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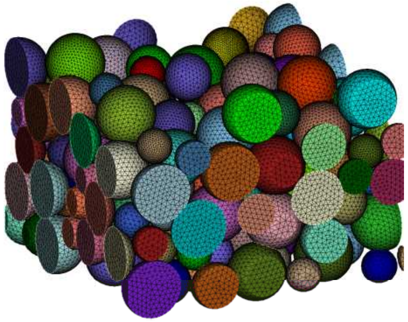

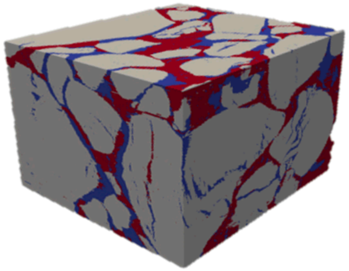

3D Printing and Digital Rock Physics for the Geosciences

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Sandia National Laboratories

Albuquerque, New Mexico

August 3, 2015

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Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

SAND2015 – xxxxx C

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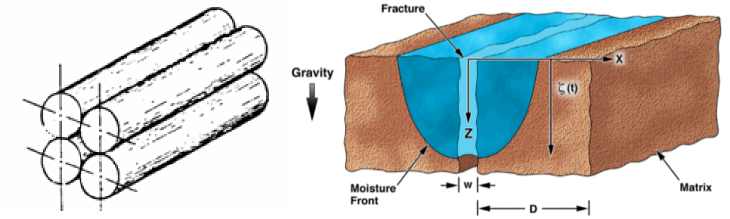
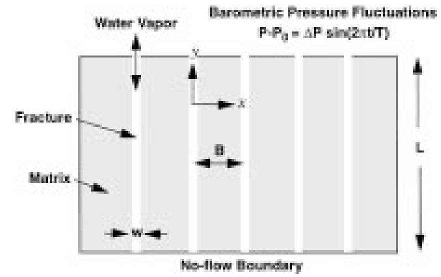
Outline

- Our motivation for 3D printing & Digital Rock Physics (DRP)
  - KEY → mesoscale to macroscale
- Digital rock physics overview and issues
  - DRP helps deal with heterogeneity, multiscale
- Digital rock physics schema can be advanced via 3D printing
- A workflow coupling 3D printing and DRP for Geosciences
- Science Challenges that can be addressed
- Additive manufacturing (3D printing) overview
- 3D printing for geosciences
- Procedure for upscaling

Shortcomings of current understanding of poromechanics

- Models of poromechanics and multiphase flow in fractured rock are based on simplistic porous texture, e.g. bundled capillary tubes, 2D slot fractures or penny-shaped cracks.
- Current understanding of poromechanics "smears" the effects of pore-scale structure
- Applicability of spatially averaged "cubic law" and Biot effective stress concepts in fractured media, and coupled effects on flow paths is poorly understood.
- Mesoscale analysis – linking discrete and complex pore-scale behavior to continuum (macroscale) reservoir response – is key, yet remains elusive as a result of the extreme heterogeneity and resulting scale dependence.

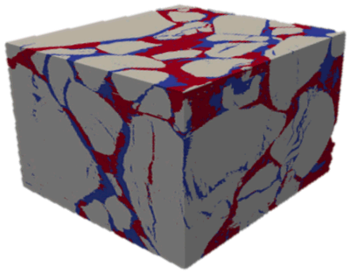




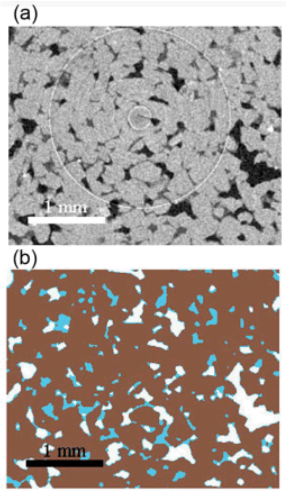
Martinez, 1999

Venerable conceptualizations of porous media

Real porous microstructure



Li-ion electrode

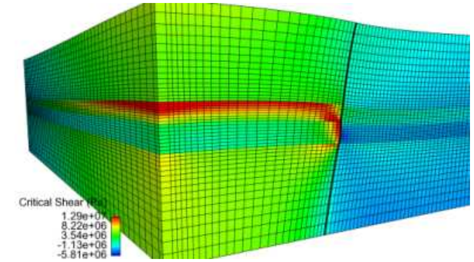


Iglauer et al 2011

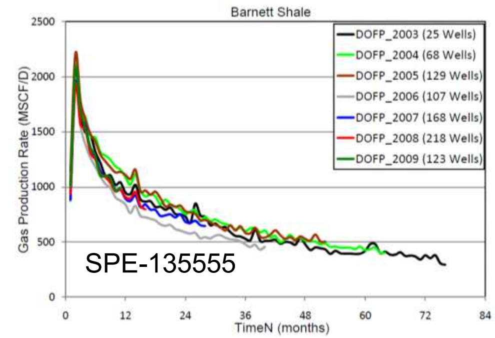
Sandstone

Research to advance our understanding of geomaterials

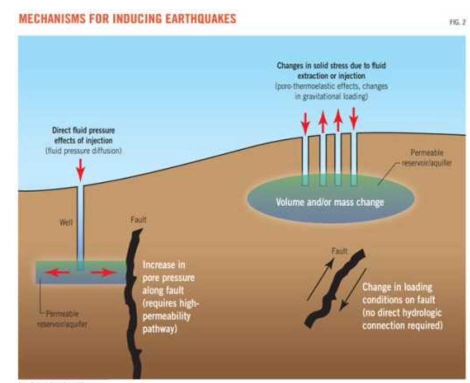
- Develop methodology to connect pore-scale structure to macro-scale behavior to advance constitutive models for poro-hydro-mechanics of fractured rock that directly impact our ability to predict:
  - aquifer response to injected fluids
  - hydrocarbon production decline,
  - efficiency of subsurface carbon storage,
  - Induced seismicity



Injection-pressure-induced deformation and shear failure

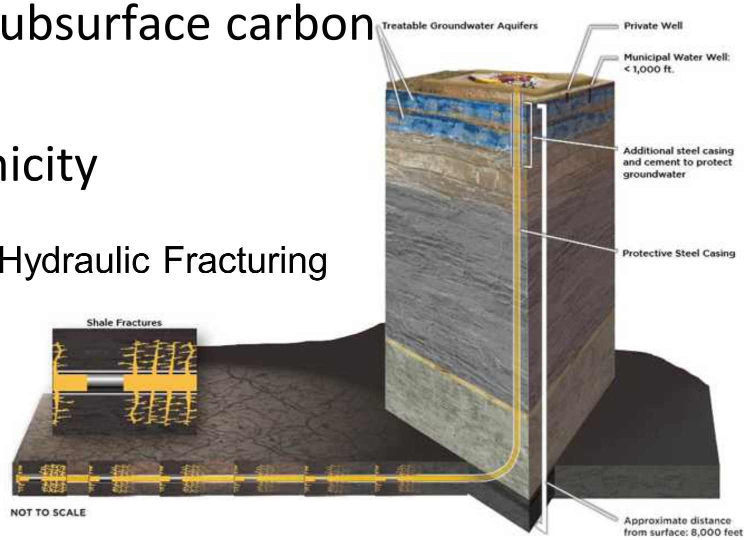


Production decline



Induced seismicity

Hydraulic Fracturing



Workflow for Digital Rock Physics

Rock Sample	Multiscale image	Image Process	Flow and Transport Properties	Static Effective Elastic Properties	Wave Propagation

- DRP can help us characterize and understand the role of heterogeneity and multiscale aspects of porous geologic media
- Multiscale imaging can support upscaling

Core (~1m)

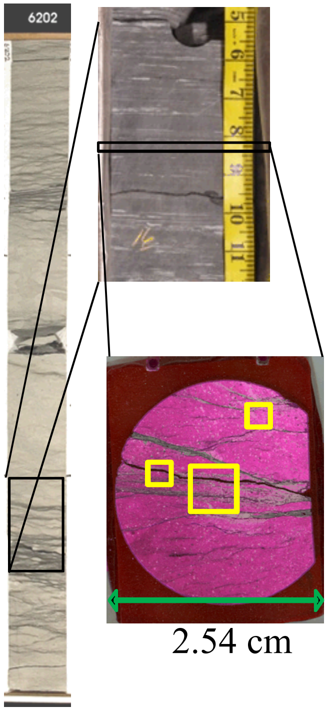


Image analysis and digital rock physics has advanced our understanding of porous media

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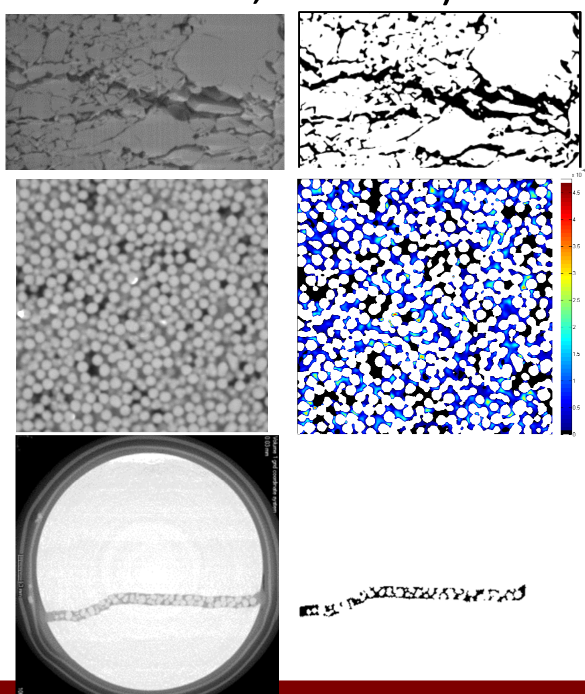
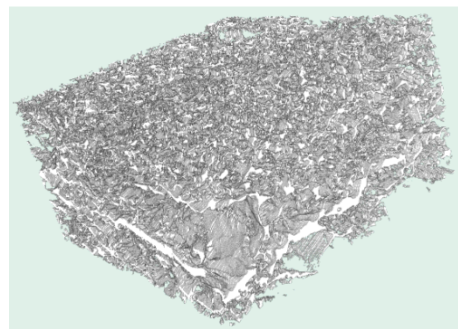
Segmentation Process

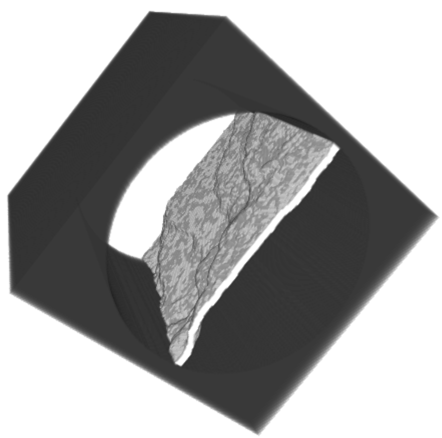
- Alignment
- Enhance contrasting
- Multiple Filtering
- Thresholding
- Post processing (e.g, dilation, erosion)



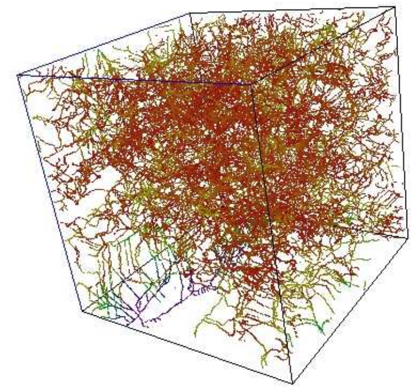
3D Digital Rock Construction

- Binary or ternary pore and fluid distribution construction



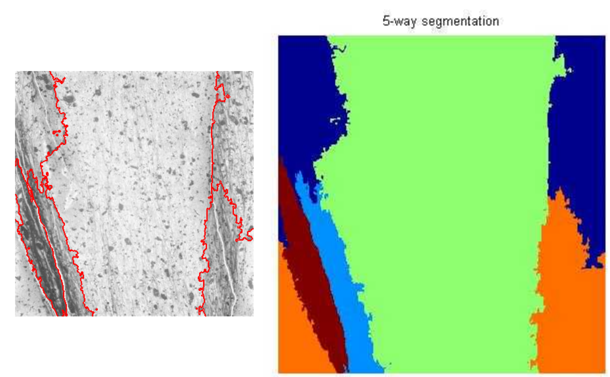


Quantitative Analysis



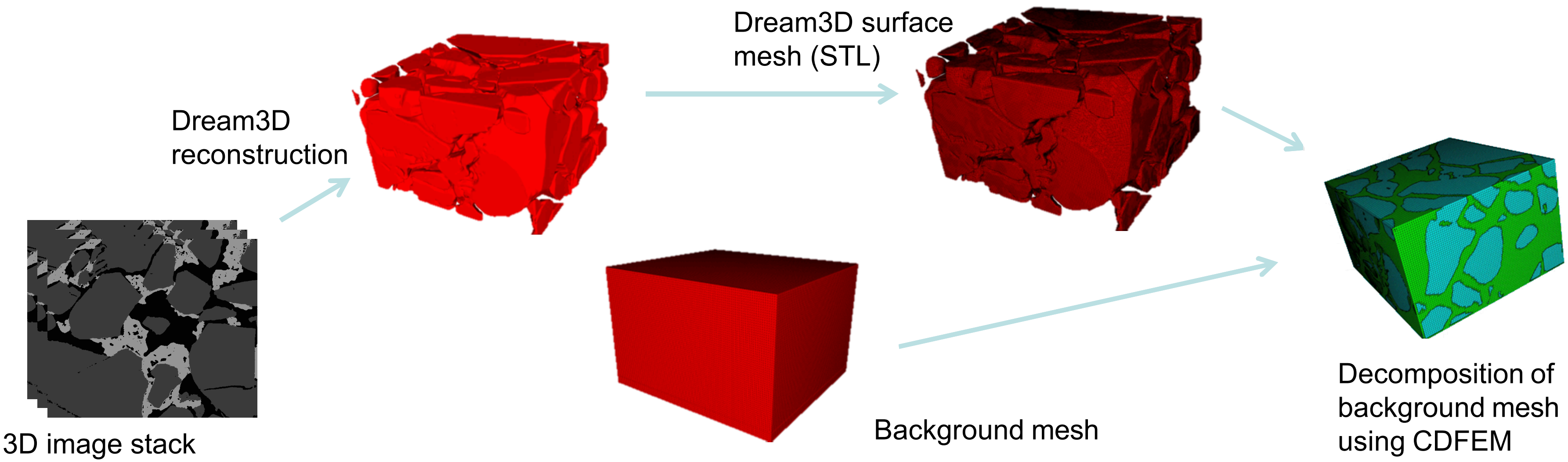
Medial Axis Analysis

Topological Analysis



Digital rock physics workflow for mesoscale simulation

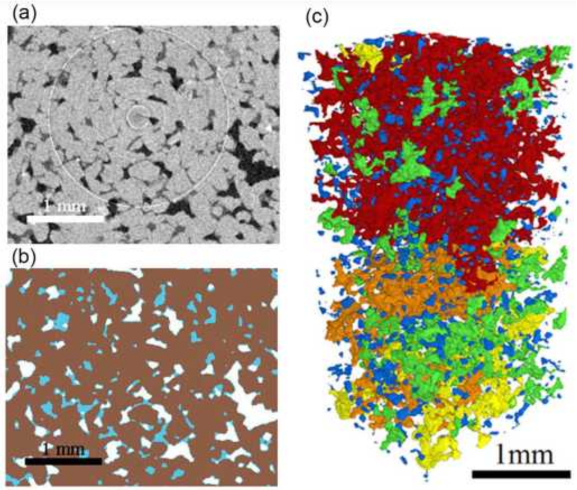
- We utilize both FEM and Lattice-Boltzmann methods, the latter can utilize voxel data directly. The former requires some form of mesh generation
- Despite the availability of commercial software for building grids based on voxel descriptions, the ability to design well-conditioned grids for modeling remains somewhat of an art.



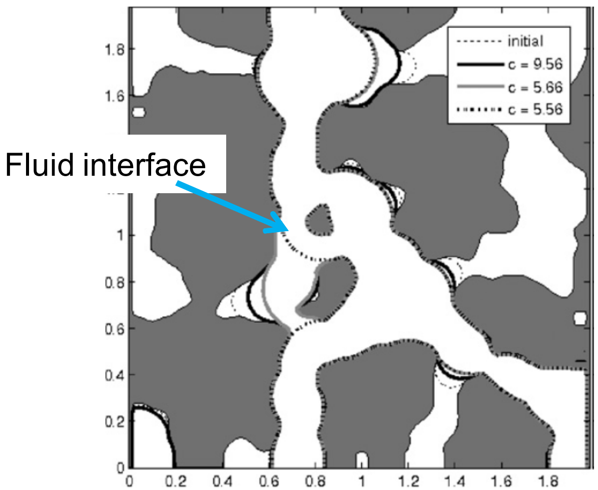
Roberts et al., 1514

Modeling at the Mesoscale

Multiphase Flow with Level Set

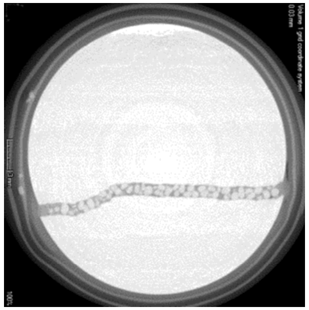


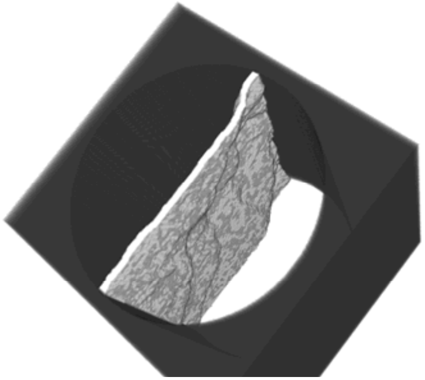
Iglauer et al 2011



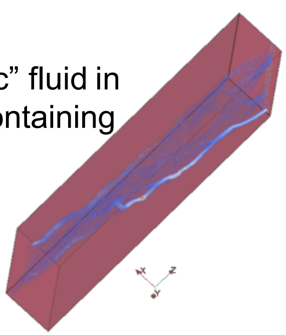
Prodanovic & Bryant 2006

Lattice Boltzmann

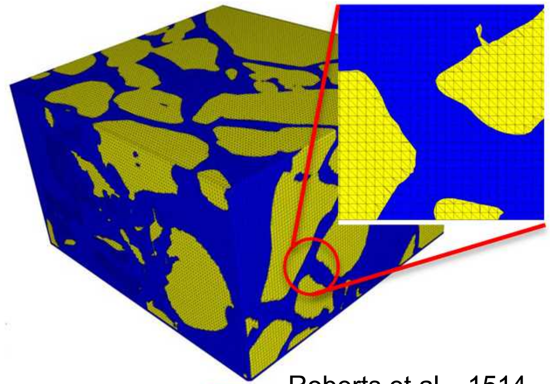




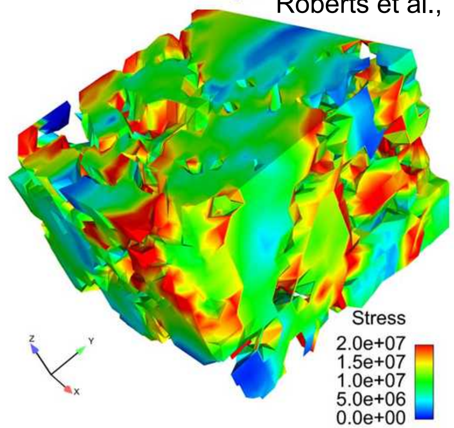
Flow of “frac” fluid in proppant-containing fracture



Sierra Mechanics/CDFEM



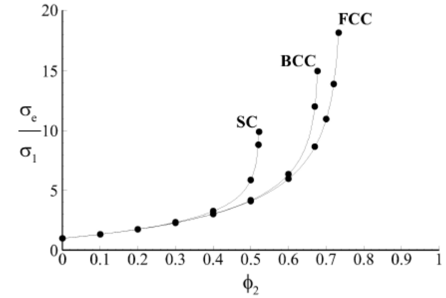
Roberts et al., 1514



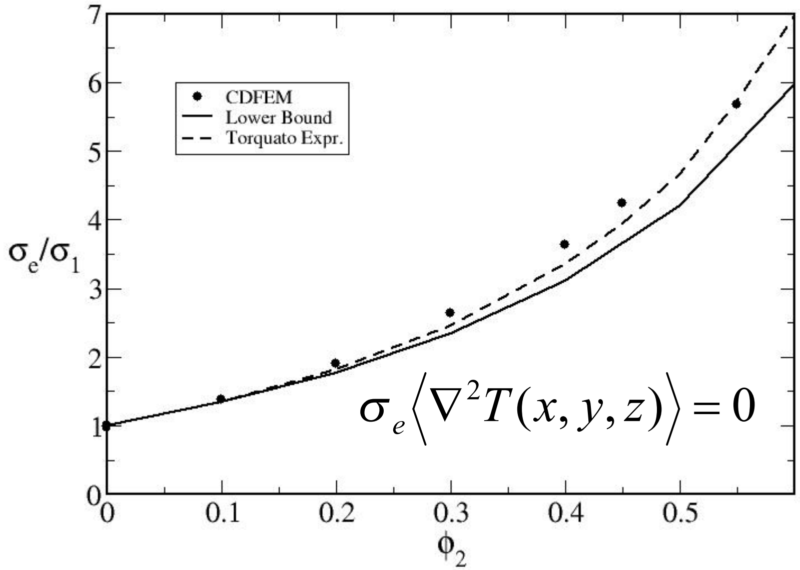
Thermal/contact stress in a reconstructed porous electrode

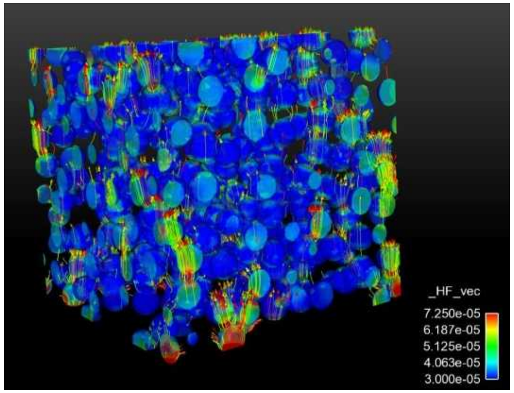
Mesoscale Example: Effective Thermal Conductivity of Particle Dispersions

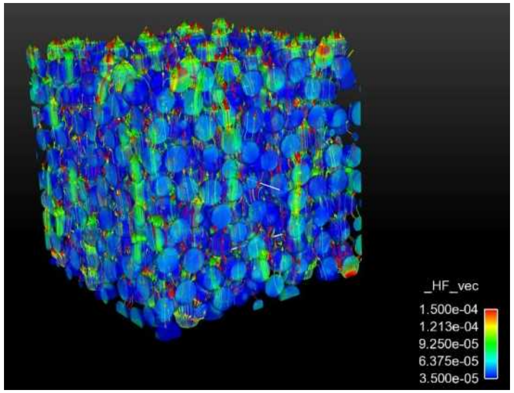
- Verification of CDFEM for Average thermal conductivity in static random dispersions
  - Particle configurations taken from Brownian Dynamics Simulations of Repulsive Colloids
  - Suspending fluid insulating, particles conductive (ratio of conductivities ~ 1000)



$$\left\langle \nabla \cdot \left(\sigma(x,y,z) \nabla T(x,y,z) \right) \right\rangle = 0$$





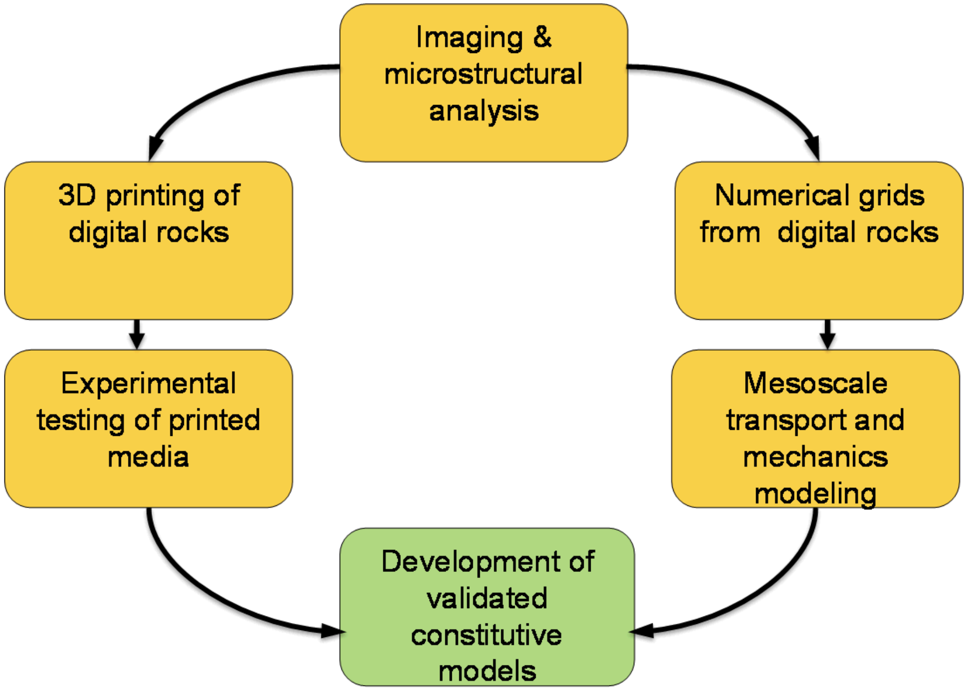


Digital rock schema could be improved with 3D printing

Reproducible synthetic media that mimic natural media, potentially enabling a limitless set of experiments benefiting all manner of scientific research

3D printing enables us to:

- surmount problems with sample-to-sample heterogeneity
- to test material response independent from pore-structure variability
- develop functional porous structures
- print porous specimen with integrated test frame
- addresses issues of scale-up



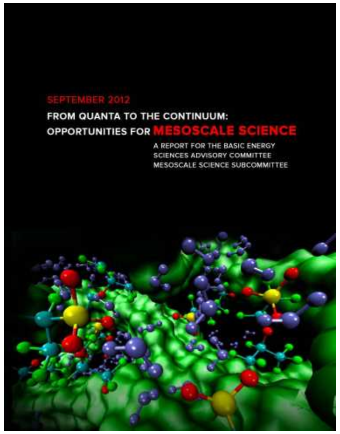
Impact:

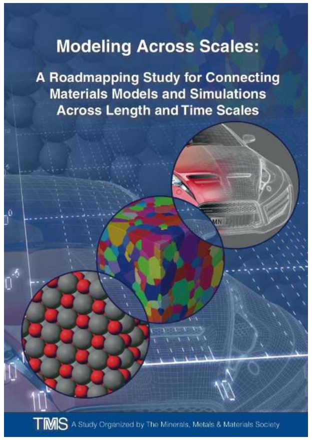
- Science-based approach to develop advanced constitutive laws
- Testing and modeling on same pore topologies and materials
- Scale dependence & model validation

Science challenges that could be addressed

Areas to impact frontiers of science and establish framework for future S&T investments:

- Ability to relate microstructure to bulk measurable properties and performance
- Understanding how to control flow in fractured media
- Testing scale-up of digital rock properties
- Develop the methodology for experimental utilization of additively manufactured copies of real rock, a potentially disruptive technology for geosciences.



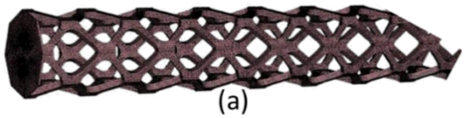


3D printing could revolutionize manufacturing

- Additive Manufacturing (ASTM F2792), aka, 3D printing is projected to revolutionize manufacturing – GE Aircraft report "… we are at the dawn of the next Industrial Revolution …"
- State of the Union Address – 3D print-driven manufacturing hub
- National Labs join America Makes (Ref: 3Dprint.com)
- Europe utilizing 3D printing in their nuclear industry
- GE's newest aircraft engine is designed with parts made from 3D printing
- Biomedical – porous lattice metallic implants and prosthetic limbs

Key benefits of AM

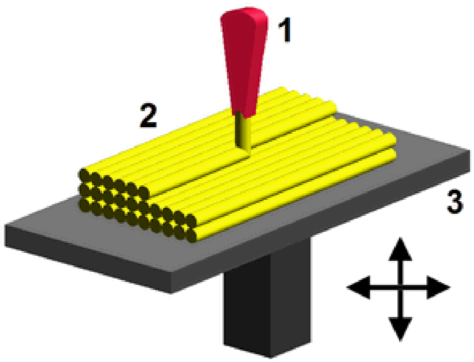
- Easily and economically build complex geometries with internal features impossible or impractical with traditional manufacturing techniques
- Parts on demand
- Adaptive Topological Optimization (shapes optimized for function)

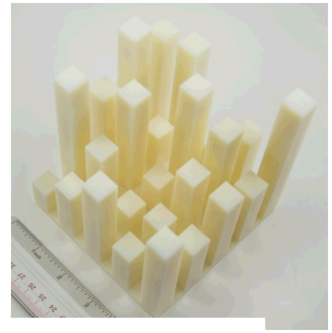


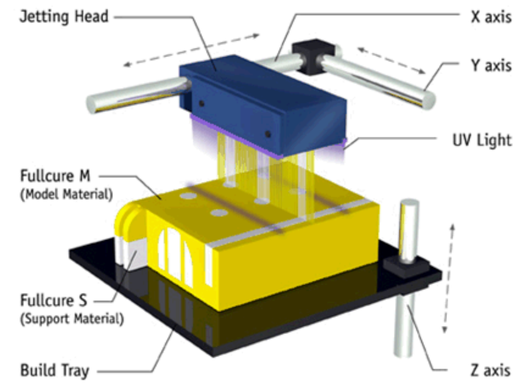
Weight-optimized torsion bar

Current research efforts provide leveraging opportunities for application of AM in the geosciences

Representative 3D Printing Process Categories

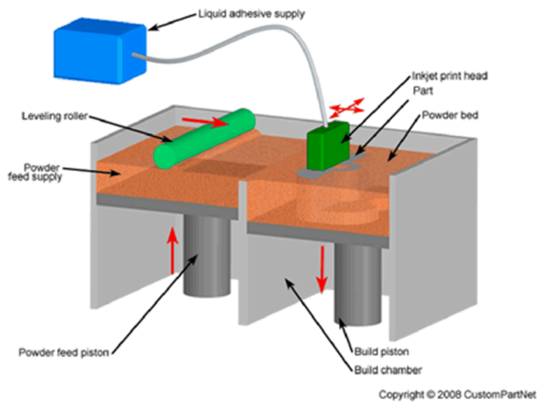


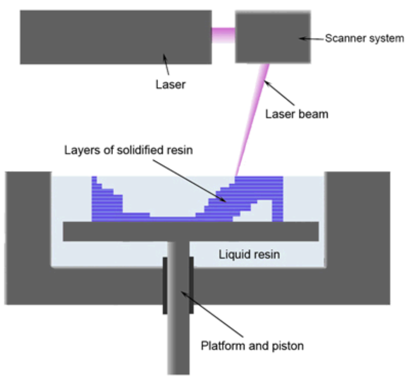


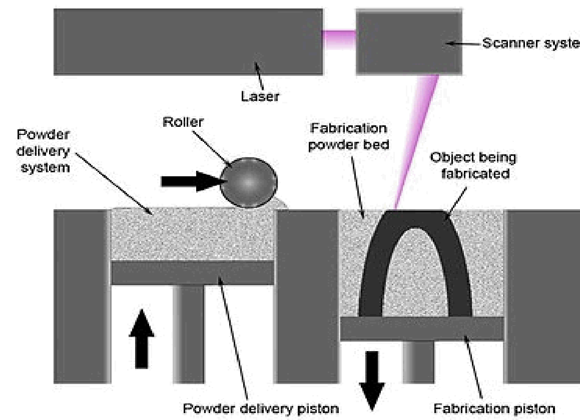


Objet material jetting, www.me.vt.edu

"**Fused deposition modelling**",
Wikipedia





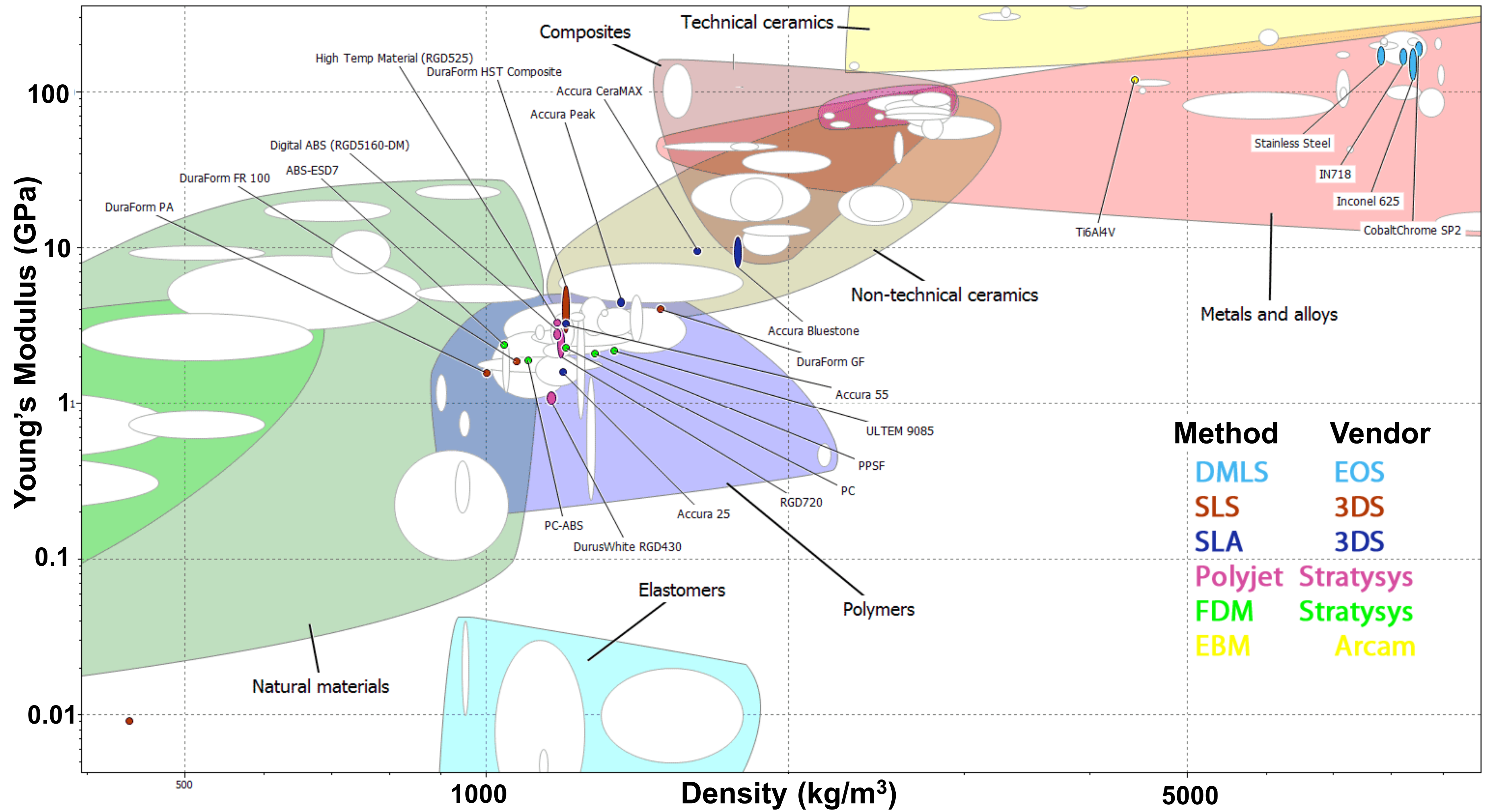


Binder jetting, www.utwente.nl

"**Stereolithography**", Wikipedia

"**Selective laser sintering**", Wikipedia

Material properties for 3D printing



Randal Schubert, HRL Laboratories @ 2013

3D printers at Sandia

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Formlabs Form 1+ (6914)

	Stratasys Dimension 1200bst	Stratasys Fortus 360mc	Stratasys Fortus 400mc	Objet Eden 260V	Objet 500 Connex3
Build Envelope	8 x 8 x 12 in	16 x 14 x 16 in	16 x 14 x 16 in	10 x 9.9 x 7.9	19.3 x 15.4 x 7.9
Layer Thickness	.010 in or .013 in	.005 in, .007, .010, and . 013 in	.005 in, .007, .010, and . 013 in	16 or 30 microns	16 or 30 microns
Modeling Material	ABSplus	ABSplus, translucent ABC	ABSplus, translucent ABC, PC	Vero family of opaque materials Tango family rubber-like flexible materials Transparent: VeroClear	Vero family of opaque materials, including multiple colors at once Tango family rubber-like flexible materials Transparent: VeroClear

Table 1 Comparison of desktop stereolithography systems *Lab Chip*, 2014, **14**, 1294–1301

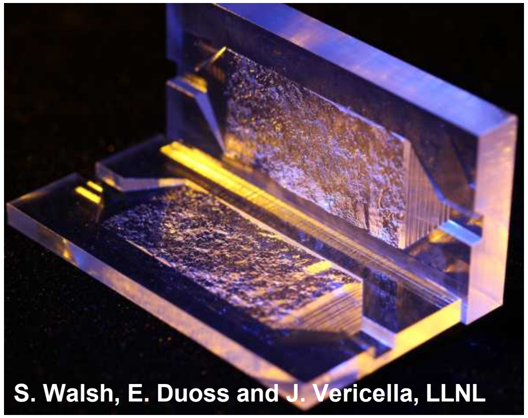
	Technology	*X–Y* resolution	Price	Open-source
Asiga Pico systems	DLP	27–39 μm	$6990–$8990	No
EnvisionTEC Micro	DLP	31 μm	€12 999	No
B9Creator	DLP	50–100 μm	$2990–$4995	Yes
MiiCraft	DLP	56 μm	$1999	Yes
3D Systems ProJet 1200	DLP	56 μm	$4900	No
Ilios HD	DLP or laser	Variable	€2805+	Yes
DigitalWax systems	DLP or laser	Many options	Many options	No
Formlabs Form 1+	Laser	25-50 μm	$3299	No

3D Printing of digital rocks

- Why 3D printing?
  - ability to design & realize complex geometries
  - engineered material control at new regimes
- Porous structure features for this work:
  - Real pore structure on specimens greater than 1 REV
  - 25-100 micron pores, 100+ micron fractures
  - ~2 cm^3 specimen
- Extensive SNL capabilities & expertise are available – leverage for Geo applications

Baker et al. (2014), Computationally generated bed (left) and 3d printed bed (right)

Technology	Materials	Min. feature size (mm)	SNL Capabilities
fused deposition modelling (FDM)	thermoplastics (ABS, PLA, nylon, PC…)	~0.5 mm	>30-40 production to consumer machines
material jetting	photocurable plastics	~0.4 mm	5-10 machines
laser sintering	metals (SS, Ti-6Al-4V, Inconel, Al…) ceramics (alumina, Ceramet, WC)	~0.2 mm ~0.5 mm	2700 purchased one
binder jet printing	gypsum / acrylate	unknown	2-3 machines
stereolithography (SLA)	photocurable resins / epoxies	<0.1 mm claimed	2-3 consumer machines, 1800 developing new μ-SLA
direct write	inks, slurries, paste, resins, etc., any material w/1-1x10^6 cPs viscosity	material dependent	multiple machine platforms w/material development support, base process invented by SNL

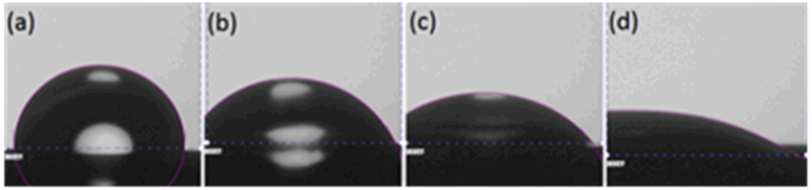


S. Walsh, E. Duoss and J. Vericella, LLNL

Collaborations with UNLV, UTEP

3D Printing in Microfluidics

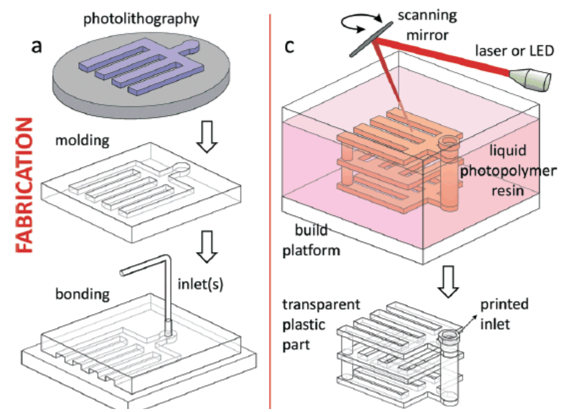
- Stereolithography(SL):
  - Rapid prototyping technique to print in transparent 3D polymer structures from a liquid photopolymer resin with a focused laser or LED
  - Printing resolution at 20-100's μm corresponding to a minimum channel width of ~200 μm
  - Simplified design processing for complex device
  - Desktop SL 3D printers are available!!
  - Printing on pre-processed surfaces (e.g., biochemically treated or nanopatterned surfaces)
  - Feasibility of imaging
  - Surface wettability can be adjusted after printing

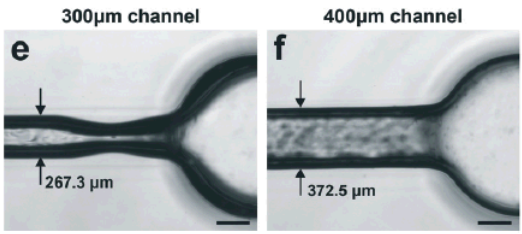


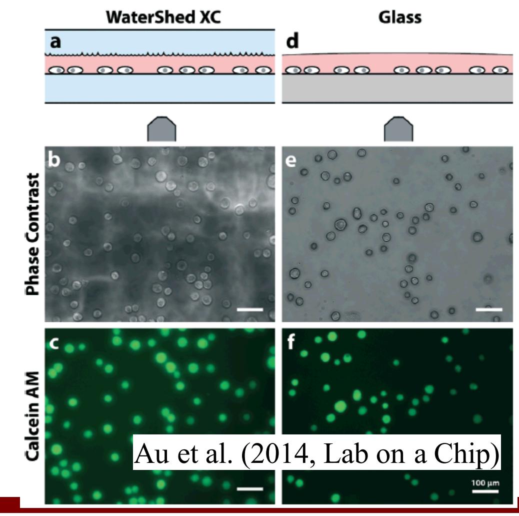
Static Water Contact Angles of self assembled nanoparticles on printed surface with variation of an additive, resulting: (a) 93°, (d) 31°.

PDMS

3D Printing







Au et al. (2014, Lab on a Chip)

3D Printing is advancing rapidly

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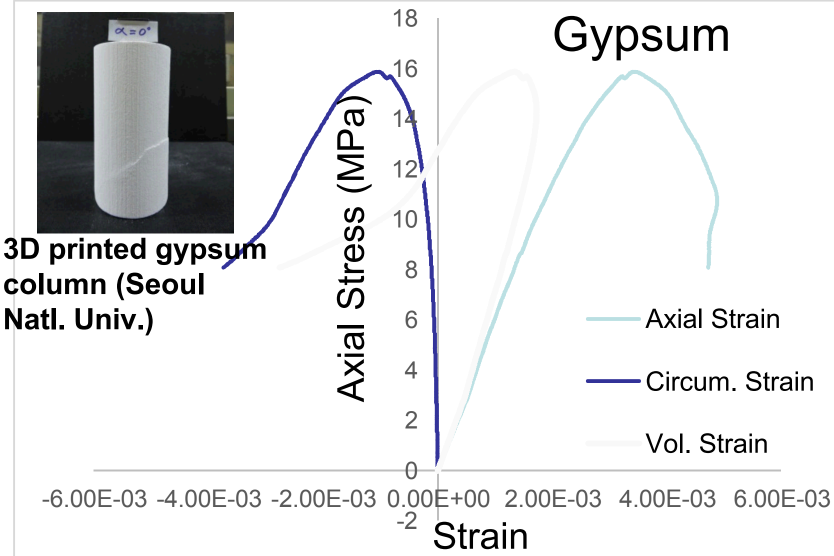
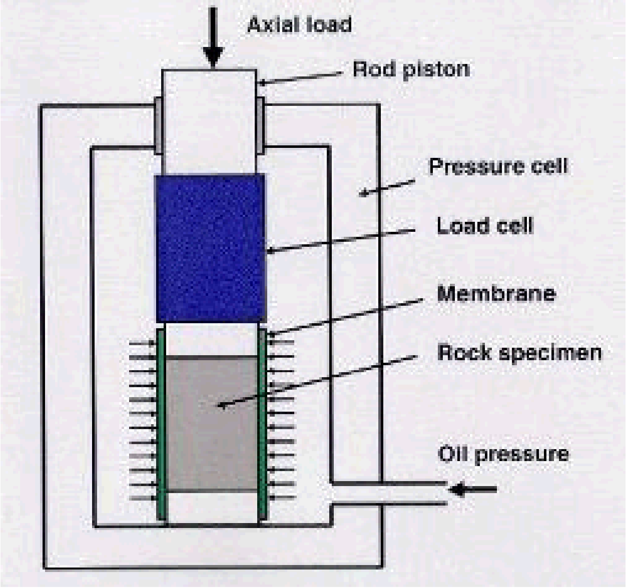
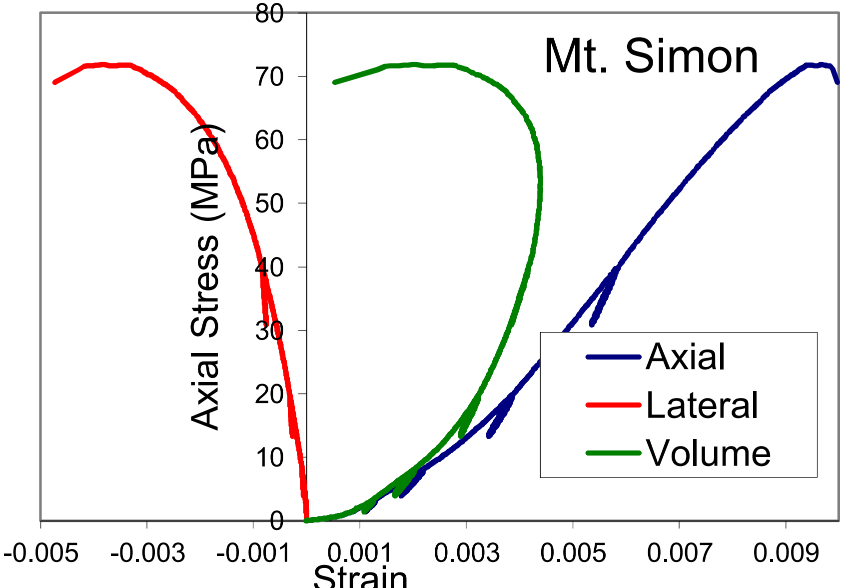
3D printed cores (Gypsum+Binder) behave like geomaterials

- Axisymmetric (triaxial) testing of 3D printed cylinder of gypsum behaves like weak sandstone (Mt Simon Sandstone, Dewers et al., 2014)
- Similarities include initial elastic behavior, yielding, and failure
- Note compaction-to-dilation “turn around”



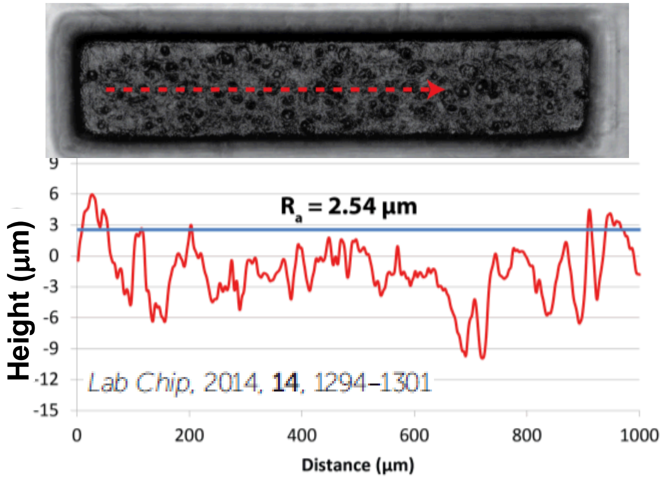


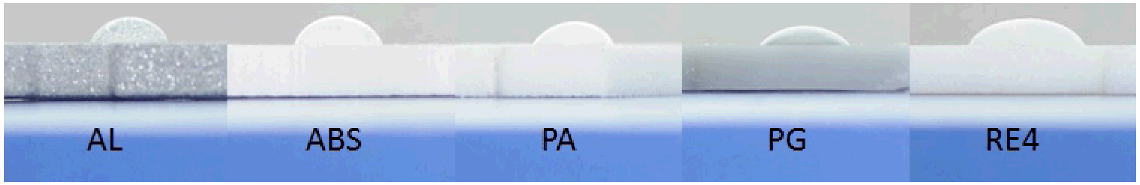


Wettability and its manipulation

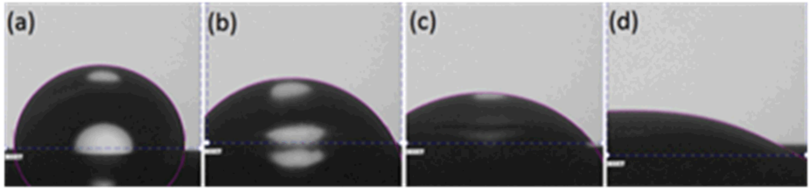
- Wettability is important for flow control and manipulation
- Wettability can be controlled by:
  - Nanoparticles
  - Surface treatments (vapor deposition)
  - Fluid additives (polymers)
  - Surrogate fluids
  - Printed materials have variable wetting characteristics
  - Surface roughness (fractures)

Surface Roughness





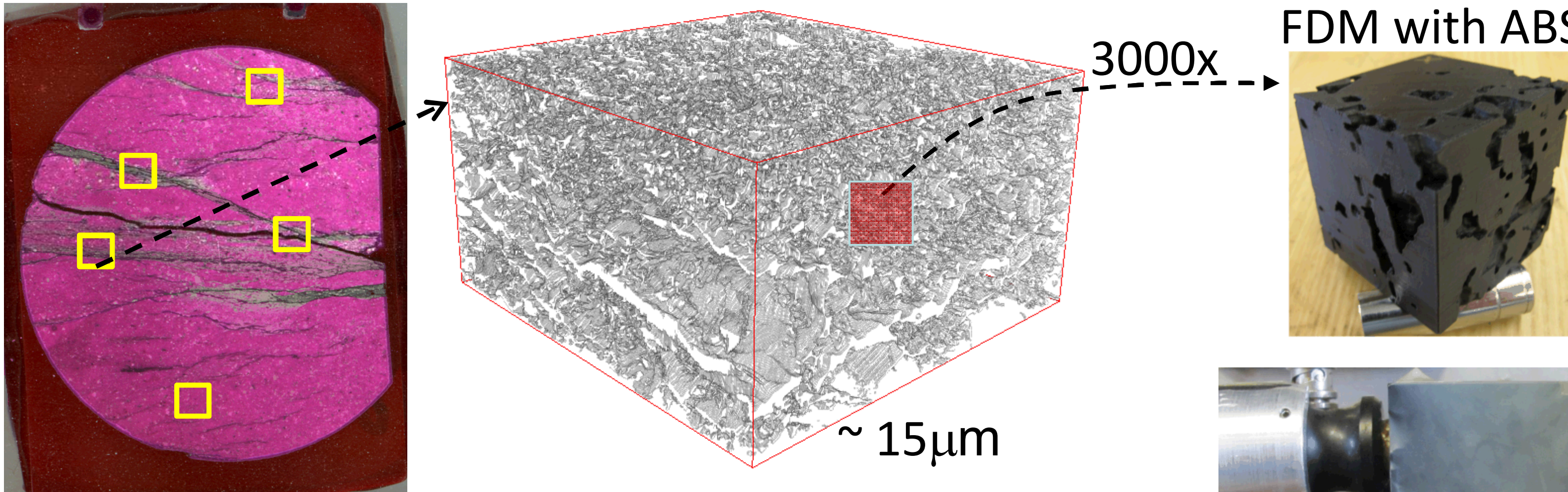
Different printing materials with a range of wetting angles (Bacher 2013, MS thesis)



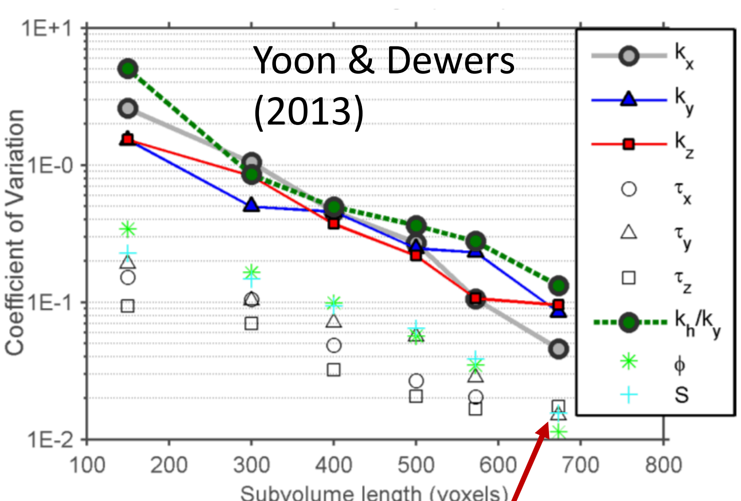
Static water contact angles of self assembled nanoparticles on printed surface with variation of an additive resulting; (a) 93°, (d) 31° (Prof. Kim, UNLV)

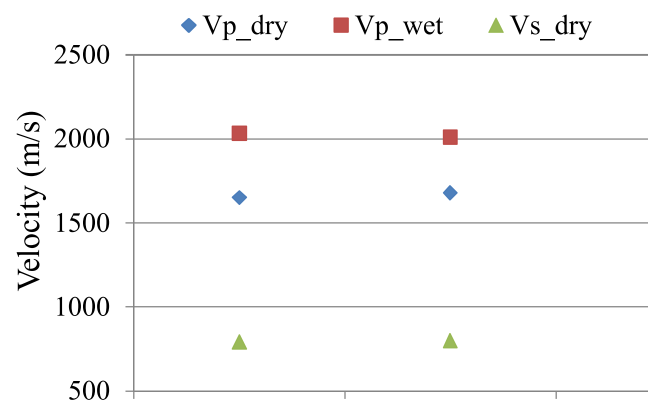
Polymers for adjusting wettability are commercially available

Digital Rock Physics with 3D printing at SNL



AE testing



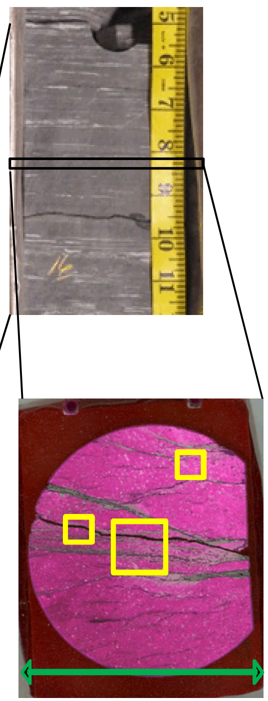


FIB-SEM sample volume has a size of statistical elementary volume at ~ 10 μm

Multi-Scale Imaging (potential for upscaling)

Characterization of pore structures, surface properties, patterns using various techniques such as optical microscopy, microCT, FIB-SEM, TEM, EDS

Core (~1m)

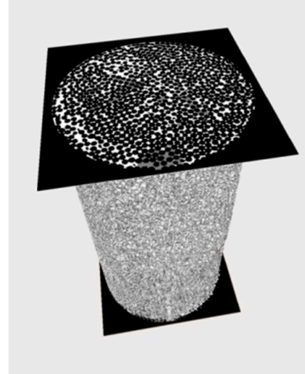


2.54 cm

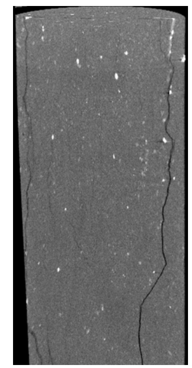
Thin Section

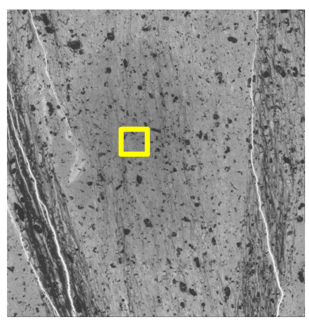
X-ray computed Tomography (CT)

Beads packing

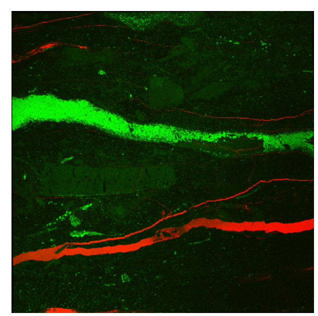


Fracturing





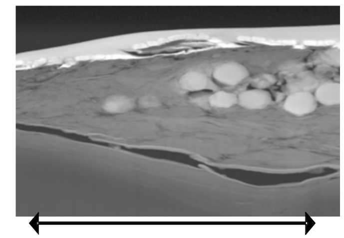
Optical Microscopy



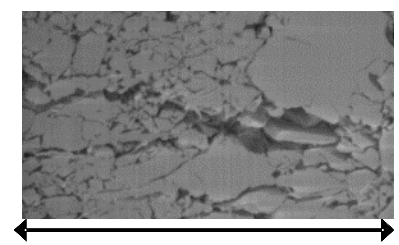
Fluorescent Microscopy

Laser Scanning Confocal Microscopy

TEM/EDS for mineral compositions



5 μm (~1 nm res.)



15 μm (~15 nm res.)

Focused Ion Beam/SEM

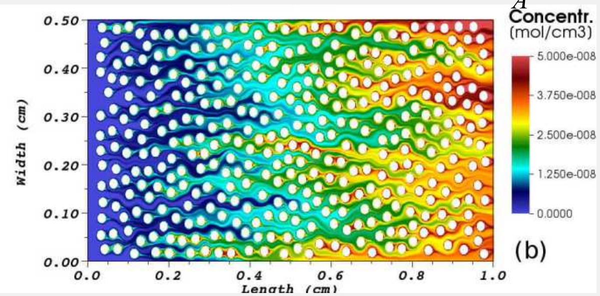
Advanced Constitutive Model Development

Methods for upscaling:

- Homogenization (multiple scale expansions)
- Moments
- Volume averaging
- Pore network models (approx. physics)
- Mass Balance principles based on pore scale models.
- Constitutive equation with closure based on detailed pore scale solutions
- Response function approach

Effective reaction rate

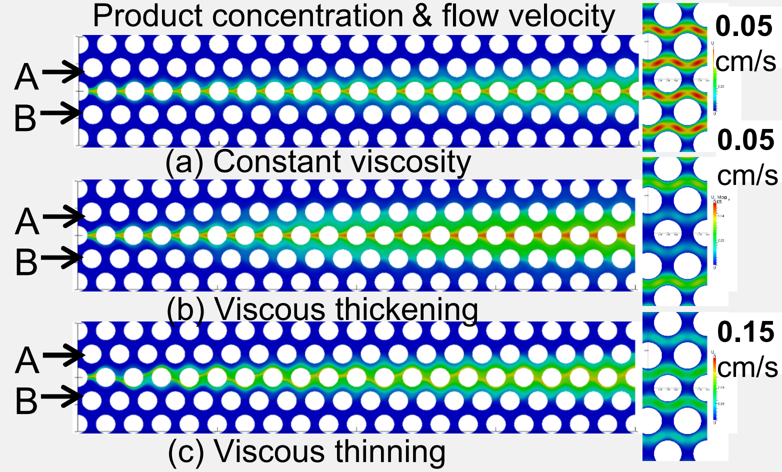
$$\dot{r}_{eff} = \frac{\left(\bar{C}_{in} - \bar{C}_{out}\right)Q}{v\,A} \qquad \bar{C}Q = \int_A \mathbf{u}c \bullet \mathbf{n}\, dS$$

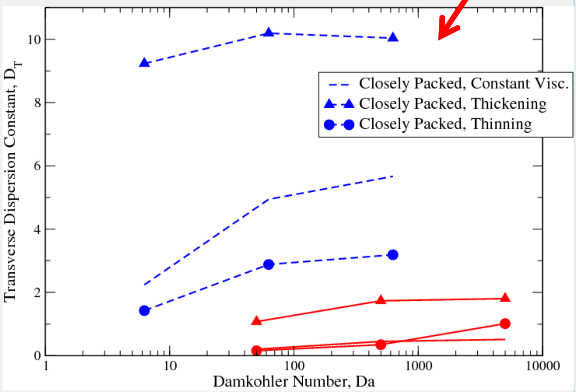


Molins et al. WRR 2012

Effective Dispersion

$$D_{T,R} = \frac{1}{X^3}\frac{9\pi v}{16 C_0^2 \varphi^2}\left[\int_0^X m(x)\,dx\right]^2$$





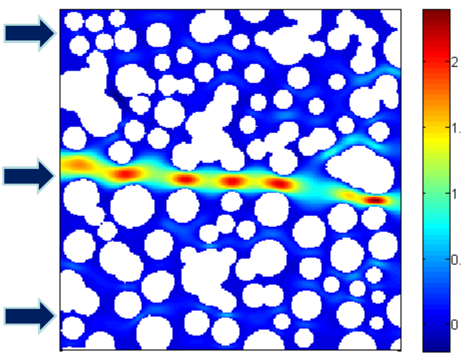
Davison, Yoon, and Martinez (2012)

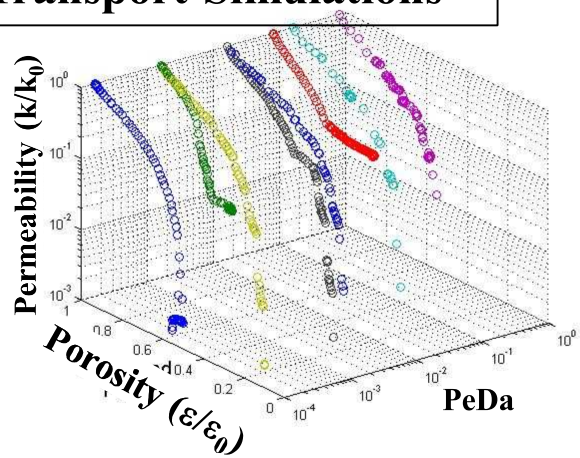
Response Surface Upscaling

- Characterize the relationship between the system's uncertain parameters (or inputs) and its performance metrics (outputs) relationship

Response Surface for Cementation based on Pore Scale Reactive Transport Simulations

Velocity

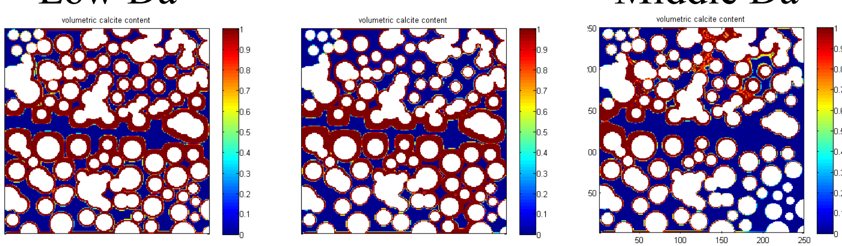




High Pe; Low Da

Middle Pe; Middle Da

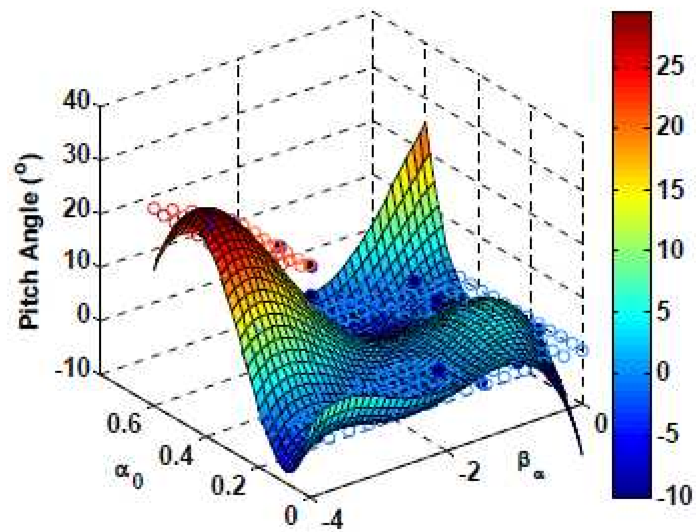
Low Pe; Middle Da



Cementation patterns for different Peclet and Damkohler numbers (bottom)

DAKOTA example for response surface approach

Nonlinear 2 DOF Airfoil problem with non-intrusive PCE method (Allen et al. 2009)



Conclusions

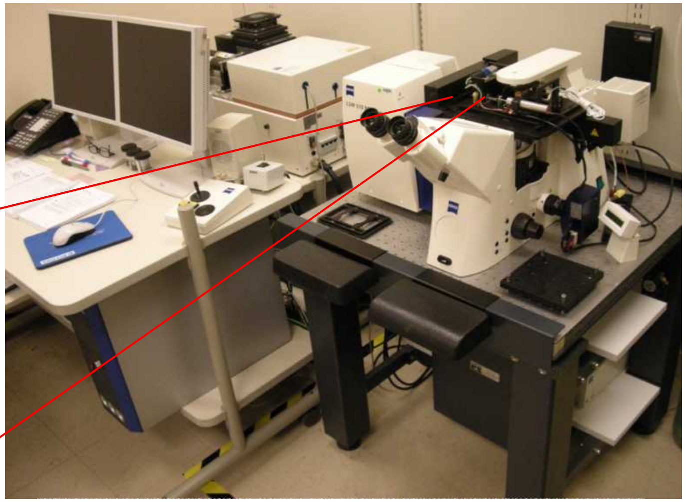
Digital rock physics augmented with 3D printing of porous structures has a lot of potential to advance our understanding of poromechanics

Backup slides

Experimental Facilities: LSC Microscope

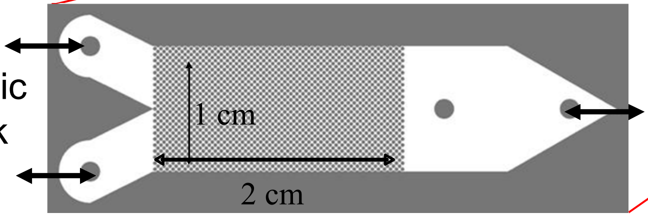
Sandia National Laboratories

- Zeiss laser scanning confocal microscope with recently updated software and hardware
- Microscope stage for real time imaging
- Tension and compression, loads to 1 ton
- Digital image correlation for strain
- Microfluidic cells for multiphase flow and transport



Zeiss 510 meta Laser Scanning Confocal Microscope

2D Microfluidic Pore Network



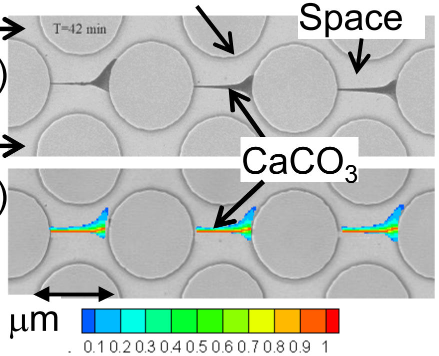
Solid Grain

Pore Space

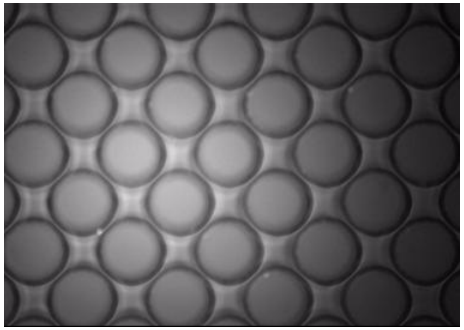
CO_3^{2-} (pH=~11)

Ca^{2+} (pH=~6)

$CaCO_3$

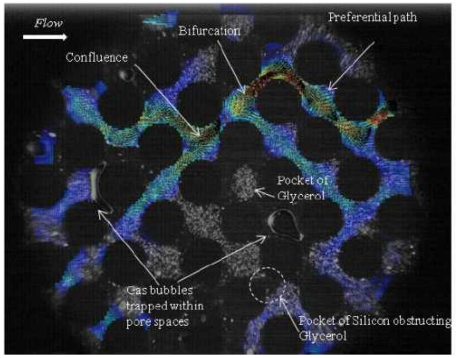


Calcite Precipitation and Model Comparison



Two phase flow

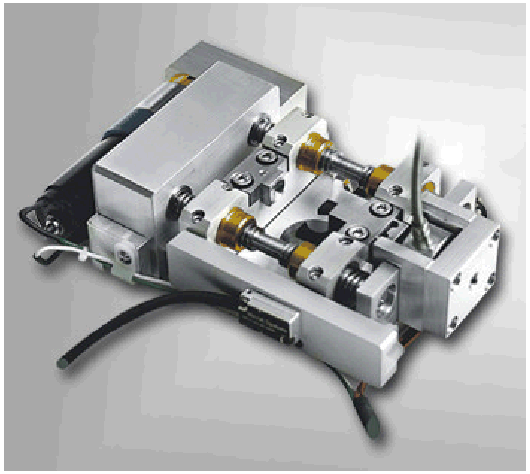
Blois et al. 2013

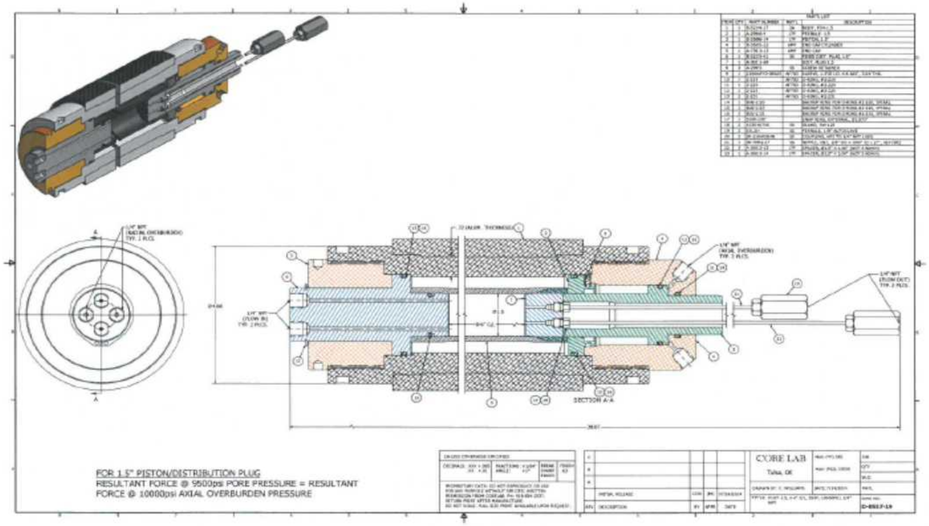


Two phase velocity vector using microscopic particle image velocimetry (μPIV) method

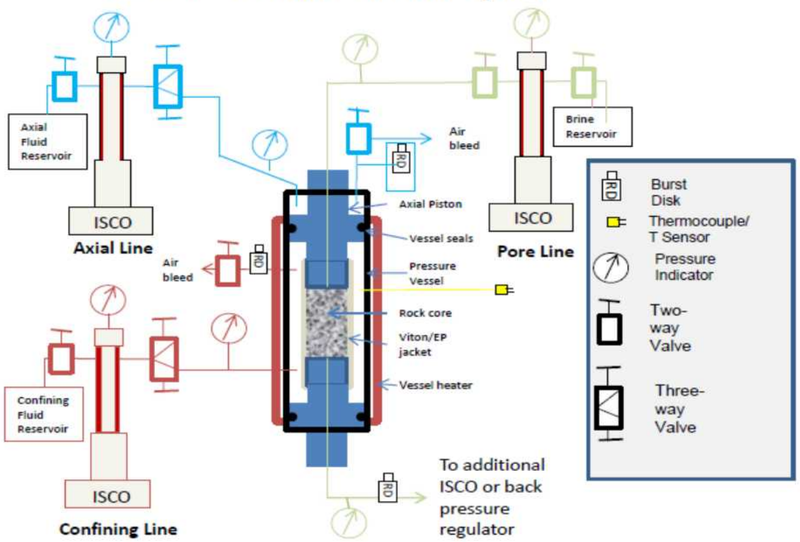
Experimental Facilities: Geomechanics

- Fullam 1-ton compression/tension load frame
- Core Labs coreholders with sonic velocity, acoustic and X-ray CT imaging capability (15,000 psi and 150^{o}C)
- Associated pressure systems for petrophysics measurements (cap pressure, rel perm etc.)
- Research code for automatic picking of arrival events from acoustic emissions

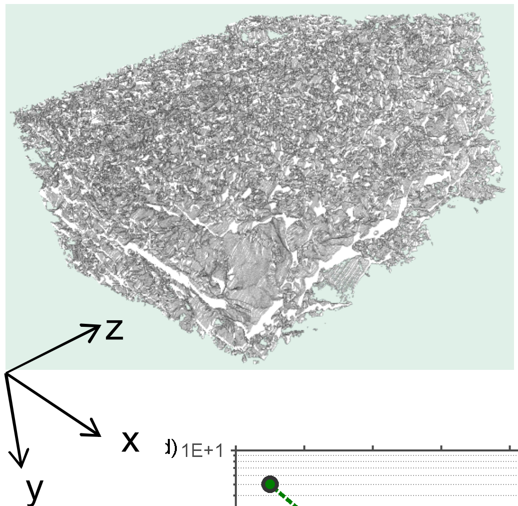


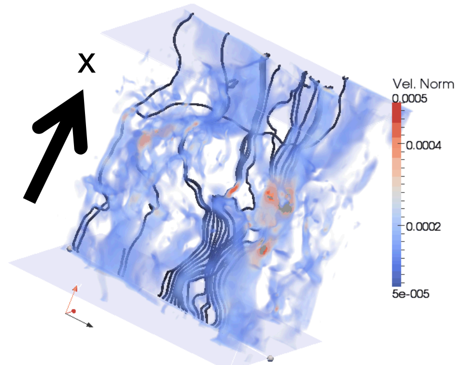


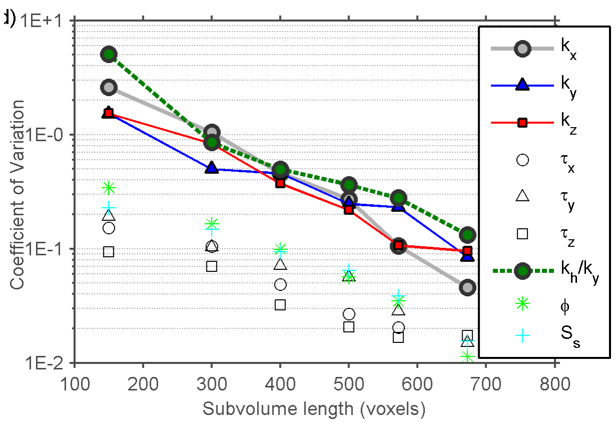
Triaxial Core Holder Pressure System

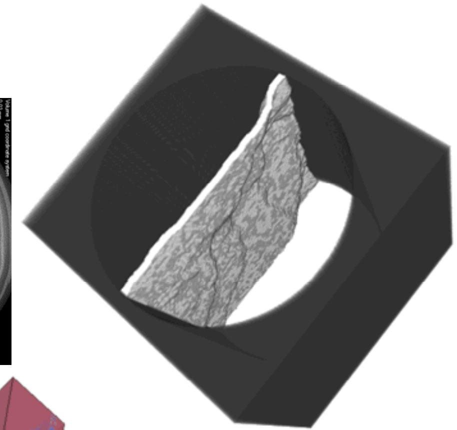


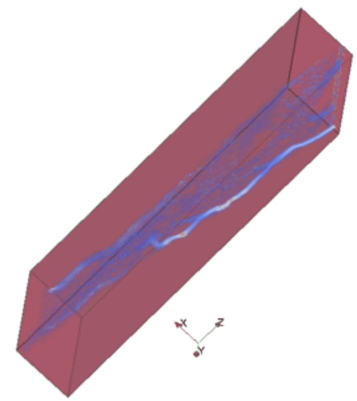
Pore Scale Lattice Boltzmann Simulations











Fracking fluid flow in the presence of proppants

- Estimation of anisotropic permeability and tortuosity at multiple scales
- Single phase flow simulations to determine a representative element volume
- Develop constitutive models for parametric models for continuum scale models - Sierra Mechanics