Flow and Transport in Fractured Granite: Modeling Studies Involving the Bentonite Rock Interaction Experiment (BRIE) and the Long Term Diffusion Experiment (LTDE)

U.S. Nuclear Waste Technical Review Board Workshop
April 25, 2019
Las Vegas, Nevada

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LA-UR-19-21112

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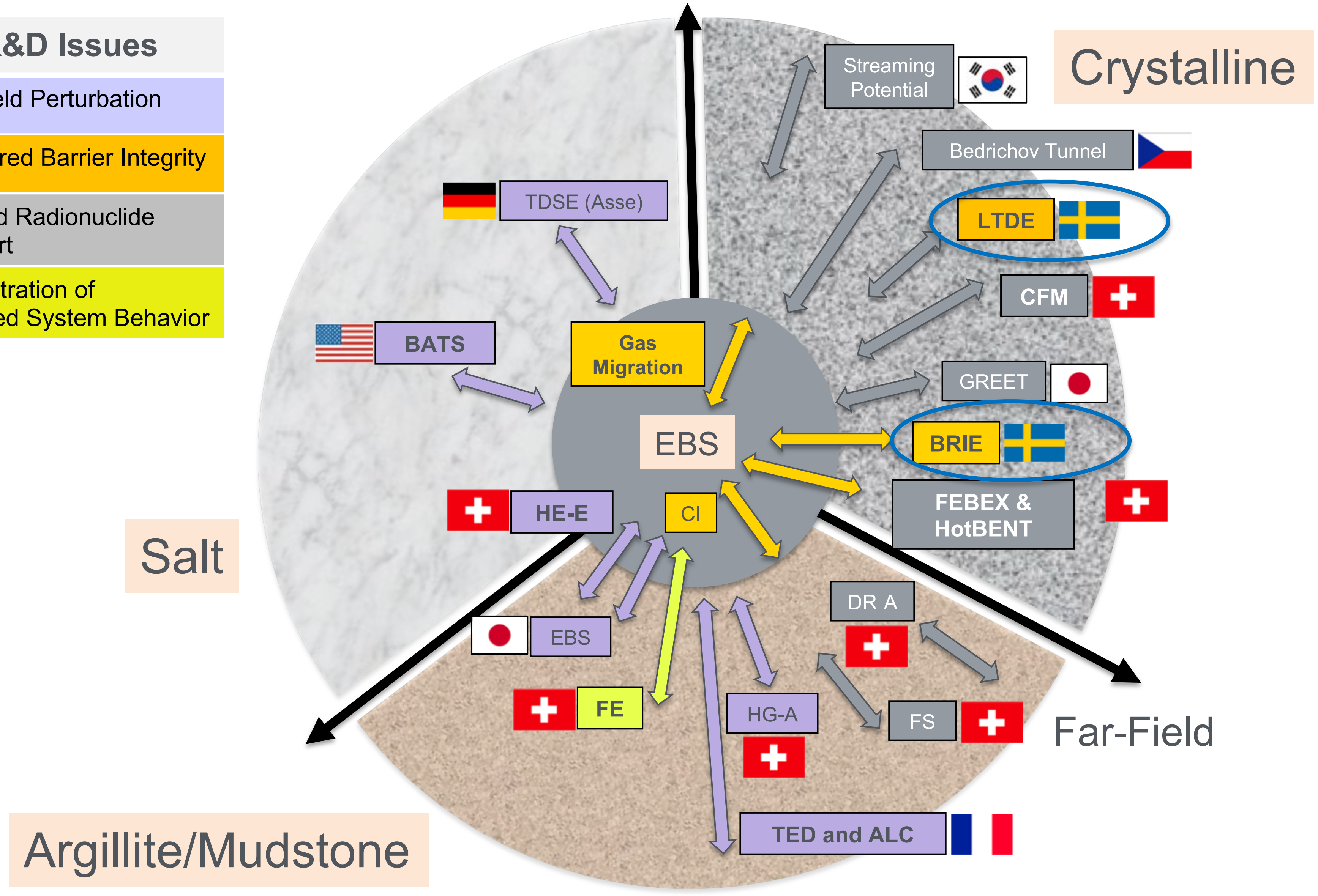
Where BRIE & LTDE Fits in the DOE URL Portfolio

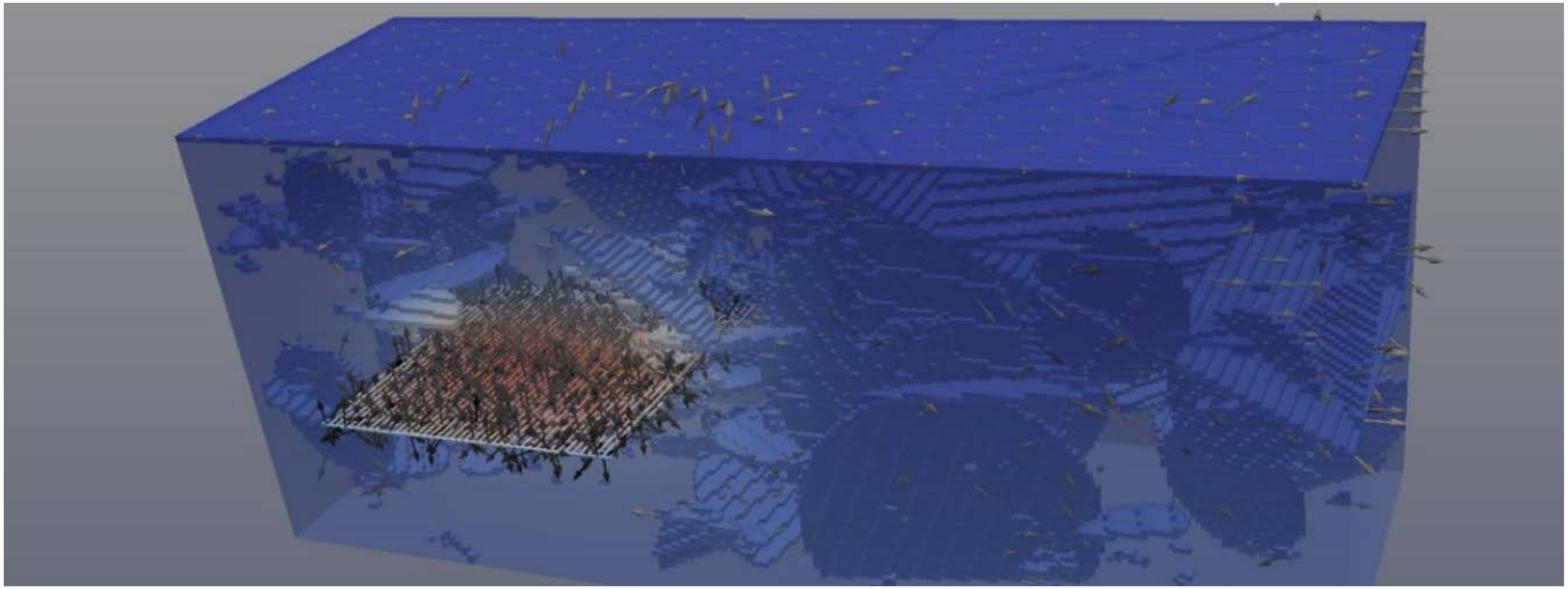
Key R&D Issues

- Near-Field Perturbation
- Engineered Barrier Integrity
- Flow and Radionuclide Transport
- Demonstration of Integrated System Behavior



Importance to Geologic Repository Post-Closure Safety

Generic Geologic Disposal Safety Assessment in Crystalline Rock



Fracture networks are one of the primary pathways for radionuclides to transport from the near field to the far field in crystalline rock.

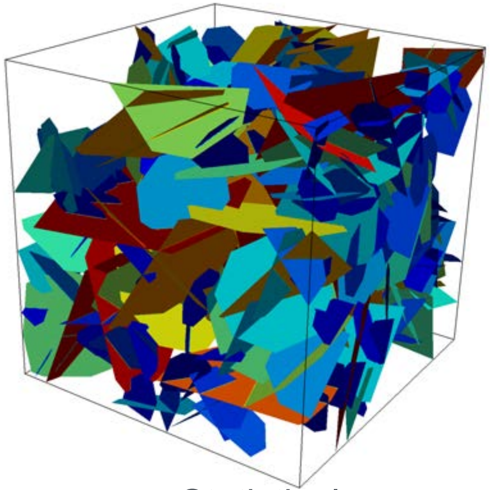
Why is crystalline rock considered for a repository?

a. Reducing conditions lead to low solubility and high retardation of many radionuclides
b. Matrix rock is very low permeability and fractures are often not well connected

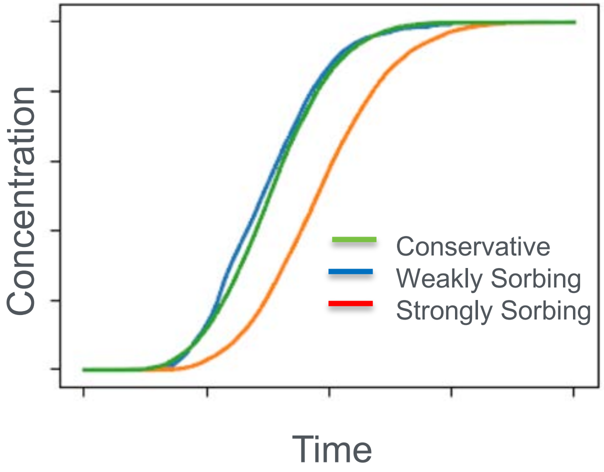
Conceptual Model

Fractured Rock
at Field Site

10 m by 10 m



Statistical
Discrete Fracture
Network Model



Typical Quantity of Interest

How these processes affect repository performance: potential for high permeability pathways to accessible environment

Fracture data needs: fracture orientation, spacing, aperture distributions, matrix diffusion

Transport data needs: same as non fractured systems, fracture roughness, surface area

R&D Context: State of the Art for Flow and Transport in Fractured Rock Systems

- Fractures are the primary flow and transport mechanism in crystalline rocks
- Discrete fracture network models, complex continuum approaches, and pipe flow models have been used to simulate these systems
- These models have evolved to include complex meshing, physics and chemistry for mechanistic representations of flow and transport in fractures

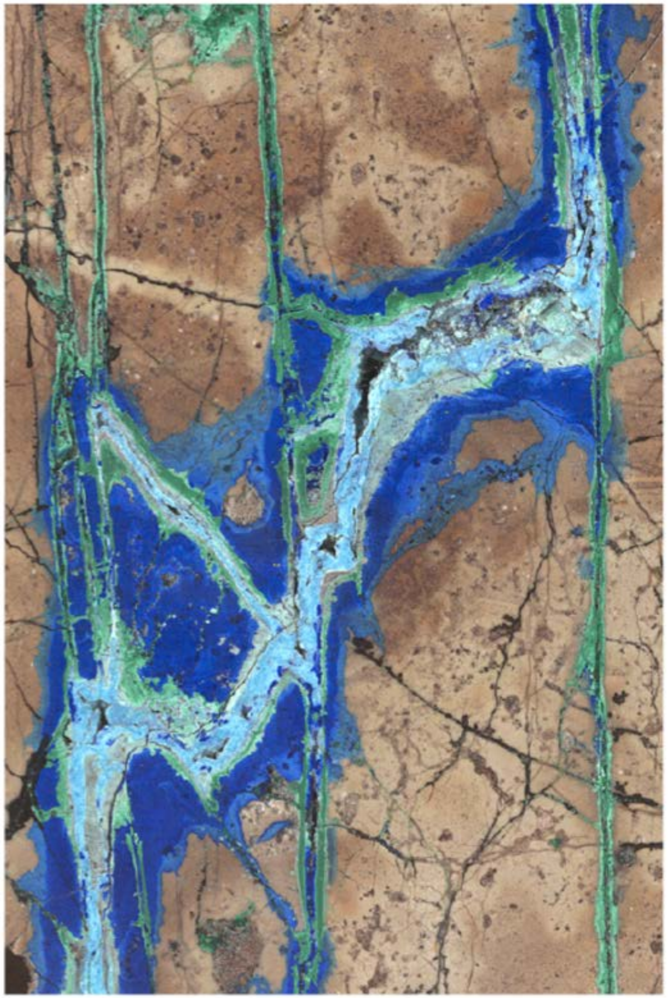


Image Courtesy of Dr. Barb Dutrow

3 cm by 6 cm

R&D Context: Representative Literature on Transport in Fractured Rock Systems

- Complex Continuum
  - Barenblatt et al., 1960
  - Neuman 2005

- Discrete Fracture Networks
  - Dershowitz et al. 1998
  - Dreuzy et al. 2014
  - Hyman et al. 2015*

- Graph-based Machine Learning Reduced Order models
  - Viswanathan et al. 2018*
  - Srinivasan et al. 2018*

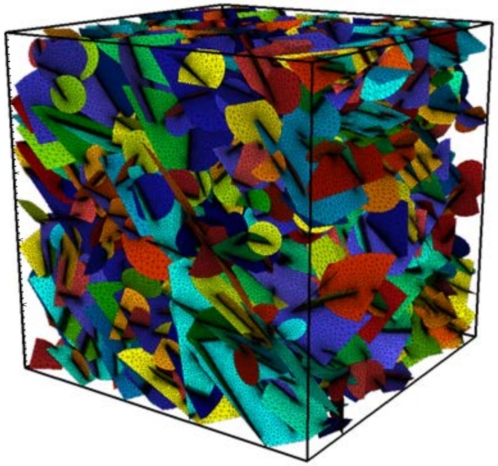
Photo by Lee Lau

*** Our teams publications**

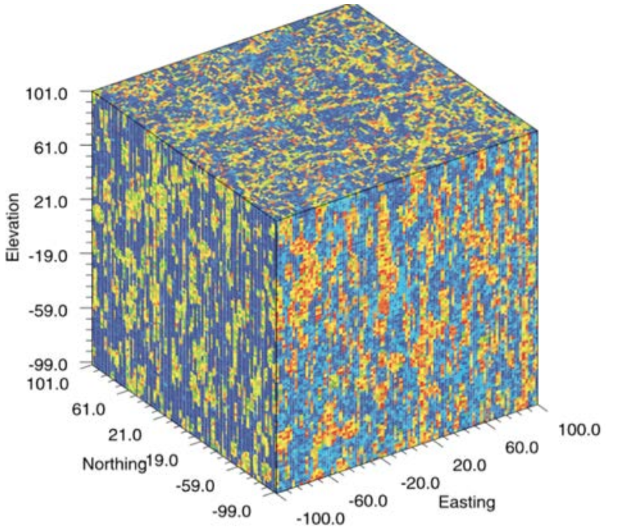
R&D Context: Outstanding Questions for Transport in Fractured Rock Systems

- Discrete fracture networks can explicitly account for topology of the fracture network but topology in the field is typically only known statistically so is this complexity warranted?
- Continuum models ”smooth” out the structure but for large scale problems are they sufficient?
- Are reduced order models (e.g. graph-based machine learning emulators) sufficient and necessary for uncertainty quantification?

Field tests are key for validation and International work has been critical



LANL Discrete Fracture Network



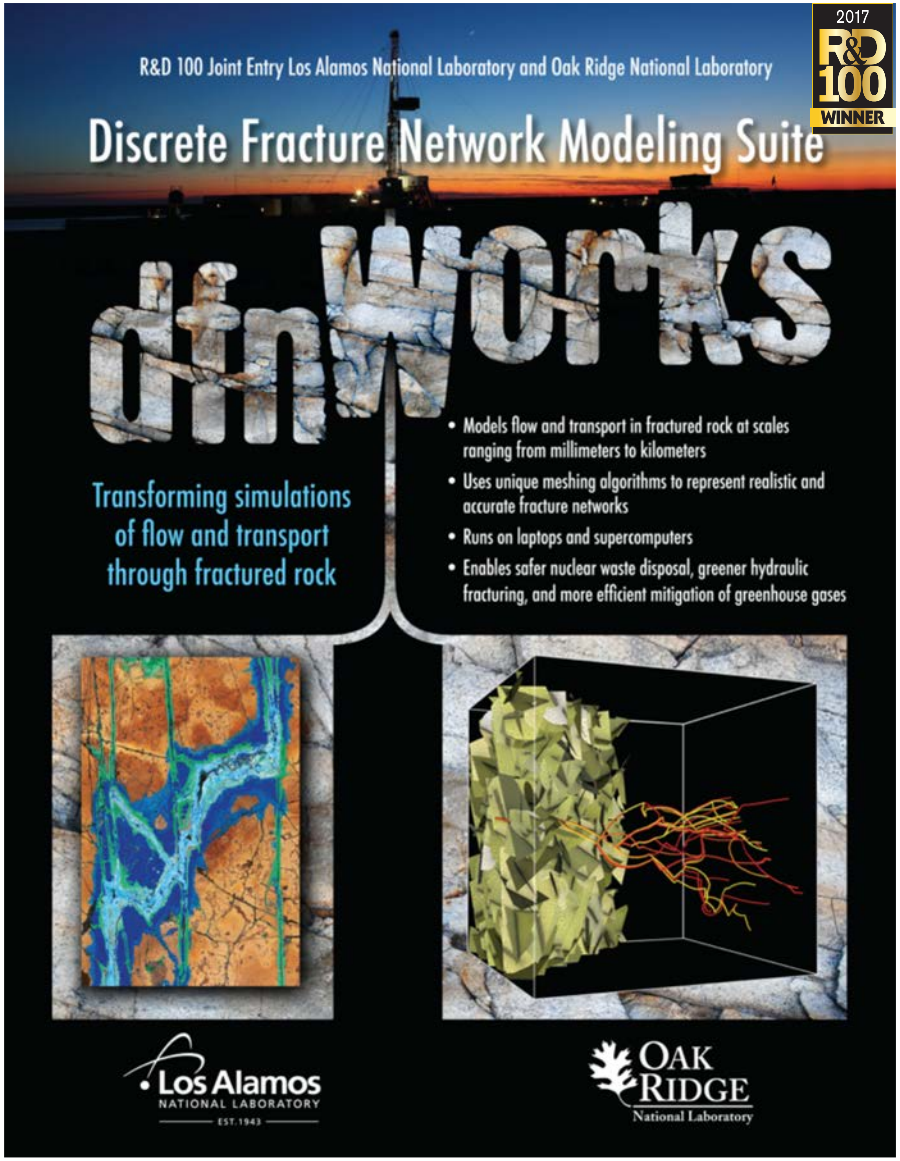
SNL Fractured Continuum Model

R&D Context: R&D gap and needs for Flow and Transport in Fractured Rock Systems

- During last decade observations at field sites improved providing rock and fracture network characteristics.
- This created a need for an advanced modeling tool for numerical representation of fracture networks, followed by accurate flow & transport simulations.
- SKB Laboratory, Sweden, provided fracture network characteristics data needed to validate numerical simulations of flow and transport through fracture networks.
- Development started in 2013 under UFD and R&D100 winner in 2017

JD Hyman, S Karra, N Makedonska, CW Gable, SL Painter, HS Viswanathan, dfnWorks: A discrete fracture network framework for modeling subsurface flow and transport, Computers & Geosciences 84, 10-19, 2015.

dfnWorks.lanl.gov



2017 R&D 100 WINNER

R&D 100 Joint Entry Los Alamos National Laboratory and Oak Ridge National Laboratory

Discrete Fracture Network Modeling Suite

dfnWorks

Transforming simulations of flow and transport through fractured rock

- Models flow and transport in fractured rock at scales ranging from millimeters to kilometers
- Uses unique meshing algorithms to represent realistic and accurate fracture networks
- Runs on laptops and supercomputers
- Enables safer nuclear waste disposal, greener hydraulic fracturing, and more efficient mitigation of greenhouse gases

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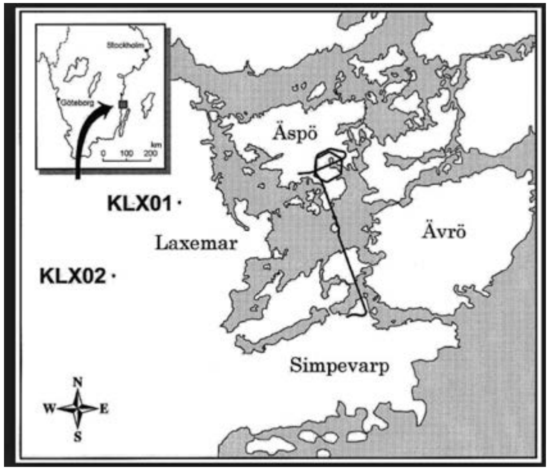
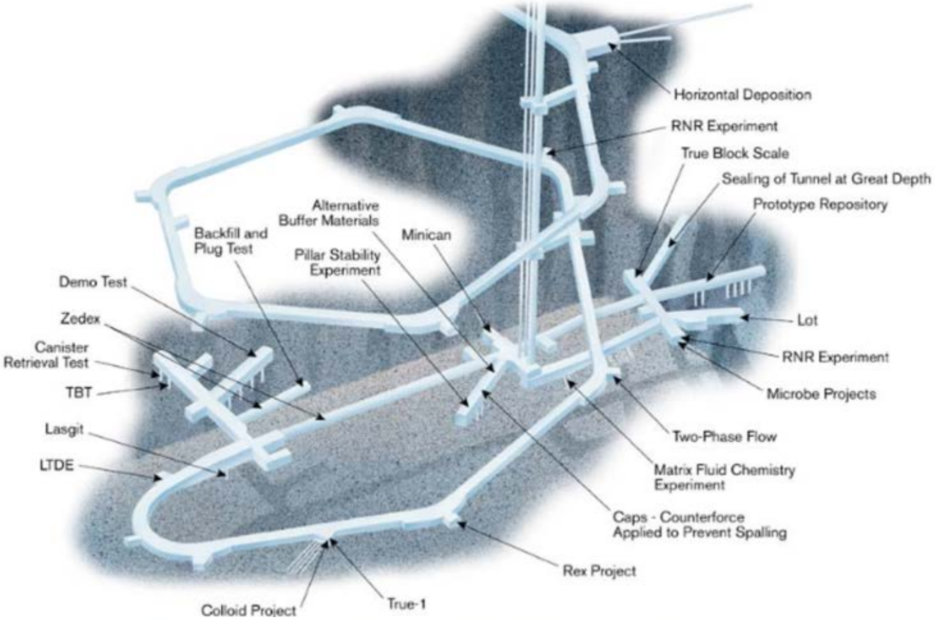
Field Tests: ASPO Hard Rock Laboratory, Sweden





Field Tests: Bentonite Rock Interaction Experiment (BRIE)

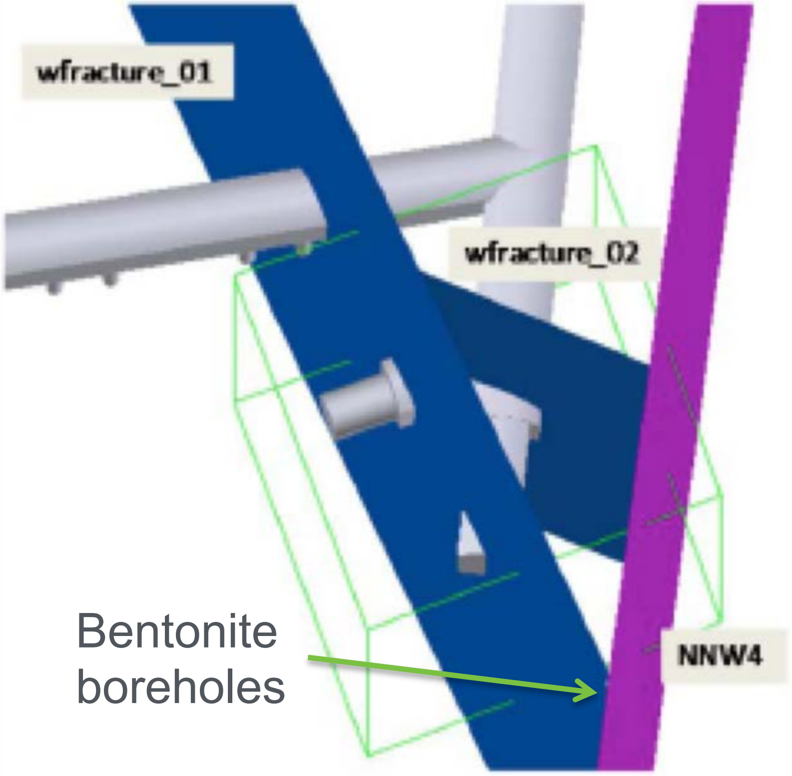
How water flows from surrounding fracture network into bentonite-filled boreholes?

Discrete Fracture Network is used to represent the fractures around borehole *(2D triangular mesh)*

3D volume mesh at the cylinder represents the borehole

DOE shaped a more integrated effort with a move toward uncertainty quantification

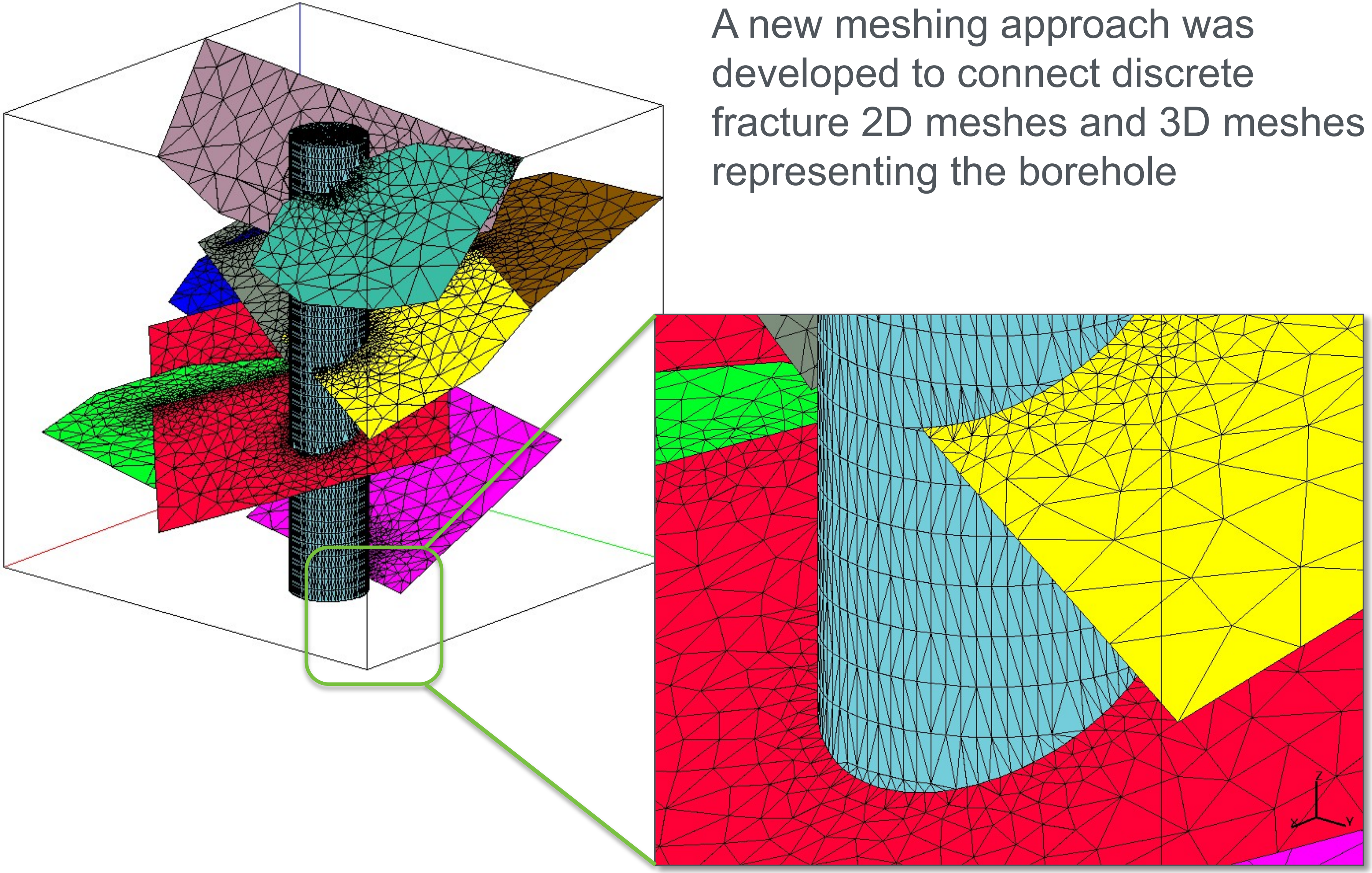
tunnels



Bentonite boreholes

Modeling domain

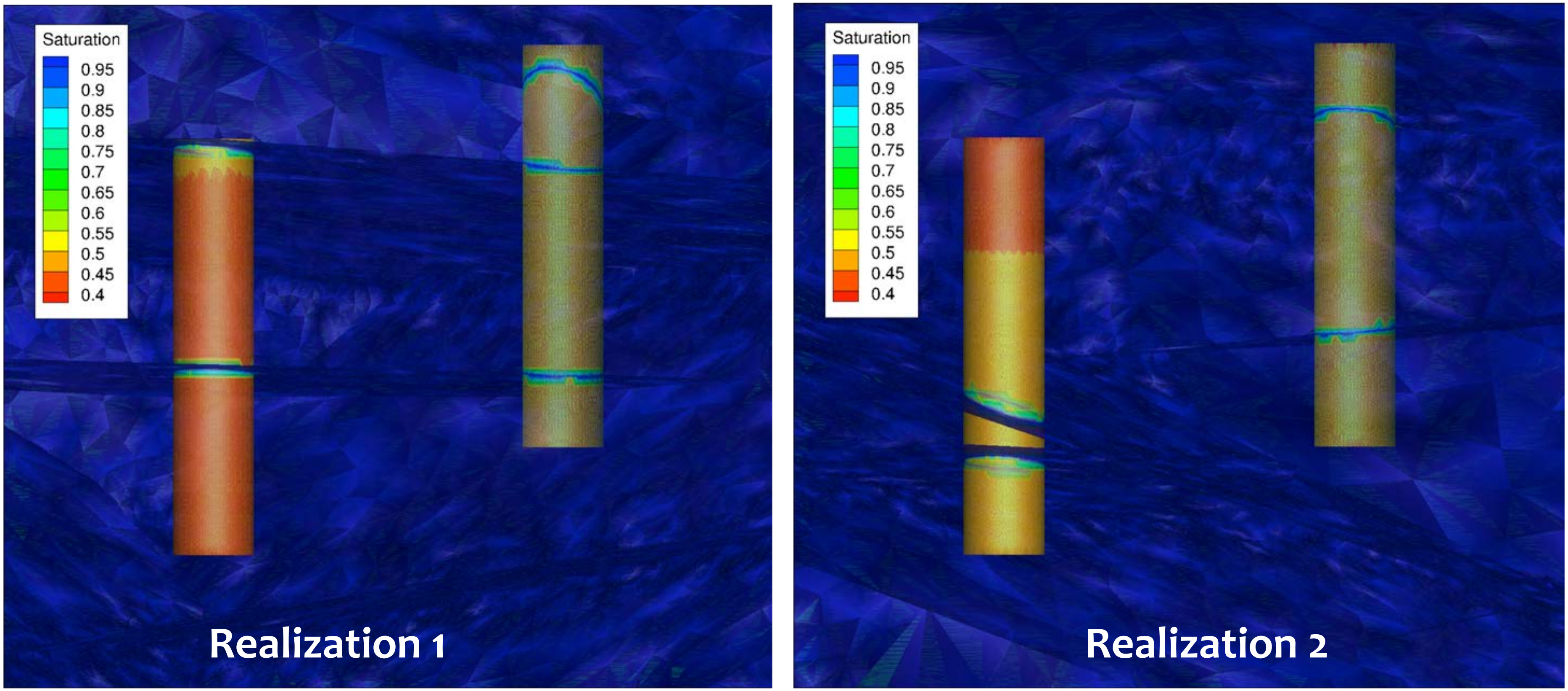
Field Tests: Bentonite Rock Interaction Experiment (BRIE)



A new meshing approach was developed to connect discrete fracture 2D meshes and 3D meshes representing the borehole

Field Tests: Bentonite Rock Interaction Experiment (BRIE)

Two phases (air and water) solution 3 months



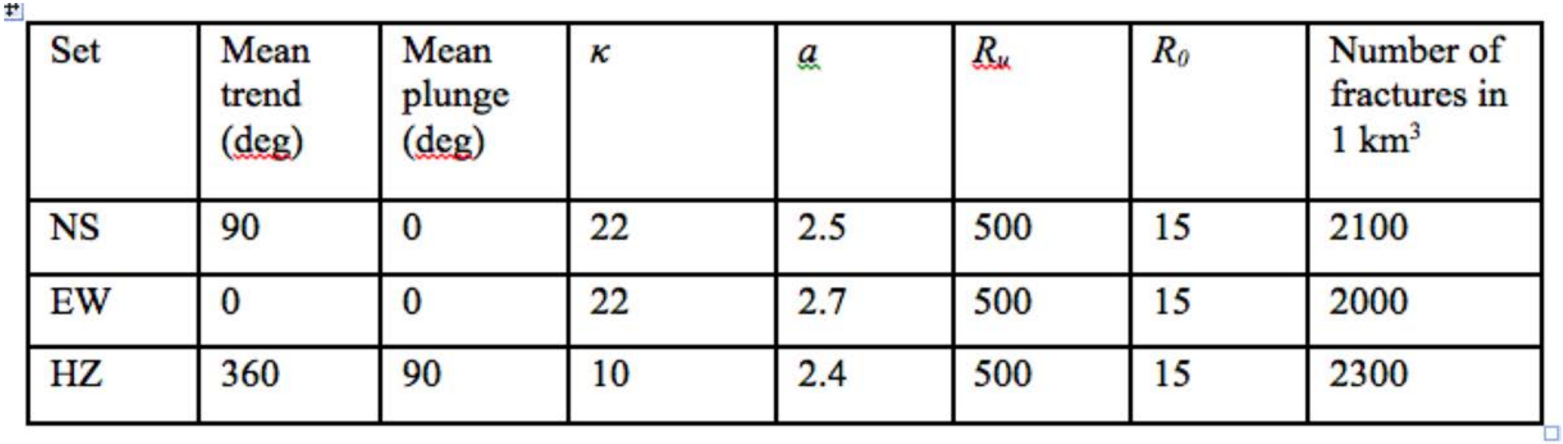
- Steep gradient in liquid saturation in the bentonite near where it intersects with fractures as observed in the field
- Bentonite rewets uniformly

First dfnWorks application to a field site in 2014

Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 1: Generate fracture networks using dfnWorks

- Three fracture sets are generated based on Forsmark site fracture characteristics (Table 6-75 SKB report TR10-52)



Set	Mean trend (deg)	Mean plunge (deg)	κ	a	R_u	R_0	Number of fractures in 1 km^3
NS	90	0	22	2.5	500	15	2100
EW	0	0	22	2.7	500	15	2000
HZ	360	90	10	2.4	500	15	2300

- Fracture transmissivity is defined as function of fracture size

$$\log(\sigma) = \log(\gamma \cdot R^{\omega}) \qquad \gamma=1.6\times10^{-9},\ \omega=0.8.$$

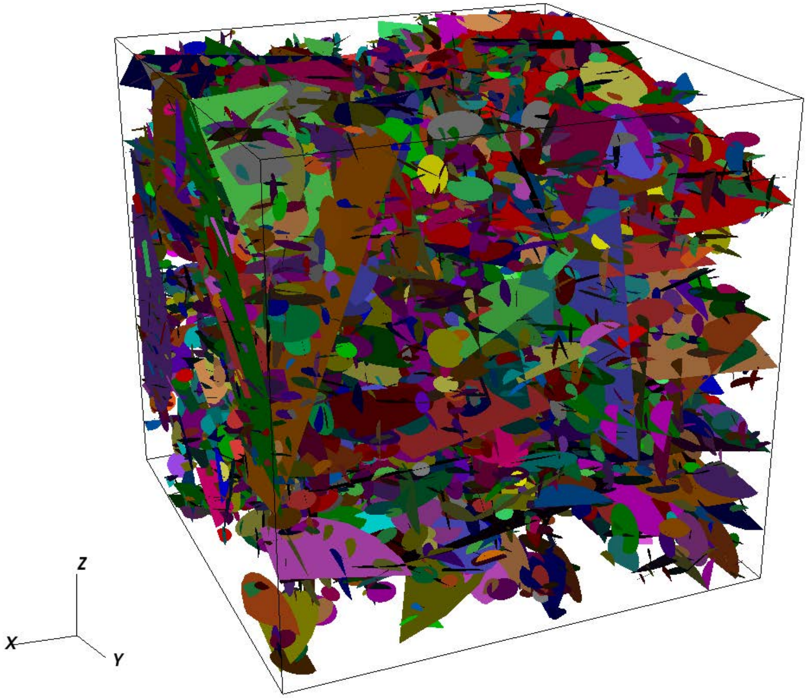
- Fracture aperture is correlated to fracture size and calculated from transmissivity using cubic law

$$\sigma = \frac{b^3}{12}\frac{\rho g}{\mu}$$

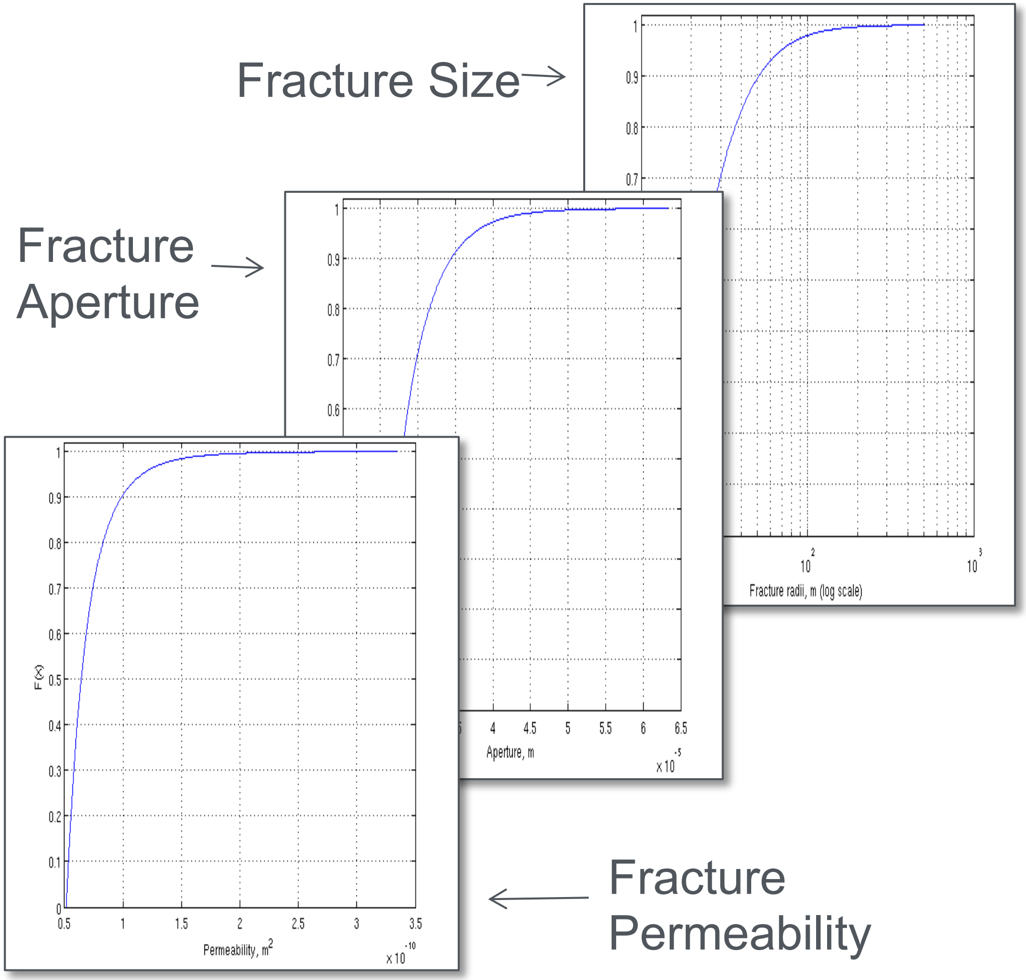
Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 1: Generate fracture networks using dfnWorks

Example of DFN realization



Statistical distributions of fracture network:



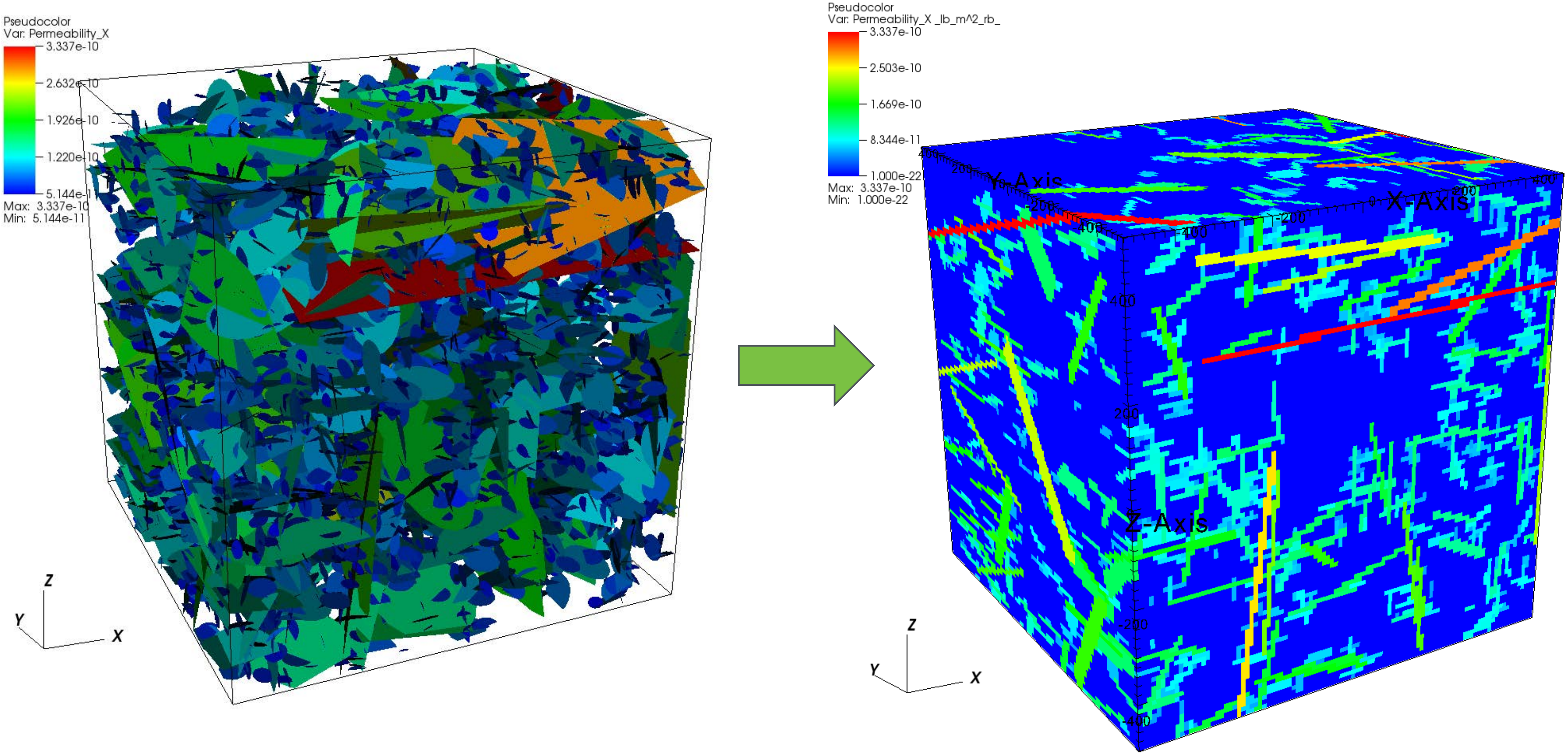
Fracture Size →

Fracture Aperture →

← Fracture Permeability

Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

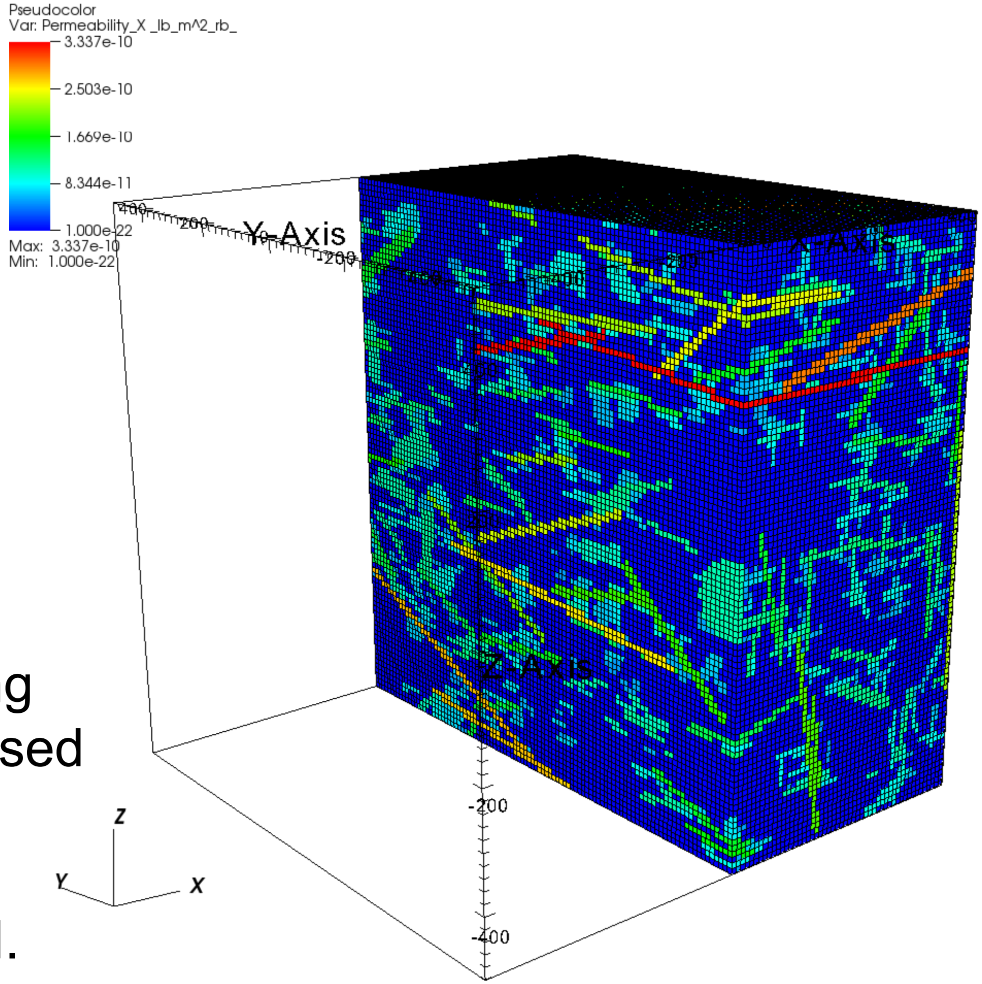
Step 2: Mapping DFN into Continuum



Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 2: Mapping DFN into Continuum

- The fracture network structure of the DFN is mapped into regular voxel mesh.
- Each voxel in the hexahedral mesh has dimensions of 10 m.



- The list of fractures intersecting each voxel is created and passed to FCM team.
- DFN team proceeds with DFN.

Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 3: Compare effective permeability of DFN and FCM

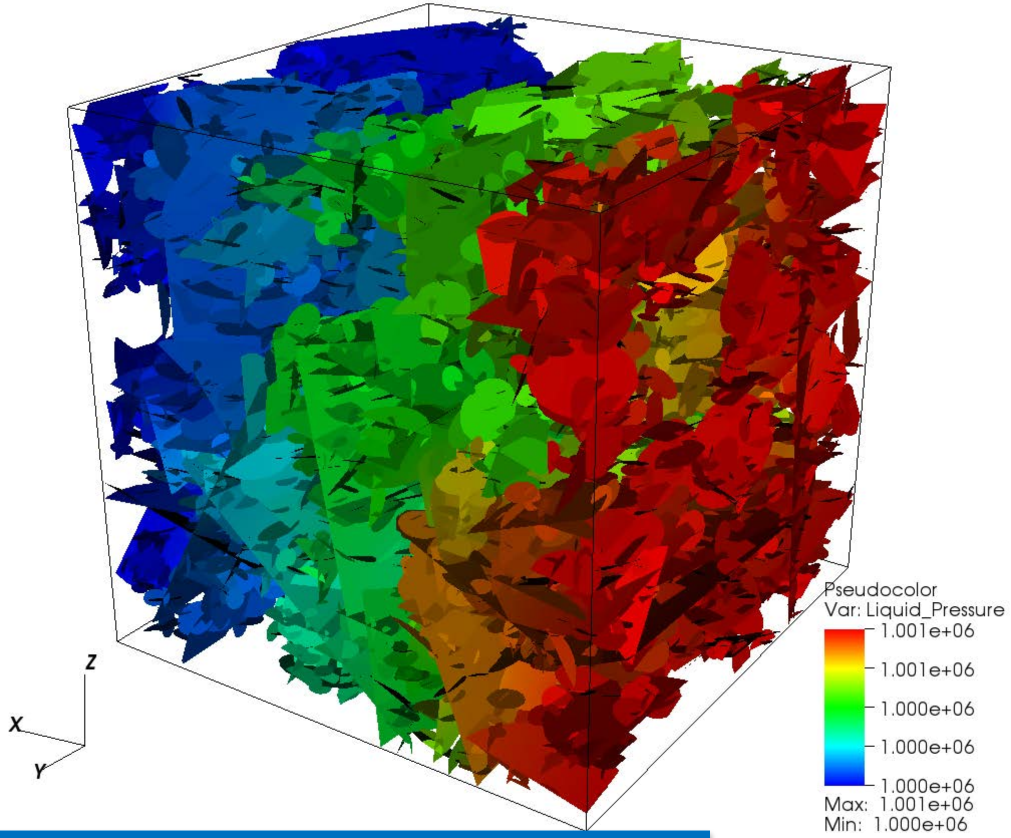
Flow direction:
West-East

Pressure gradient:
10^3 Pa

Compare Effective Permeability of DFNs and FCM:

Effective permeability of 5 realizations is in the range:

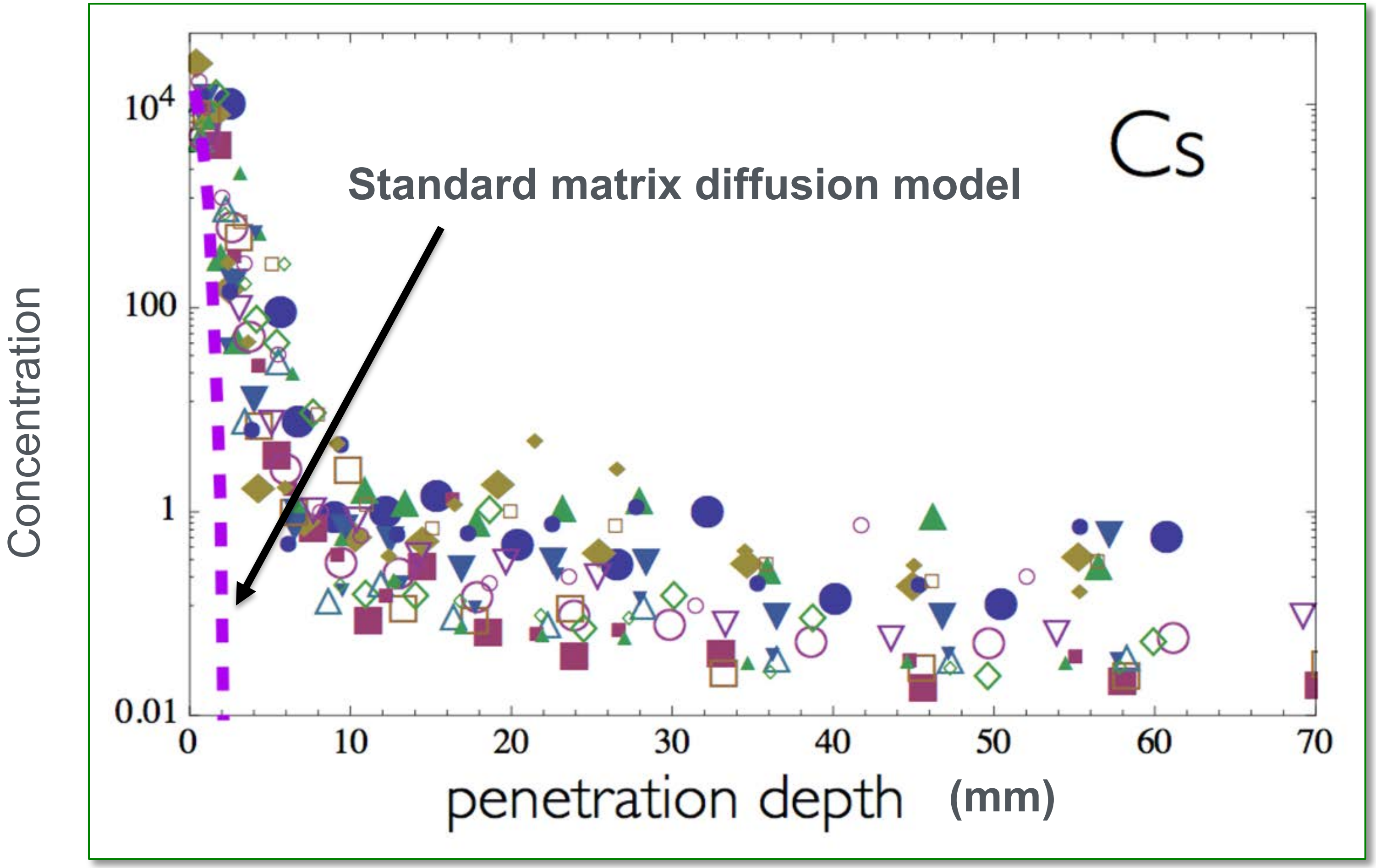
DFN 3.347 e-17 – 4.242 e-17 m^2
FCM 3.68 e-17 – 4.67 e-17 m^2



Both models result in similar effective permeabilities

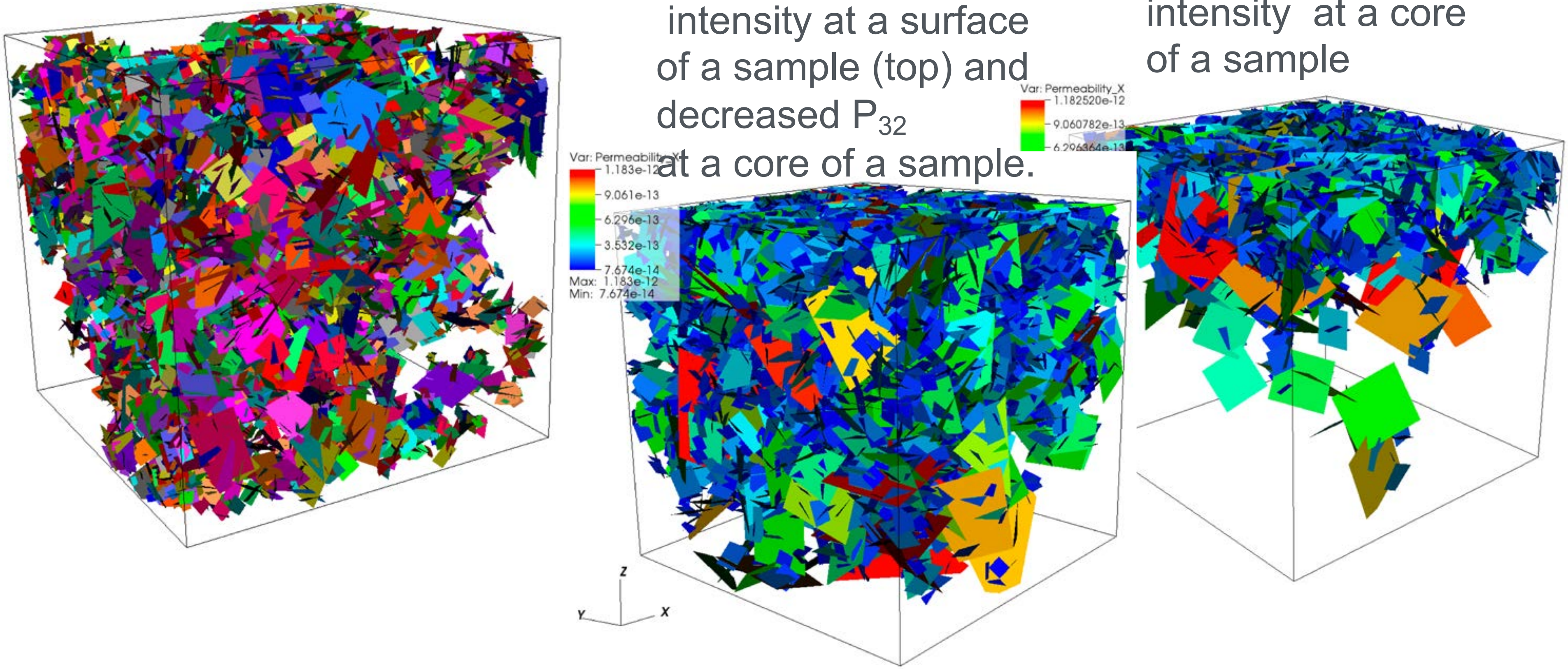
Field Tests: Long Term Diffusion Experiment (LTDE)

Penetration Profile in Long-Term Diffusion Experiment



Enhanced penetration of cesium was measured into the crystalline rock

Field Tests: Long Term Diffusion Experiment (LTDE)



1. DFN of high uniform micro-fracture intensity

2. DFN of high micro-fracture intensity at a surface of a sample (top) and decreased P_{32} at a core of a sample.

3. DFN of significantly low intensity at a core of a sample

Three DFN configurations

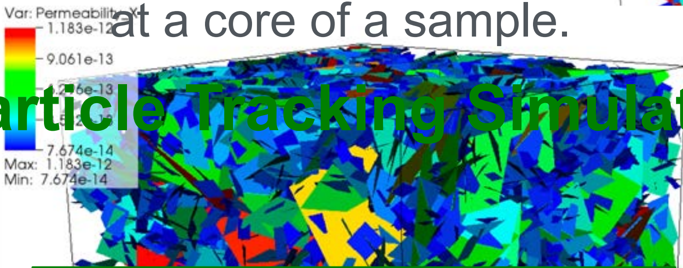
Field Tests: Long Term Diffusion Experiment (LTDE)

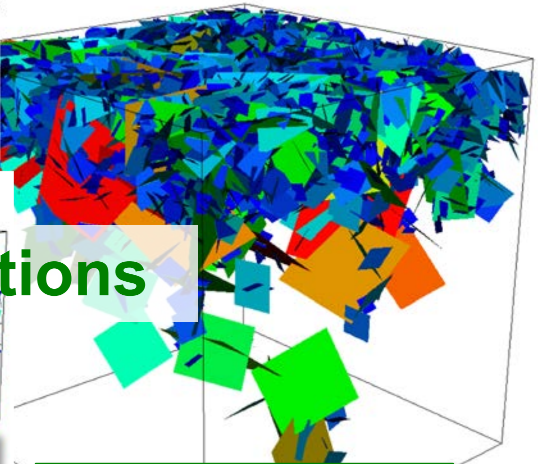
1. DFN of high uniform micro-fracture intensity

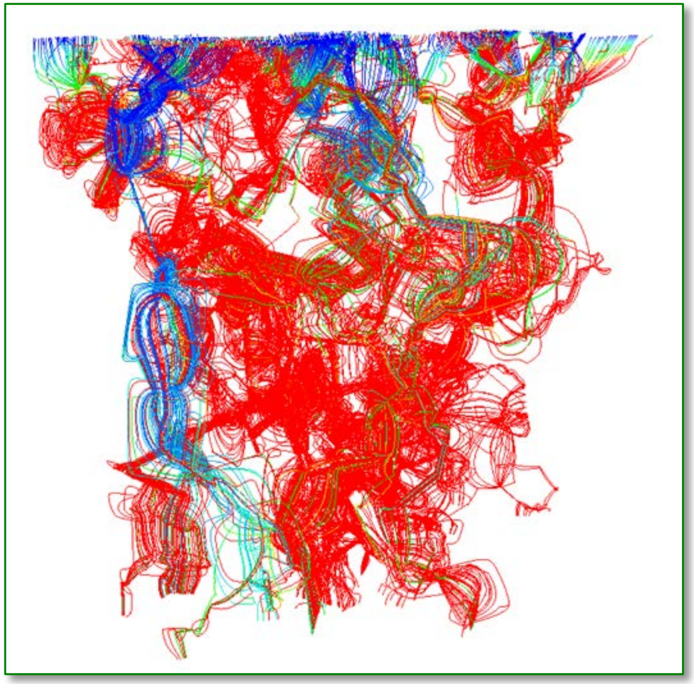
2. DFN of high micro-fracture intensity at a surface of a sample (top) and decreased P_{32} at a core of a sample.

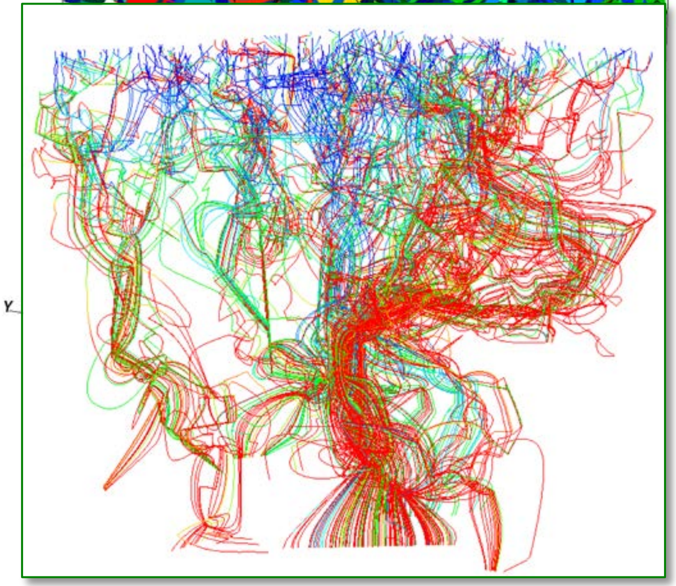
3. DFN of significantly low intensity at a core of a sample

Perform Particle Tracking Simulations



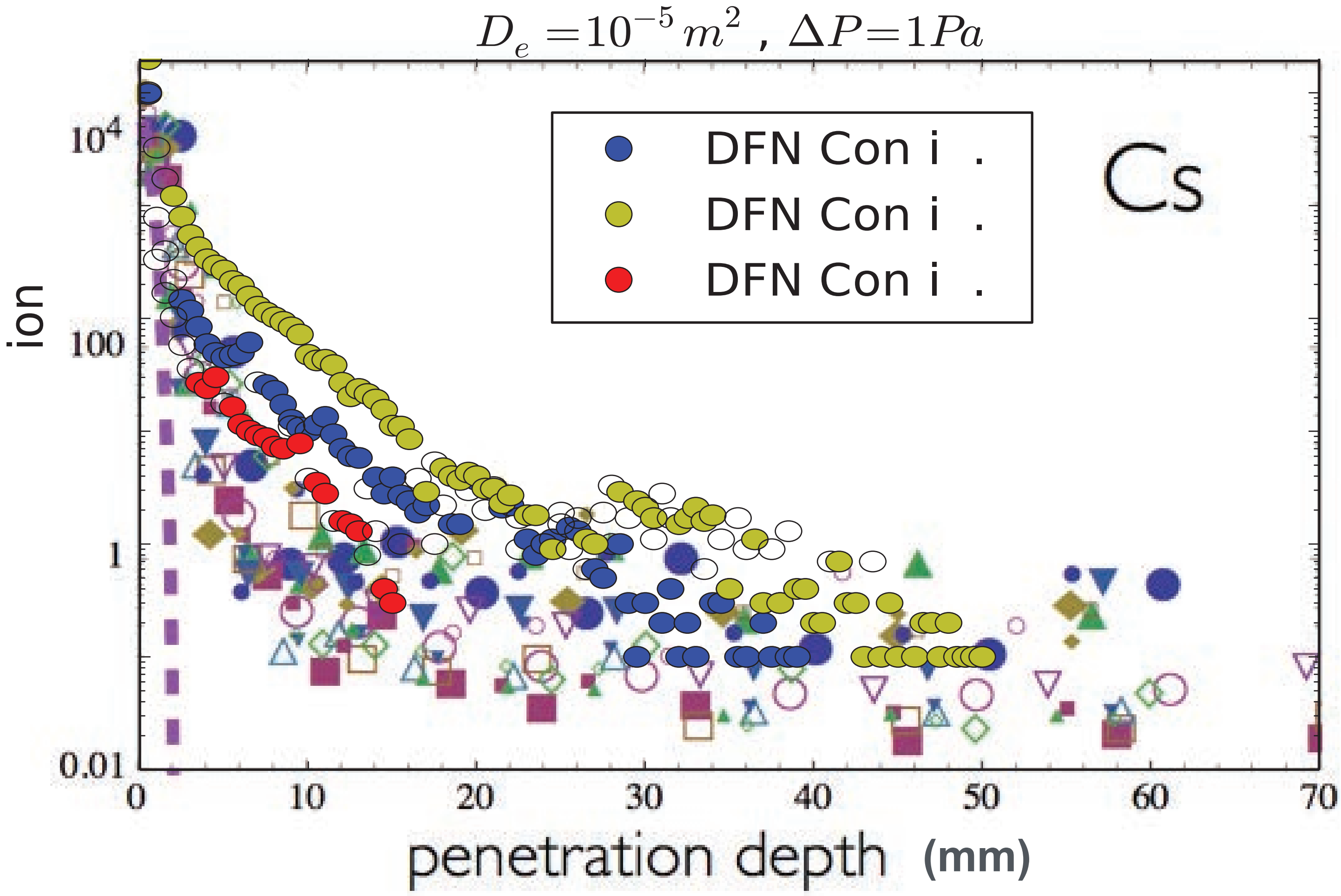






The team has published more than 60 manuscripts (42 cited in Section 7) in the area of fracture formation and fluid flow in fractures systems.

Field Tests: Long Term Diffusion Experiment (LTDE)

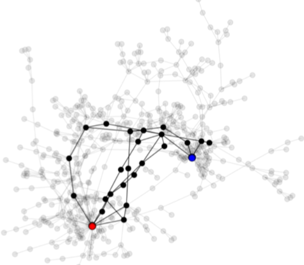


Microstructure can explain increased Rn penetration

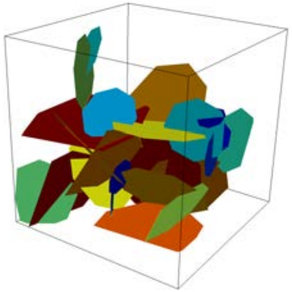
Incorporation into GDSA and the Safety Case

Fractured Rock
at Field Site

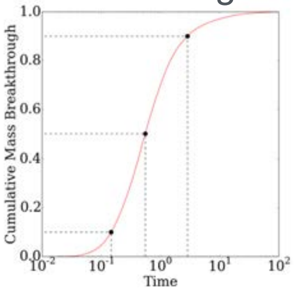
Pruned Graph



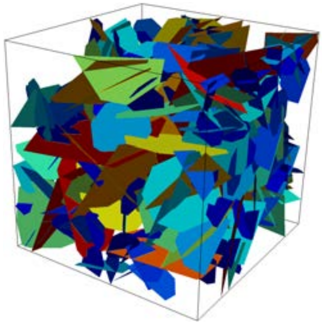
Pruned DFN



QOI -
Breakthrough

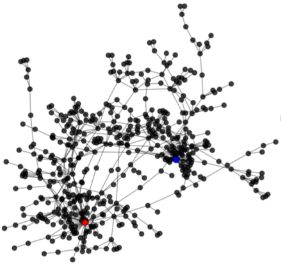


ML / Physics
Informed Pruning

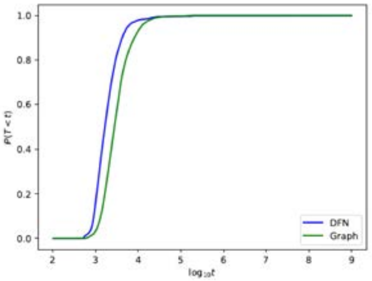


High Fidelity
DFN

Physics
on Graph

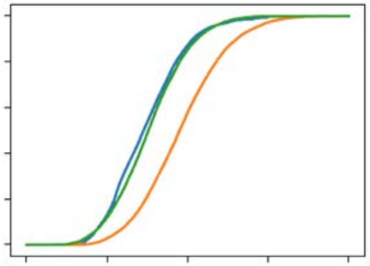


Graph
Representation



QOI -
Breakthrough

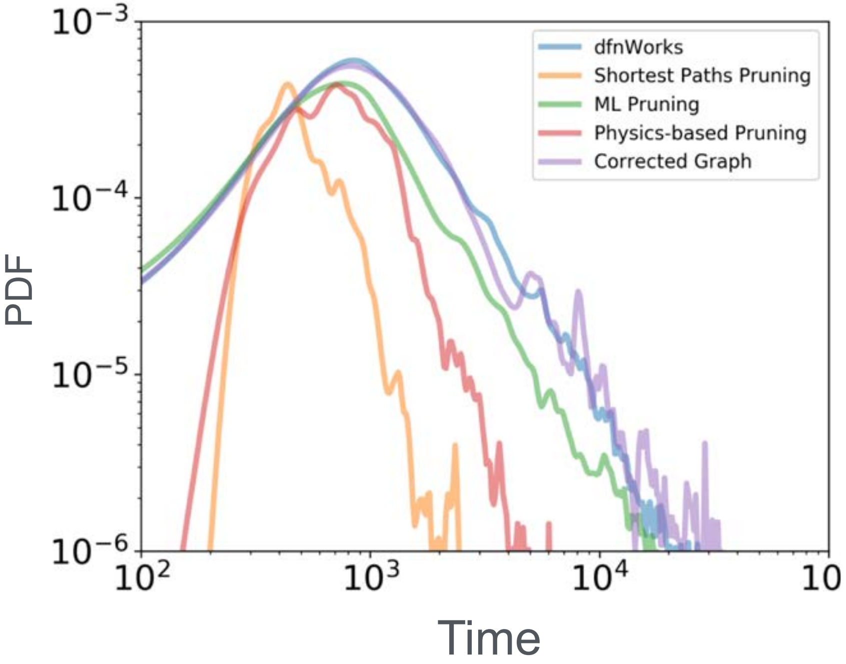
UQ / Bias
Correction



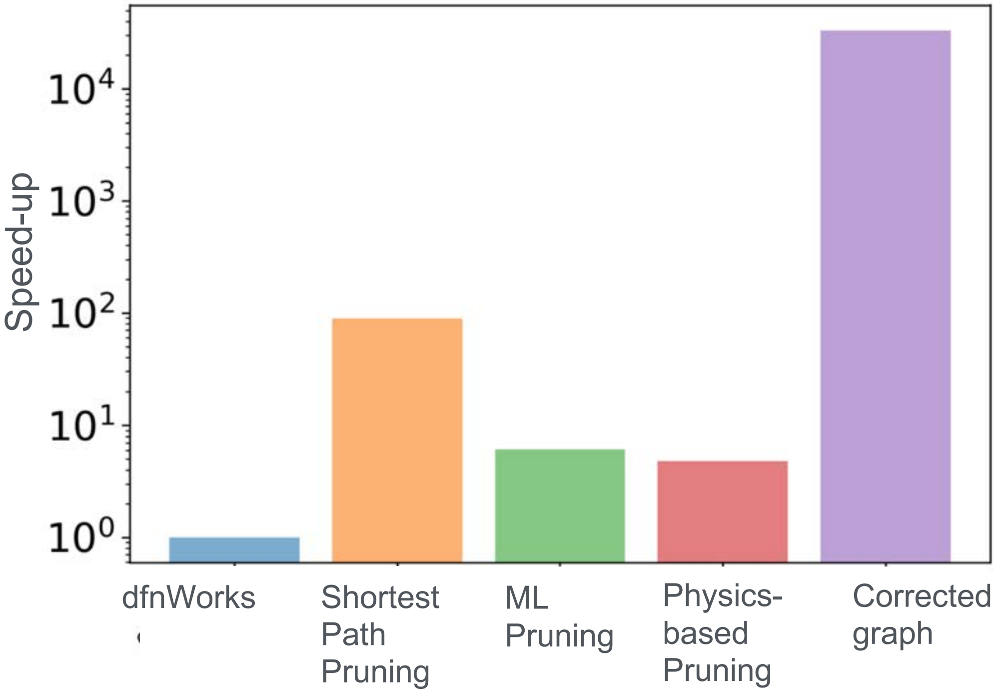
Corrected
Breakthrough

Reduced order models of fracture flow and transport using machine learning

Incorporation into GDSA and the Safety Case



QOI: Breakthrough Curves



Computational Performance

We can tailor the reduced order model depending on the QOI:

- » Quick shortest path calculation if only early arrival is needed
- » ML or physics-based pruning is effective but still requires mapping back to DFN(10X-100X speedup)
- » Transport on the graph is 4 orders of magnitude faster but accurate for more complex cases?

Incorporation into GDSA and the Safety Case

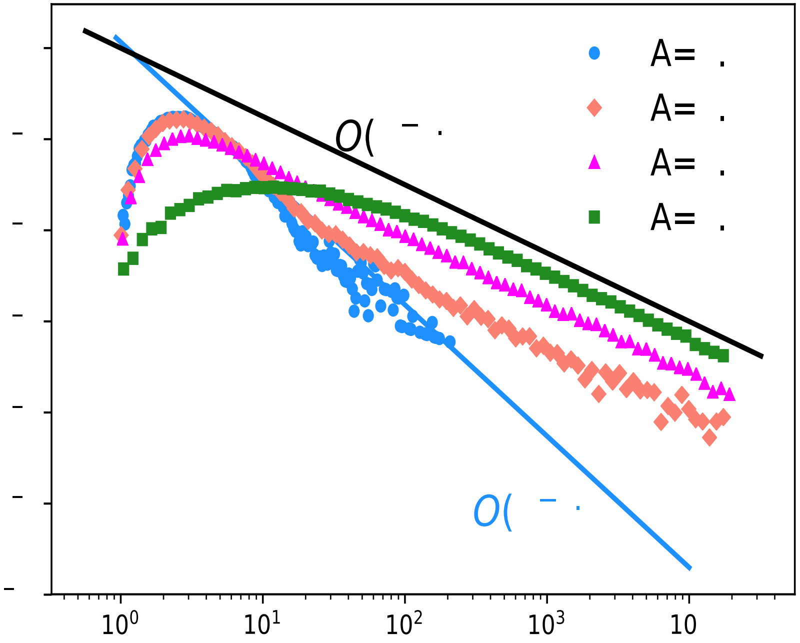
- Time Domain Random Walk
- Interaction with the rock matrix surrounding the network is currently not considered in dfnWorks

- We've including matrix diffusion into dfnWorks simulations using a Lagrangian approach

- Can also be included into graph transport using the same approach

- Verification of matrix diffusion -> recover classic -3/2 slope

- Will be compared with DFM models



Matrix Diffusion in Fractured Media: New Insights into Power-Law Scaling of Breakthrough Curves, JD Hyman, H Rajaram, S Srinivasan, N Makedonska, S Karra, H Viswanathan, G Srinivasan. In prep for Geophysical Research Letters

Matrix diffusion included in dfnWorks for fracture-matrix interactions

Benefits of Participation

- International program has provided comprehensive field tests for detailed validation of fracture networks models in different types of geologic media
- International collaborations have pushed the need to develop new capabilities (e.g. dfnWorks, fracture continuum model) that utilize high performance computing, multi-physics and multi-scale methods
- International programs have many world leaders in flow and transport in fractured systems
- DOE is an important contributor in areas of physics-based, HPC simulation methods, uncertainty quantification and reduced order models

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External References

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Questions?

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