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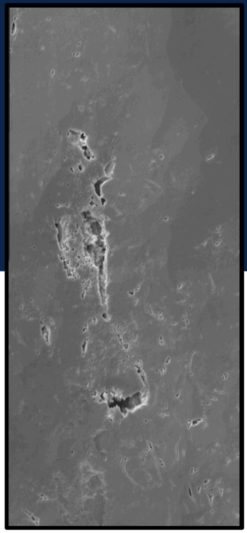

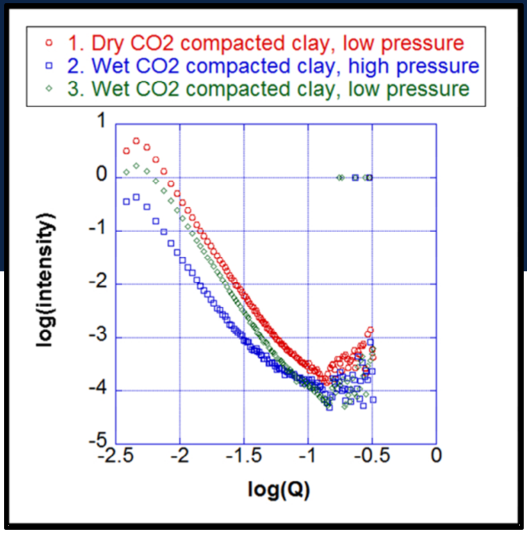

A Whirlwind Tour of Geoscience for the Working Mathematician

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Presented December 1, 2016, to the BYU Math Department

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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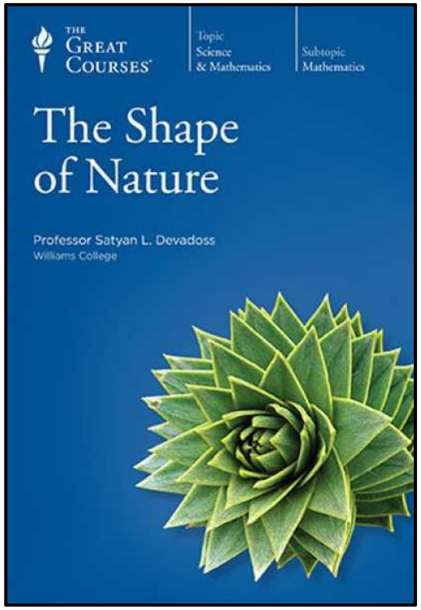
Outline

1. Introduction
2. The whirlwind tour
3. Future directions and collaborations

Outline

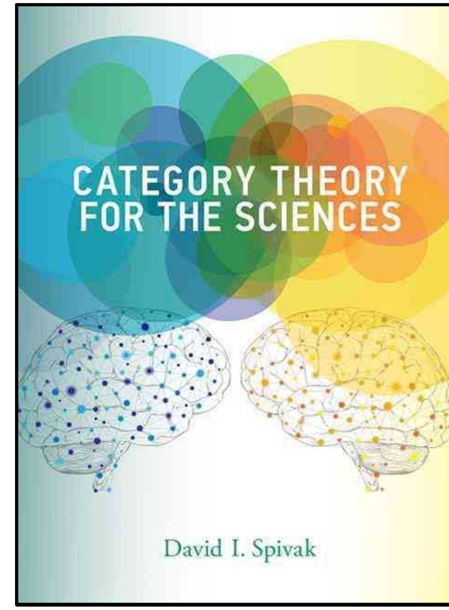
1. Introduction
   - Goal: better collaboration between mathematics and geoscience
   - What is Geoscience?
   - Domains of Math related to Geoscience
   - Amazing geology nearby
2. The whirlwind tour
3. Future directions and collaborations

Goal: better collaboration



Interviewer to Geologist:
What is 2+2?

Geologist (beginning to sweat):
Well, uhhh, it's more than 3 and it's less than 5… awww shoot! That's about as good as I can get.



Form and Function
Language of shapes
Knots, links, and braids
Vector fields on shapes
Bending chains and origami
Surface reconstruction
Notions of equivalences and groups
Configuration spaces

Ontology logs (ologs)
Sets, functions, products, coproducts
Pullbacks, pushouts
Spans, experiments, and matrices
Monoids, groups, graphs, orders, sheaves
Database schemas
Categories, functors,
Natural transformations

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What is Geoscience?

Philosophical approaches and classification:

- Geology vs chemistry and physics
- Geology as a historical and hermeneutic science
- “Strong Inference” and multiple working hypothesis

NSF view on the disciplines of geoscience:

Geology, geophysics, hydrology, oceanography, marine science, atmospheric sicne, planetary science, meteorology, environmental science, and soil science

Main geo-departments at Sandia:

Geomechanics, Geophysics, Geochemistry, Geophysics, Geotechnologies and Engineering, and Atmospheric Sciences

Domains of math related to geoscience

Three main categories of mathematics according to S. Devadoss

What “bins” do each geoscience discipline and faculty member predominantly go into?

Geoscience disciplines

Hydrology, Seismology

Geophysics, Geochemistry

Geotechnical engineering

Structural geology, Geodesy

Geomorphology, Geomechanics

Stratigraphy, Paleontology

Sedimentology, Petrology

Mineralogy

Analysis (change)

Algebra (structure)

Geometry (shape)

BYU Math Department

Mark Abramson
Roger Baker
Blake Barker
James Cannon
Jasbir Chahal
Shue-Sum Chow
Gregory Conner
John Dallon
…

Finding where we connect is the fiber product

$$\begin{array}{ccc} X \times_Z Y & \xrightarrow{\pi_2} & Y \\ \pi_1 \downarrow & & \downarrow g \\ X & \xrightarrow[f]{} & Z \end{array}$$

What about foundations, probability and statistics, and computational sciences?

Amazing nearby geology

Virgin Anticline, east of Saint George, UT

Image sources: Left: from the GEO 1001 website of the University of Utah's College of Mines and Earth Sciences, and specifically from www.mines.utah.edu/geo/courses/UOnline/slideshow/folds_6.html. Above: an illustration from Hamblin and Christiansen's Earth's Dynamic Systems (seventh editon) used on Terry J. Boroughs's Geologic Structures Diagrams webpage at www.arc.losrios.edu/~borougt/GeologicStructuresDiagrams.htm .

http://www.gly.uga.edu/railsback/VFT/VFTVirginAnticline.html

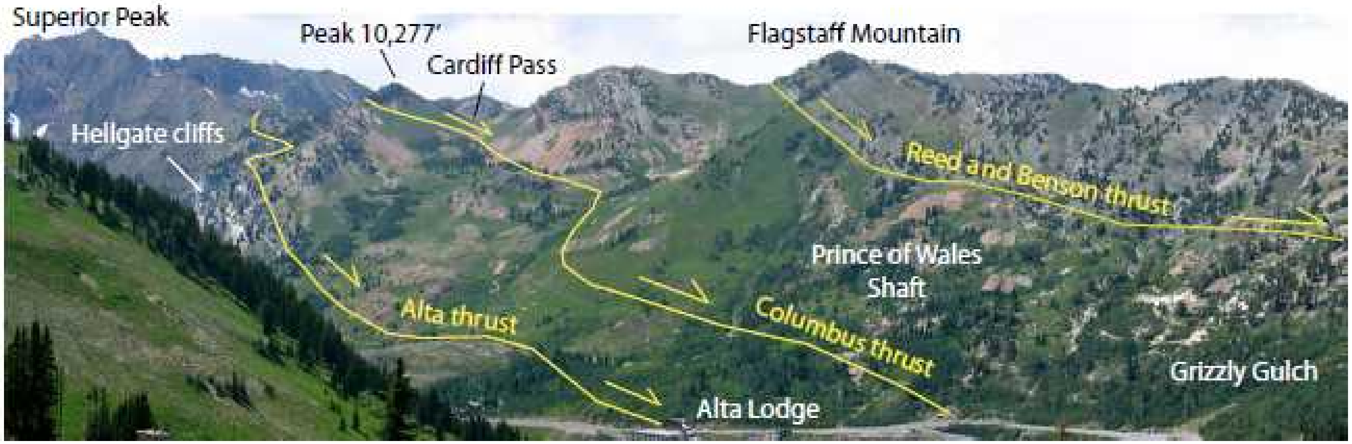

Figure 6. Looking north from the Catherine Pass trail head near the Sunnyside Lift parking area or Alta Resort. The Cambrian to Mississippian section is repeated three times by thrust duplexing.

Figure 7. Looking north at recumbent folds of Precambrian Mineral Fork Tillite at the structural base of the Alta thrust. Strain is partitioned into clay rich units, such as the tillite, which records up to 50% shortening near thrust faults. Fold asymmetry indicates top-to-the-east-northeast sense of shear (067-110°).

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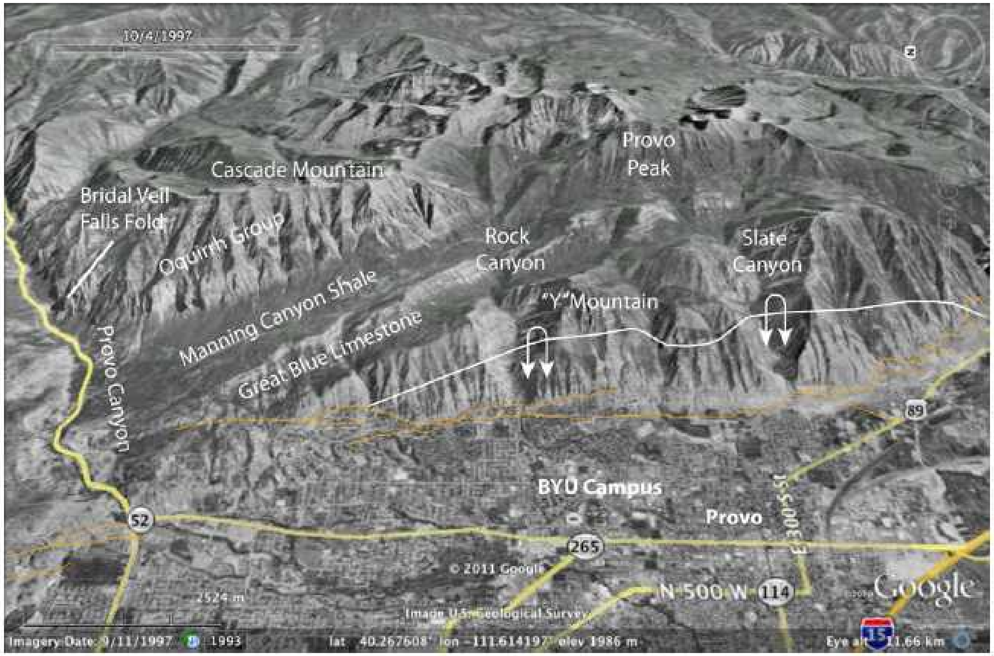
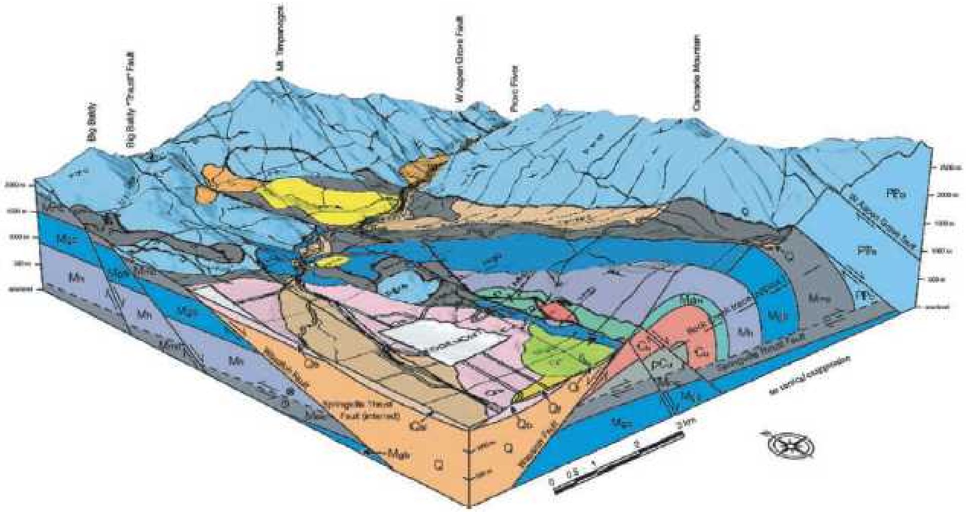


Figure 9. Location map of the "Y" Mountain anticline near Provo (oblique view looking east). Note plunge to the north and south, and strike valley of Manning Canyon Shale.



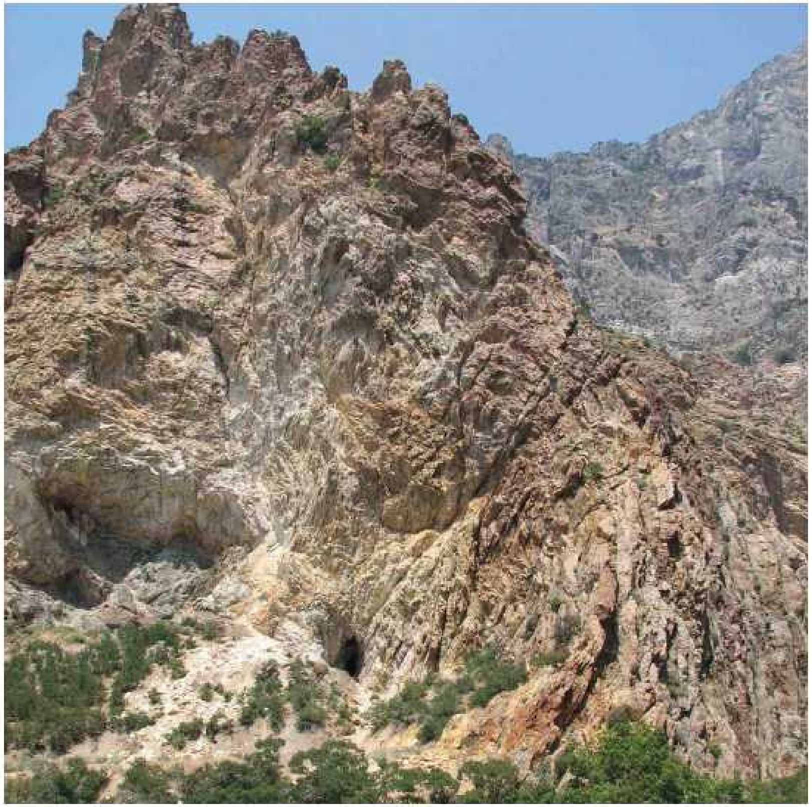


Figure 12. Hinge zone of the "Y" Mountain anticline in Rock Canyon looking east. Closely spaced bedding planes in the Tintic Quartzite change from near horizontal to vertical and overturned from left to right. In shade at far left are opposing thrust faults that bring tillite over quartzite.

Figure 13. Looking south along strike at the vertical to slightly overturned beds of the "Y" Mountain anticline. "Y" Mountain is right of center. Provo Peak (11,068 feet elevation) is on the far left. The strike valley of the Manning Canyon Shale is at the base of Provo Peak (see figure 9). Flexural slip along the weakest units moves structurally higher dip domains over lower ones, which accounts for the abrupt shallowing in dip across these horizons upsection (see explanation in Bridal Veil Fall fold).

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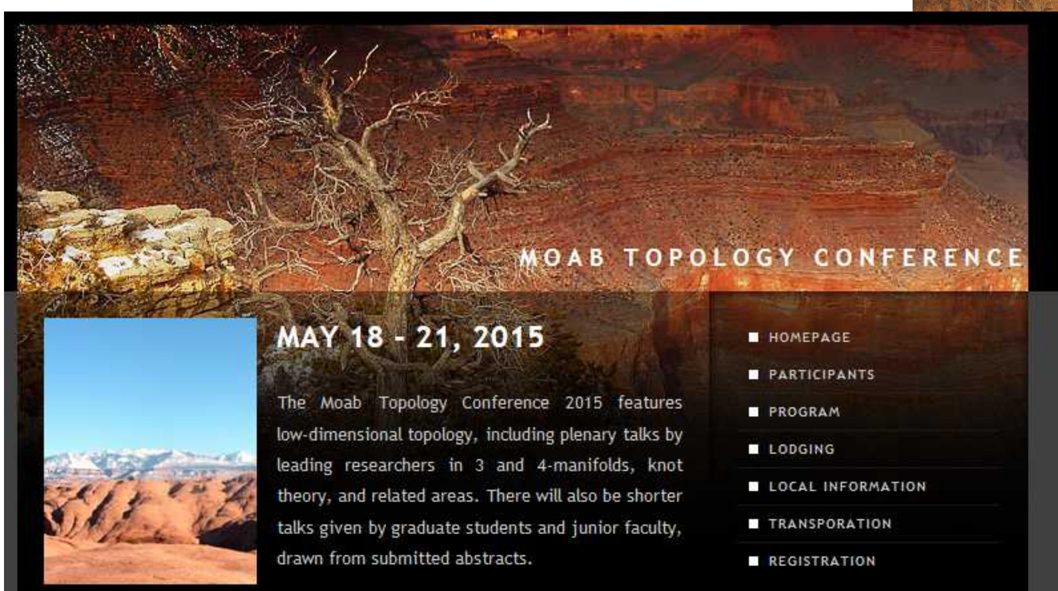

Southern Utah

Geology and Topology…

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Raduha et al., 2016, Potential Seal Bypass and Caprock Storage… Geofluids Journal.

Outline

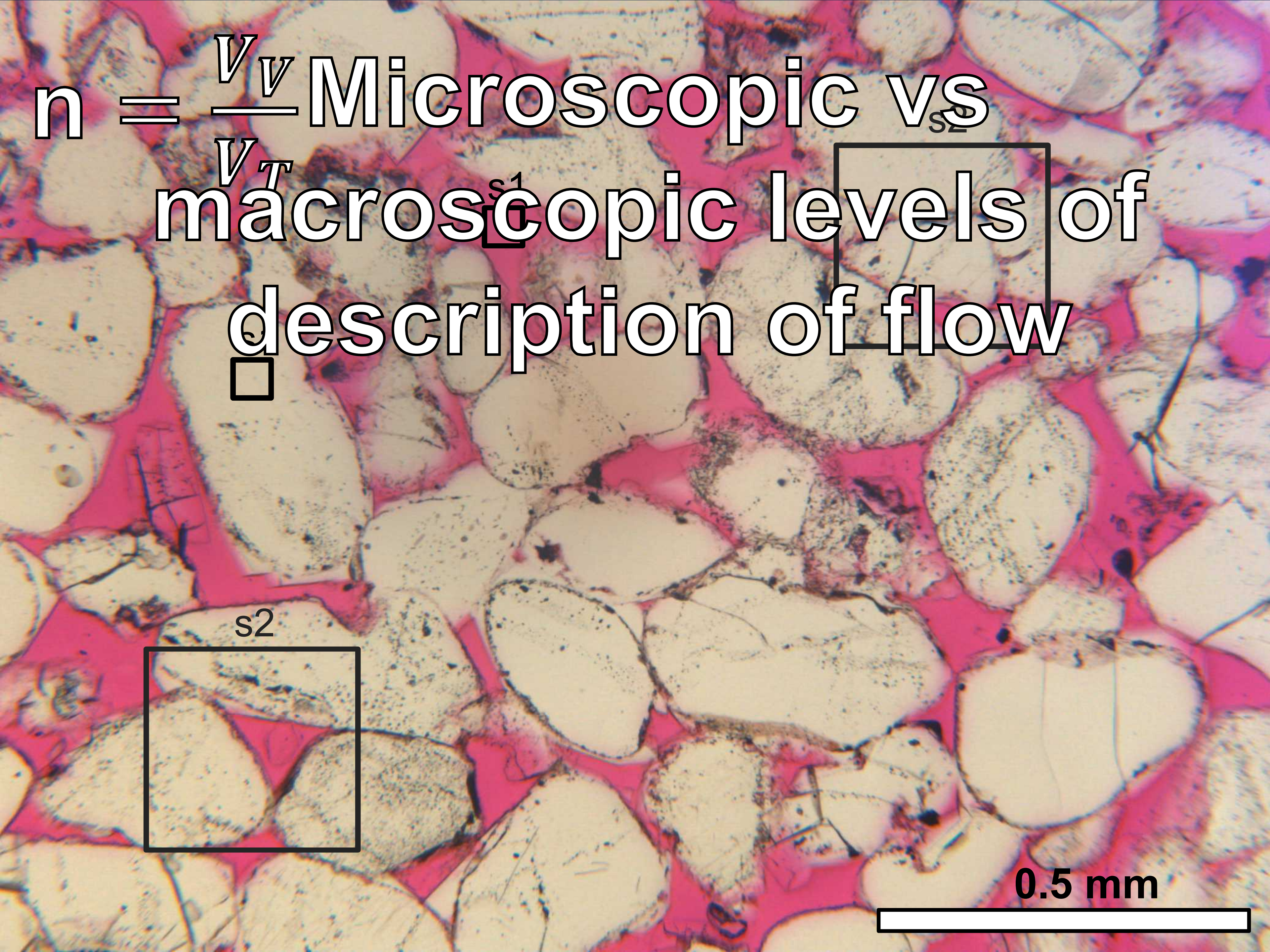
1. Introduction
2. The whirlwind tour
   - Broad research challenges of the geosciences
   - Examples of applications and mathematical approaches
     - Underground storage of CO_2
     - Fluid mixing in salt caverns of the US DOE's Strategic Petroleum Reserve
     - Shale as a energy resource
3. Future directions and collaborations

2. The whirlwind tour: broad research challenges

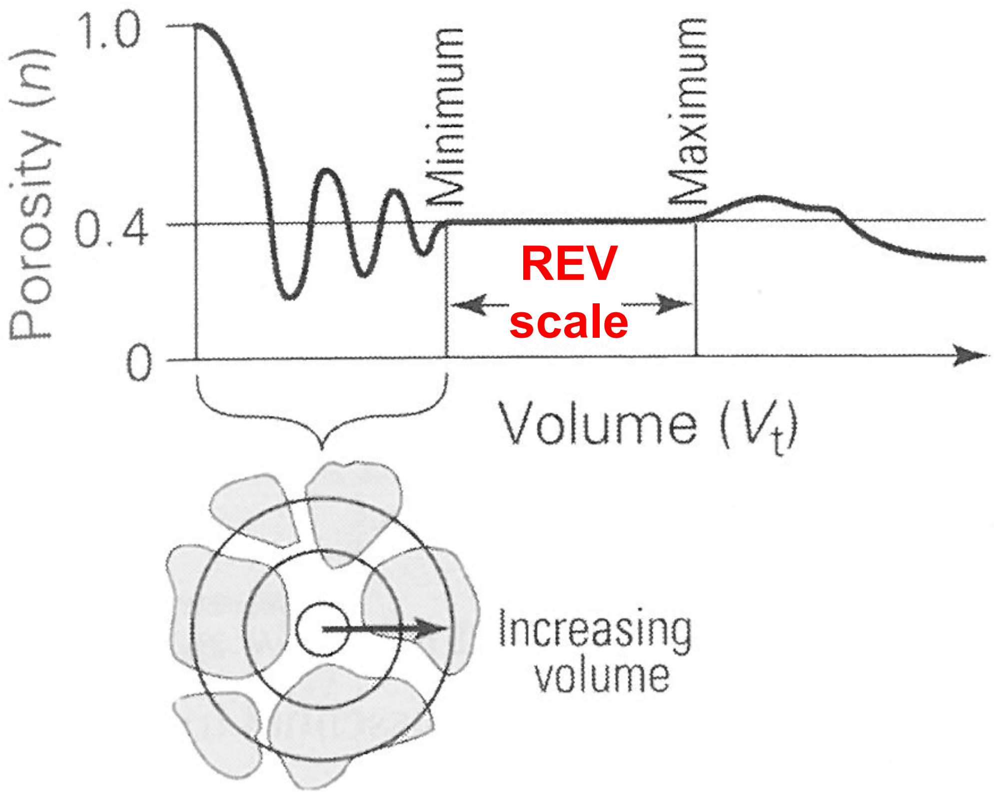
- Heterogeneity in properties
- Sparse data - especially for the subsurface
- Too much data
- Limitations (?) of continuum approaches
- Inability in reproduce many phenomena in lab

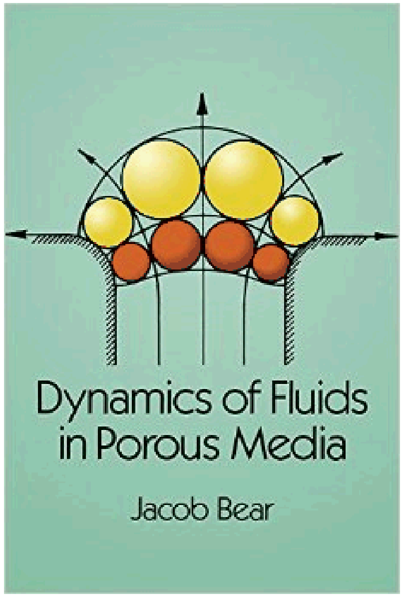
$$n = \frac{V_V}{V_T}$$

Microscopic vs macroscopic levels of description of flow



Representative elementary volume





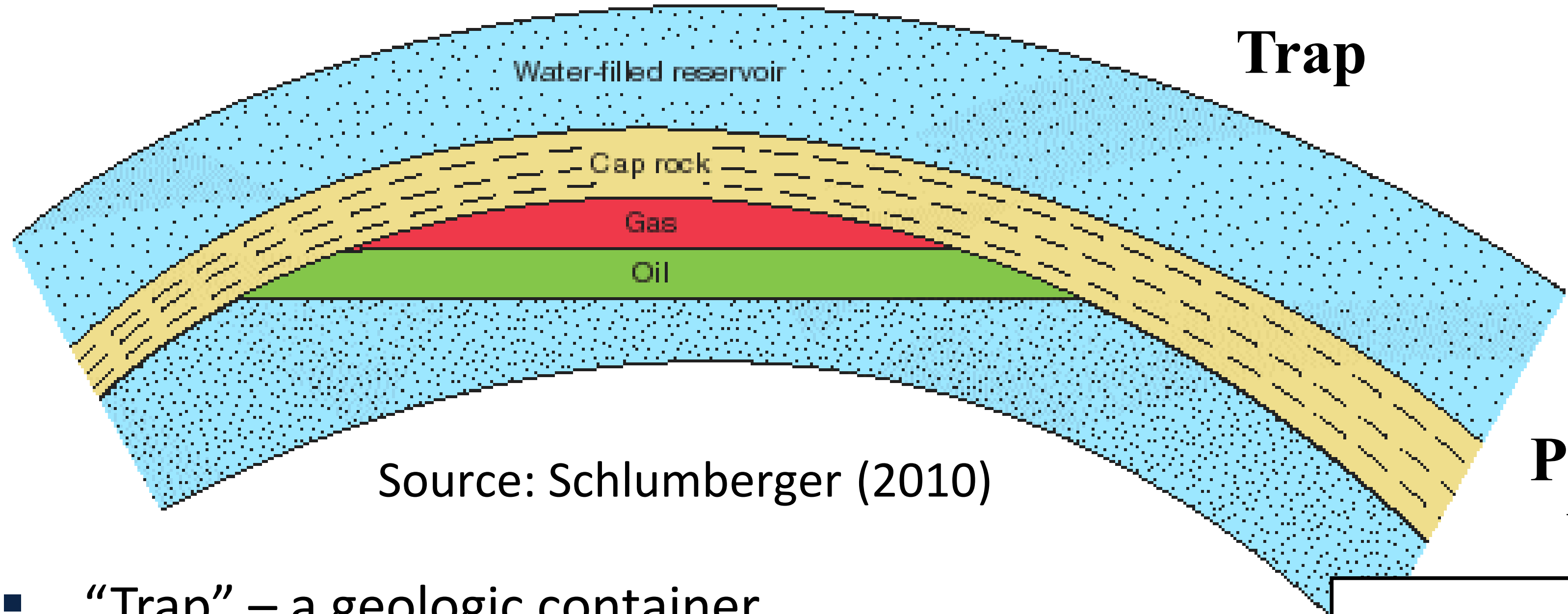
Advection-dispersion equation

$$\nabla \cdot (n_e \rho \bar{D} \nabla C) - \nabla \cdot (n_e \rho v C) + Q_s = \frac{\partial (n \rho C)}{\partial t}$$

2. Applications and mathematical approaches

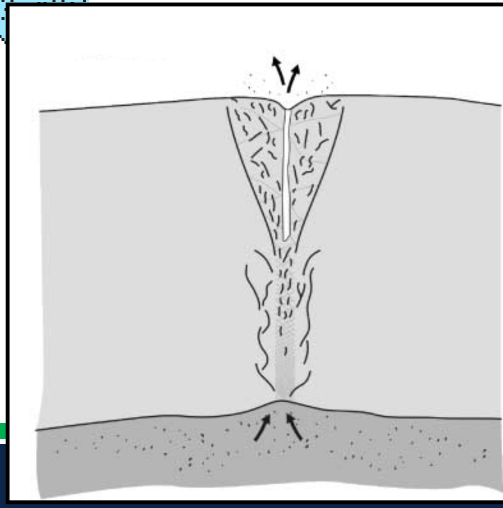
Underground storage of CO_2

Trap



Source: Schlumberger (2010)

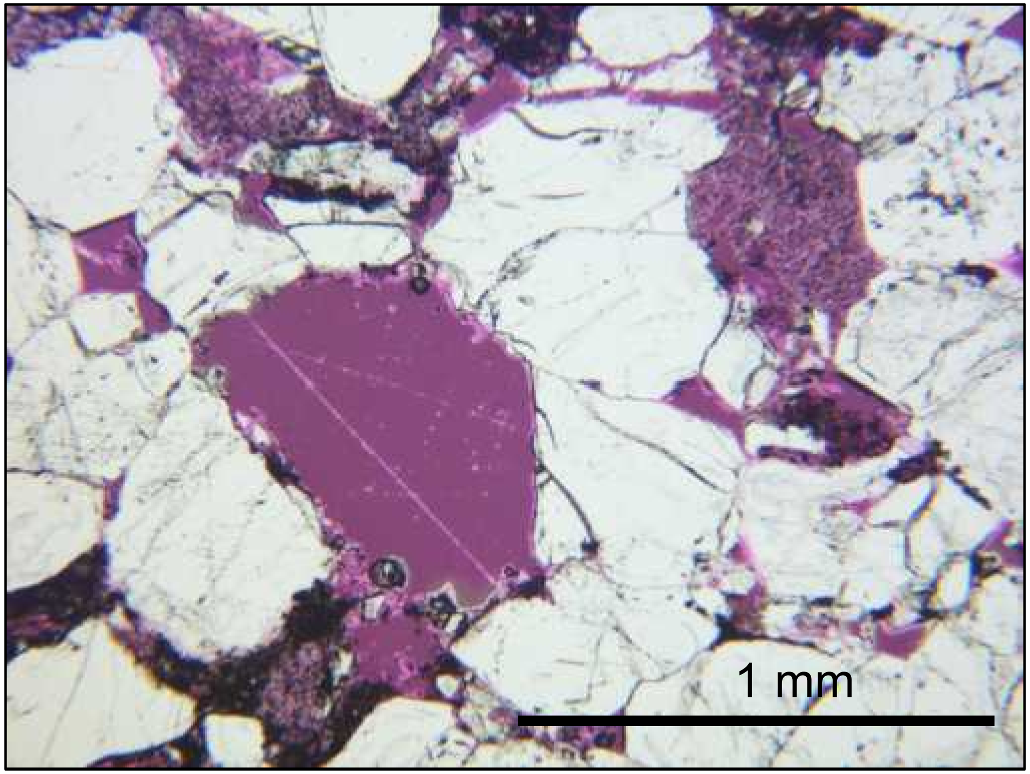
Pipe-type bypass



- "Trap" – a geologic container
- Sealing behavior
- Concept of caprock depends on time scales
- "Seal bypass systems" (see Cartwright et al., 2007)

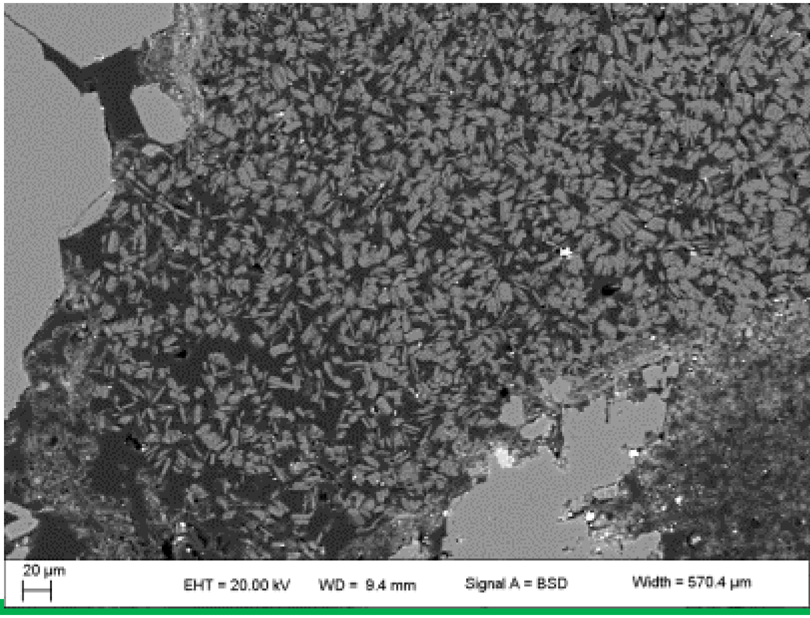
2. Applications and mathematical approaches

Underground storage of CO_2 – example from Farnsworth Unit, TX

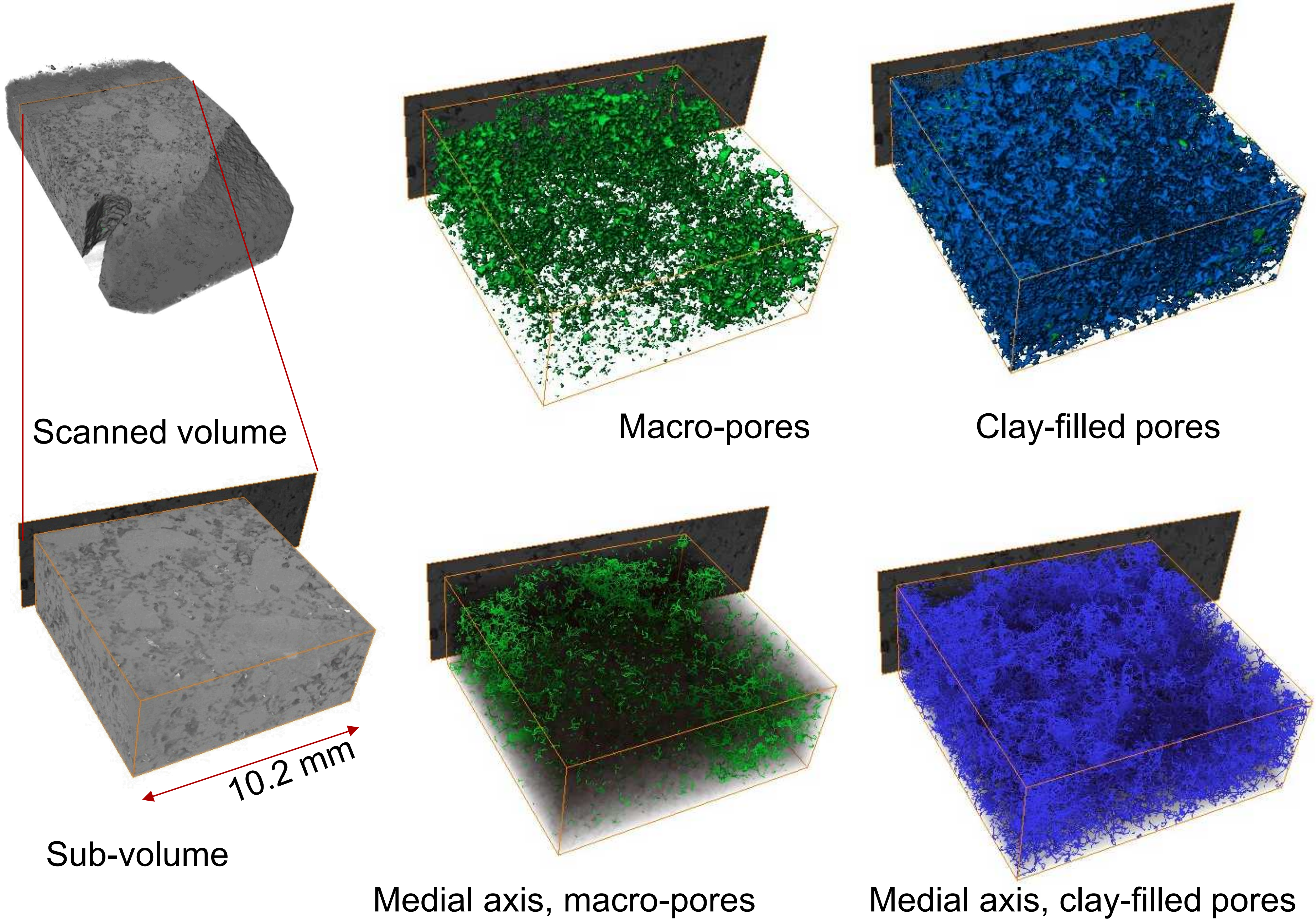


Common features:

- “clean” macro or oversized pores
- authigenic clays with microporosity



What is the core-scale connectivity of macropores and clay-associated micropores?

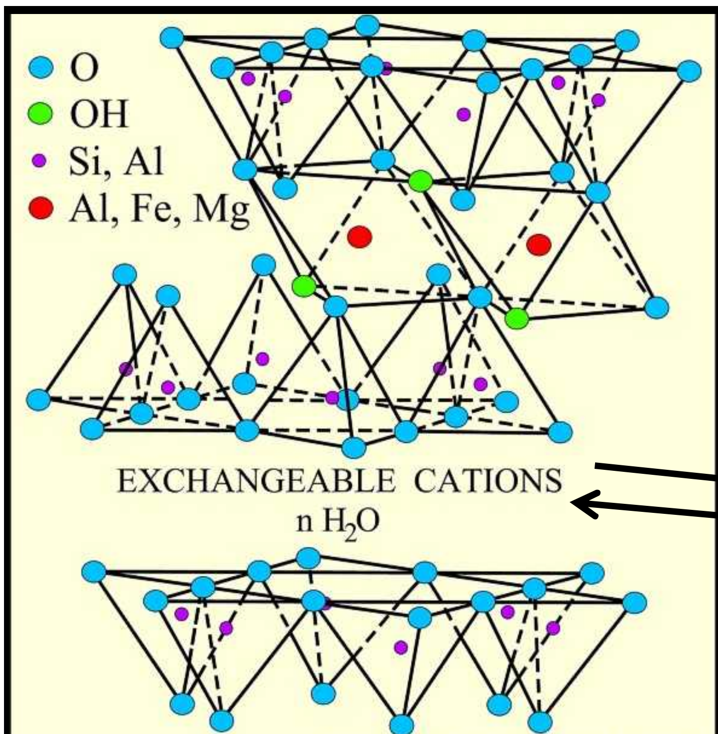


Scanned volume
10.2 mm
Sub-volume
Macro-pores
Clay-filled pores
Medial axis, macro-pores
Medial axis, clay-filled pores

What is the change in pore structure of montmorillonite (SWy-2) as a function of non-hydrostatic stress conditions and dissolved water in CO_2?

Approach:

- Measure compaction or swelling with oedometer, coupled to SANS
- Take the same clay sample through a stress path with different pore fluids (dry and wet CO_2) and measure pore structure with SANS



H_2O?

CO_2?

Initially dry supercritical CO_2 in pores

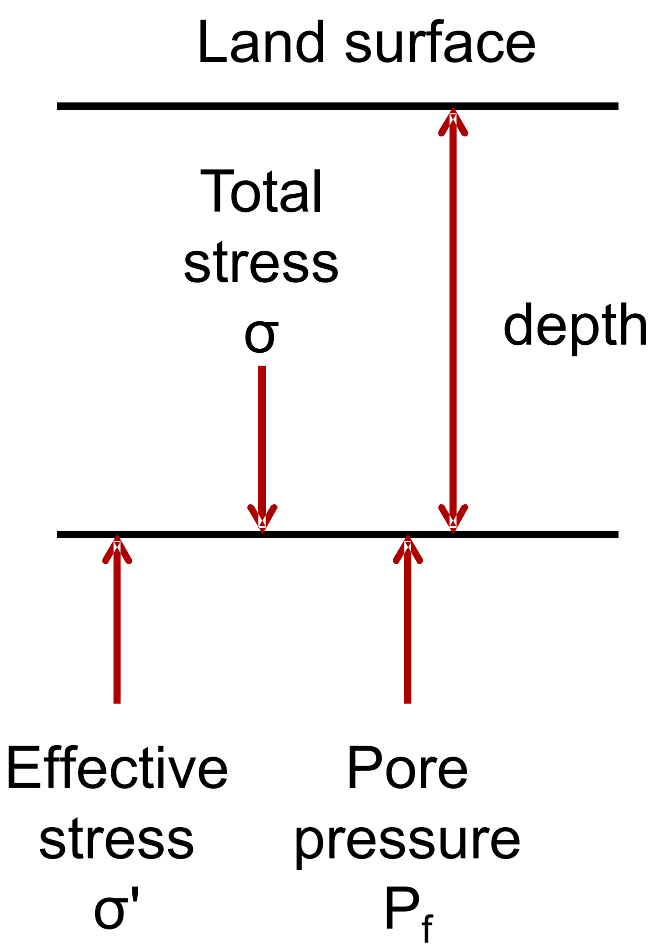
Oedometric SANS

Key advances:

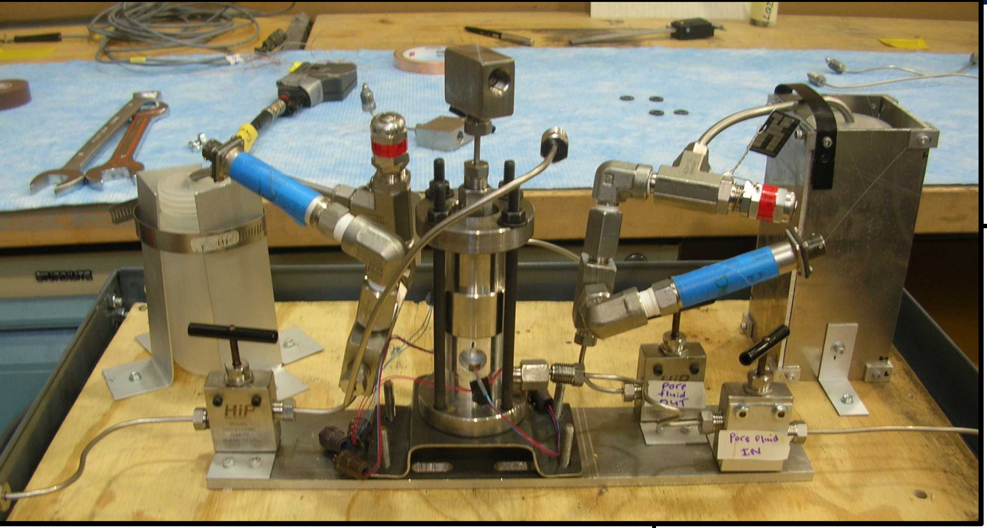
- Data collection over 1 to 1000 nm (or to 10s of microns if used with USANS)
- Accommodates pore fluids at high pressure and temperature
- Non-hydrostatic stress state applied to sample

Difficulties and opportunities:

- We are developing oedometer v4.0…
- Sample preparation for *in situ* fluids, pressure, and temperature at beam facilities (LANSCE; NIST with USANS); thin sample
- Data interpretation – you don't "see" pores

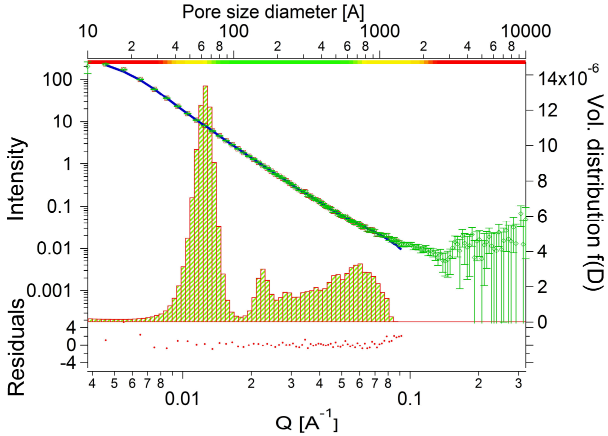


Oedometer v2.0

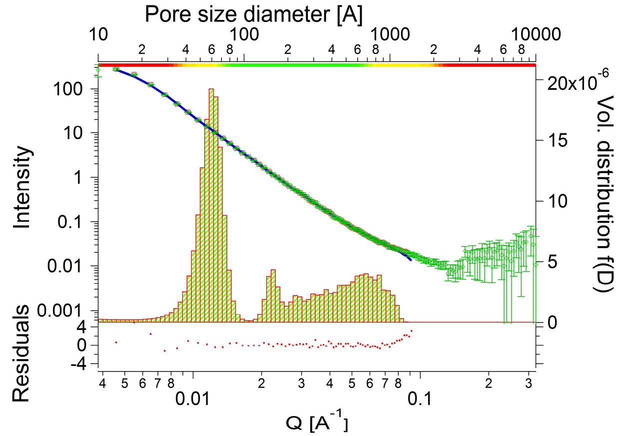


- MAWP: 6.89 MPa
- Al window; steel
- Designed for SANS neutron optics
- Drawback: “penny-shaped” crack in metal…

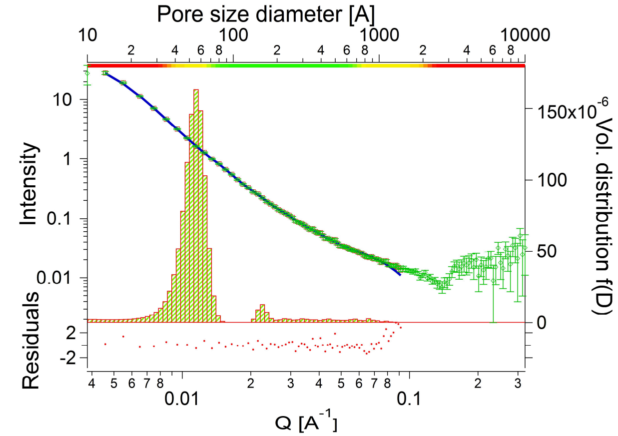
I



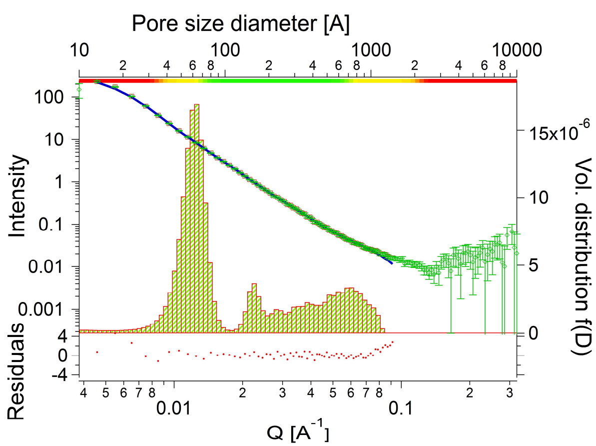
II



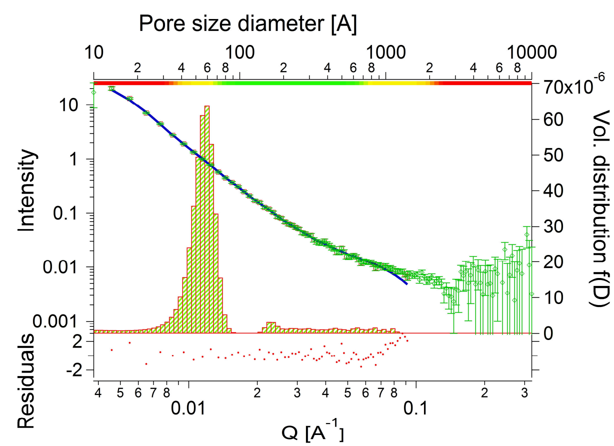
III



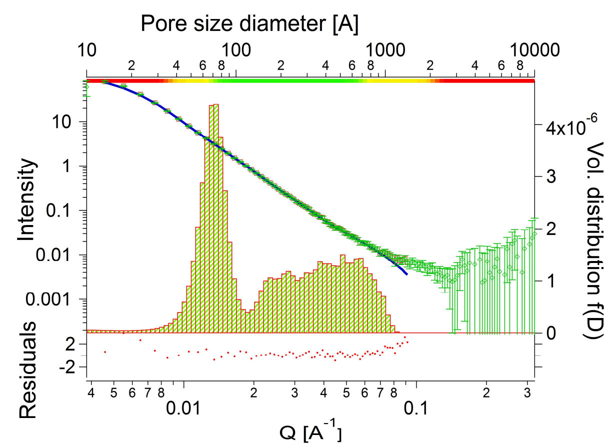
IV



V



VI

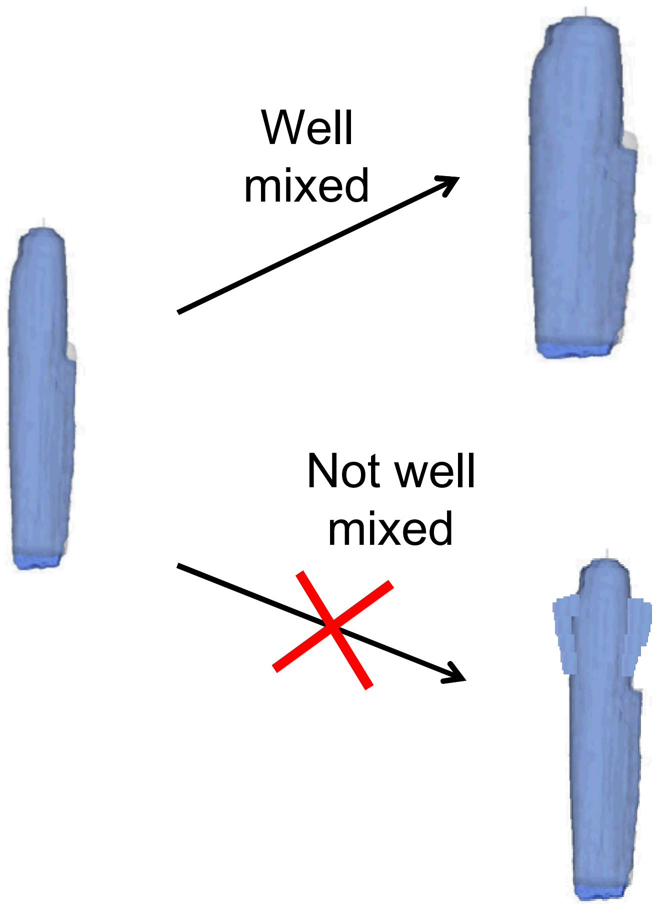


PSD obtained with: Irena Tool Suite: Ilavsky and Jemian, P.R., 2009

2. Applications and mathematical approaches

Fluid mixing in salt caverns for the USDOE SPR

Under what conditions does fresh-water injection into a cavern containing saturated brine lead to complete mixing?

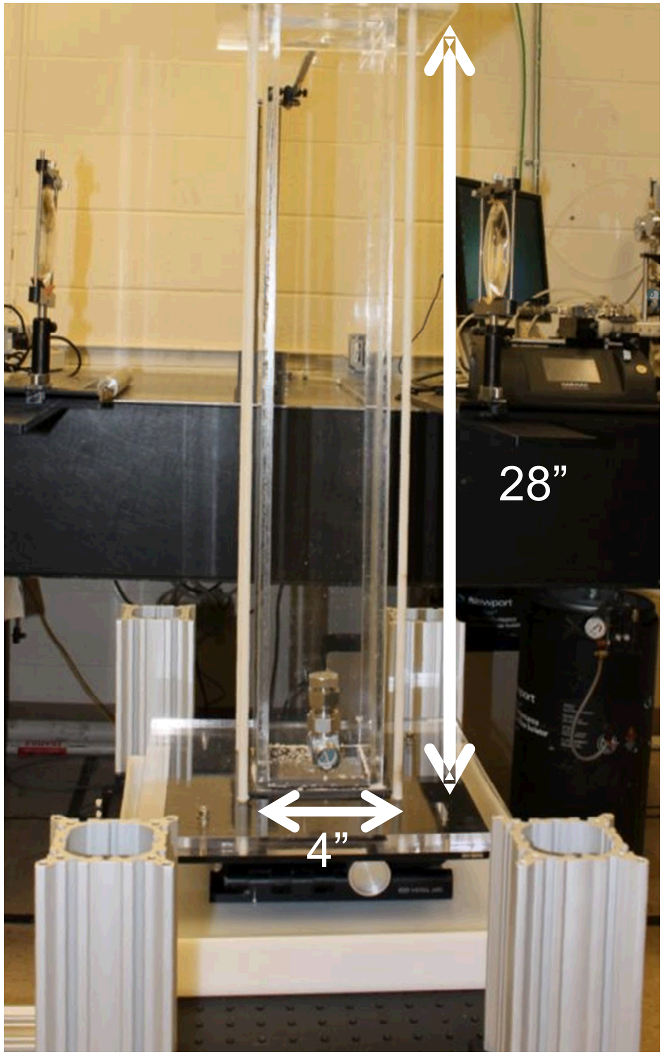


Complete mixing throughout the cavern leads to even dissolution of cavern walls above the injection point

Incomplete mixing has the potential to give the cavern “wings” at the oil-brine interface, causing potential salt fall

Material on SPR work from Heath et al., 2015

Experimental Design



- **Original Hypothesis:**
  1. If the fresh water jet spreads to fill the entire plan view (4” x 4”) then maximum mixing will occur.
  2. Incomplete mixing leading to a layer of fresh water at the top of the tank will occur at a some flow rate below 1.
- **Experimental Method:**
  A. Observe the plume width versus time to determine flow conditions that lead to a plume that fills the plan view of the tank.
  B. Determine conditions that lead to a fresh water cap.
  C. Correlate A. and B.

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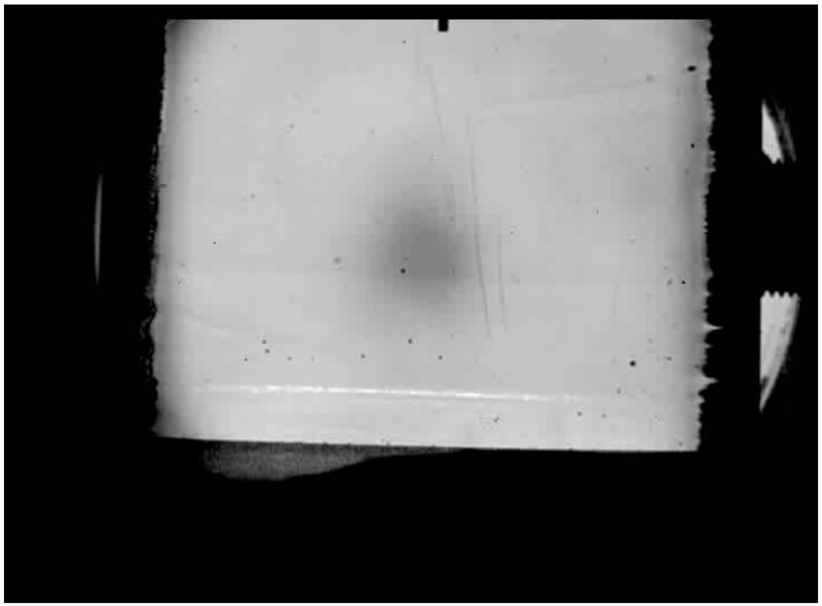
First Round of Experiments

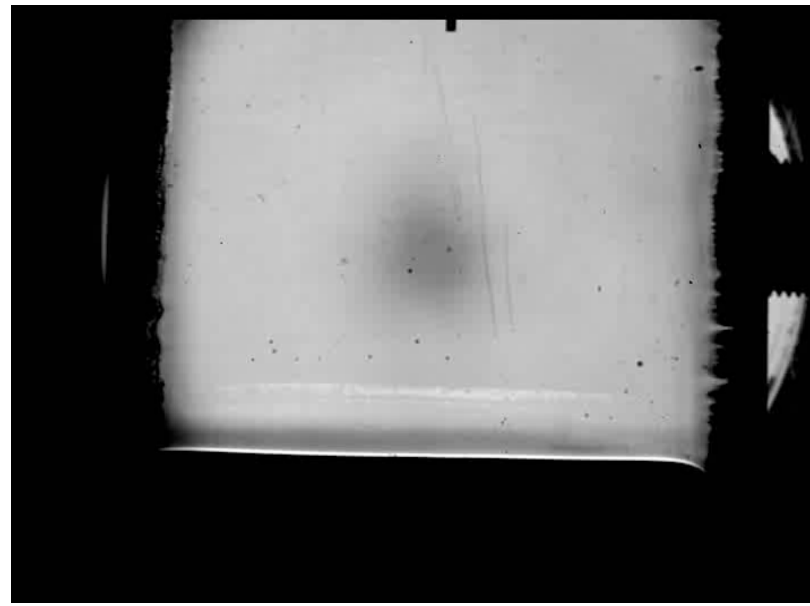
Observe bottom of the tank, determine controls on plume spreading

Non-impinging



Nozzle is 3” from bottom
Height of brine column: 26”
Orifice diameter: 0.06”
Flow rate: **52.5 ml/min**
Velocity: 0.5 m/sec

Impinging



Nozzle is 3” from bottom
Height of brine column: 26”
Orifice diameter: 0.06”
Flow rate: **210 ml/min**
Velocity: 2 m/sec

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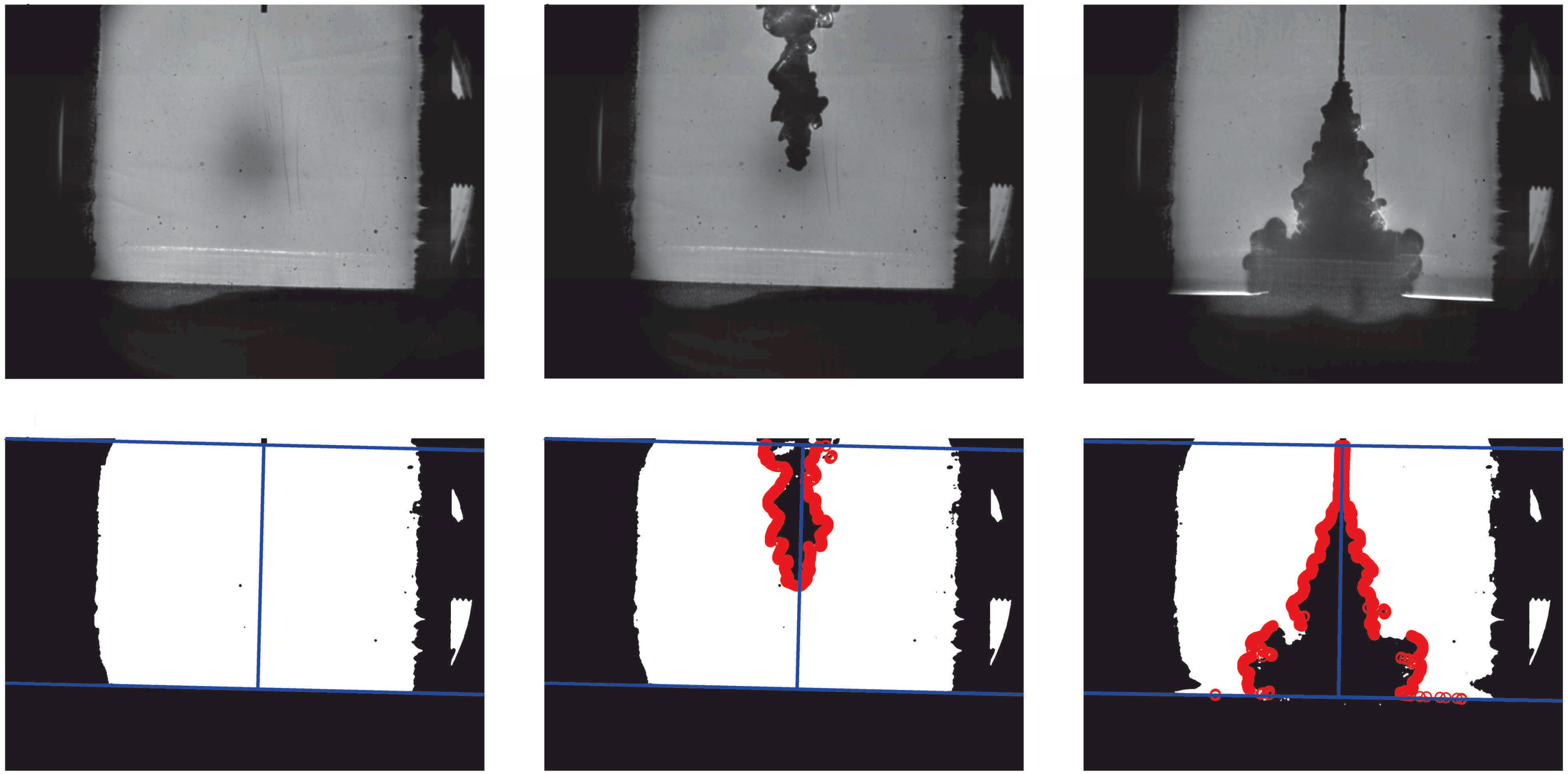
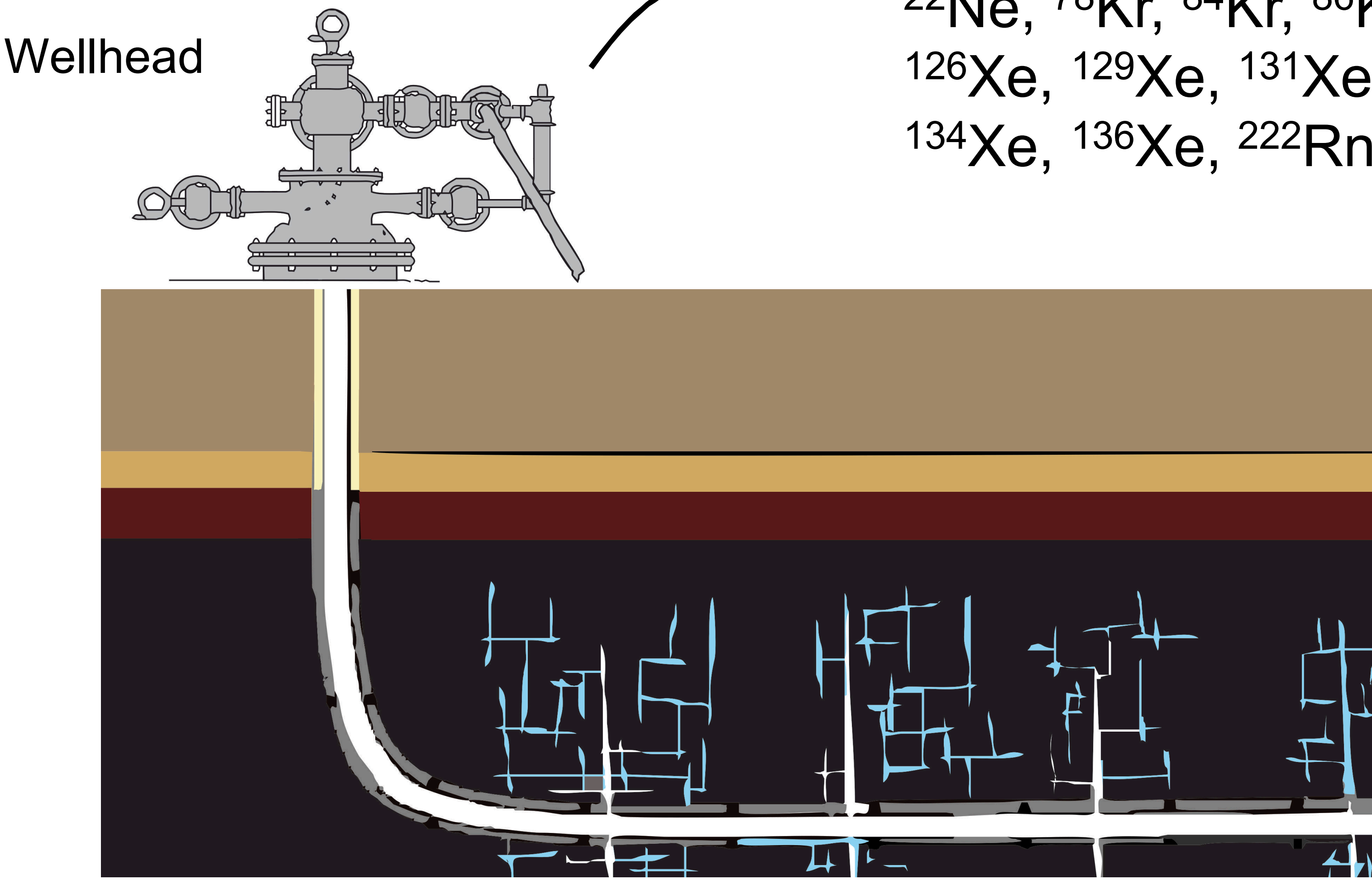


- Image processing determines the plume width versus time
- Scripts automatically threshold and measure plume width for every frame

2. Applications and mathematical approaches

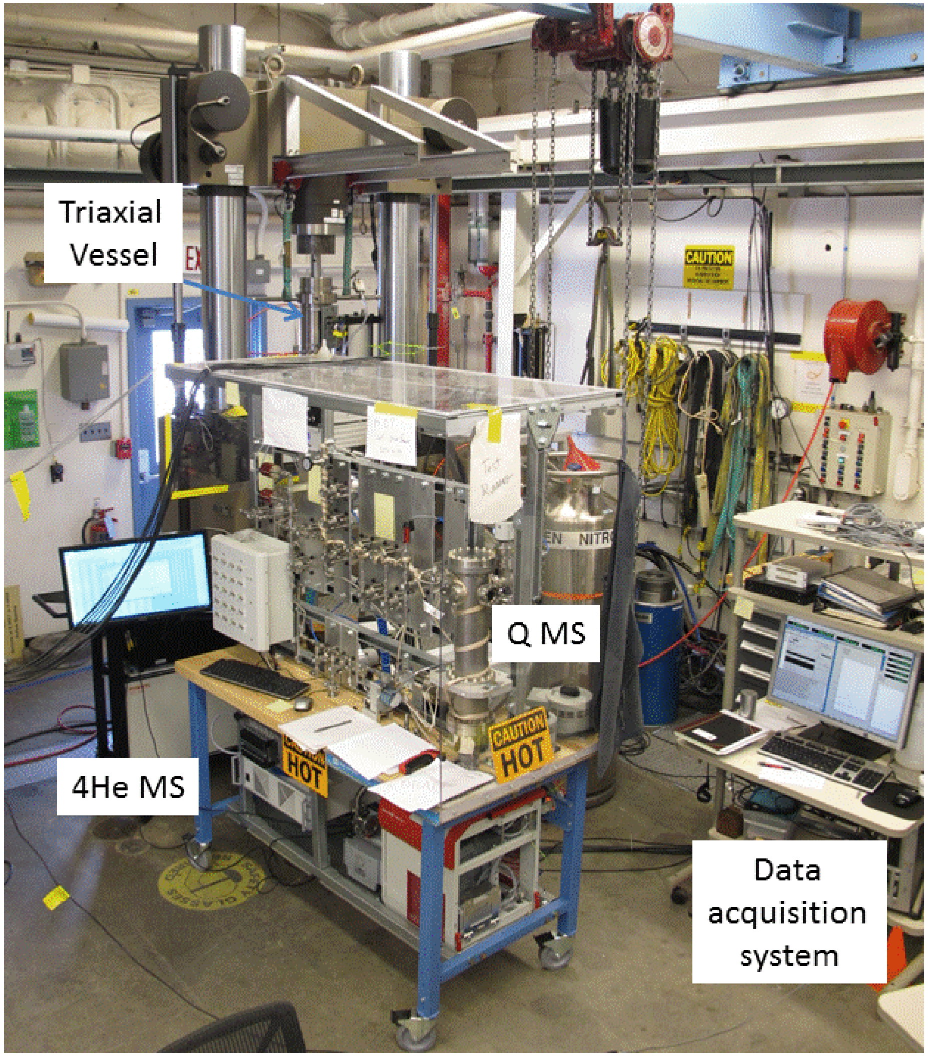
Shale as an energy resource



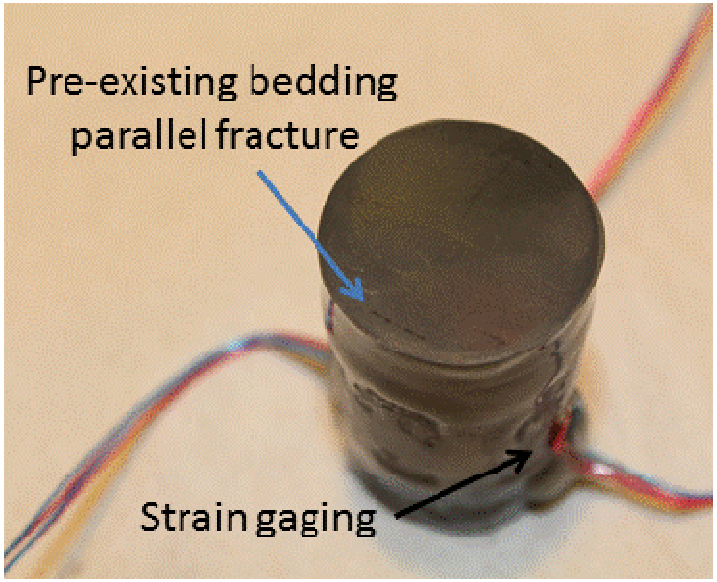
^{3}He, ^{4}He, ^{36}Ar, ^{40}Ar, ^{20}Ne, ^{22}Ne, ^{78}Kr, ^{84}Kr, ^{86}Kr, ^{126}Xe, ^{129}Xe, ^{131}Xe, ^{132}Xe, ^{134}Xe, ^{136}Xe, ^{222}Rn

(modified from King, 2010)

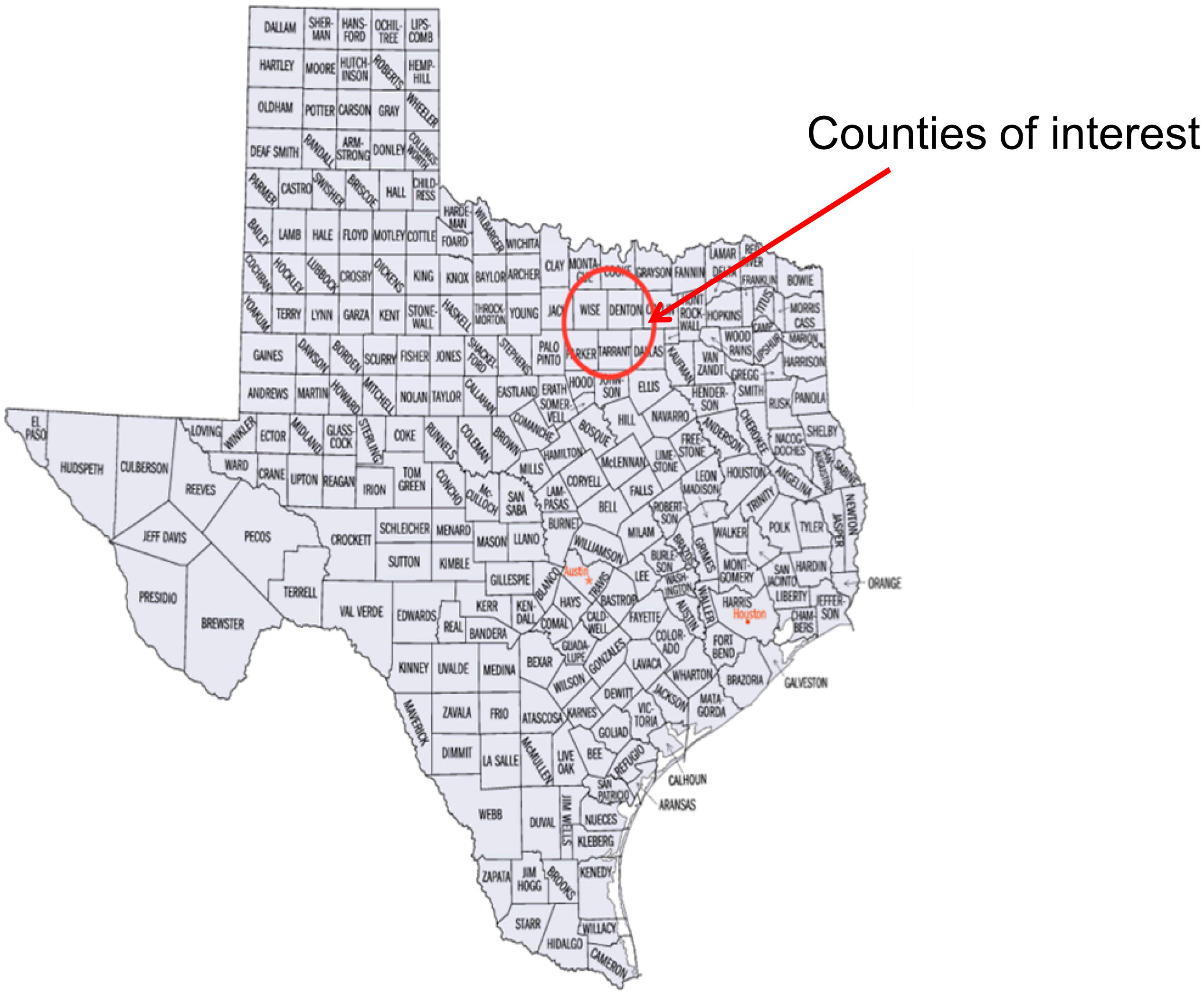
Gas release and flow measurements at elevated pressure and differential stress



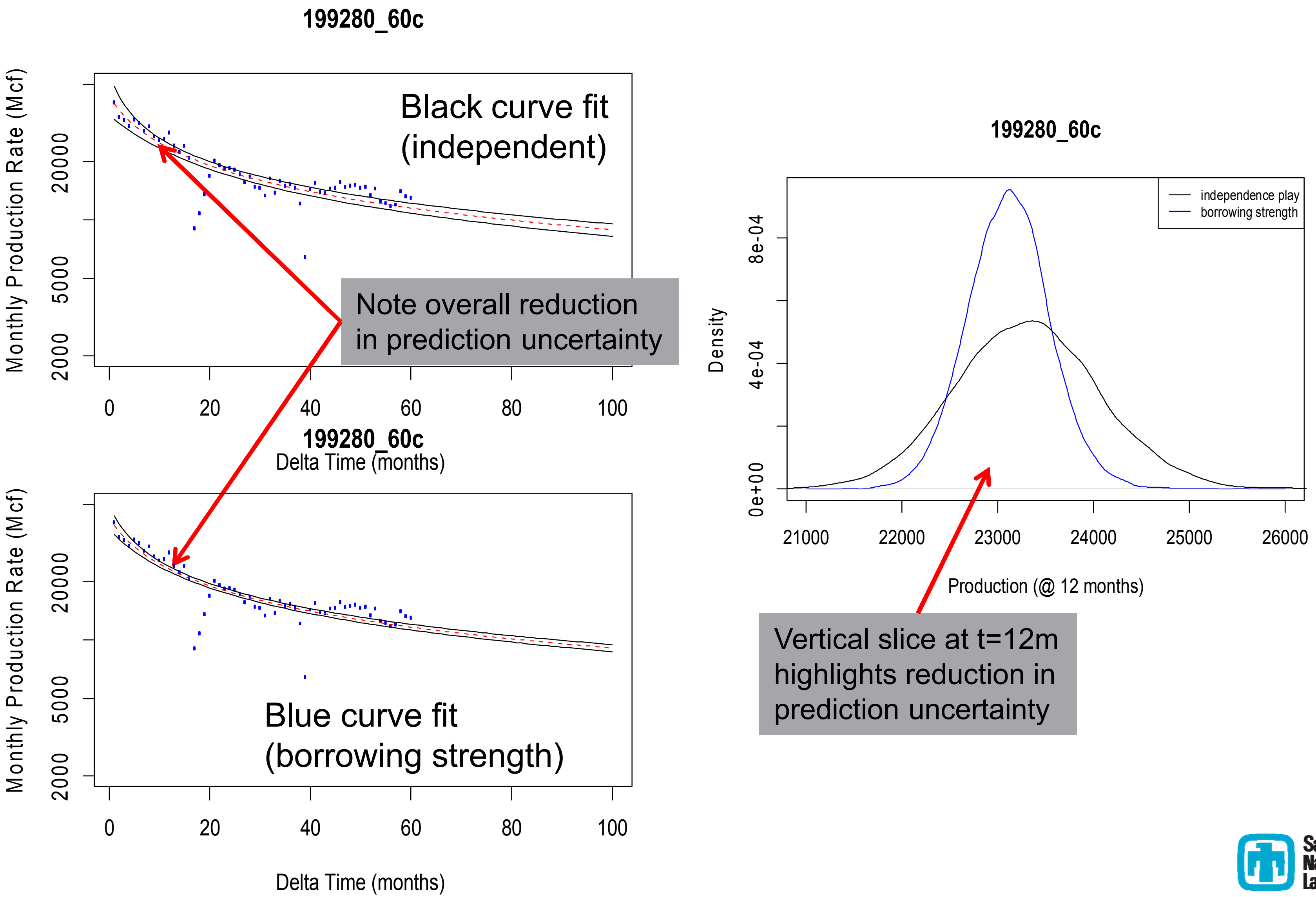
Helium mass spectrometer and quadrupole mass spectrometer used to
measure gas release and
flow through shale at
simulated downhole conditions



Bayesian Data Analysis: 197 TX wells



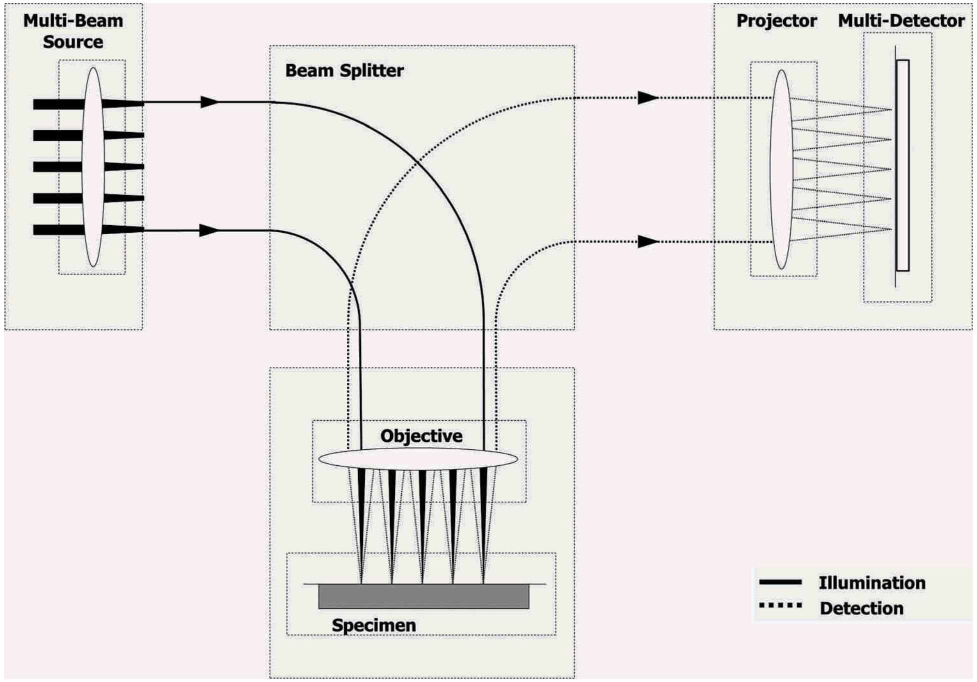
Borrowing Statistical Strength



Multibeam SEM of Porosity: REV and Scale Separation

Research questions:

- Do REV concepts apply to shale?
- What is an REV for flow and/or mechanical processes?
- Do hierarchical pore structures have “scale separation?”



Methods:

- Multibeam SEM
  - 61 simultaneous electron beams
  - 1.22 GPixels/s over mm areas at 4 nm resolution!
  - Secondary electrons
- Different shale types
  - Homogeneous: Siliceous shale (like Mowry)
  - Heterogeneous: Mancos
- Multiscale mechanical testing

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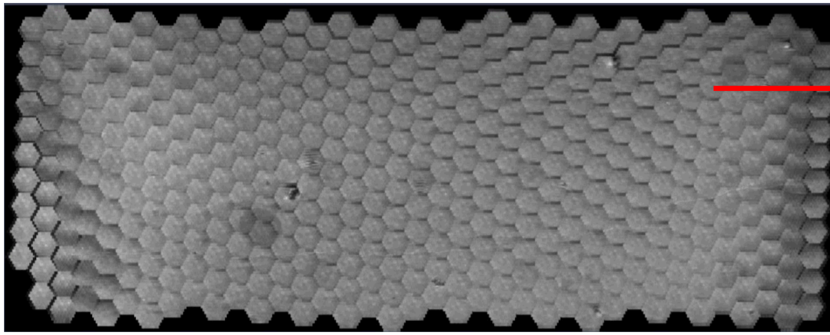
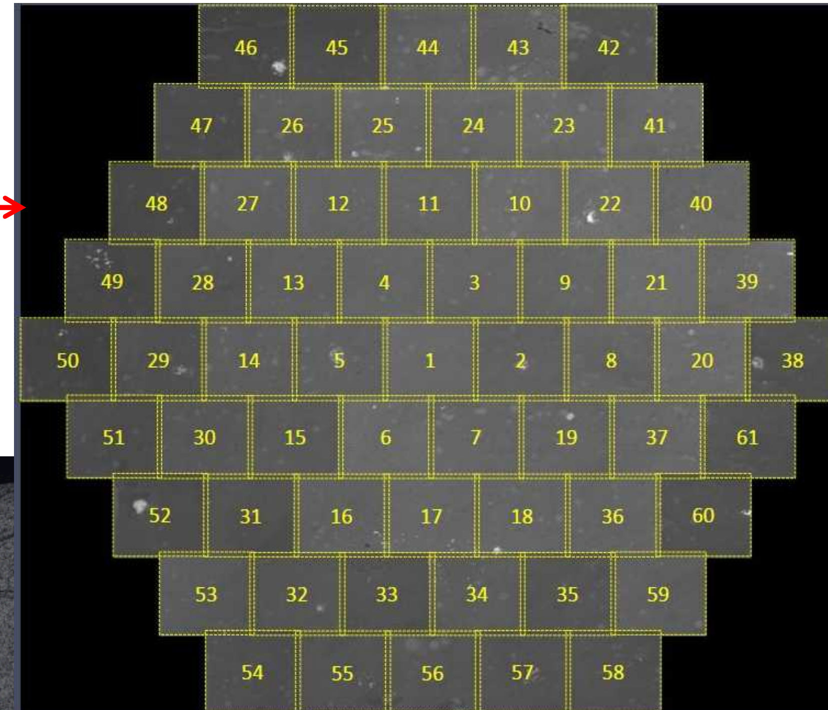
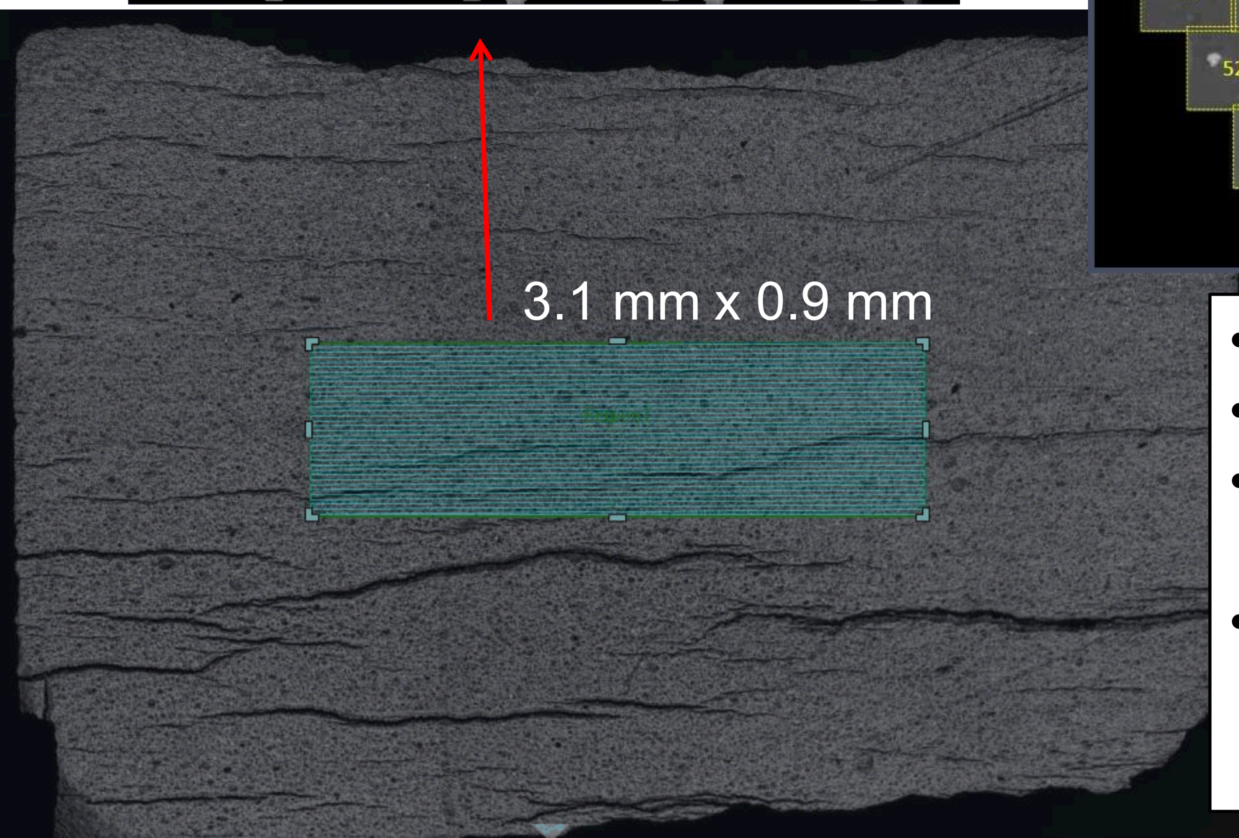
Initial Application of mSEM to siliceous shale

Broad ion beam polishing on sample from K. Milliken, TX-BEG



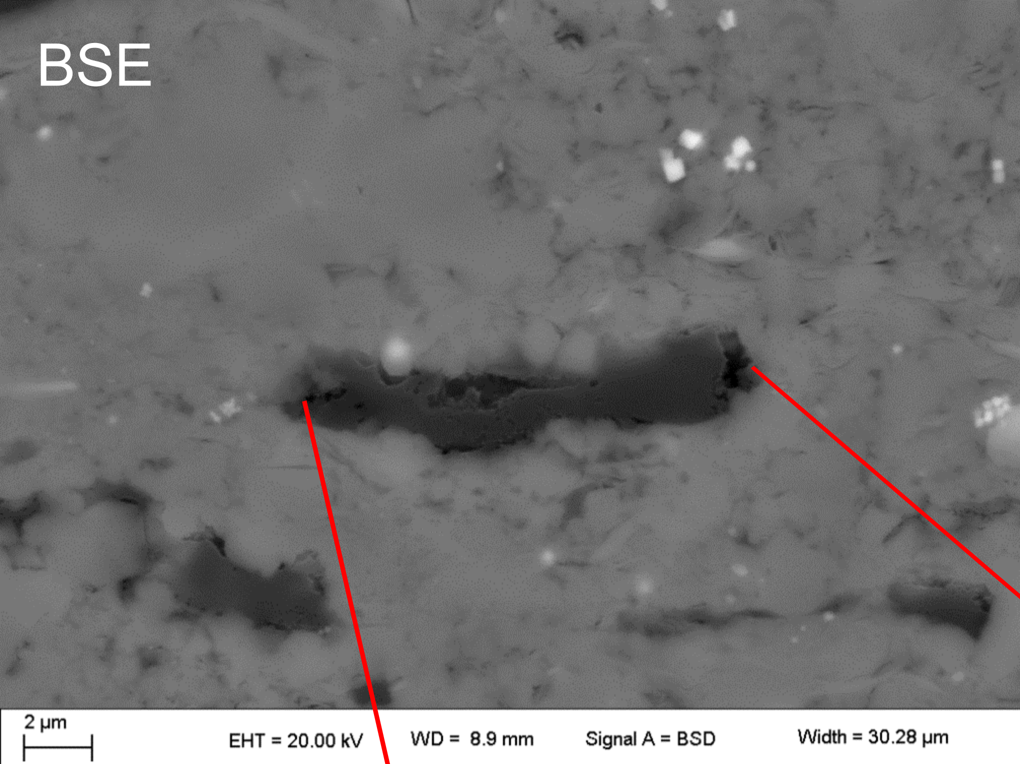


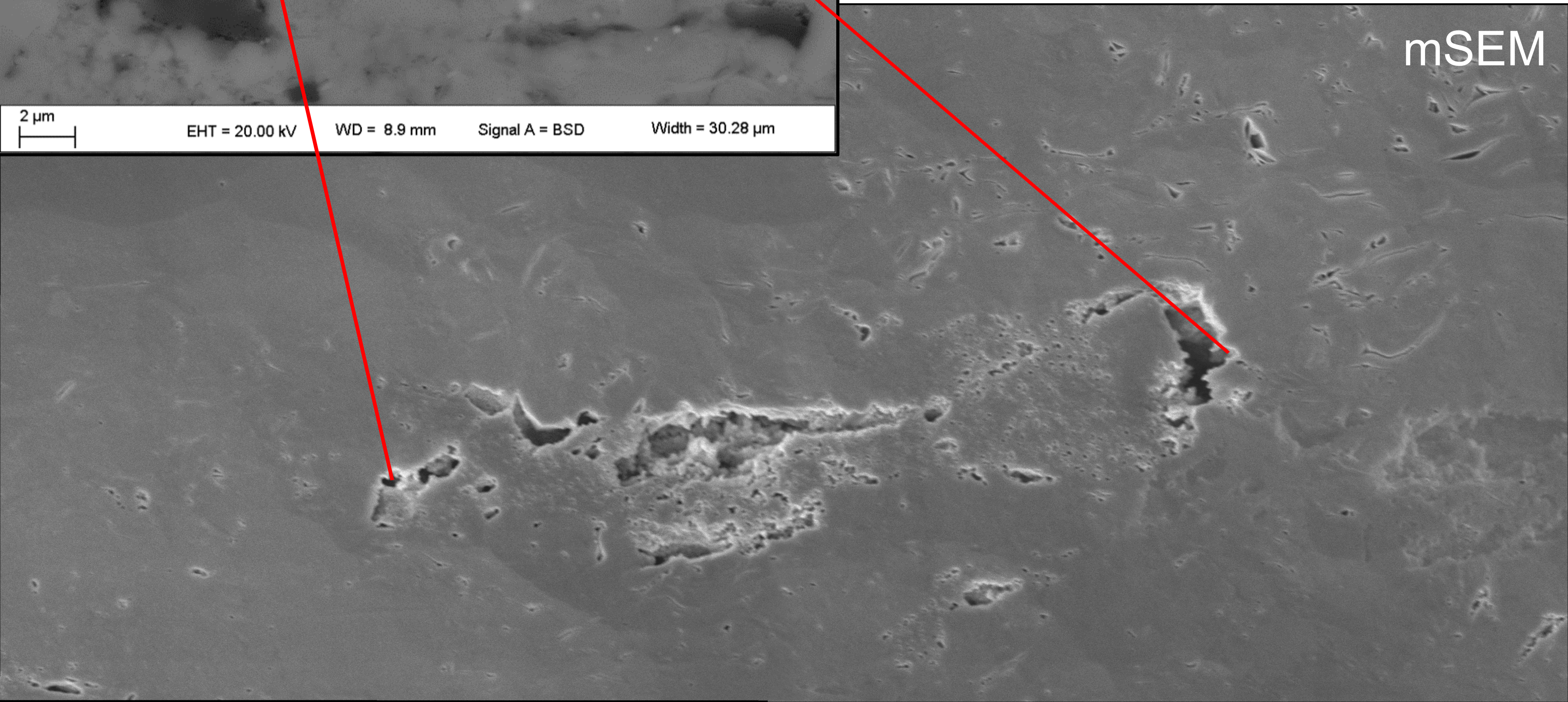


- ~ 3 x 1 mm area
- 4 nm resolution, 3 keV
- Data collection time: 16 min.
- 26,657 images
    - Single image: 12.5 x 10.9 µm

mSEM compared to BSE

- Pores on margins of organics, BSE
- Organics do not show up well at low keV in mSEM, but pores are clearly visible
- Non-epoxied, ion-milled very flat samples required for mSEM





Outline

1. Introduction
2. The whirlwind tour
3. Future directions and collaborations
   - Algebraic Topology and Rocks
   - Category Theory, conceptual models, and the pipeline to mathematics
   - Origami and geoscience
   - Thoughts on collaborations between BYU and SNL

Future directions and collaborations

Algebraic Topology and Porosity of Rocks

Can we do better than gridblocks and “enriched” FEM methods?

Ideas for future work

Goals:
- Create novel barcodes or “fingerprints” for rocks
  - Underlying hypothesis: unique “barcodes can be identified because of the following:
    - depositional setting → diagenesis → pore structure and pore-lining phases → fluid flow and mechancial reponse
- Predict performance

Foundational Math and Simulation:
- Homology (Algebraic Topology) measures number of pore shells, cycles, and connected components.
- Persistent homology measures global connectivity changes as local connections are made.
- Mechanical (force chains) behavior and multiphase fluid flow can drive those local connections, giving us a view into how a rock type responds.

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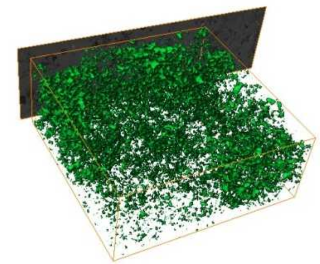
Persistent Homology and Barcodes

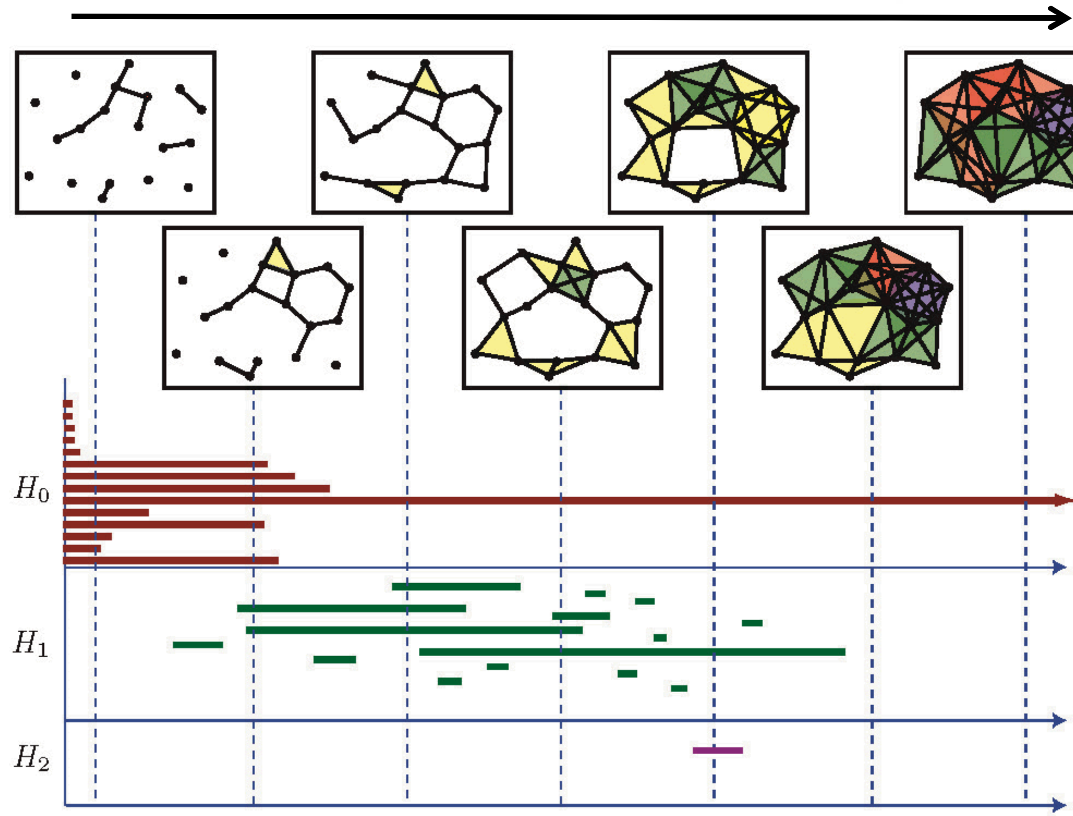
(Established math tool. Relevance to *this* application TBD.)



Persistent homology describes **connectivity** at different force chain pressures
(or spatial resolutions, ...)

Major connectivity shows up as long-lived lines in barcode

Increasing connections



Homology

H_0 isolated pore volumes

H_1 flow path cycles

H_2 filled cycles

Force Chain Pressure

(from Ghrist, 2008)

Thesis: barcode is a kind of "digital-fingerprint" identifying how a rock type reacts

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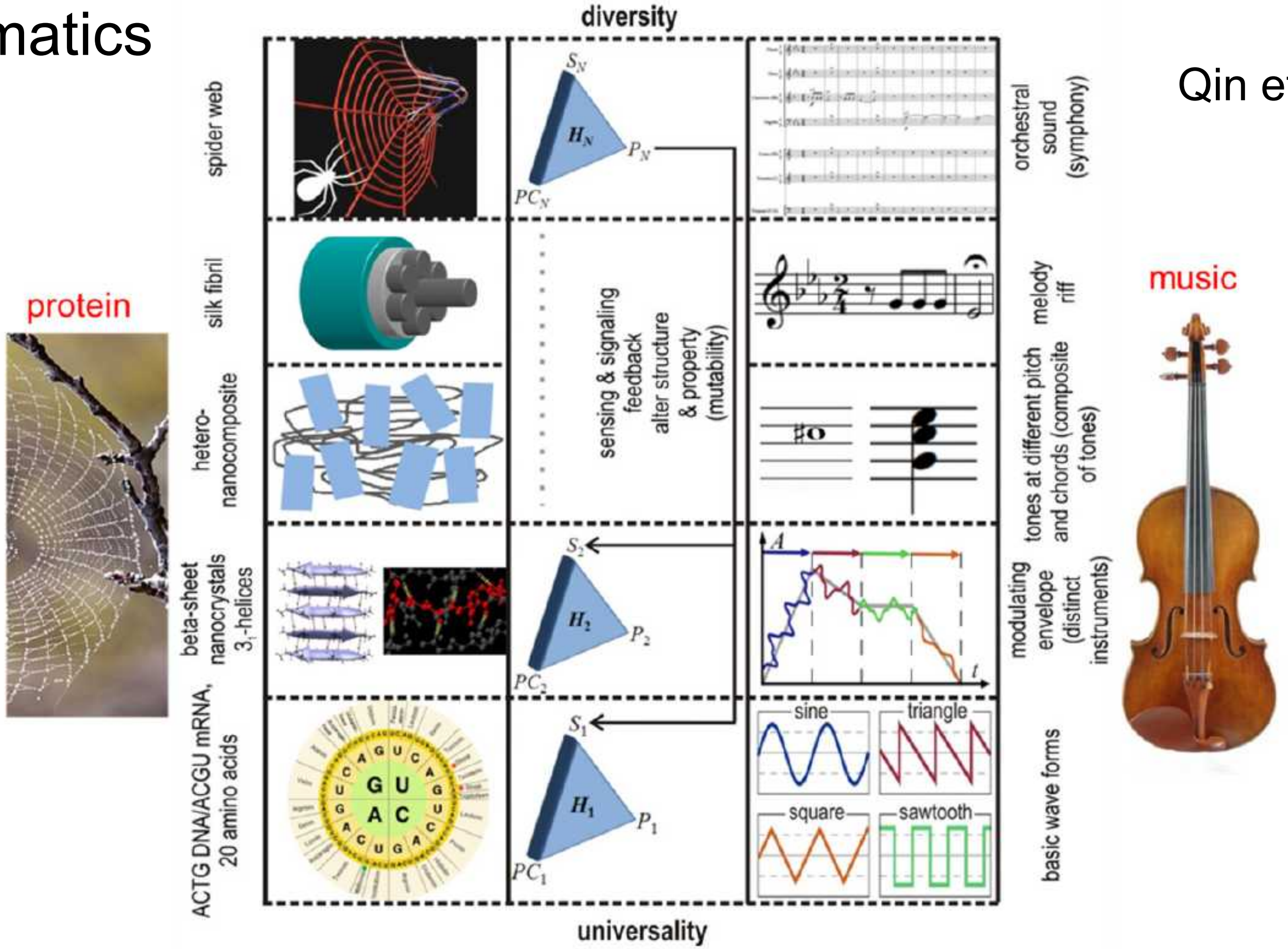
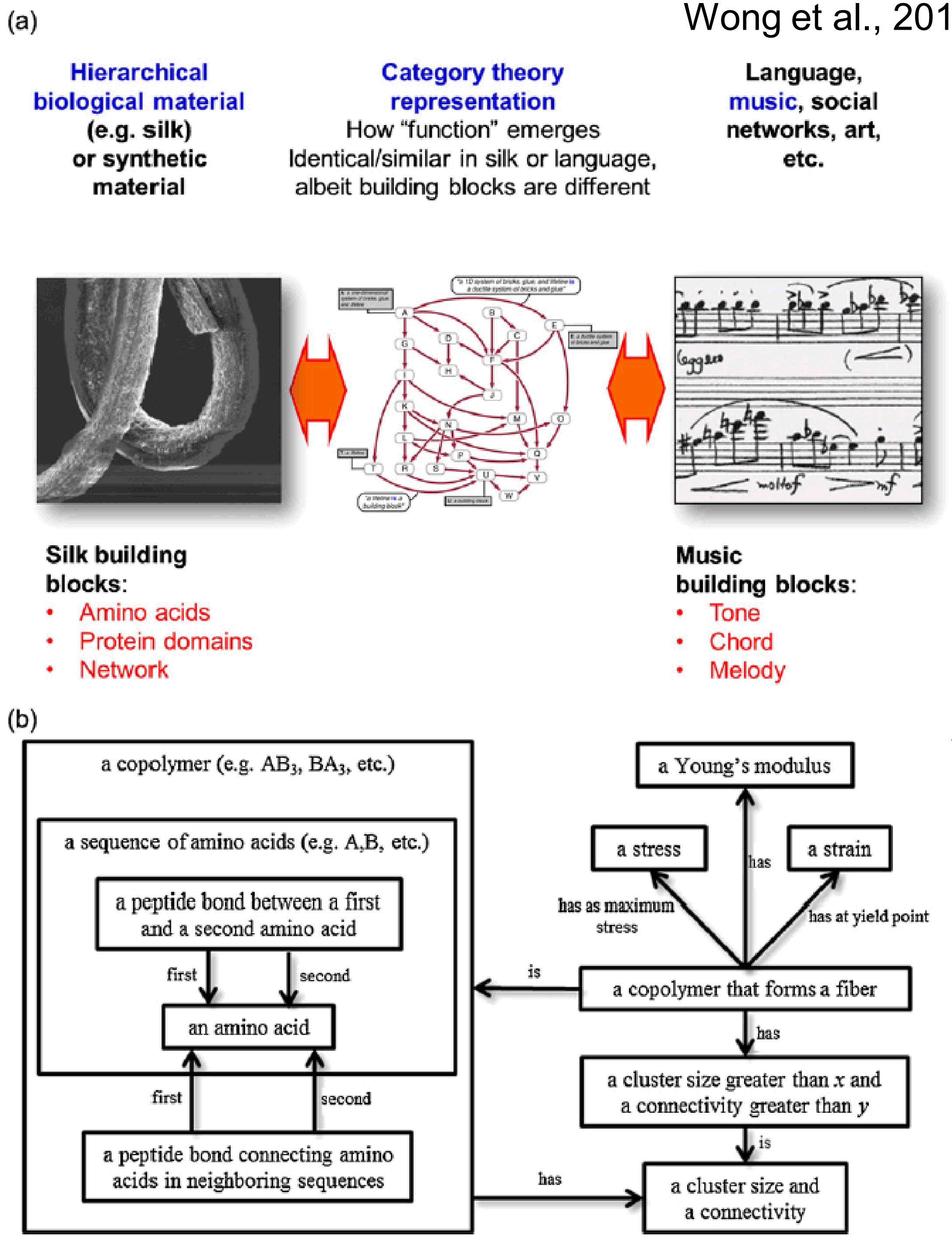
Future directions and collaborations

Category Theory, conceptual models, and pipeline to mathematics

Qin et al., 2012



Wong et al., 2012



Hierarchical material olog (ontology log)

Add certain components and rules, and you have a database schema

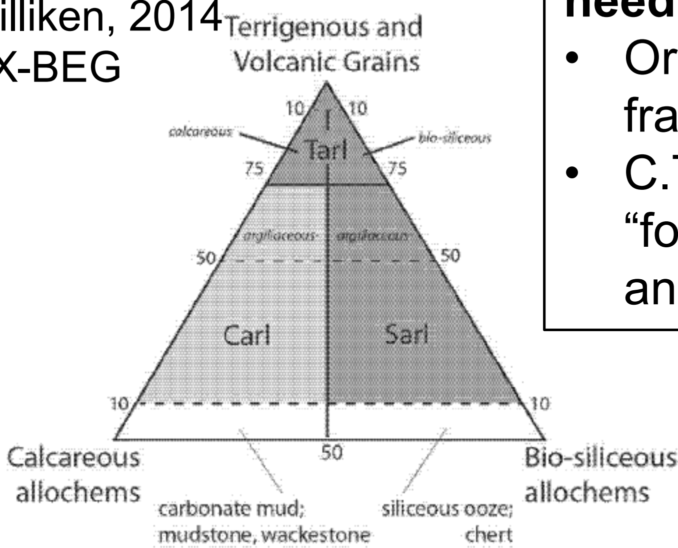
Dream paper:

Category Theory for Mudstones *(or EOR)*: Classification Schema and Structure of Coupled Processes

Current mudstone classification schemes lack formal mathematical structure – hard to tell how what “morphisms” apply to link to coupled process, for example:

(modifiers) Tarl, Carl, and Sarl

Milliken, 2014
TX-BEG

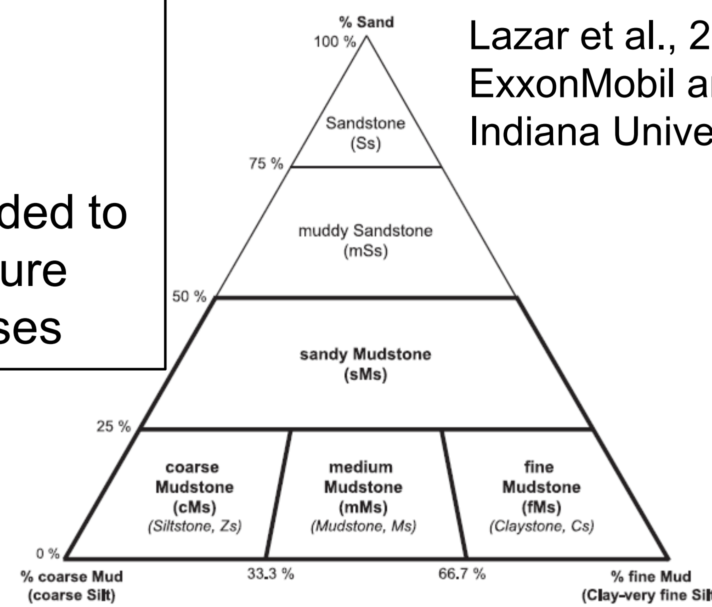


Current mudstone classifications lack or need:

- Order Hierarchical framework
- C.T. structure is needed to “forward map” structure and coupled processes

(composition, texture, bedding) mudstone

Lazar et al., 2015
ExxonMobil and
Indiana University



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Future directions and collaborations

Origami and Geoscience

1. Spatial self-organization in geologic systems

- *Far from equilibrium, coupled processes, and feedback*
- Folding of rocks is an example
- Global “self-folding” being applied to electronics, etc…

2. Engineering geoscience needs origami principles

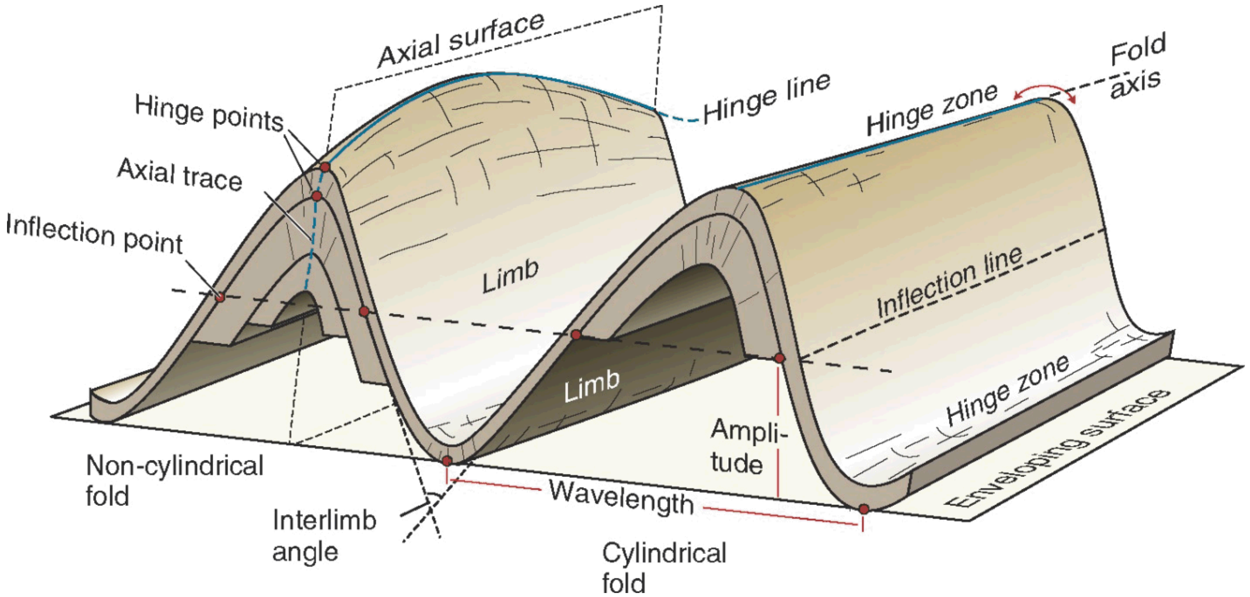
- Compact yet deployable
- Controlled self-assembly
- Multi degree-of-freedom (DOF) devices for reconfiguration
- Tailored origami (micro) structure for creating desired macro-behavior or metamaterials

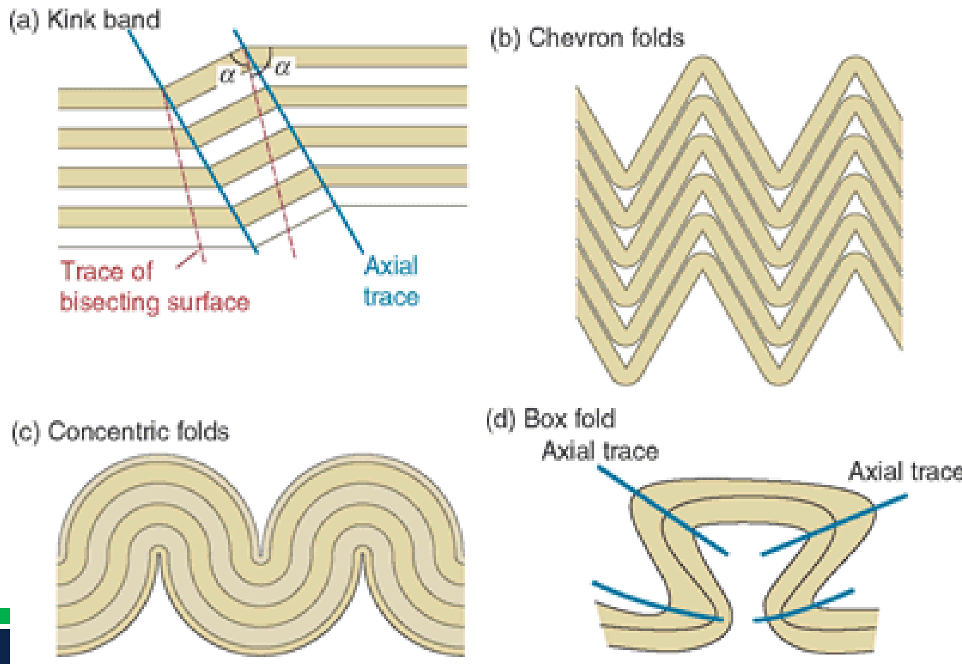
Folds in Rocks

http://myweb.facstaff.wwu.edu/talbot/cdgeol/Structure/Strain/Folds.html

Geometric descriptions
Types of folds
Mechanisms and processes

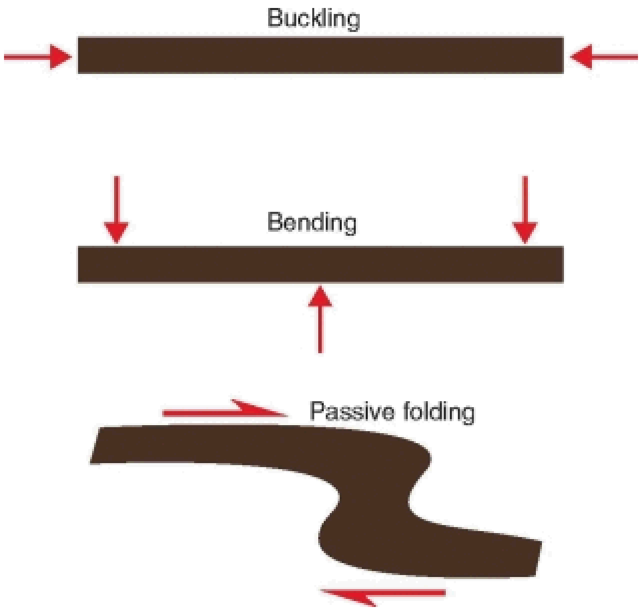
Fossen, 2014, Structural Geology





Folding mechanisms

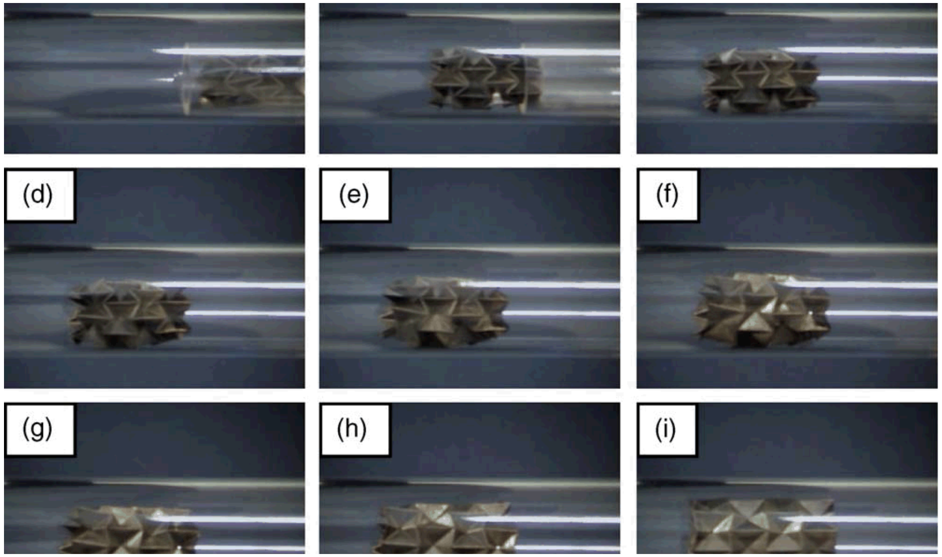
- Active folding or buckling
- Passive folding
- Bending



Active folding: wavelength and layer thickness

http://folk.uib.no/nglhe/PhotoAlbum/Folding%20Chapter%2011/index.html
Chapter 11, Fossen, Structural Geology

Partially opened model of the HanaFlex array and truss. Zirbel et al 2015



Series of frames from video recording showing self-deployment of the stent (side view): (a) stent graft which is folded and backed into a small acrylic tube of 13mm radius was inserted into another acrylic tube of 25mm radius and (b) the small acrylic tube was removed and (c–i) the stent graft was self-expanding at above Af (319 K). Kuribayashi et al 2006

Sandia National Laboratories

Future directions and collaborations

Thoughts on collaborations

- Joint Moab Topology and Geology Conference?
- LDRD program
- Other proposals
- Student interns for projects

Thanks for the opportunity to speak!

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