Year 1 of 3 SAND2020-0772D

Computational Analysis of Coupled Geoscience Processes in Fractured and Deformable Media

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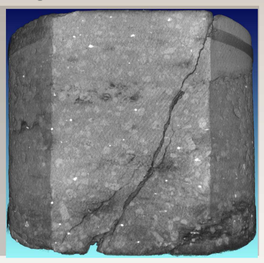
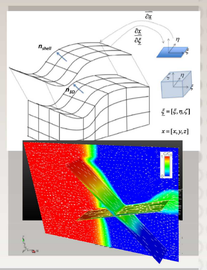
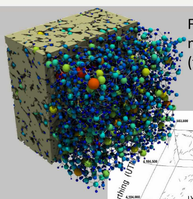
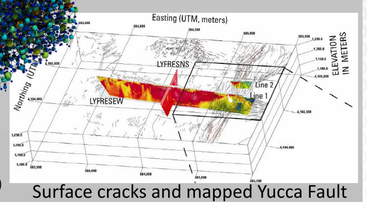


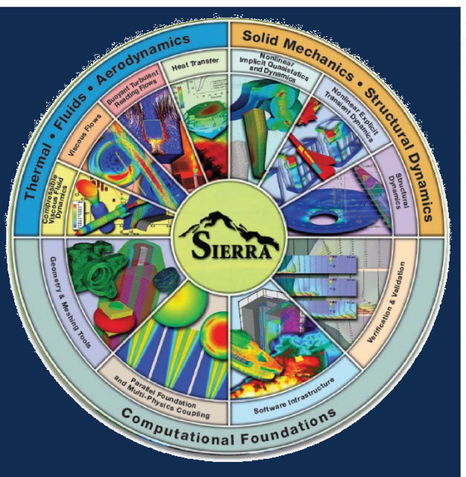




Fracture/pore multiscale graph network (from OpenPNM)



(USGS-OF08-1346) Surface cracks and mapped Yucca Fault



Science Challenges & Objectives

Challenges: Path-dominant and discontinuous features of fractured deformable media pose significant challenges to understanding and control of coupled flow and transport processes that are important for monitoring of nuclear explosion test, subsurface energy resources recovery, and nuclear waste disposal.

Objectives: Advance computational capabilities for coupled earth science processes in fractured deformable porous media, integration of high-fidelity predictive simulation with experimental data, and machine learning based reduced order model approach.

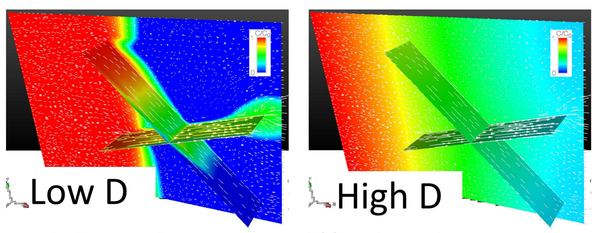
The larger aim is to lay the foundation for a high performance computing (HPC) software platform for the future needs of earth science R&D for global security, national defense, and energy security programs.

Sandia SIERRA coupled physics software for massively parallel HPC applications

- Sandia's computational framework for engineering science mission for multiphysics and multiscale applications
- Platform for integrating research in numerical mathematics and algorithms for chemically reactive multiphase and solid mechanics with advanced scientific computing research in adaptive coupled solution control and framework architecture

Enhancement in Sierra-Aria/Solid Mechanics for Coupled Processes

Curvilinear shell elements for 3D fractures/faults



- Advection and diffusion in two fractures (100x:10x perm to matrix)

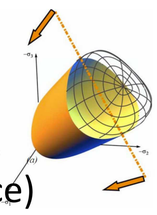
- Meshing for complex fracture network
- High aspect ratio of fracture/faults
- Easy implementation for aperture distribution
- Coupled THMC models

Enhancement

- Chemical reactive transport
- Coupled mechanics with shell elements
- Interactions between fracture and matrix (e.g. multirate diffusion models)

Material property library

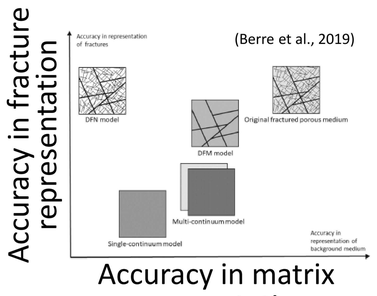
- Library of Advanced Materials for Engineering (LAME): Bulk Constitutive Properties for plasticity, effective stress, Biot coeff, etc.



- Kayenta geomaterial model (e.g., 3D view of continuous yield surface)

Multiscale multiphysics in fractured media

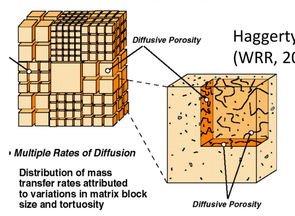
- Prediction of stress-permeability relations in fractured media is a fundamental challenge under different models (multi-continuum, DFN, and DFM)
- Prediction of flow and reactive transport processes and interactions between fractures and surrounding media (e.g. multirate diffusion)



Fracture network

(copied from dfnworks manual)

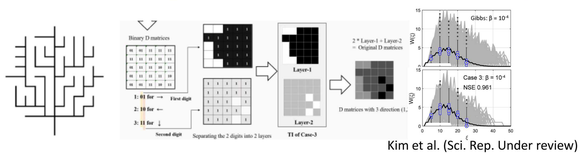
Multirate diffusion model



Haggerty et al. (WRR, 2001)

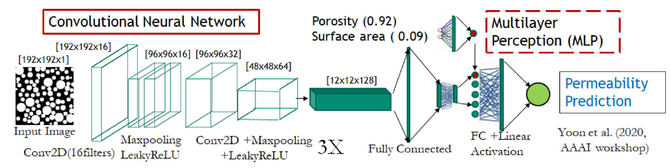
Physics-Informed machine learning

- Network generation (DCGANs)



Kim et al. (Sci. Rep. Under review)

- Permeability prediction (CNN+MLP)

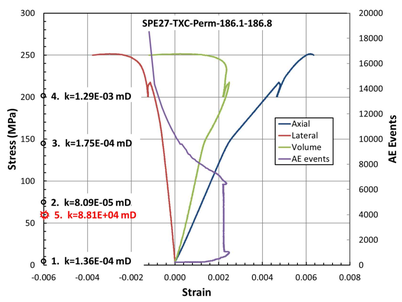


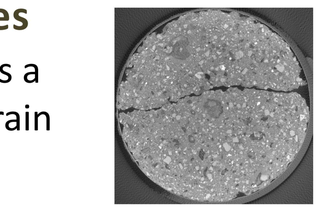
Yoon et al. (2020, AAAI workshop)

Applications of multiphysics toolkit for coupled processes

(T)-H-M processes

Permeability evolution as a function of stress and strain

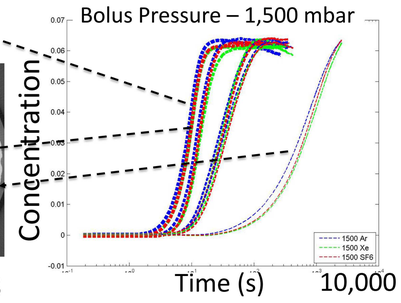




Various testing samples

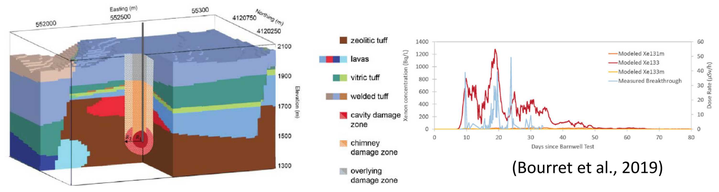
(T)-H-C processes

Gas species dependent transport properties in different materials



(T)-H-M-C processes

Effect of fractured porous media permeability on noble gas and gas tracer transport (Xe, Ar, SF6, CF4)



(Bourret et al., 2019)

- Validation of multiphysics models against experimental data both at laboratory and field scales obtained from a part of a U.S. DOE NNSA non-proliferation campaign
- A suite of core testing, microCT imaging, geomechanical, hydrogeological, petrophysical analysis at the laboratory and well testing results at the Nevada field site will be used

Exceptional service in the national interest

Sandia National Laboratories

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