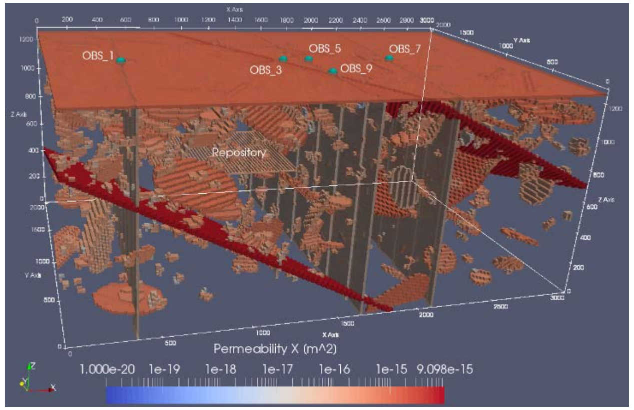

Physical and Geochemical Processes that Impact Flow and Transport in Crystalline Host Rock

U.S. Nuclear Waste Technical Review Board
May 21-22, 2024
Knoxville, TN

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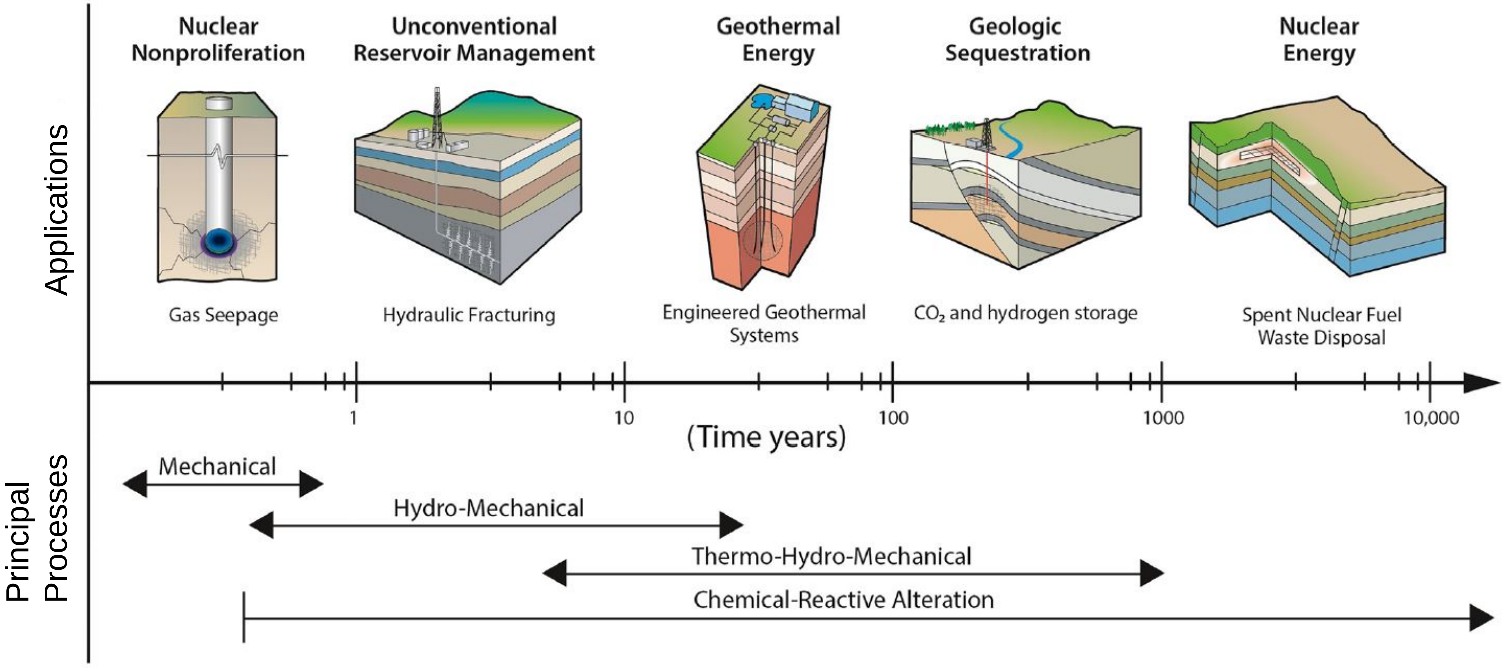
Motivation: Subsurface Fractured Systems

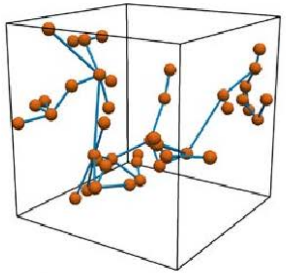


Viswanathan et al., (2022)

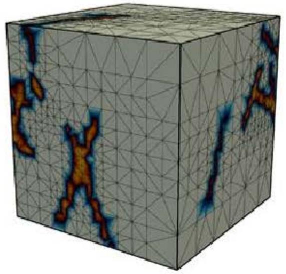
- Range of DOE application spaces involve subsurface flow and transport in fractured porous rocks
- Fractures often dominate flow and transport behavior
- Physics-based models can be constrained by field and lab measurements
- Machine learning models can be used to accelerate physics-based models for robust uncertainty quantification

Current Methodologies for RTM in Fractured Media

- We can build fracture networks from length, aperture, fracture spacing, spatial and orientation distributions measured at the field and core scales, but uncertainty persists
- Run models in ensembles to describe ranges of possible behavior and develop uncertainty bounds and statistics
- Characterizing the effects of coupled processes (e.g., thermal, mechanical, chemical) is even more challenging
- There are a lot of computer models with various strengths and weakness to model reactive transport (RTM) in fractured media
    - Discrete fracture networks
    - Channel / Pipe networks
    - Upscaled Continuum models
    - Discrete fracture matrix models

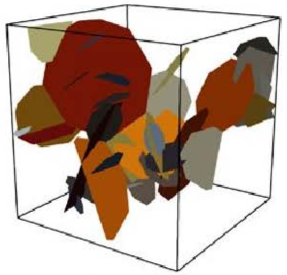


Channel Network

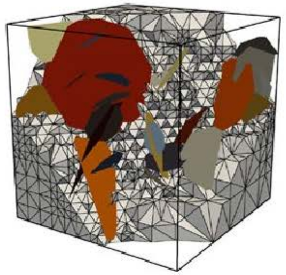


Continuum Methods

Fractured Rock



Discrete Fracture Network

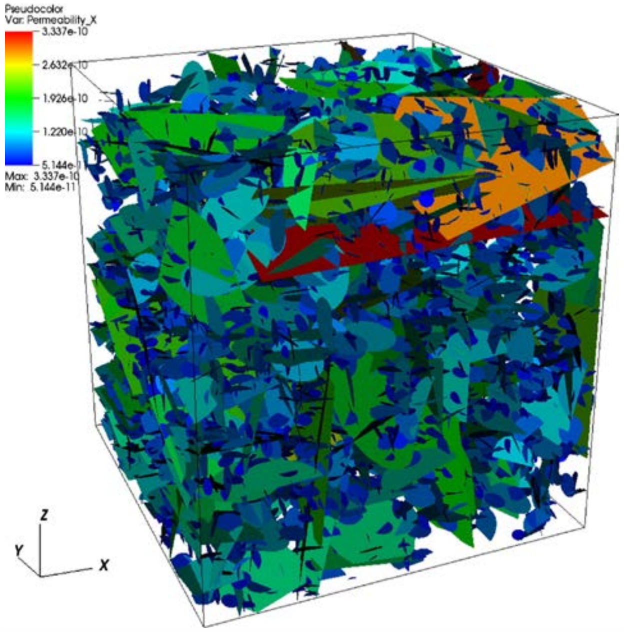


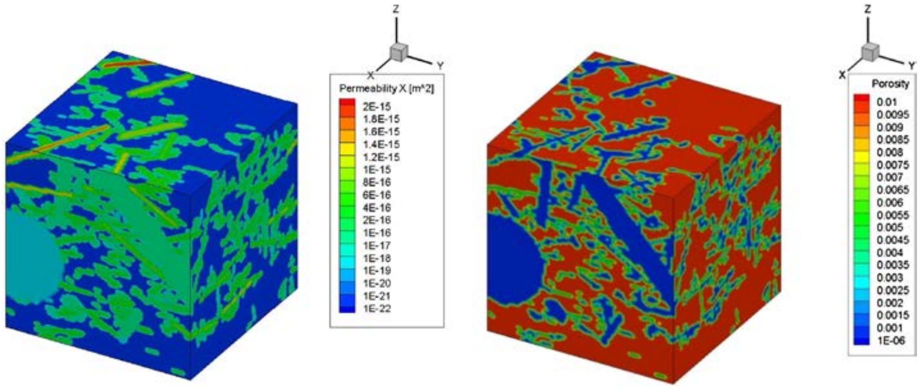
Discrete Fracture Matrix

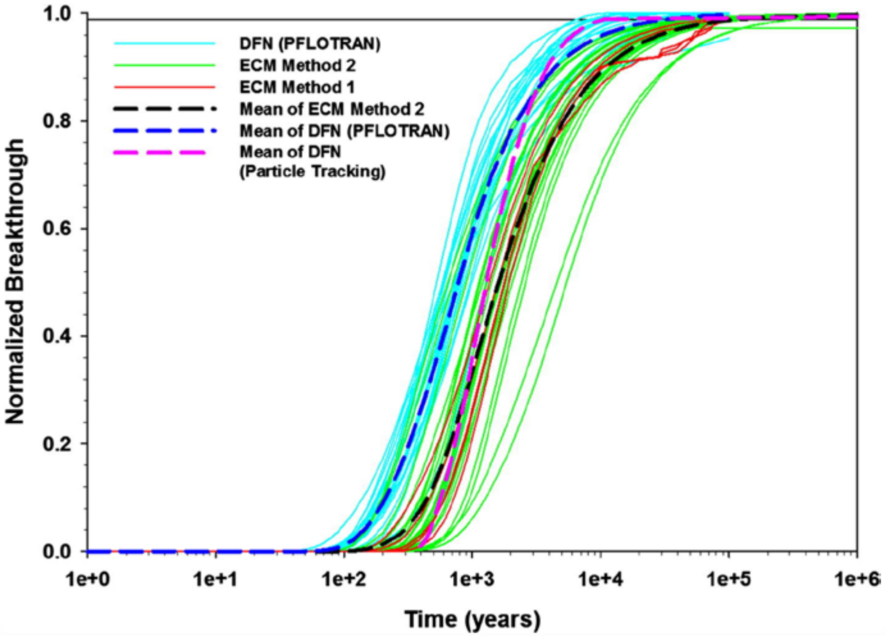
Implicit/Continuum vs Explicit/DFN Approaches

- Models differ in representation of fractures and hydraulic parameters, as well as representation of surrounding rock
- Model choice should be made based on problem and quantity of interest, i.e., *What problem are you trying to solve?*
- Success of continuum approaches to reproduce underlying fracture network behavior has been mixed, but overall positive

DFN → Upscale hydraulic parameters → Run flow and transport







Hadgu et al., (2017)

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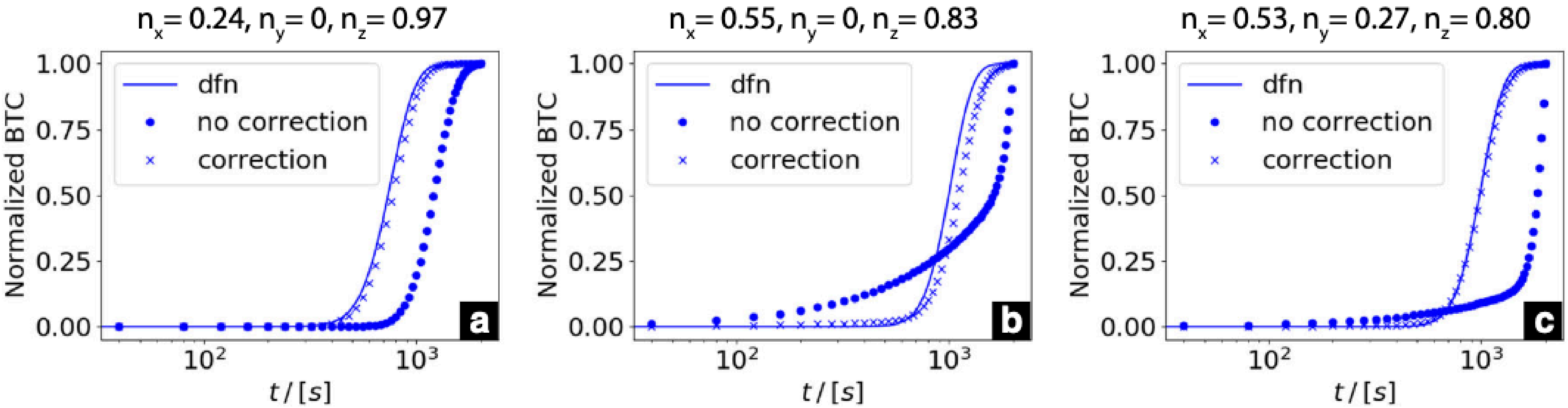
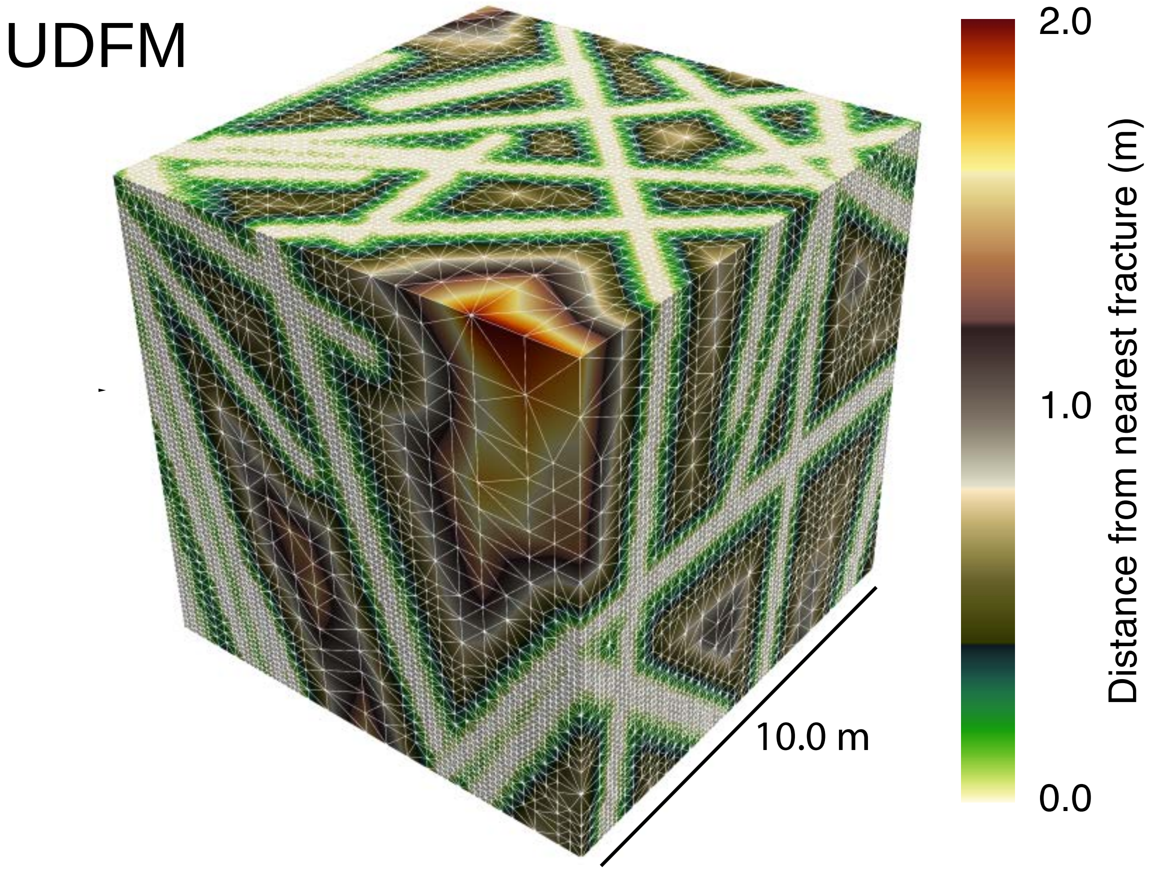
Bias between DFN and Continuum can be corrected



Sweeney et al., (2020)

Upscaling Methods from a DFN to a Continuum

- “Fracture cells” get fracture/matrix properties and “matrix cells” get matrix properties
- Single and dual continuum is readily used in PFLOTRAN
- Mesh resolution can greatly impact transport properties
- Methods in dfnWorks
  - UDFM
    - Octree variable resolution / refined next to fractures (fewer unknowns for solution)
    - High cost of meshing
  - mapDFN
    - Uniform hex mesh (trivial meshing)
    - More DOFs in solver
- Used in DECOVALEX Task F1



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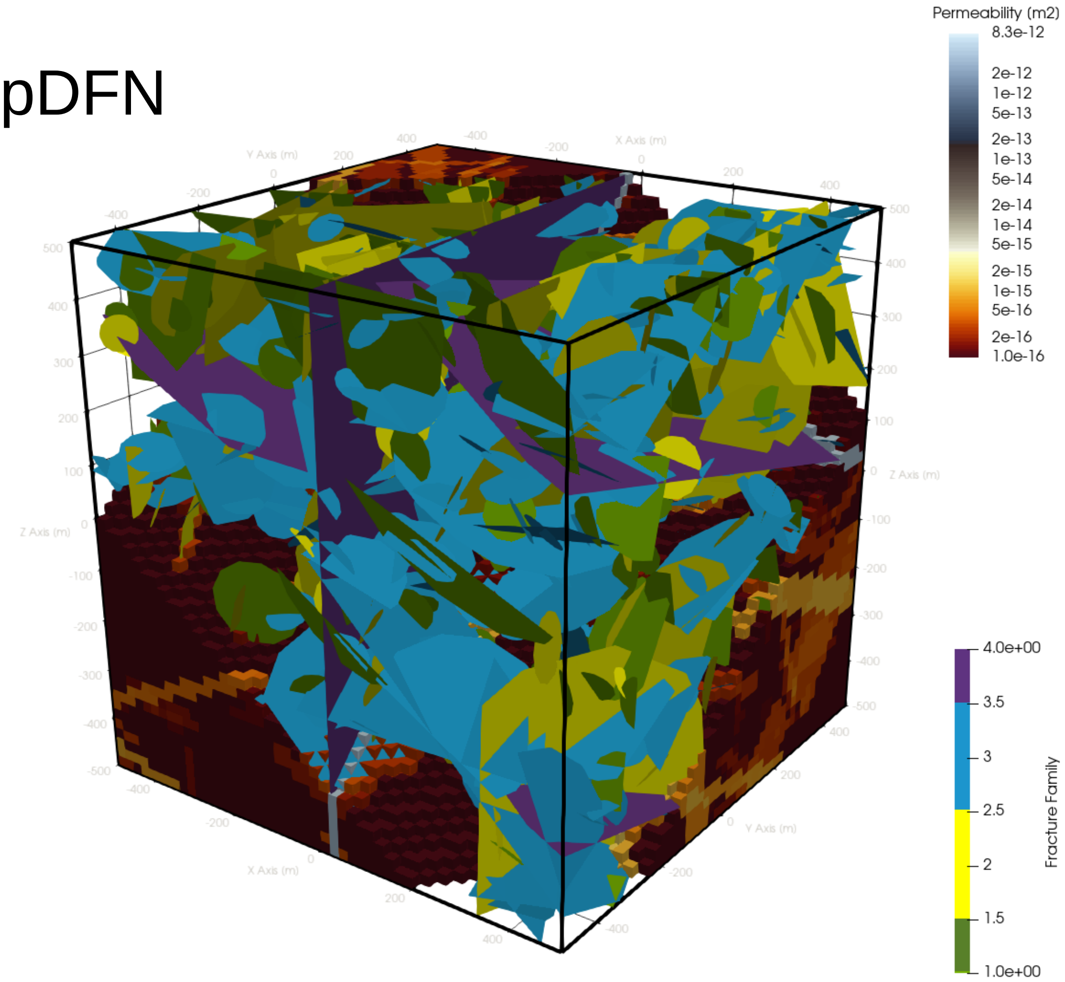
mapDFN



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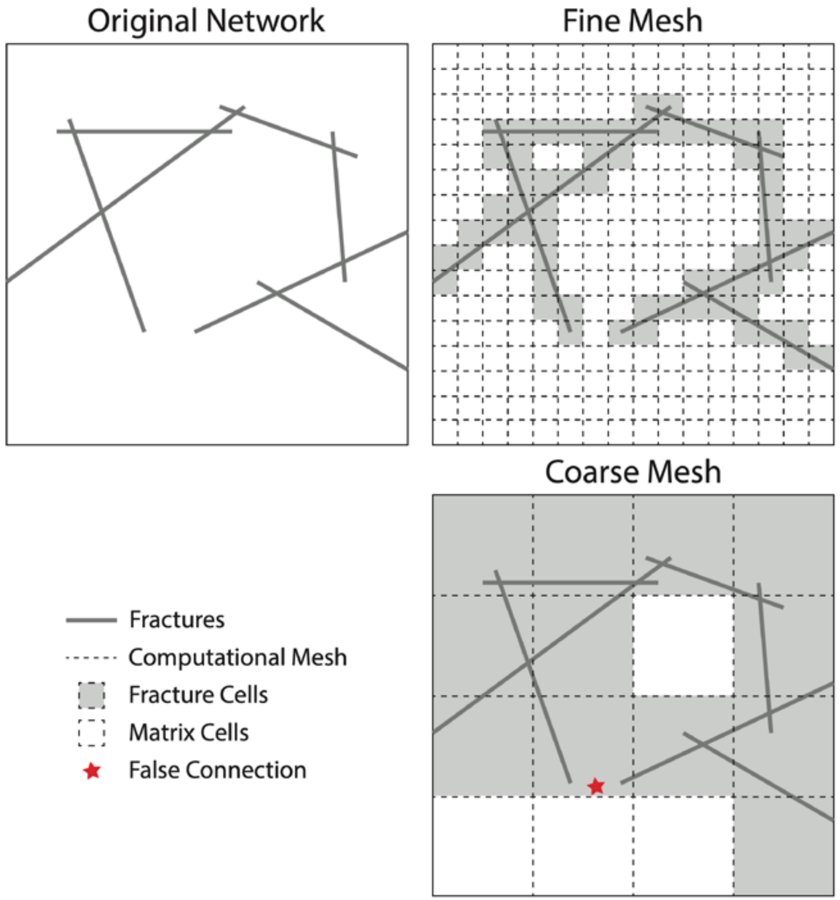


Pachalieva et al., (2023)

How Does Dissolution Influence Flow Channelization?

Flow and reactive transport simulations

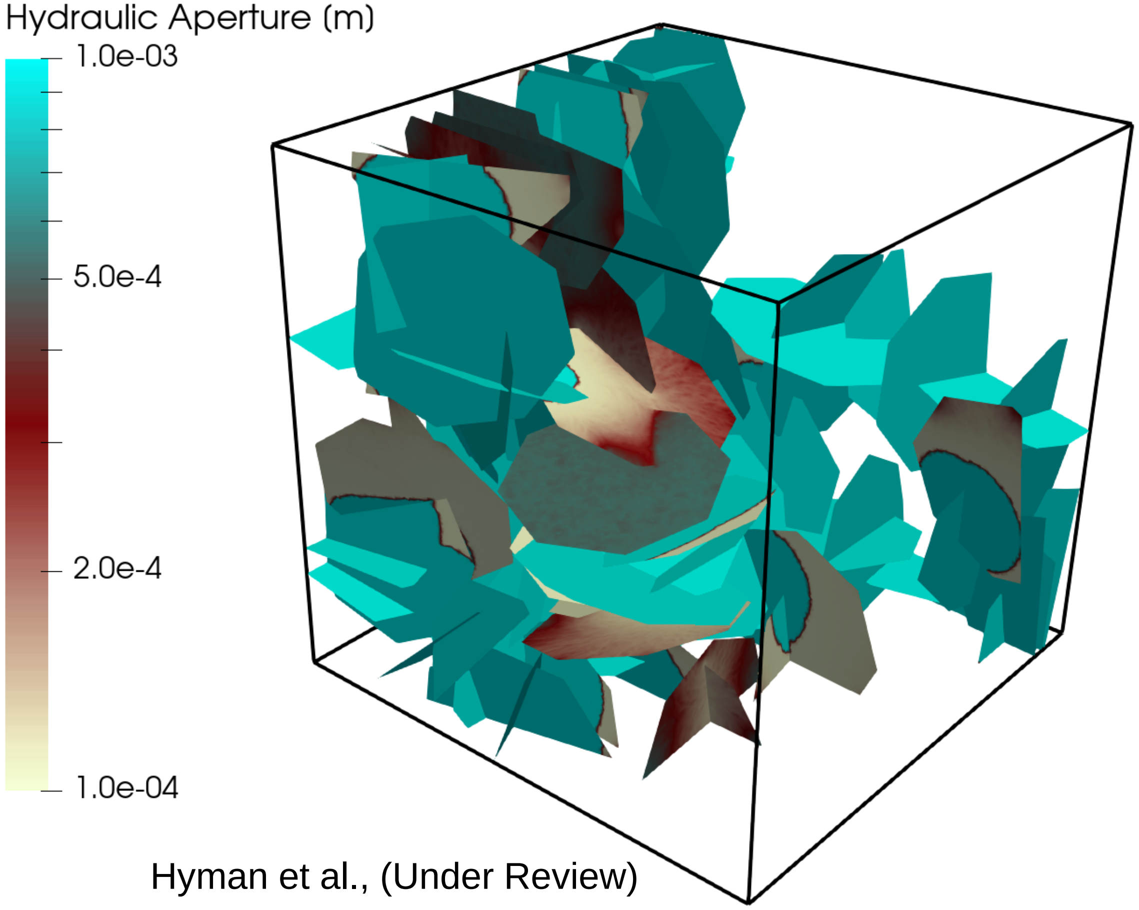
- Performed flow and transport using PFLOTRAN with the Hanford dataset and dfnWorks for DFN realizations
- Quartz dissolves to produce aqueous silica
- Dynamic update to hydraulic properties (volume of quartz, permeability, porosity, and mineral surface)
- Passive particle tracking performed in the unreacted and dissolved networks

Results

- Increased effective block permeability
- Decreased active surface area
- Decreased first arrival time / Faster Transport

Implications

- First RTM in 3D DFNS
- Dynamic geochemistry resulting in spatially variable aperture



Hyman et al., (Under Review)

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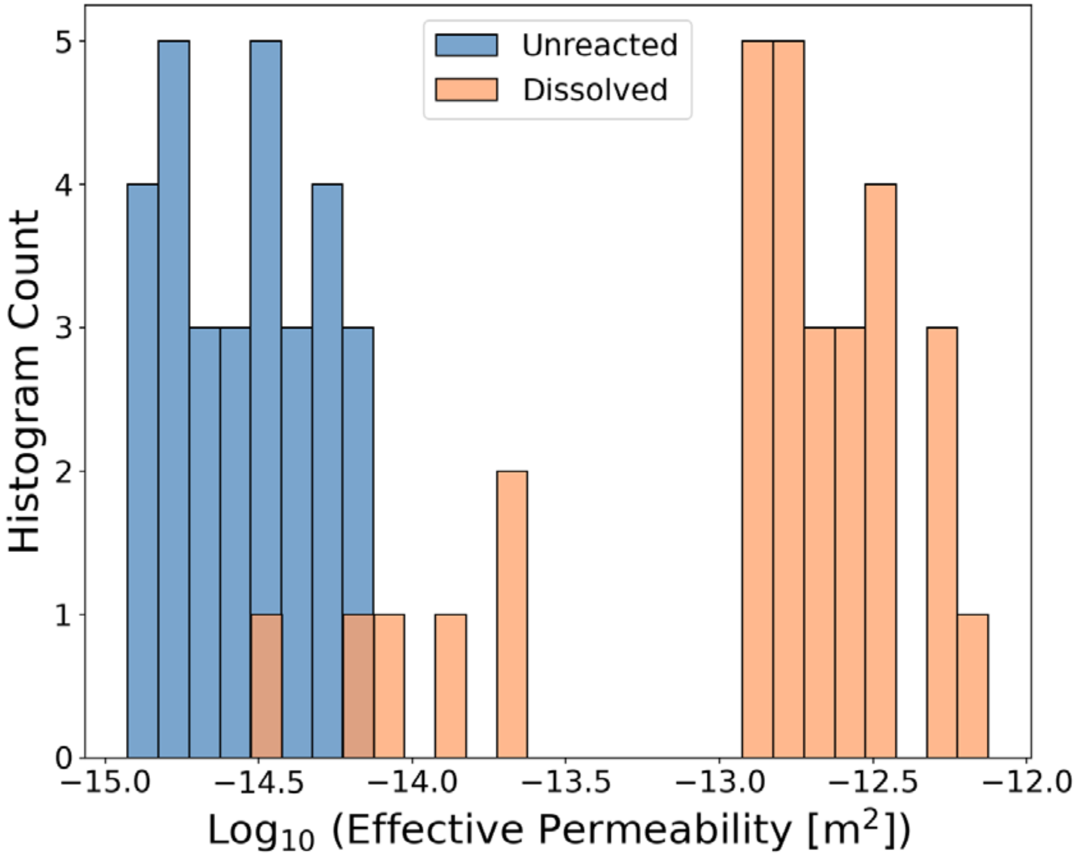

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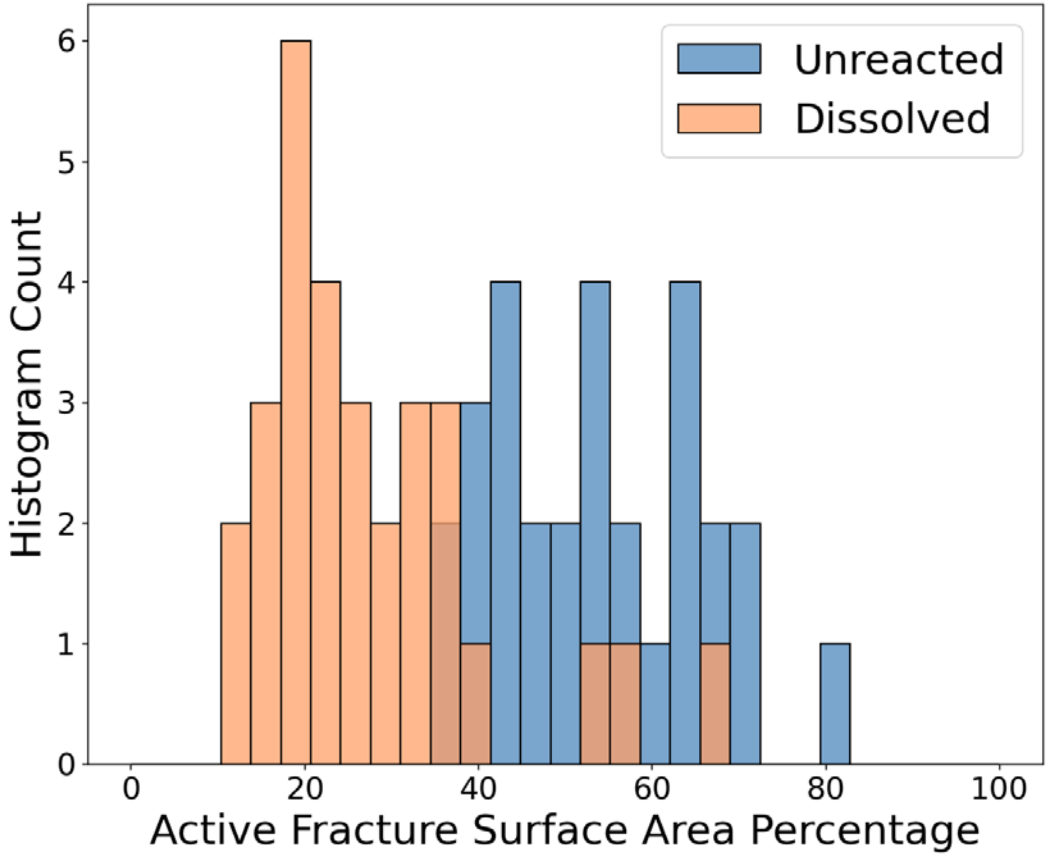

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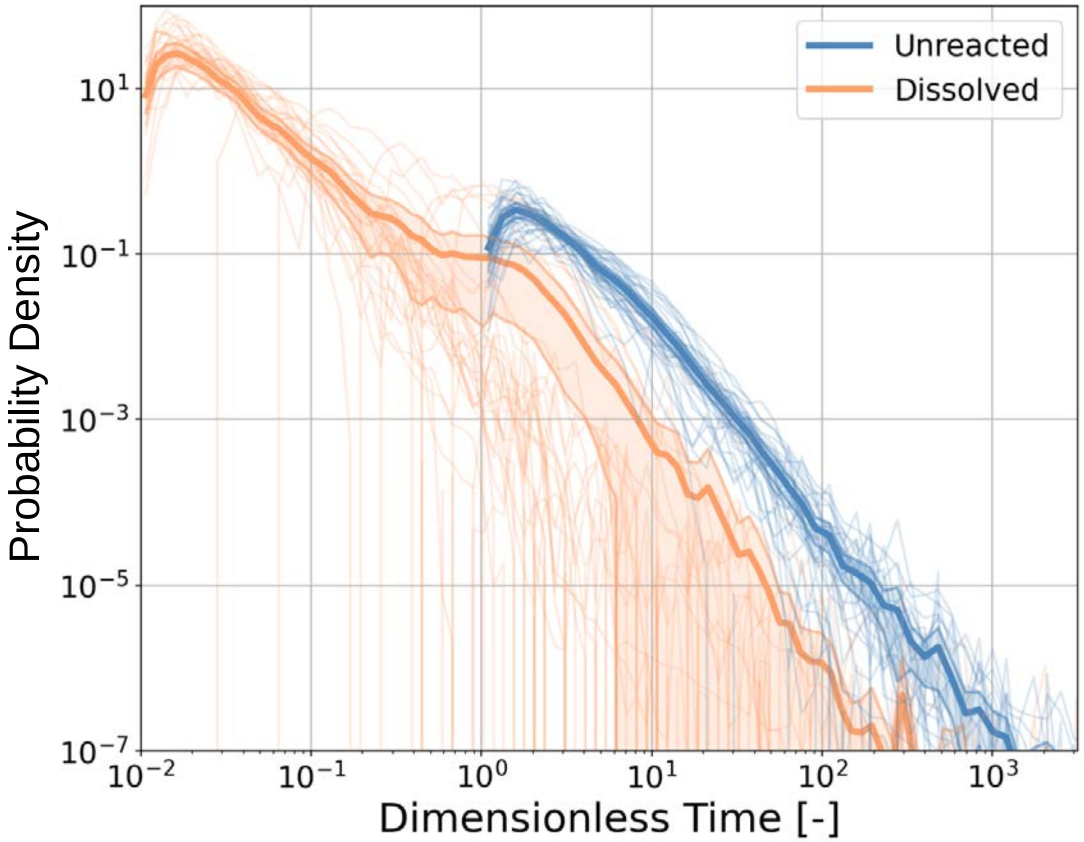
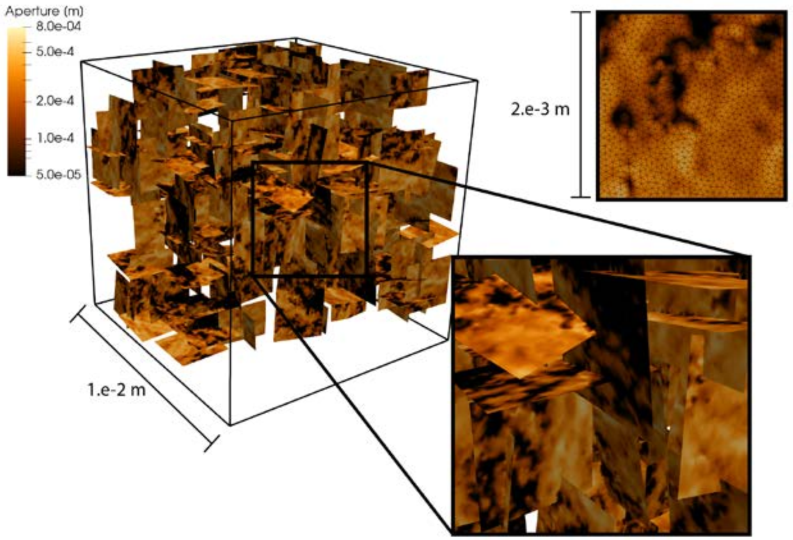
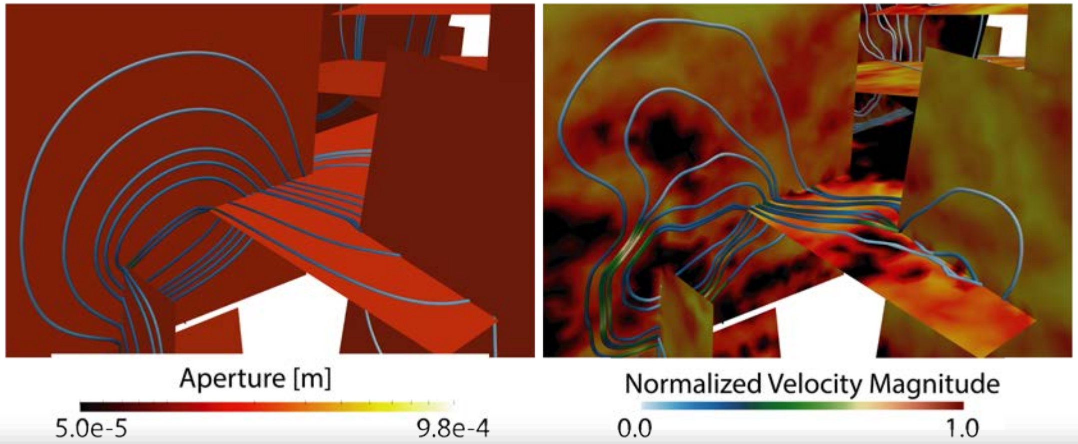
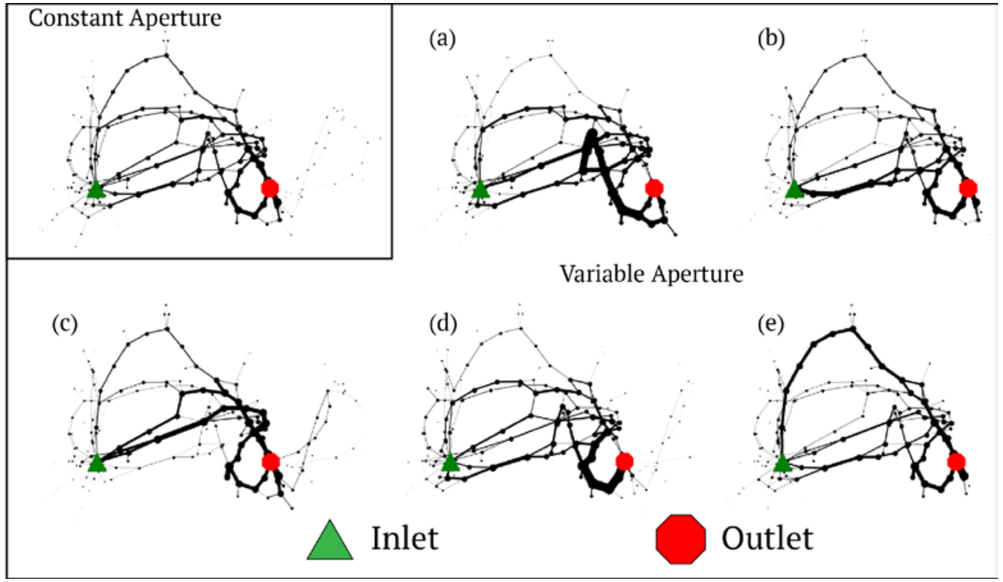


In-fracture Aperture Variability in Networks





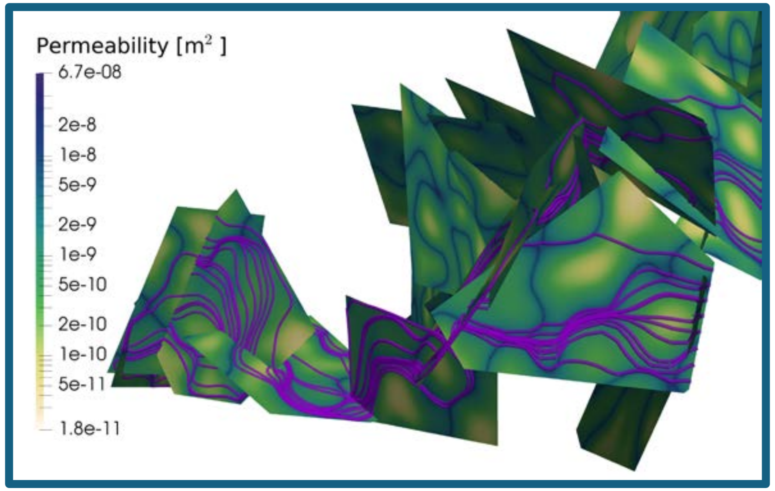


- Variations in the local hydraulic aperture not only modifies the local flow field within a single fracture but can also restructure the network-scale flow
- These changes alter particle transport and would thereby alter retention processes of a chemical species passing through the network
- The active surface area is reduced compared to reference networks with constant aperture
- **In-fracture aperture variability increases network scale flow channeling, which could decrease the host rock barrier capability**

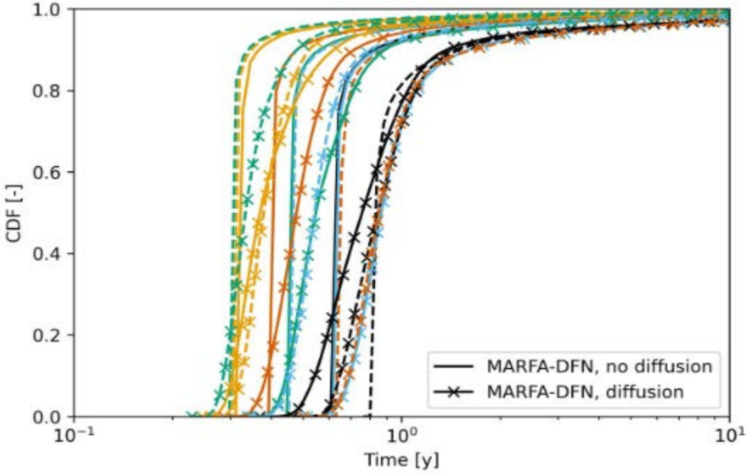
Hyman et al., (2021)

Particle Tracking with MARFA in a DFN

- Internal velocity field pathline tracking
- Integration with Migration Analysis of Radionuclides in the Far Field (MARFA)
- Multi-scale dispersion
    - In-plane (aperture variations)
    - Taylor Dispersion
    - Longitudinal Transverse
    - Molecular Diffusion
- Sorption / Matrix diffusion retention
- Internal aperture variability
- Undergoing a refactor and port to C++ for parallelization and tight integration with MARFA



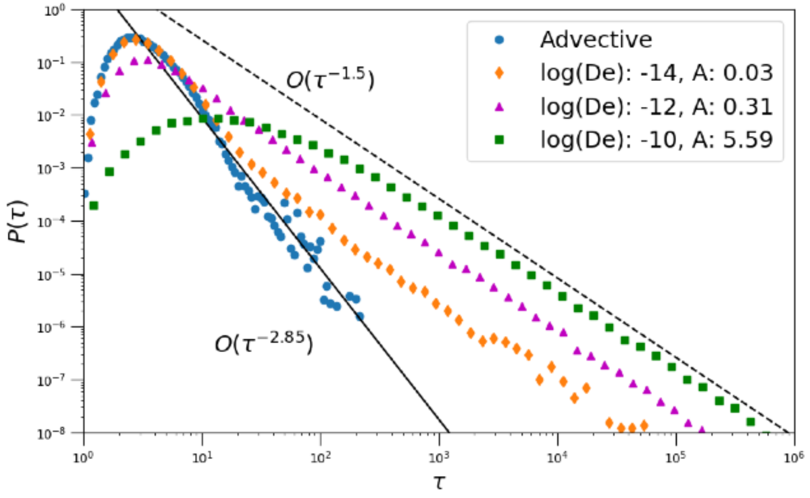
Sanglas et al., (2024)



These are all fundamental processes and phenomenon which support GDSA and radionuclide transport

Having a Lagrangian transport model supports benchmarking and verification of Eulerian models

Hyman et al., (2019)



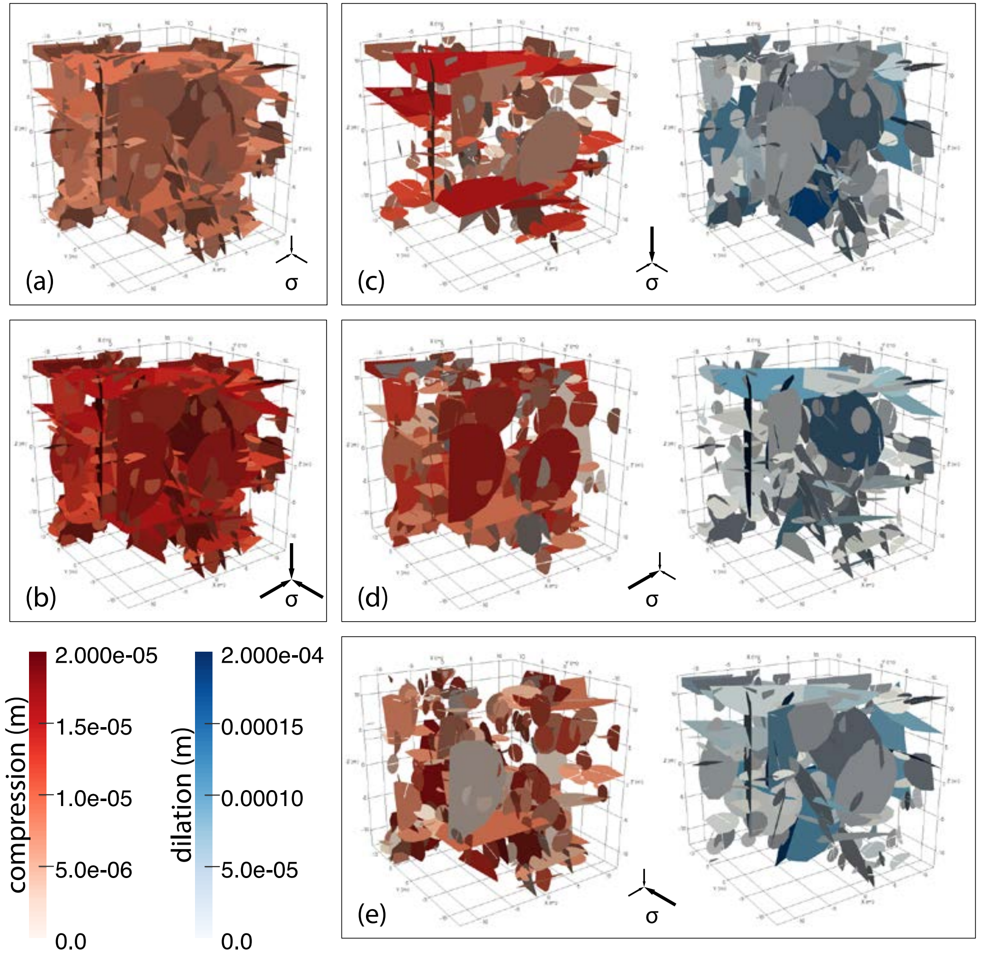
Inclusion of Background Stress in a Fracture Network

- The relationship between dilation/compression of a fracture's hydraulic aperture and the stress field is computed analytically by means of projection of the stress tensor onto the orientation of the fracture to compute the normal stress, Barton Bandis Model

- When the network is subjected to anisotropic stress regimes, the flow field and associated transport behavior can be dramatically altered.

- These changes are characterized by a broadening aperture distribution, which can result in early time arrival of particles or solute. However, in most cases we observed delayed arrival and long tailing behavior due to increases in tortuosity and changes in the network backbones.

- Stress changes could impact flow and transport around repository if stress regime changes during lifetime (e.g., isostatic rebound)



Sweeney et al., (2020)

Summary

- Model choice for RTM in fracture networks needs to be made with problem and quantity of interest in mind, (e.g., time and length scales, arrival of solutes, coupled processes)
- Relationship between field, core, and lab measurements and generating numerical representations is an active area of research
- Continuum models can reproduce much of the flow and transport behavior of higher resolution DFN models, but can not resolve high fidelity in-fracture scale processes
- Lagrangian particle tracking can be used in conjunction with Eulerian models to understand repository performance
- Long term stress changes could impact flow fields around repositories

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