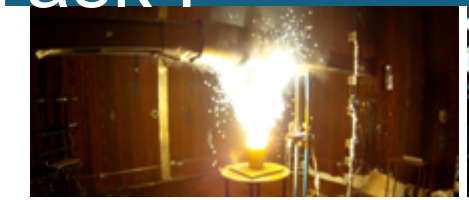
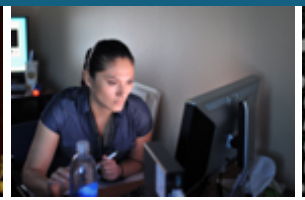
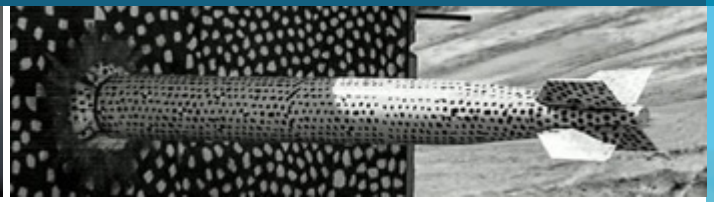
SAND2020-12883PE

# Flow and Transport Modeling in Fractured Crystalline Rock Using PFLOTRAN and dfnWorks: Crystalline Task F







*Rosie Leone and Teresa Portone*

11/19/20

DECOVALEX-2023 November 2020 Virtual Meeting

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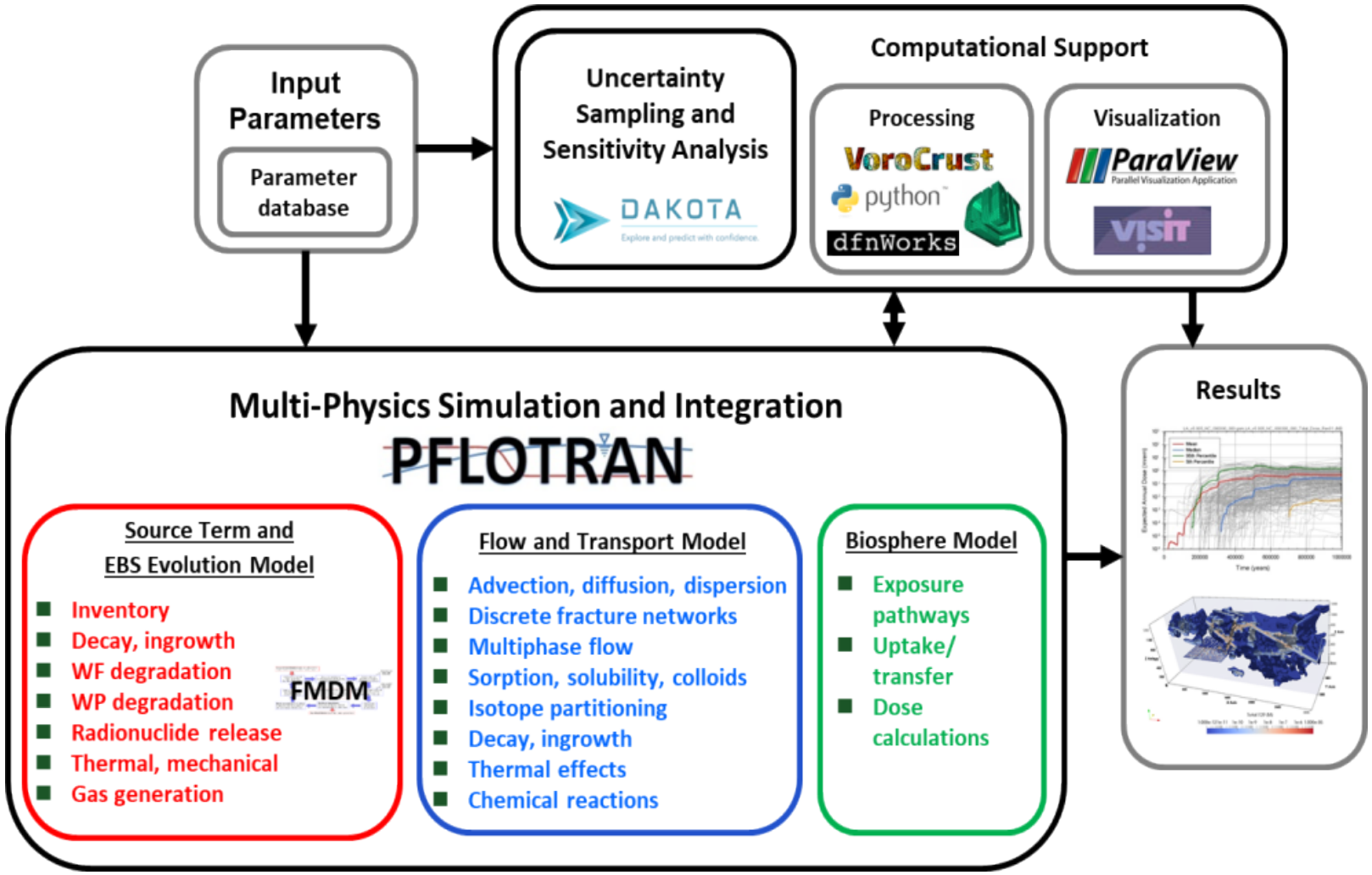
# Geologic Disposal Safety Assessment (GDSA) Framework

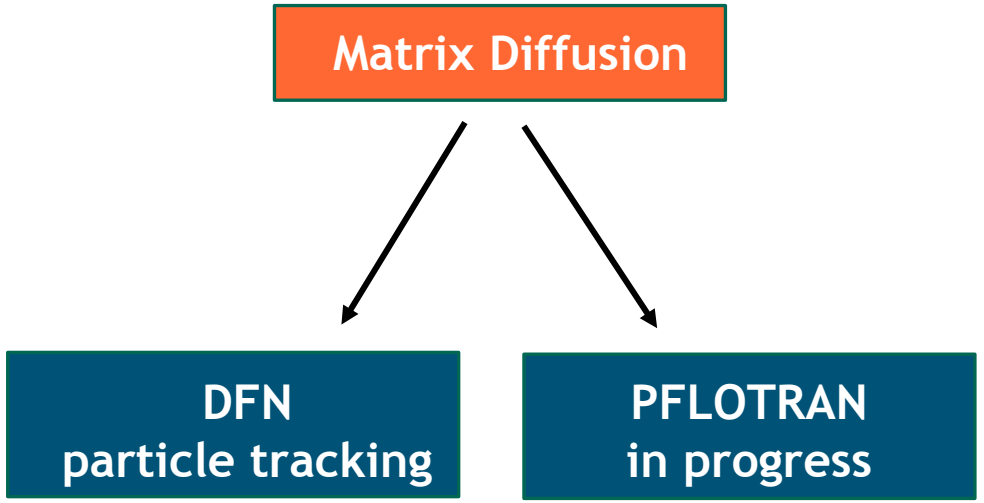



https://pa.sandia.gov

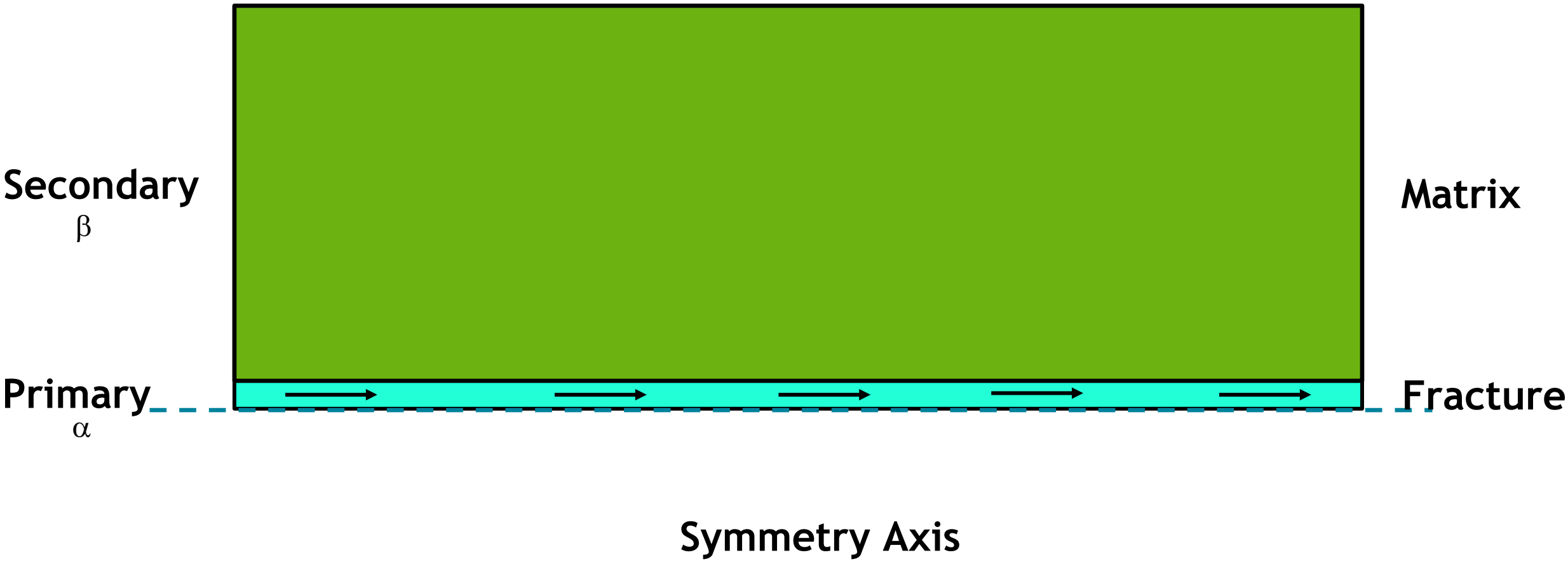
# Flow/transport options considered in crystalline fractured rock

- Fracture transport with matrix diffusion (No advection in matrix)
  - Implementation in PFLOTRAN (in progress) with single fracture
  - dfnWorks particle tracking with four fractures
- Flow and transport
  - Meshing options
  - Transport options
  - Previous crystalline reference case

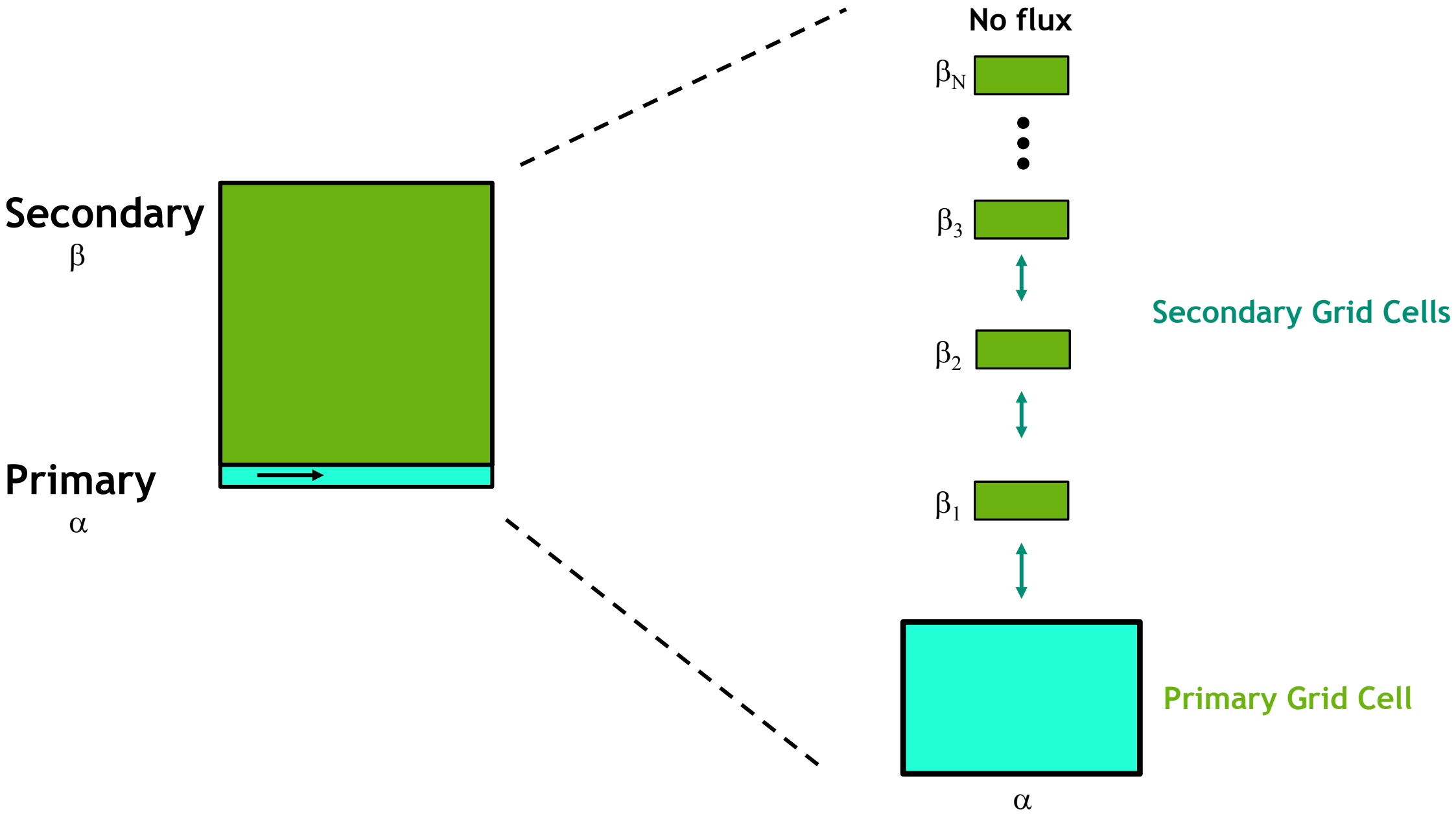
# Matrix Diffusion



# Single Fracture with Matrix Diffusion Benchmark in PFLOTRAN



# Dual Continuum Disconnected Matrix Model (DCDMM)



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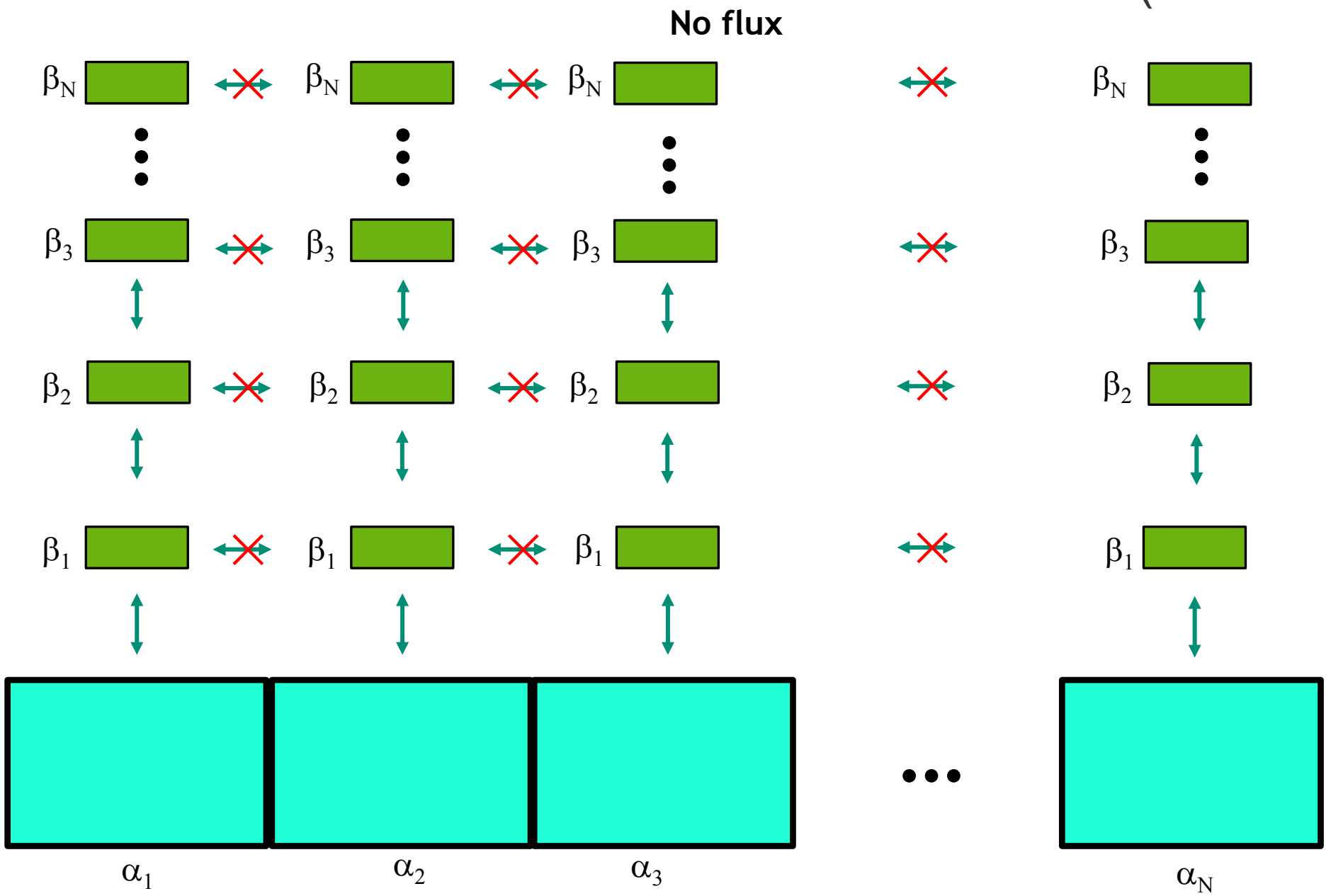
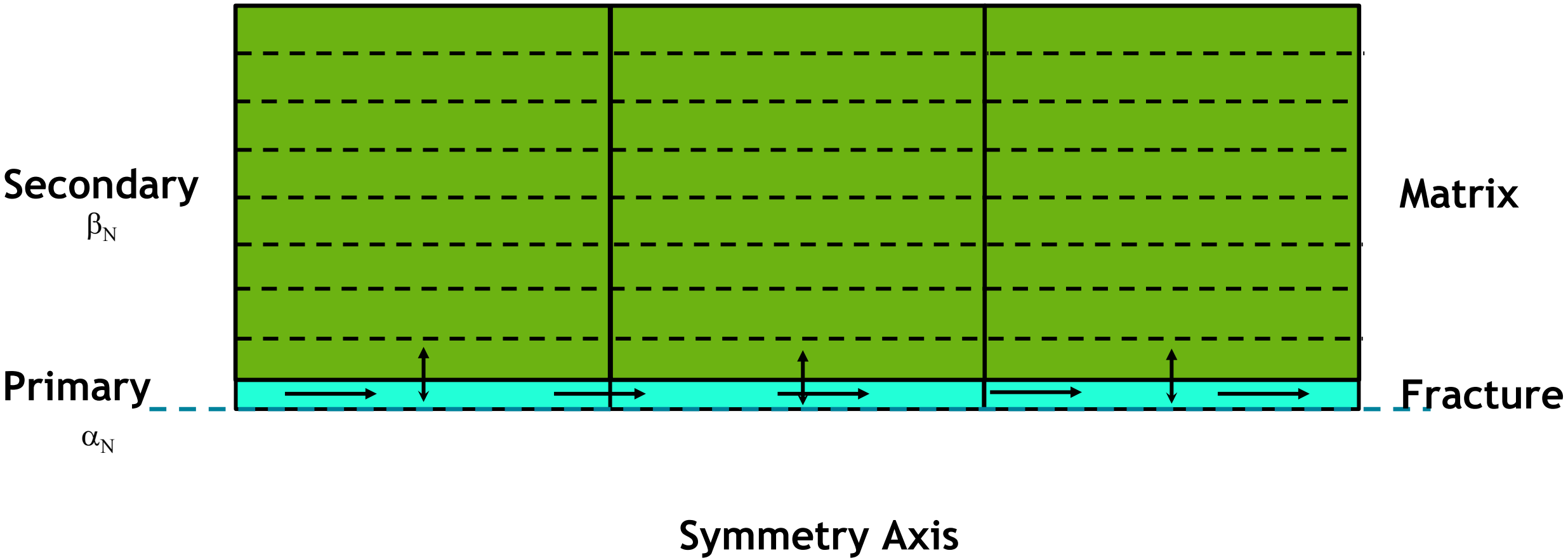


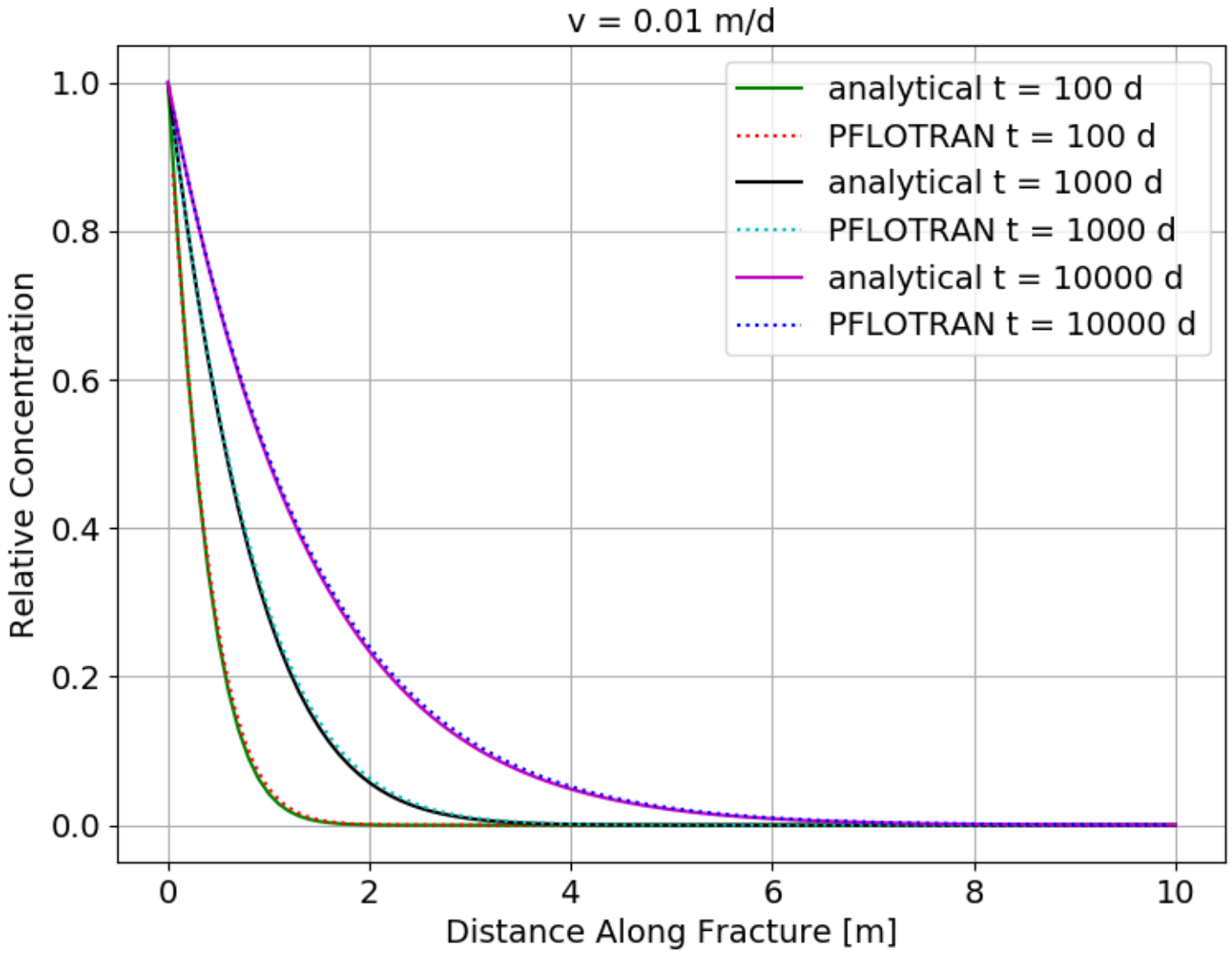
# Single Fracture Benchmark Set Up




Transport in fracture due to advection & dispersion
Transport in matrix due to diffusion only (diffusive flux occurs perpendicular to fracture wall)

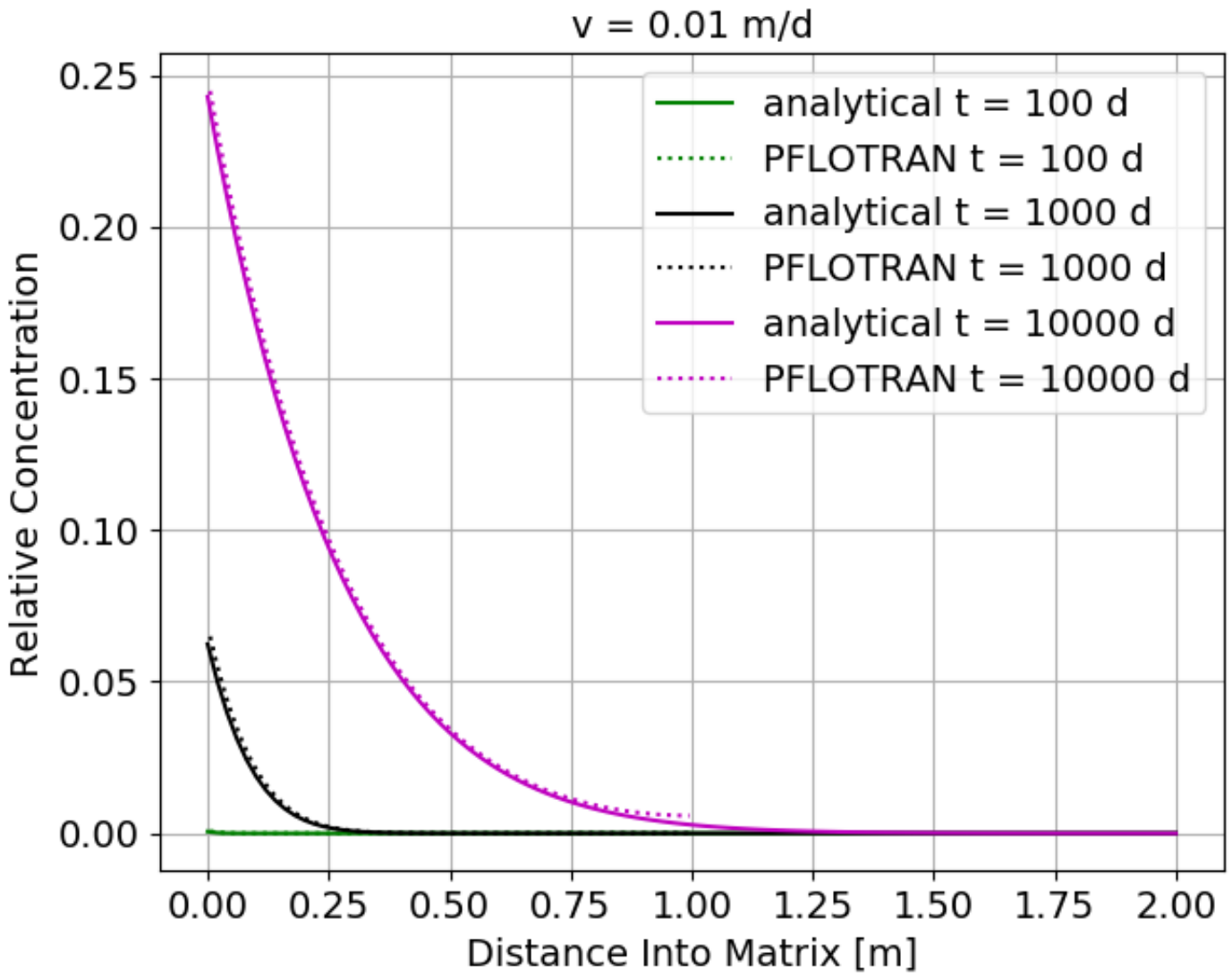
# Single Fracture Benchmark Comparison in Fracture

- 100 primary grid cells
- 100 secondary grid cells per primary cell
- Time step: 0.01 d
- Analytical solution by Tang et al. (1981)
  - Assumes direction of mass flux in porous matrix to be perpendicular to fracture axis



# Single Fracture Benchmark Comparison in Matrix

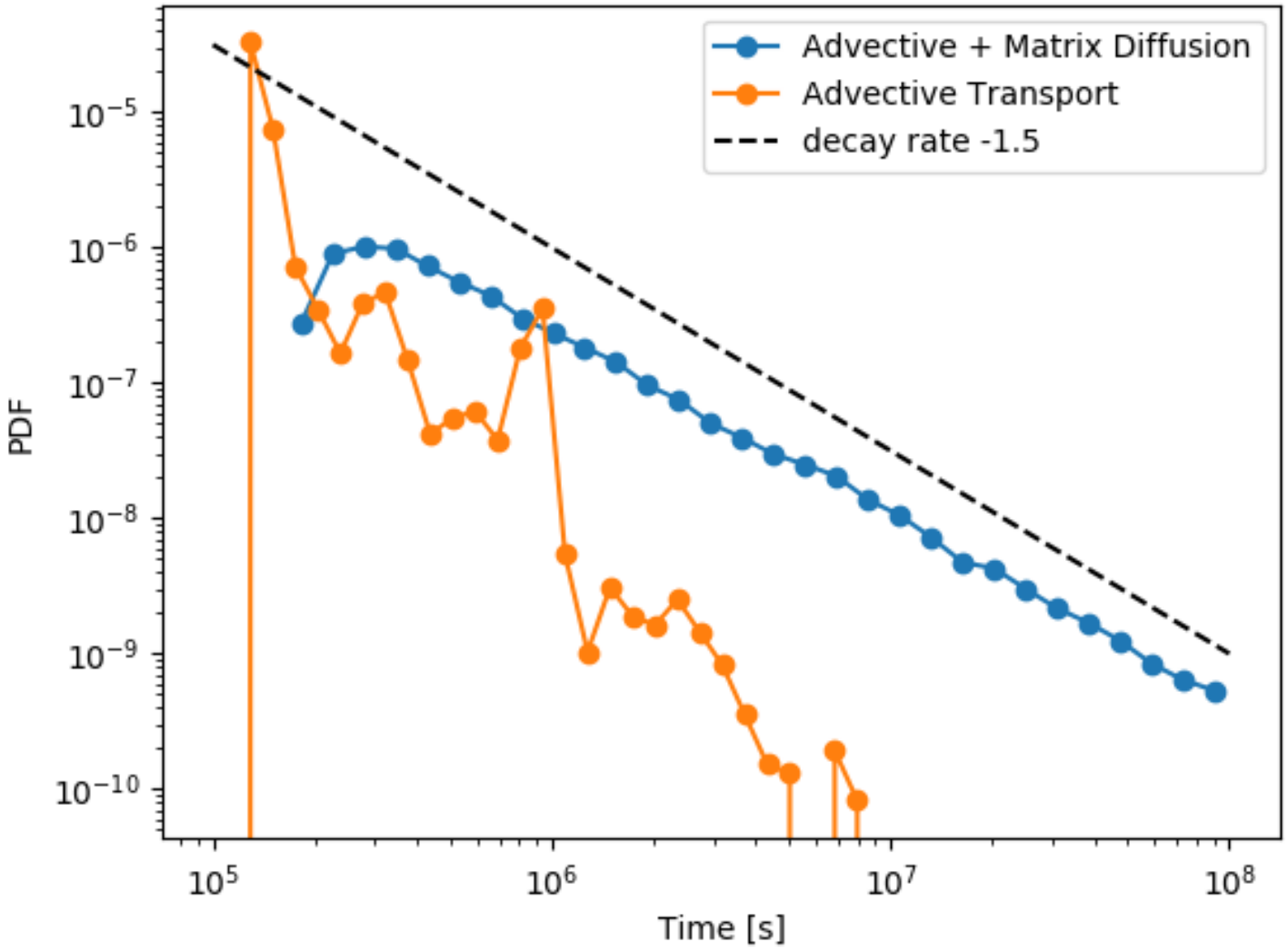
- 100 primary grid cells
- 100 secondary grid cells per primary cell
- Time step: 0.01 d
- Analytical solution by Tang et al. (1981)
  - Assumes direction of mass flux in porous matrix to be perpendicular to fracture axis



# Matrix Diffusion in DFN Particle Tracking

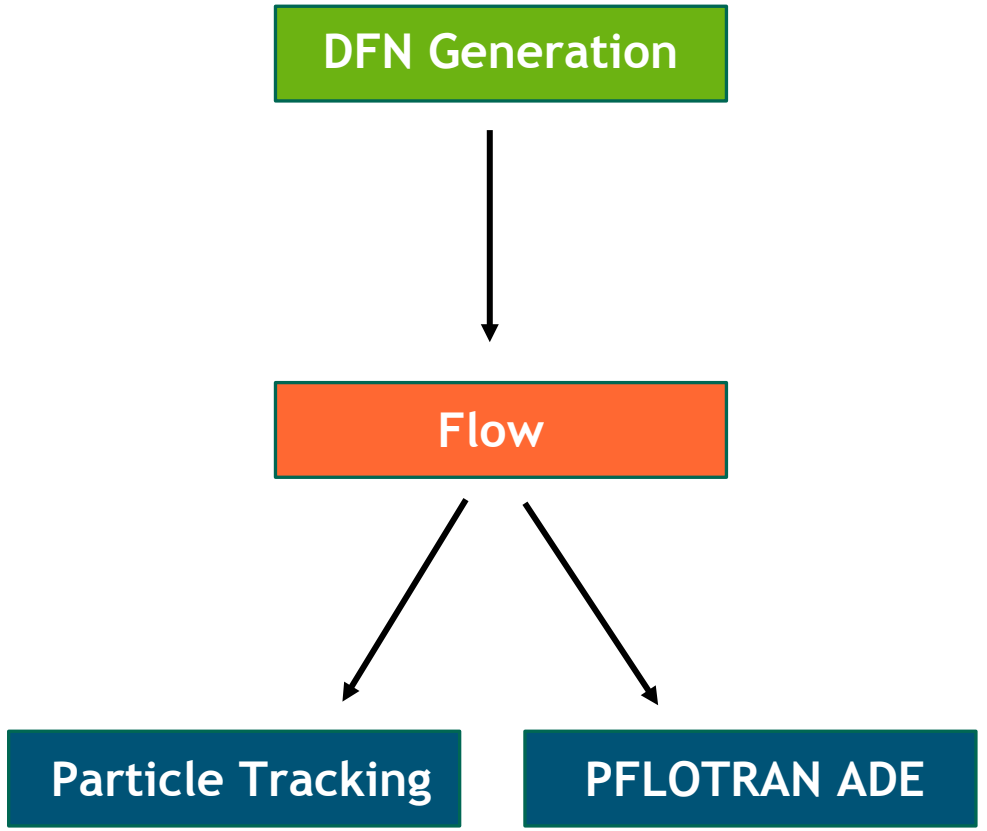
- 4 elliptical fractures
- 1 m cubic domain
- Impulse injection
- 10000 particles
- Matrix Porosity: 0.01
- Diffusion Coefficient: 1 x $10^{-11}$ $m^2/s$
- Inflow Pressure: 1.01 x $10^6$ Pa
- Outflow Pressure: 1 x $10^6$ Pa

Probability Density Function (PDF) of particles exiting domain



# DFN Flow & Transport

- Discrete Fracture Network (DFN) generation
  - dfnWorks
  - Equivalent Continuous Porous Medium (ECPM) or DFN
- Flow simulation
  - PFLOTRAN
- Transport simulation
  - ECPM with PFLOTRAN advection-diffusion equation (ADE)
  - DFN with PFLOTRAN advection-diffusion equation (ADE)
  - Particle Tracking (dfnTrans)

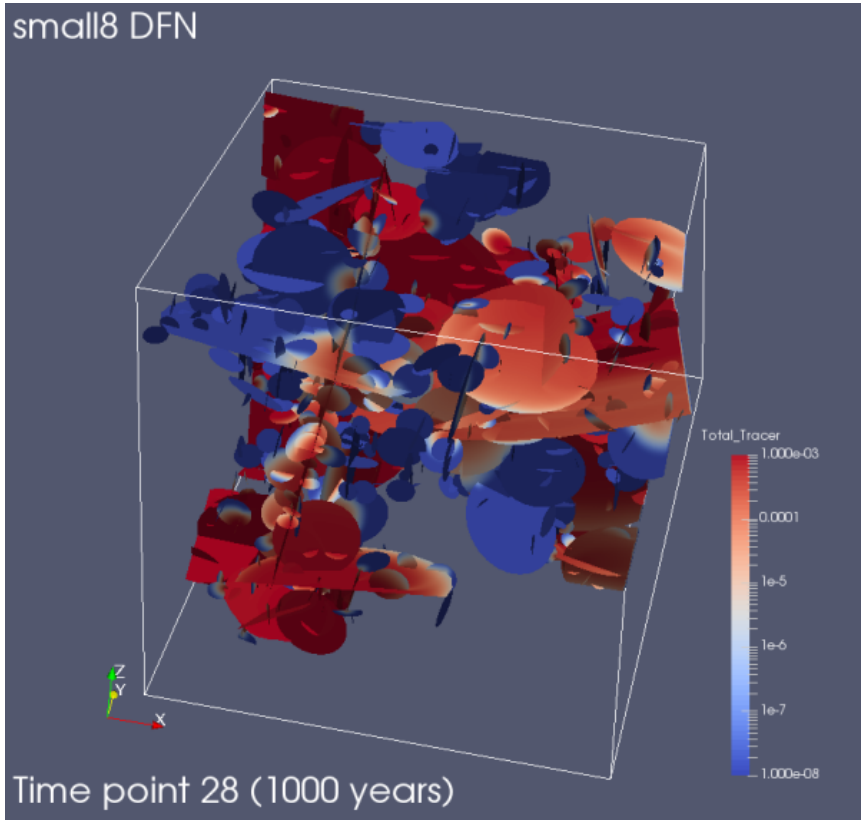


# Meshing options

**Domain:** 990 m/side.
**Options:** 1) Mesh the DFN and solve ADE on DFN 2) Convert to ECPM

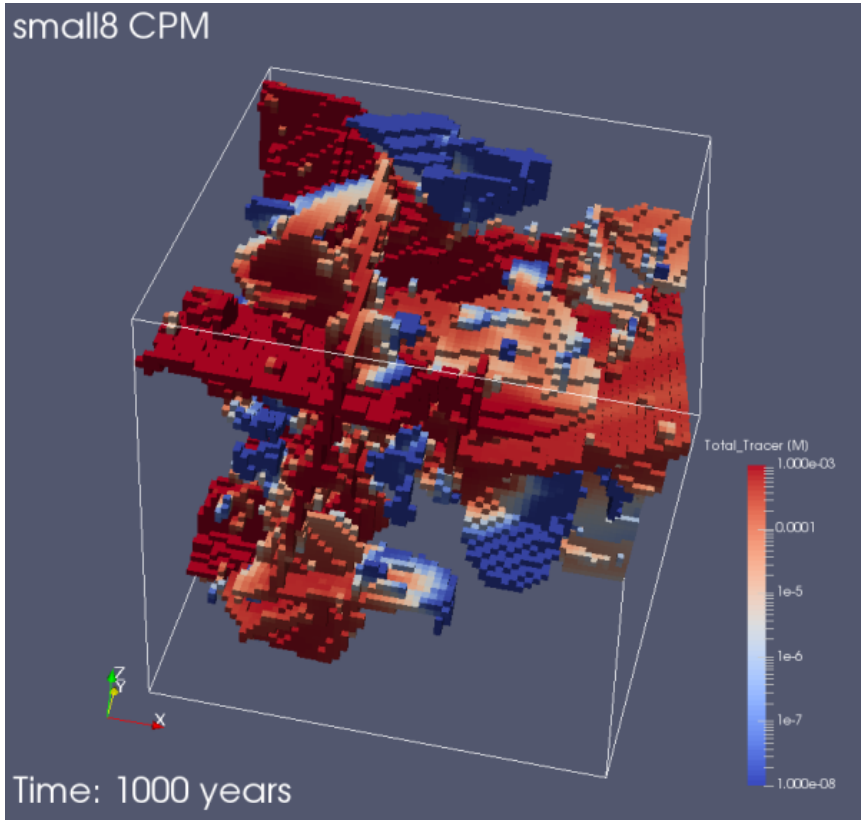
## DFN

~1.7 million cells, 103 minutes to 1 My




## ECPM

287,496 cells, 1.9 minutes to 1 My




Stein, Emily, et al. *Modeling Coupled Reactive Flow Processes in Fractured Crystalline Rock.* No. SAND2017-0230C. Sandia National Lab.(SNL-NM), Albuquerque, NM (United States); Sandia National Laboratories, Las Vegas, NV, 2017.

# ECPM meshing options

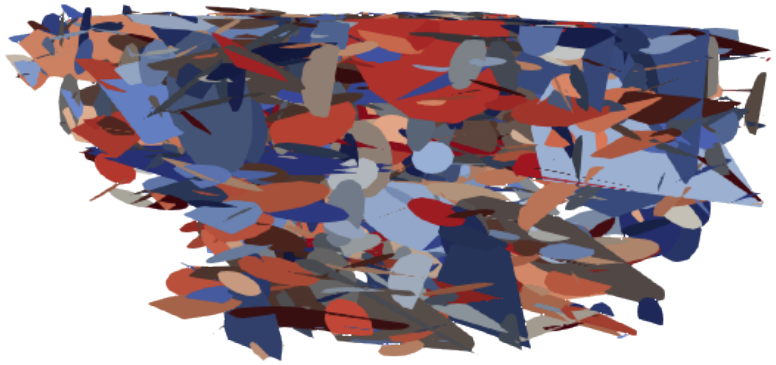
1000 x 1000 x 500 m domain
Fracture statistics taken from Forsmark

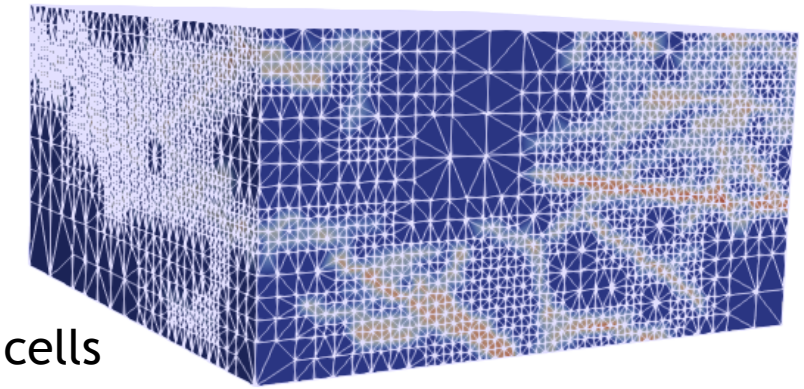
**dfnWorks octree meshing**

- Only refines where there are fractures.
  - Save cost if network is sparse, or
  - Mitigate false connections for same cost
- Largest cell size 125 m; 3 refinement levels = ~15 m cells
- Tetrahedral mesh; have to deal with diagonal faces for continuous properties; makes anisotropic K challenging in PFLOTRAN.

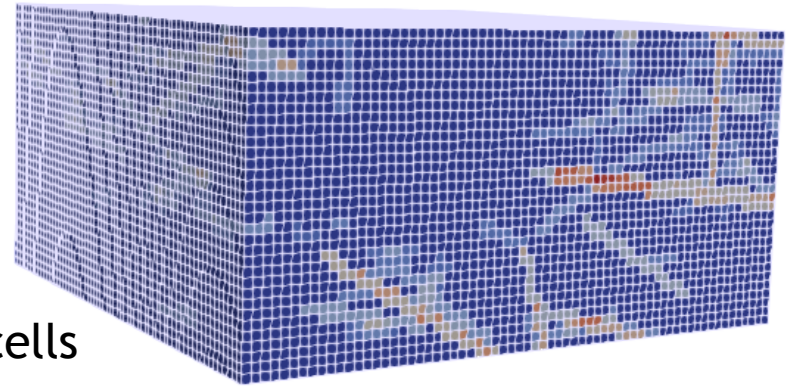
**mapdfn.py**

- Uniform mesh.
- 15 m cubic cells.
- Tensor properties directly map to faces of cells; makes anisotropic K possible (still only diagonals) in PFLOTRAN.





108285 cells



143748 cells

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  - DFN with PFLOTRAN advection-diffusion equation (ADE)
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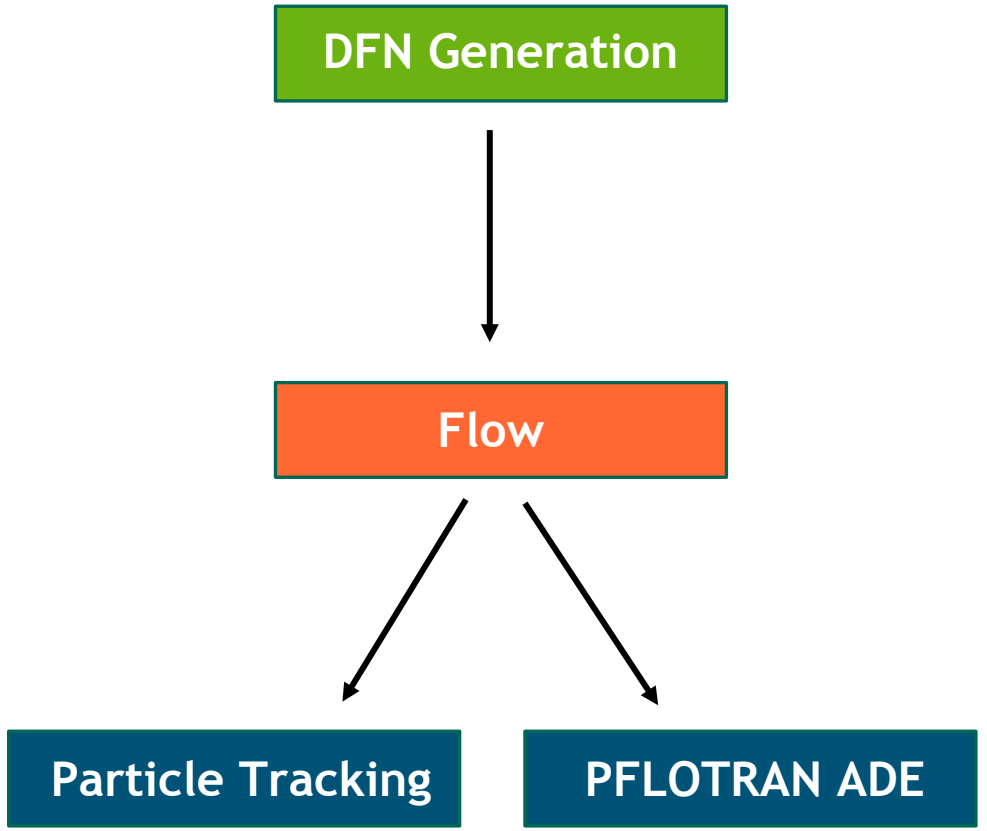
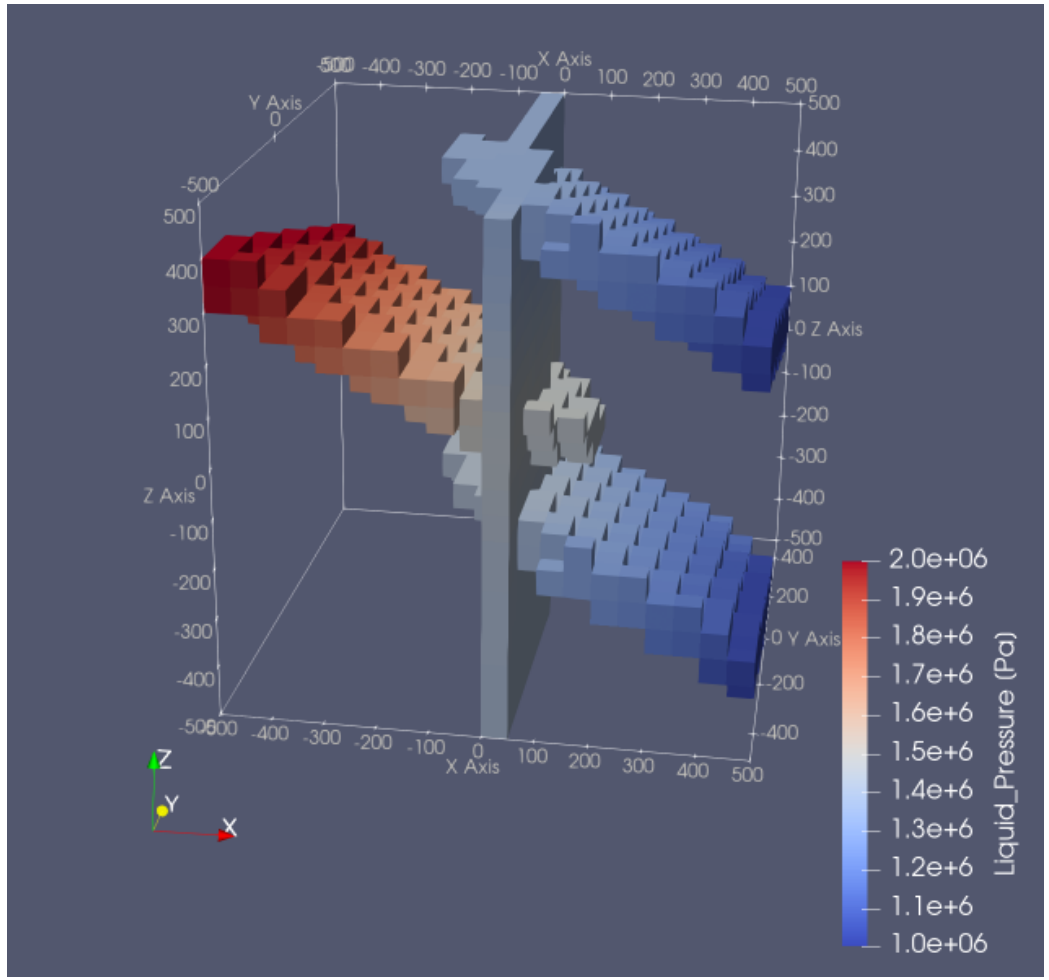


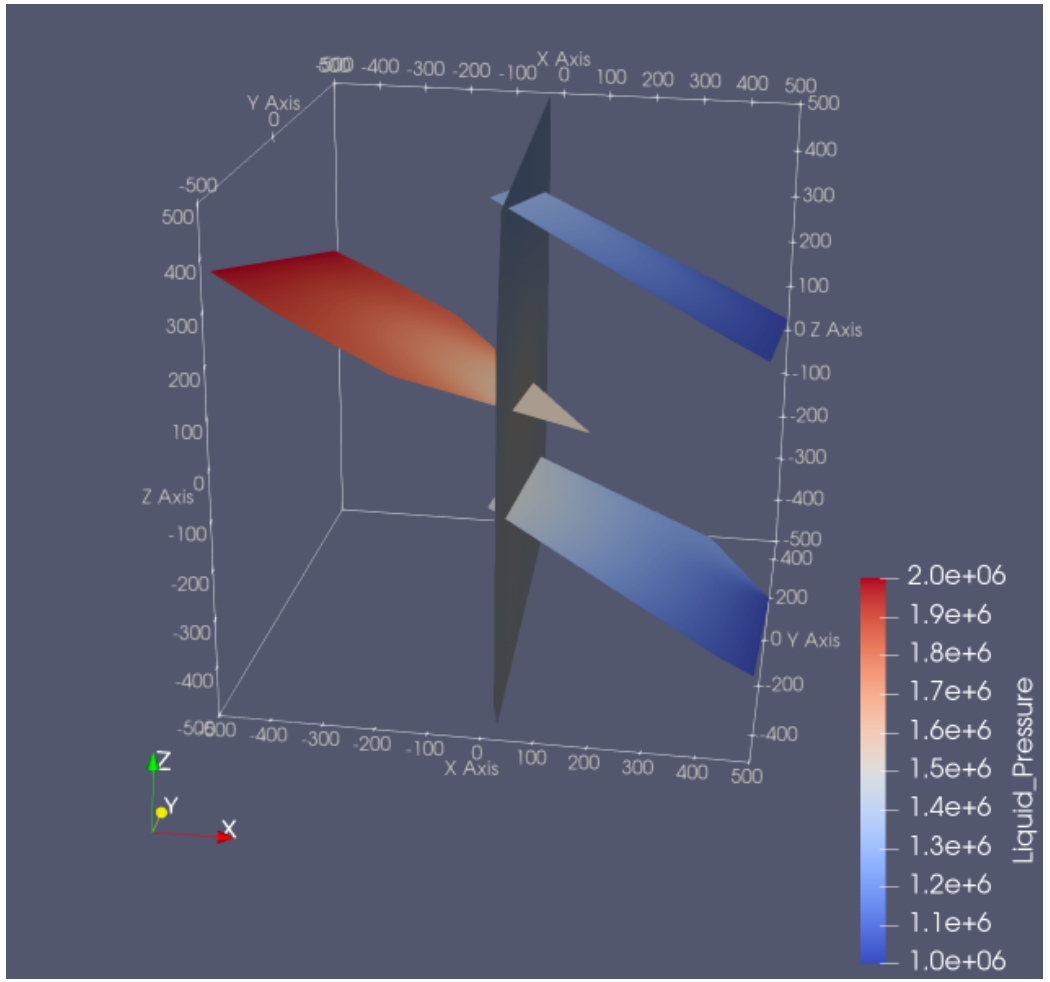
# DFN Flow: 4-Fracture Benchmark Case

Modeled via Darcy's Law

**ECPM**

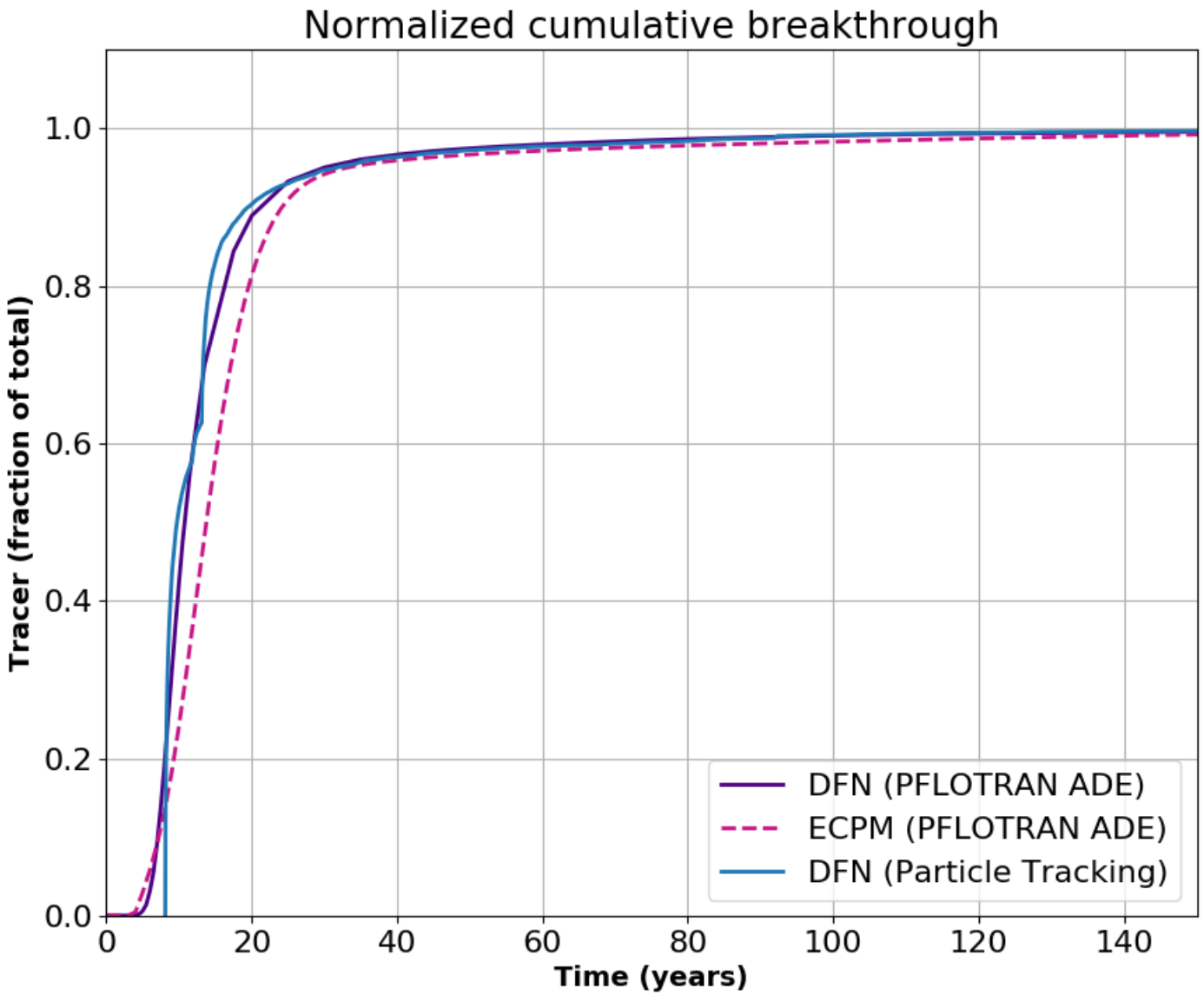



**DFN**



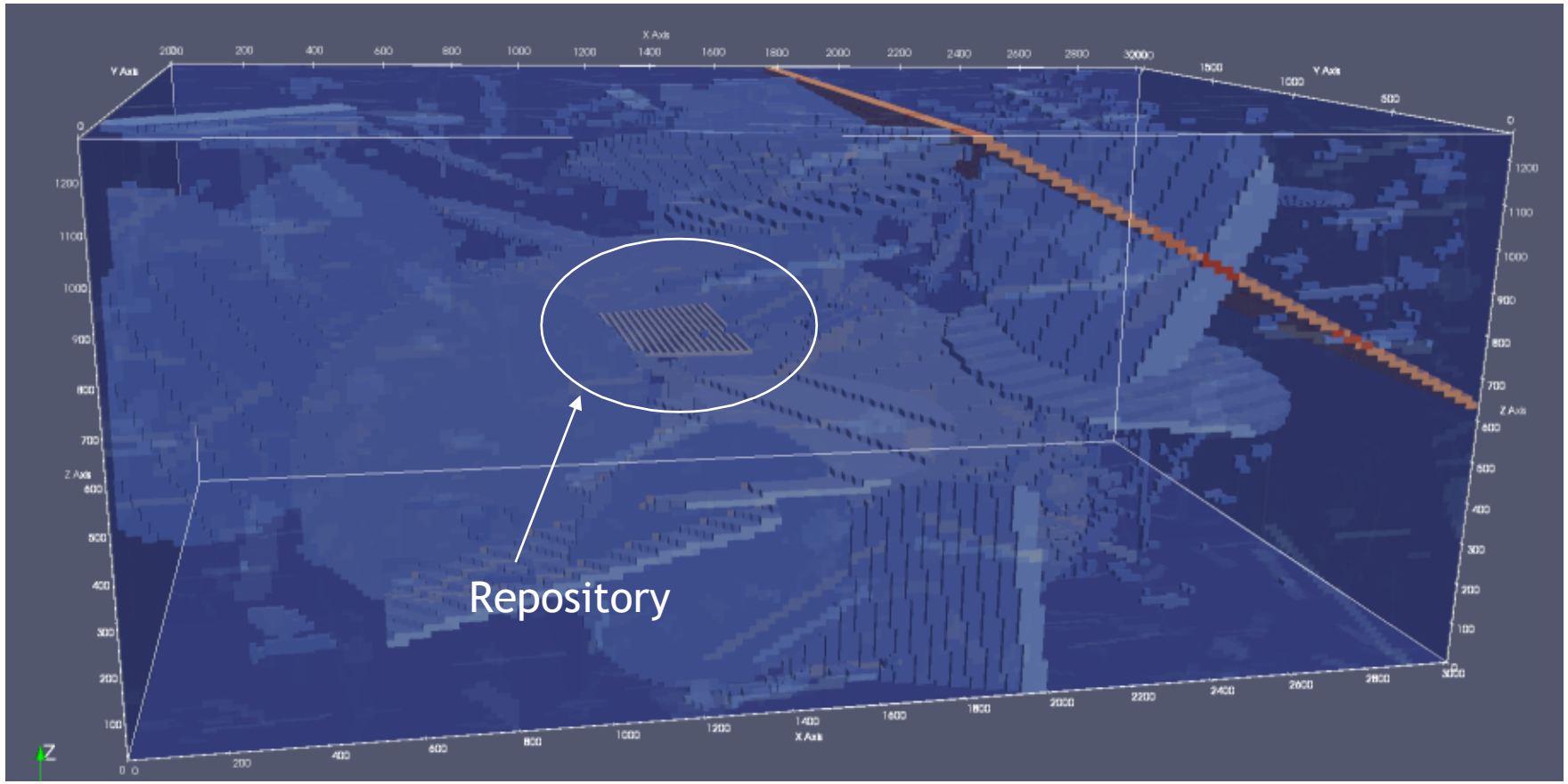
# DFN Transport : 4-Fracture Benchmark Case

- Steady-state flow field
- 10000 particles
- Impulse tracer injected in fractures
- 20 m cell size in ECPM

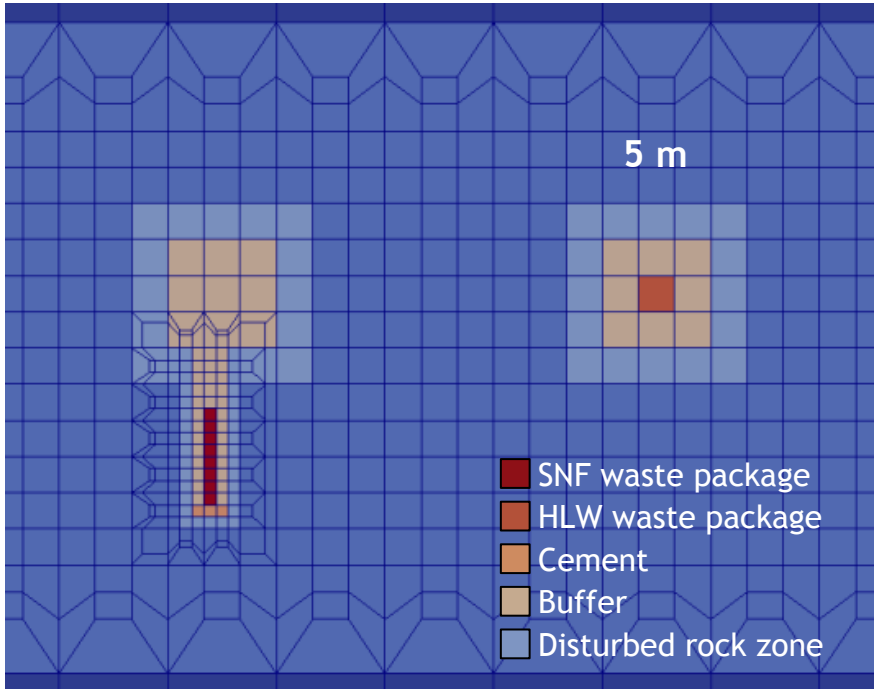


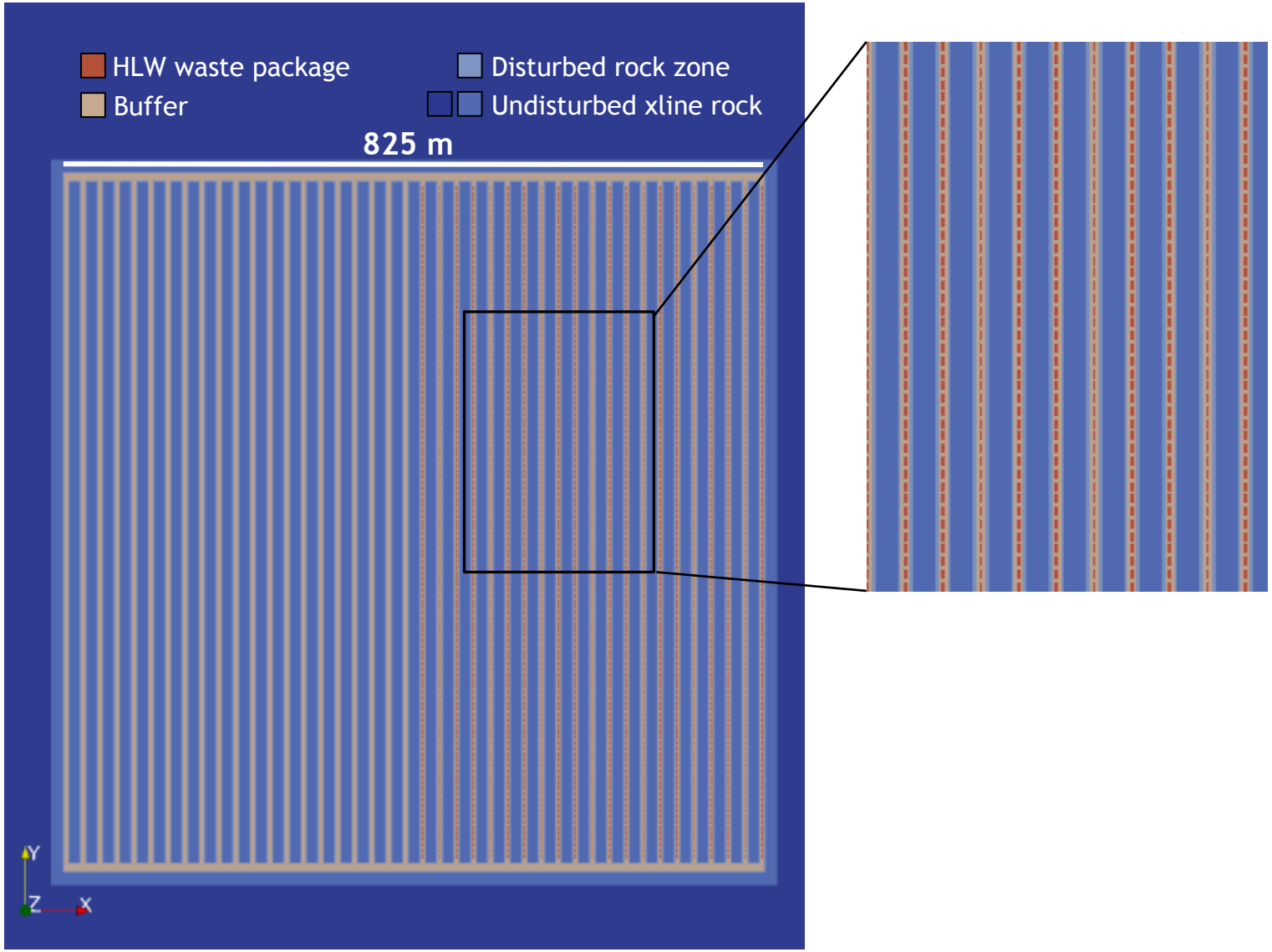
# Modeling the repository

Repository is refined even further to 1.67 m for in-drift waste package and to 1.67/3 m for vertical deposition holes.



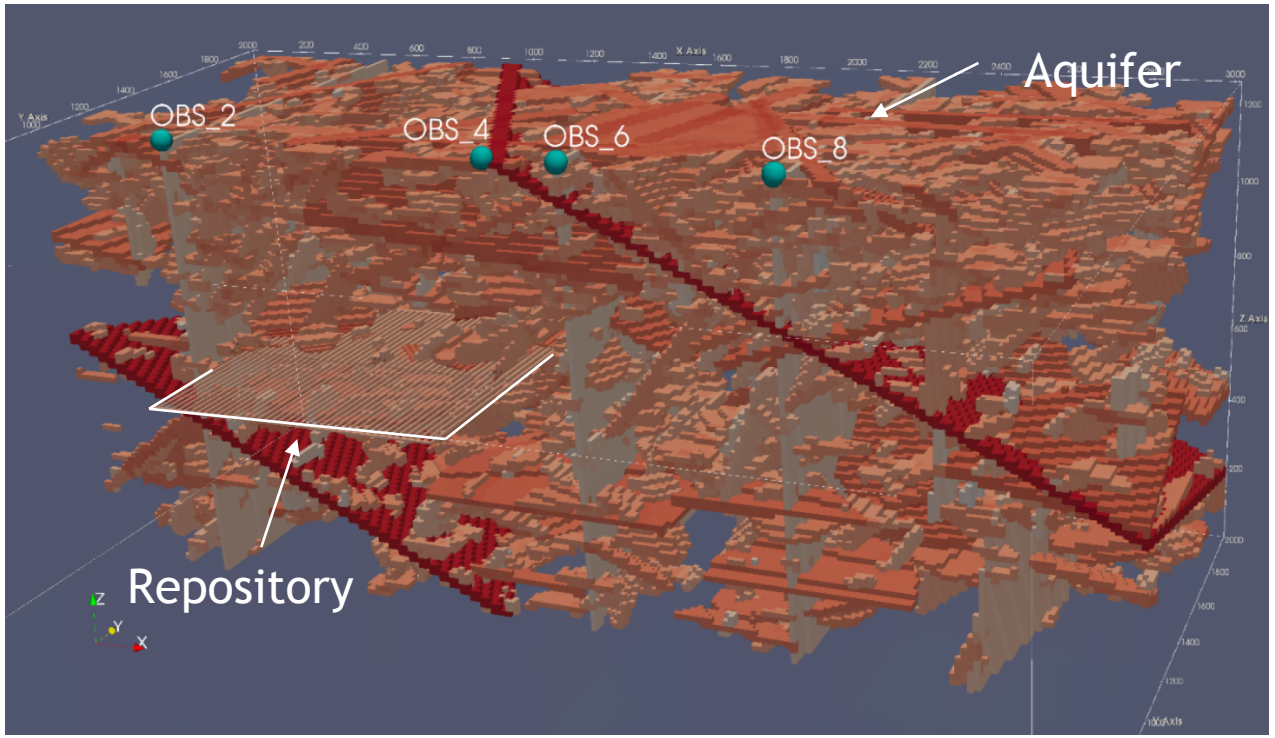
# Meshing the repo



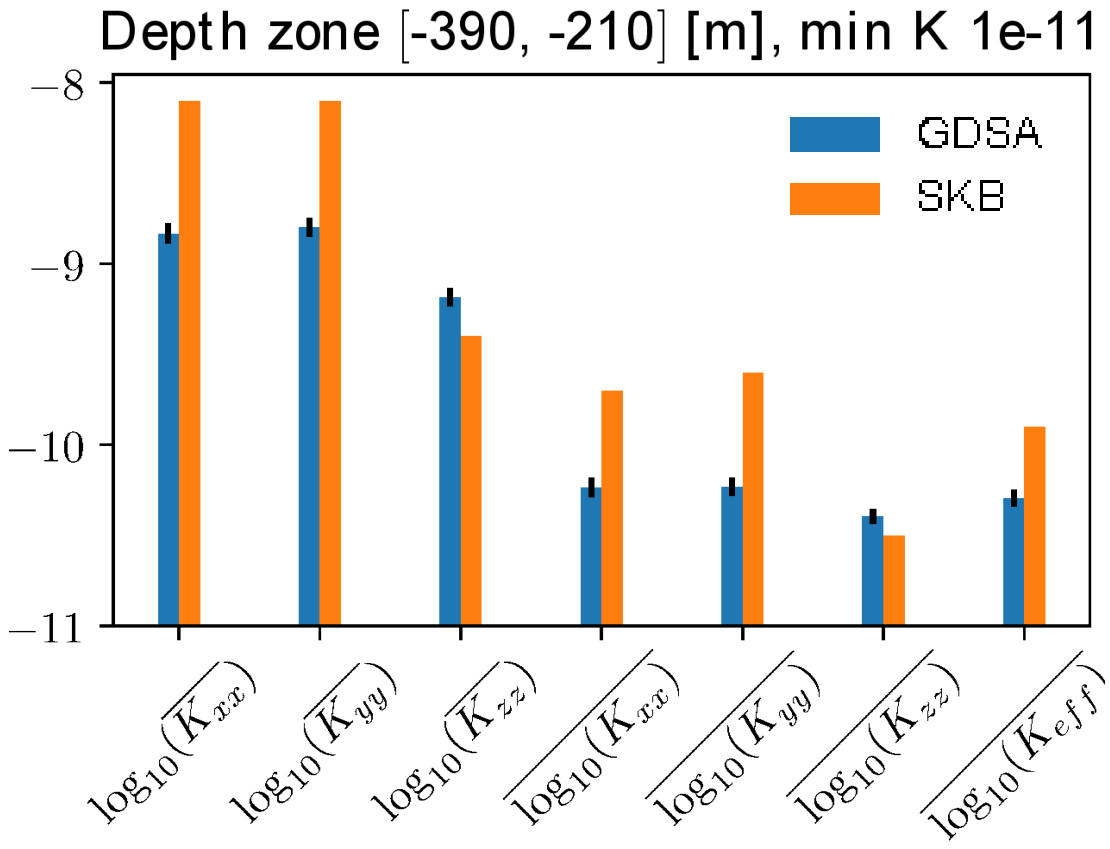
# Sandia's previous crystalline reference case

- DFN based off fracture statistics for Forsmark site
- 3015 x 2025 x 1260 m
- Mapped to ECPM with mapdfn.py
- Meshed DFN: 2,279,340 degrees of freedom
- Meshed repository: 187,974
- Runs out to 1 million years.
- 1152 cores ~1.5 hours to run



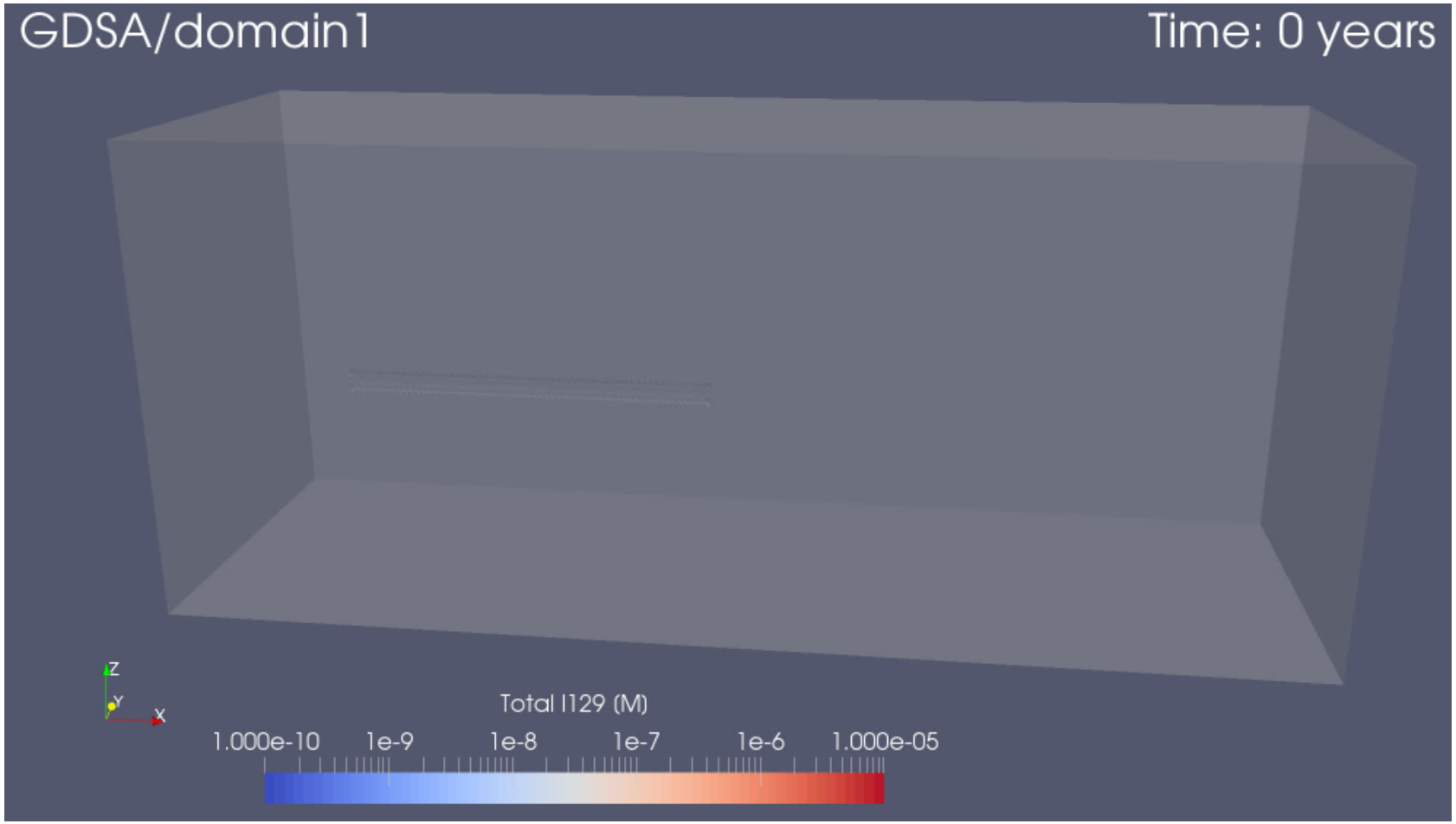
# CPM Verification Exercise

- Performed a verification exercise to ensure our ECPM permeabilities were similar to those produced by SKB.
- Averaged hydraulic conductivity over middle depth zone for Forsmark.
- Expected our **K** to be less conductive overall. Our grid was finer and they included fractures of smaller radius in their DFNs.
- In general we saw our **K** were in line with their values or slightly lower.




**SKB statistics provided by:** Lee Hartley and Steven Joyce. Responses to SSM on Hydrogeology, SKBdoc 1396325 ver 1.0, Svensk Kärnbränslehantering AB., 2013. SKBdoc documents will be submitted upon request to document@skb.se.

# $^{129}$I concentration in similar domain




$^{129}$I concentration over 1 million years in Forsmark-based crystalline case. General corrosion rate assumed such that median WP failure time is around 23,000 years.