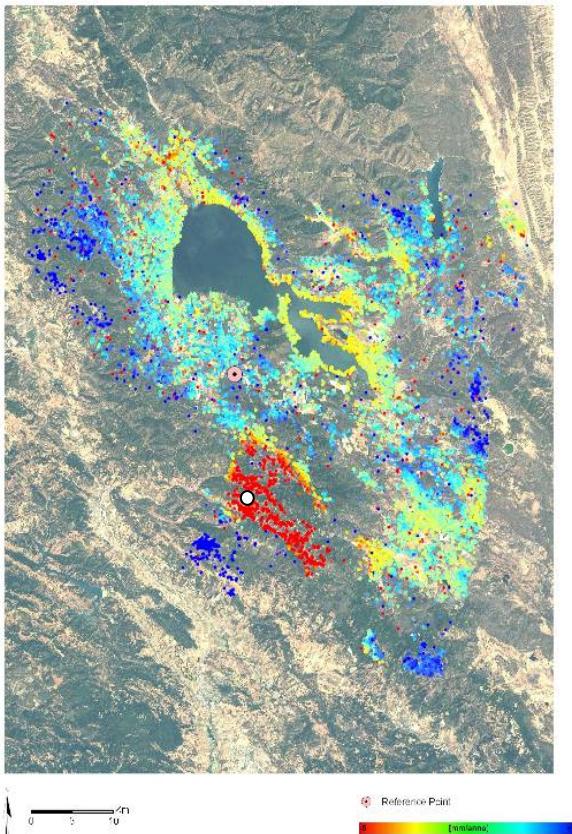


What is EGS

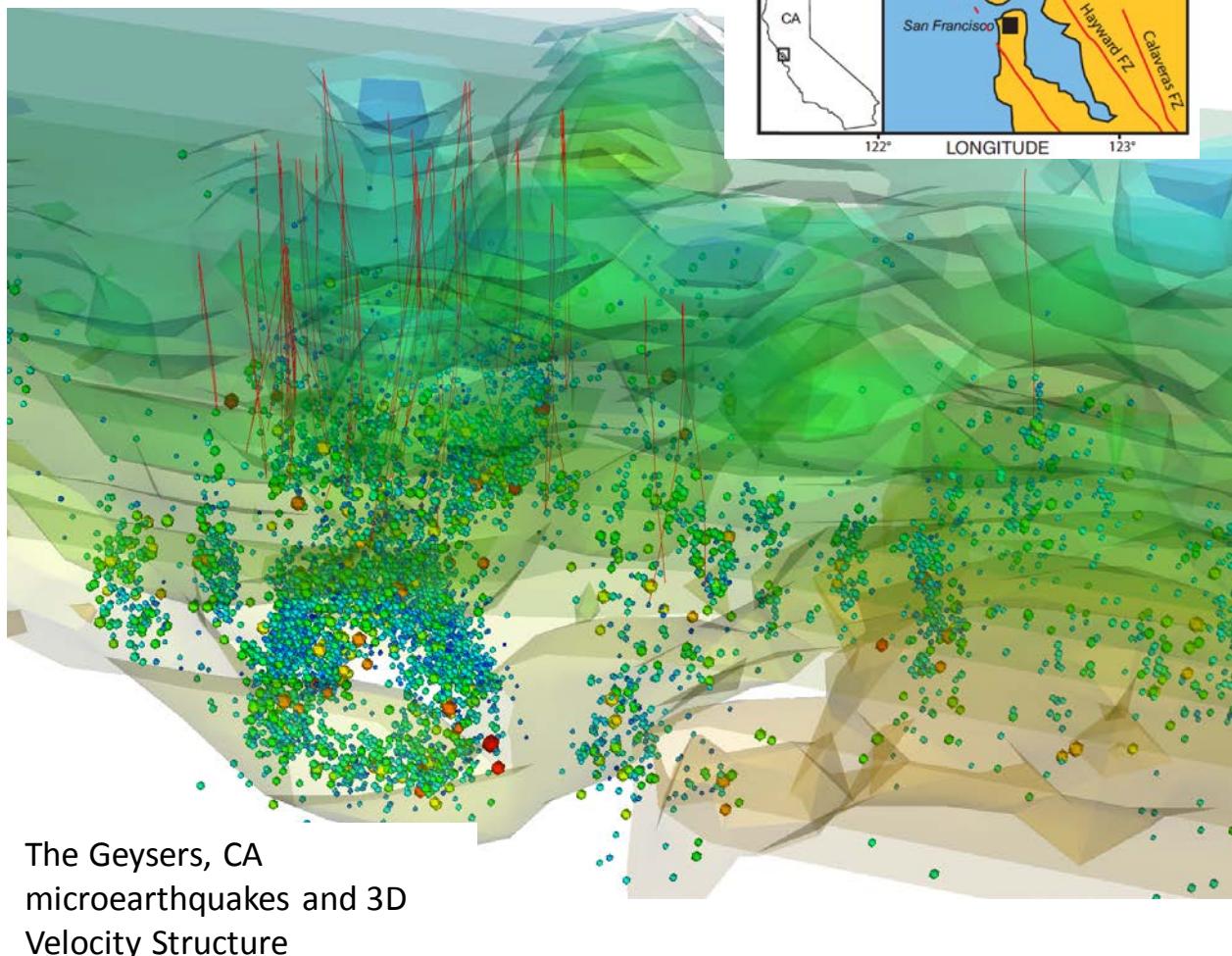
- Artificially create/enhance a fracture network by hydraulic fracturing and/or chemical mechanisms in high temperature, low permeability rock.
- Transfer heat to surface by circulating fluid through the fracture network with injection and production boreholes.

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

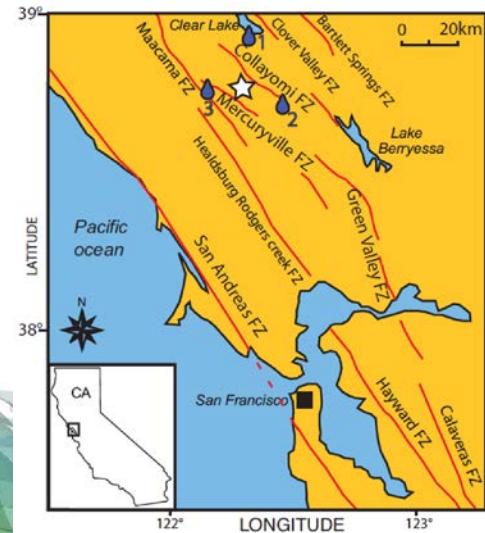
The Geysers geothermal field in Northern California is “enhanced” in that fluid is being added to a natural system



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

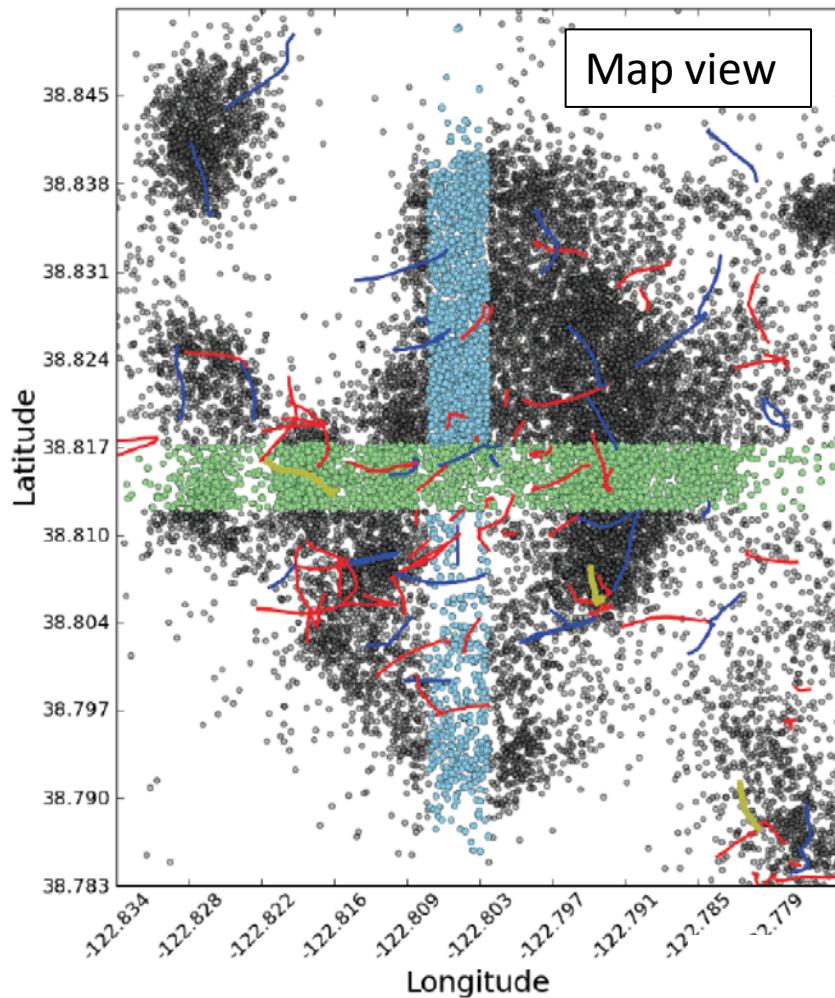


The Geysers, CA
microearthquakes and 3D
Velocity Structure

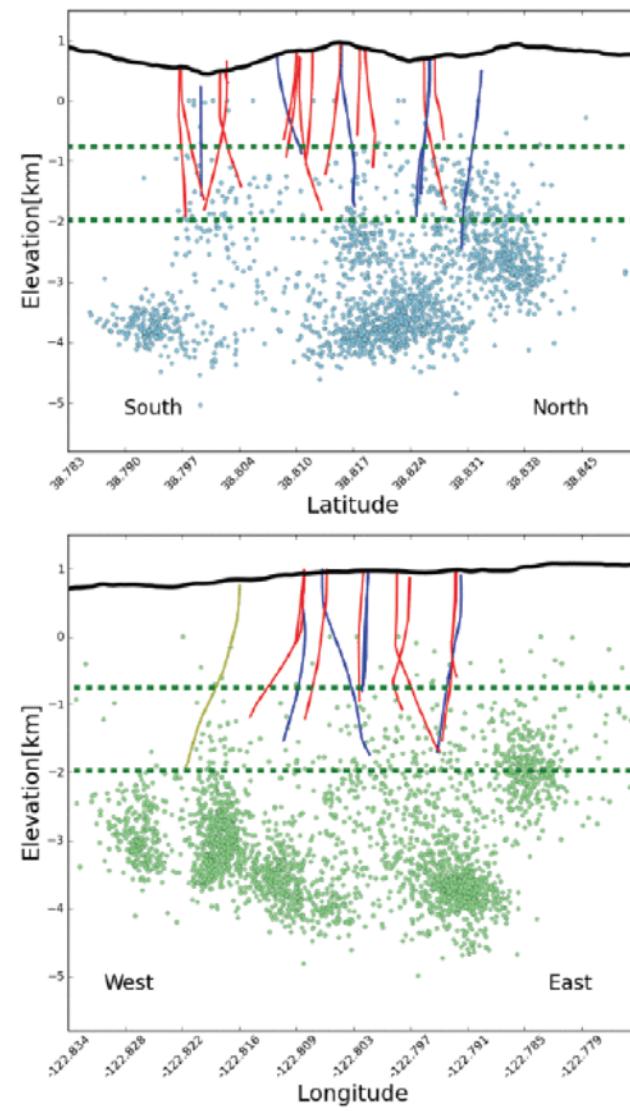


Geysers earthquakes are not clustered at the points of injection

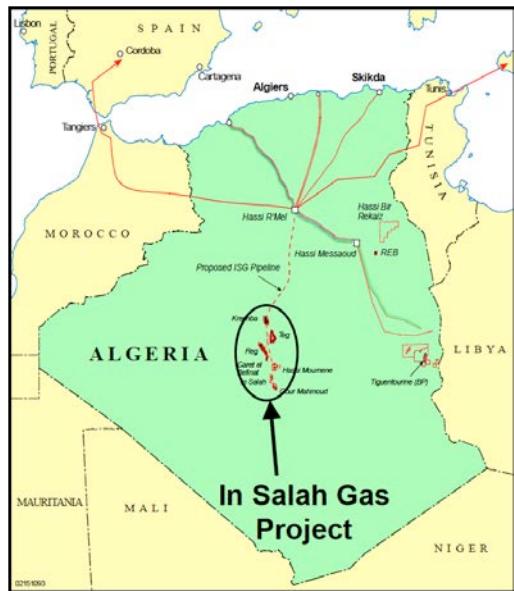
Microearthquake locations



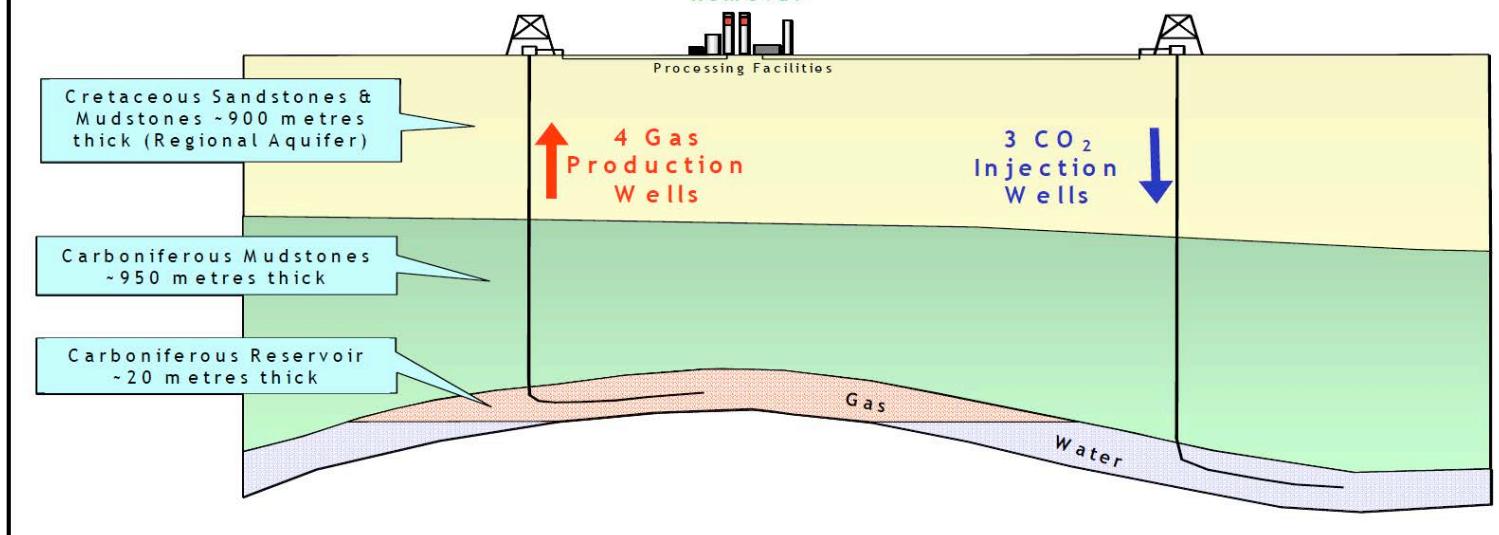
Cross sections



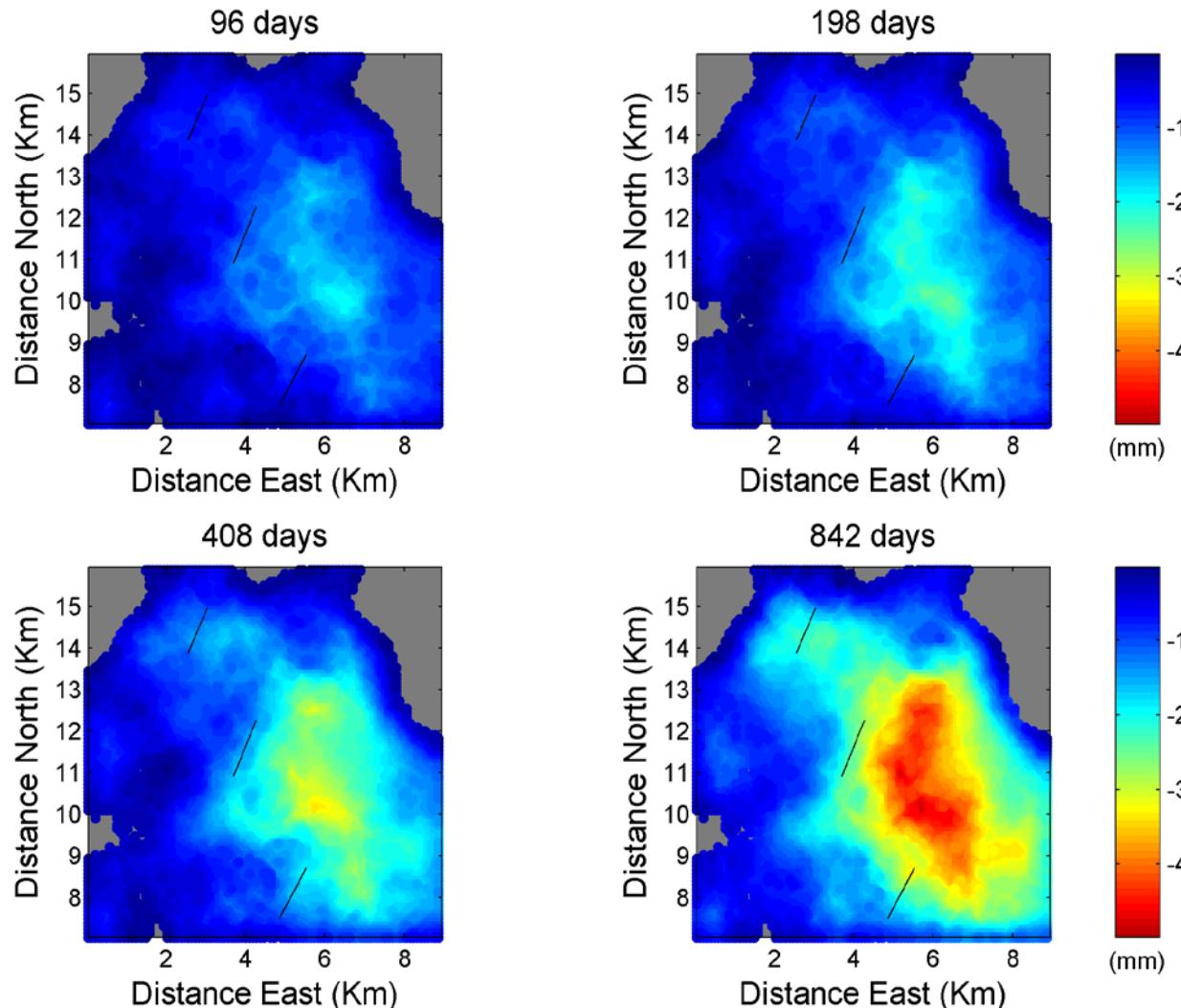
CO₂ storage experiment at Krechba gas field in Algeria: Another way to observe deformation related to subsurface stress distribution – ground surface uplift



CO₂ separated
from natural
gas re-injected
at 1.9 km
depth



Ground surface uplift (in mm) following injection of CO₂ 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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Crosscutting themes and approaches

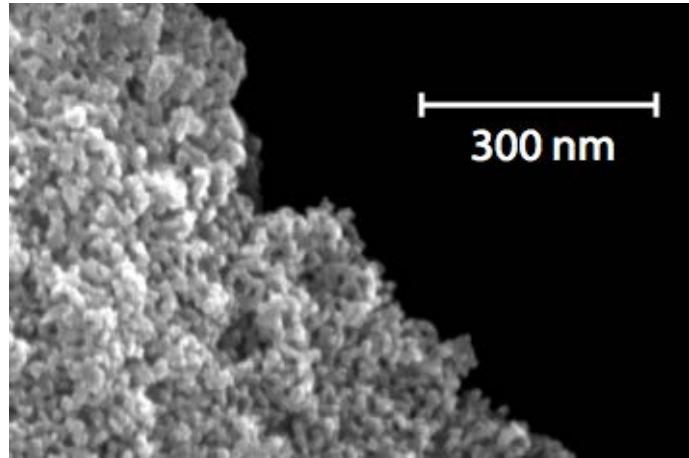
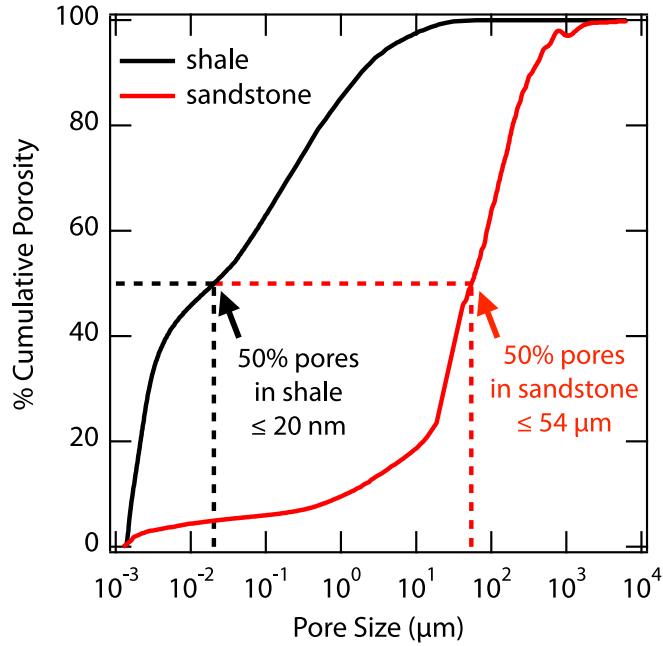
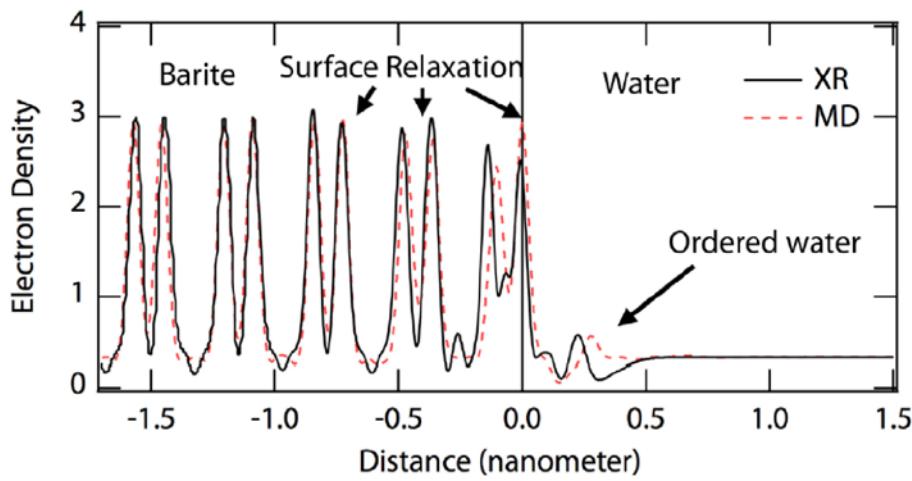
- Advanced computational methods for heterogeneous time dependent geologic systems
- Architected geomaterials to address heterogeneity and scaling

Nanoporous geomaterials – reactivity, flow and mechanics

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

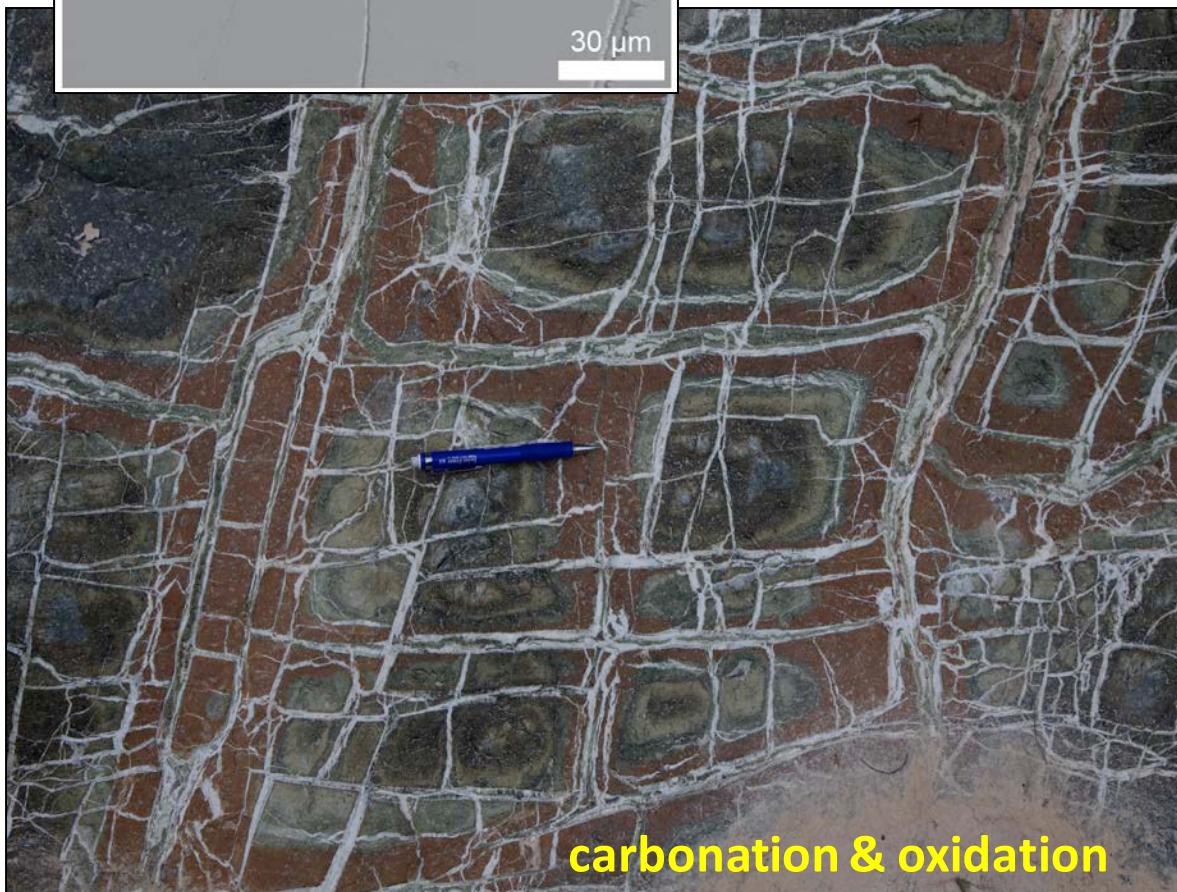
- **Problem:**

- 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**

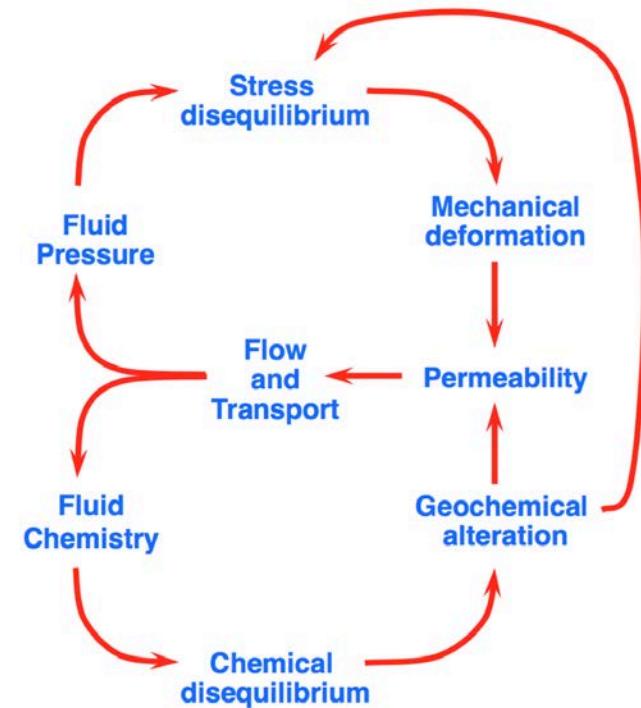
- New capabilities for measuring rates of chemical reactions and 3D imaging of response to applied stresses (Xrays, neutrons)
- Increased computing power combined with algorithm development
- New purpose-built experimental systems designed to be compatible with imaging tools for real time monitoring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

f Reaction Driven Cracking



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

Stress must be inferred from observed material responses

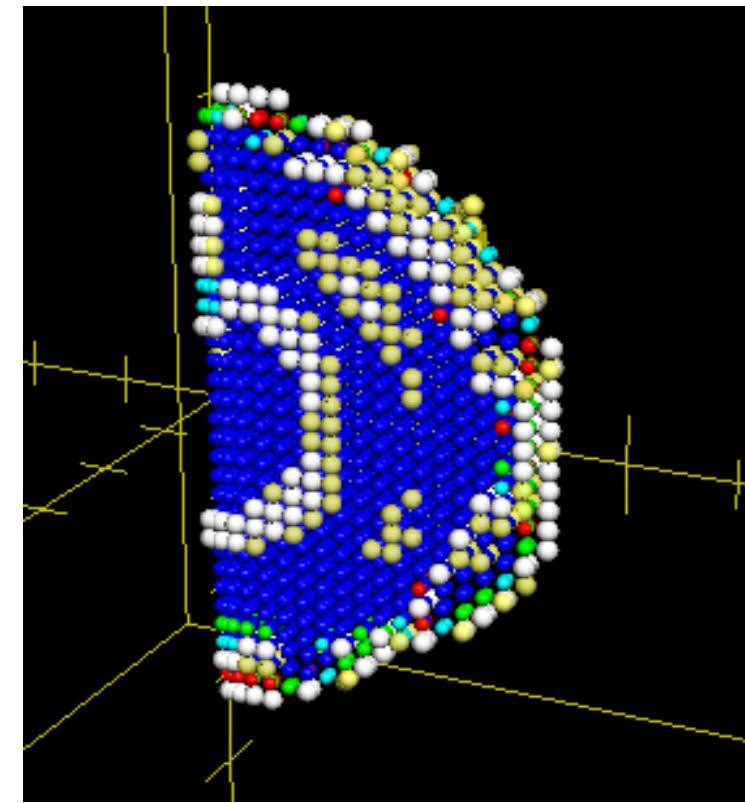
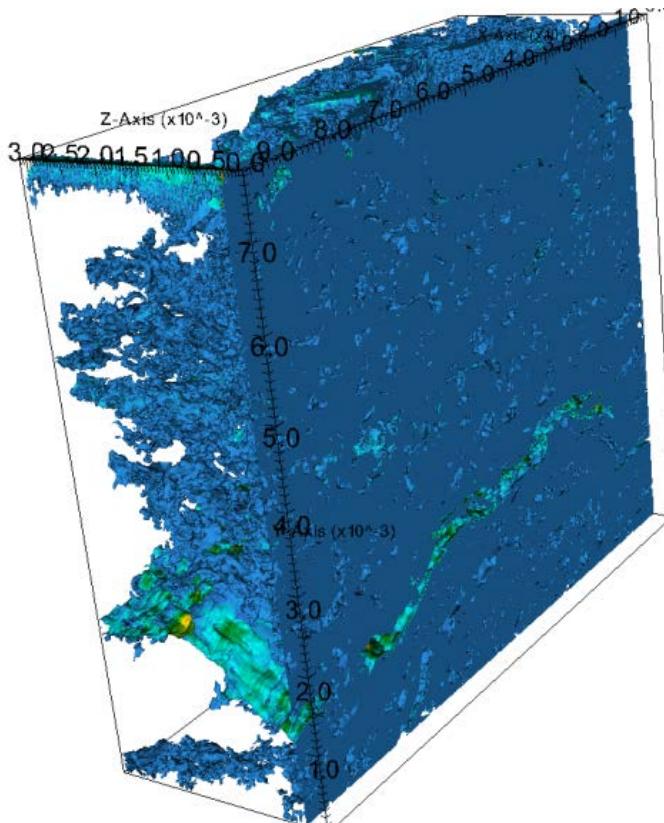


*Components of a coupled modeling strategy
Detwiler, 2015*

Advanced computational methods

- **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



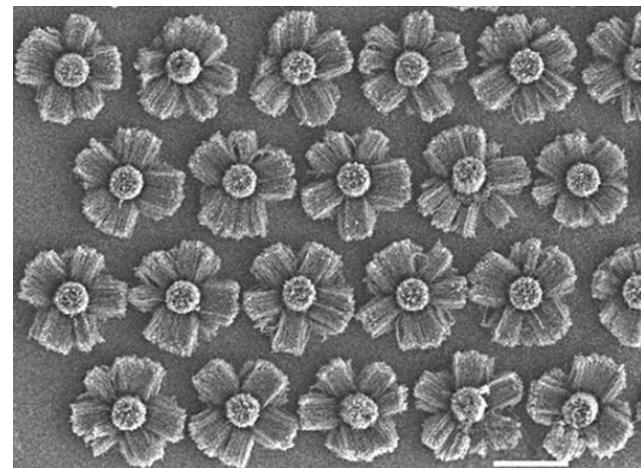
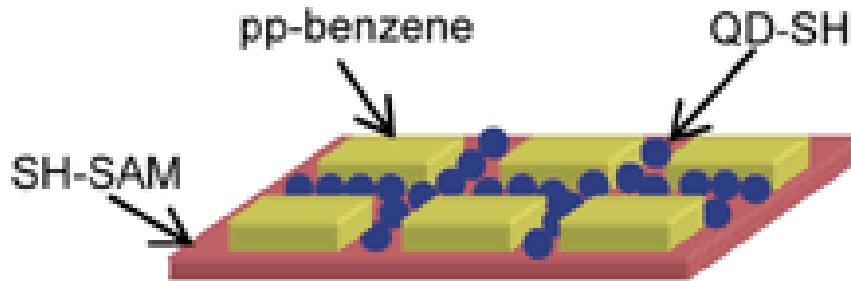
Simulation of flow in a previously imaged sample of fractured Marcellus shale using 60,000 cores of NERSC Hopper and the software package Chombo-Crunch.

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

- 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

	Wellbore Integrity	Subsurface Stress & Induced Seismicity	Permeability Manipulation	New Subsurface Signals
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

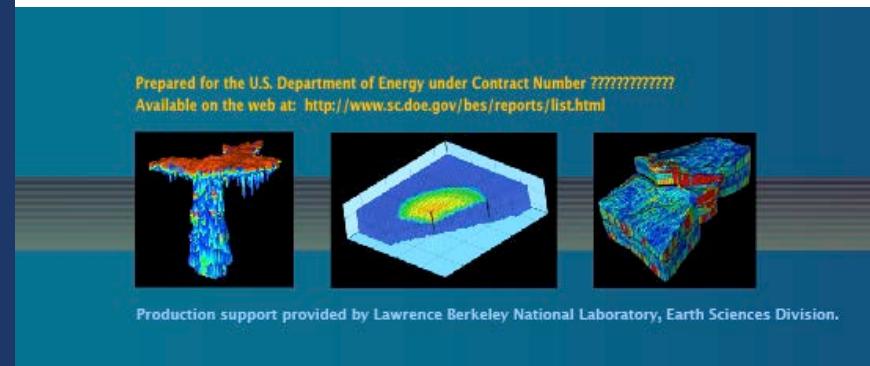


Basic Research Needs in Geosciences: Facilitating 21st Century Energy Systems
Sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences

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)



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



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

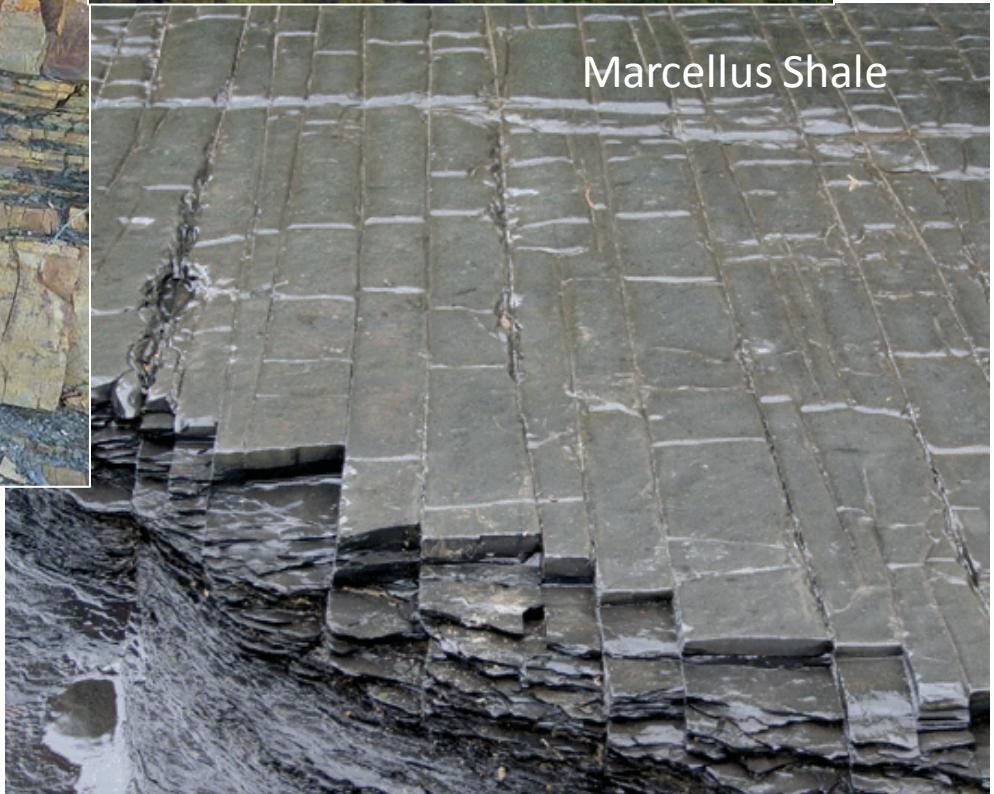
- Mineral-fluid interface complexity and dynamics
- Nanoparticulate and colloid chemistry and physics
- Dynamic imaging of flow and transport
- Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization
- Fluid-induced rock deformation
- Biogeochemistry in extreme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

- Develop and test methods for assessing storage capacity and for monitoring containment of CO₂ 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.



Marcellus Shale



Thank You

Additional reference slides

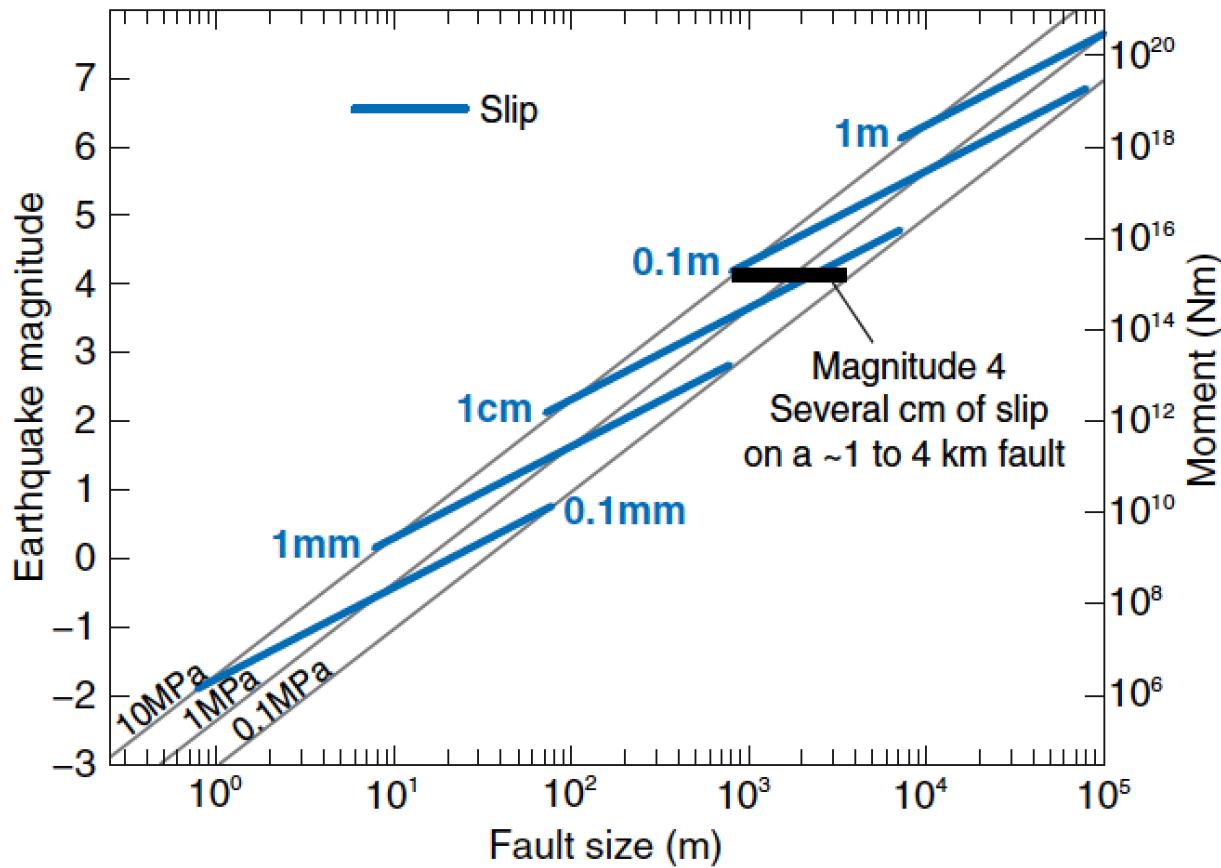
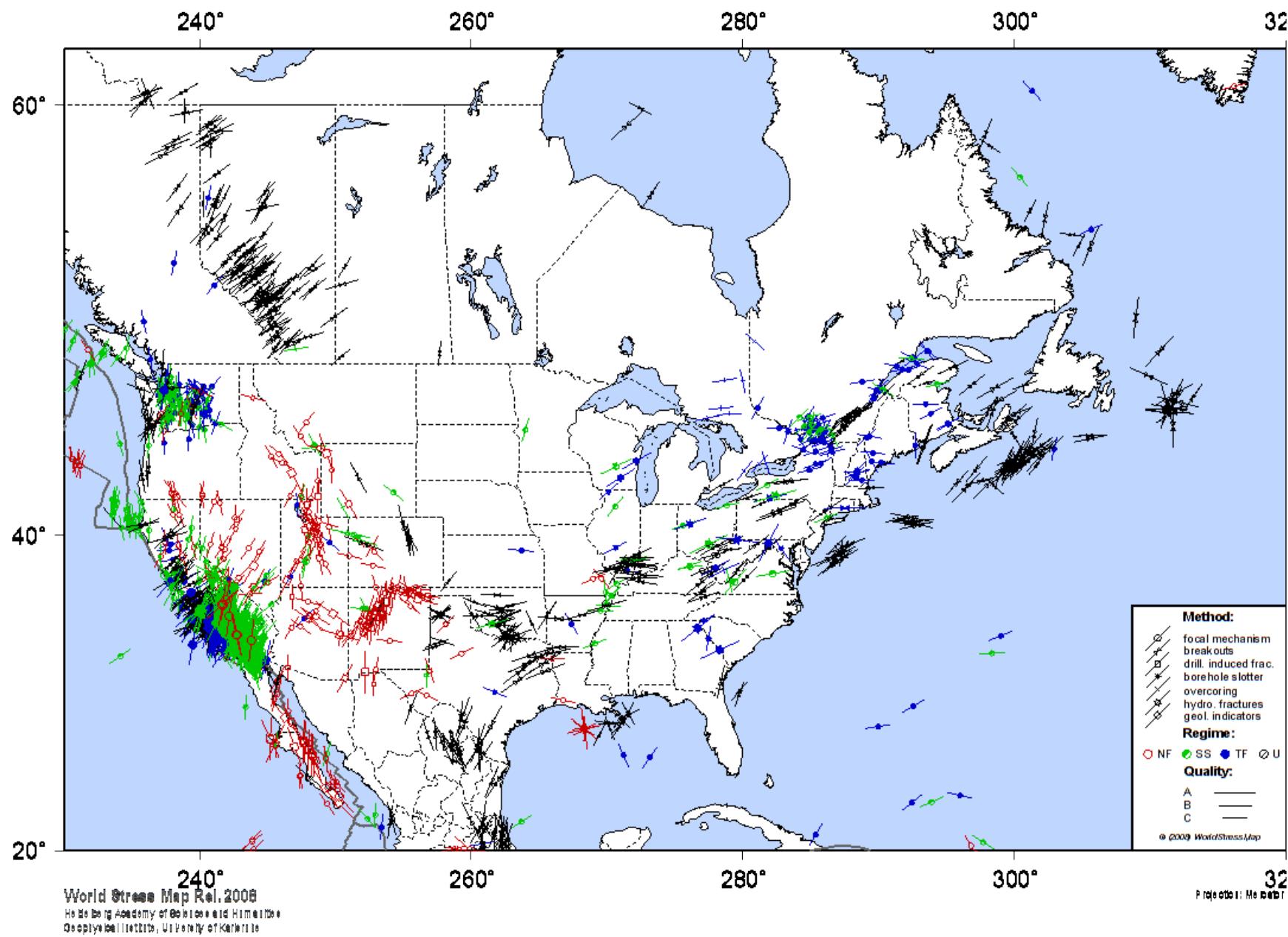


Fig. 2. Relationships among various scaling parameters for earthquakes. The larger the earthquake, the larger the fault and amount of slip, depending on the stress drop in a particular earthquake. Observational data indicate that earthquake stress drops range between 0.1 and 10 MPa.



From Alt and Zoback, 2014

