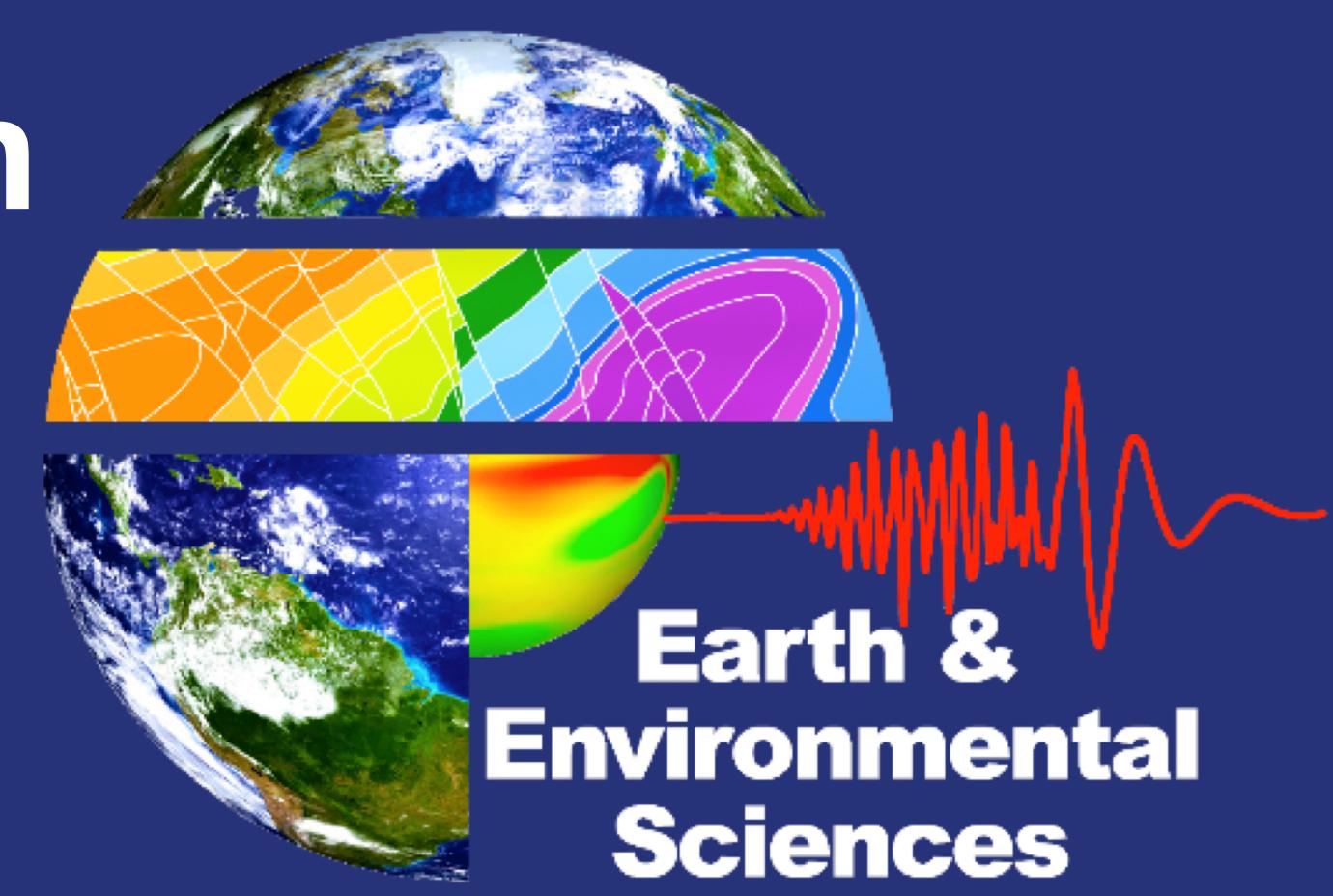


# Coupled discrete fracture and 3D continuum domain representation to efficiently capture gas transport from underground cavities

John P. Ortiz, Dylan Harp, Phil Stauffer, Carl Gable, and Nataliia Makedonska  
*Los Alamos National Laboratory, Computational Earth Science (EES-16), Los Alamos, NM*

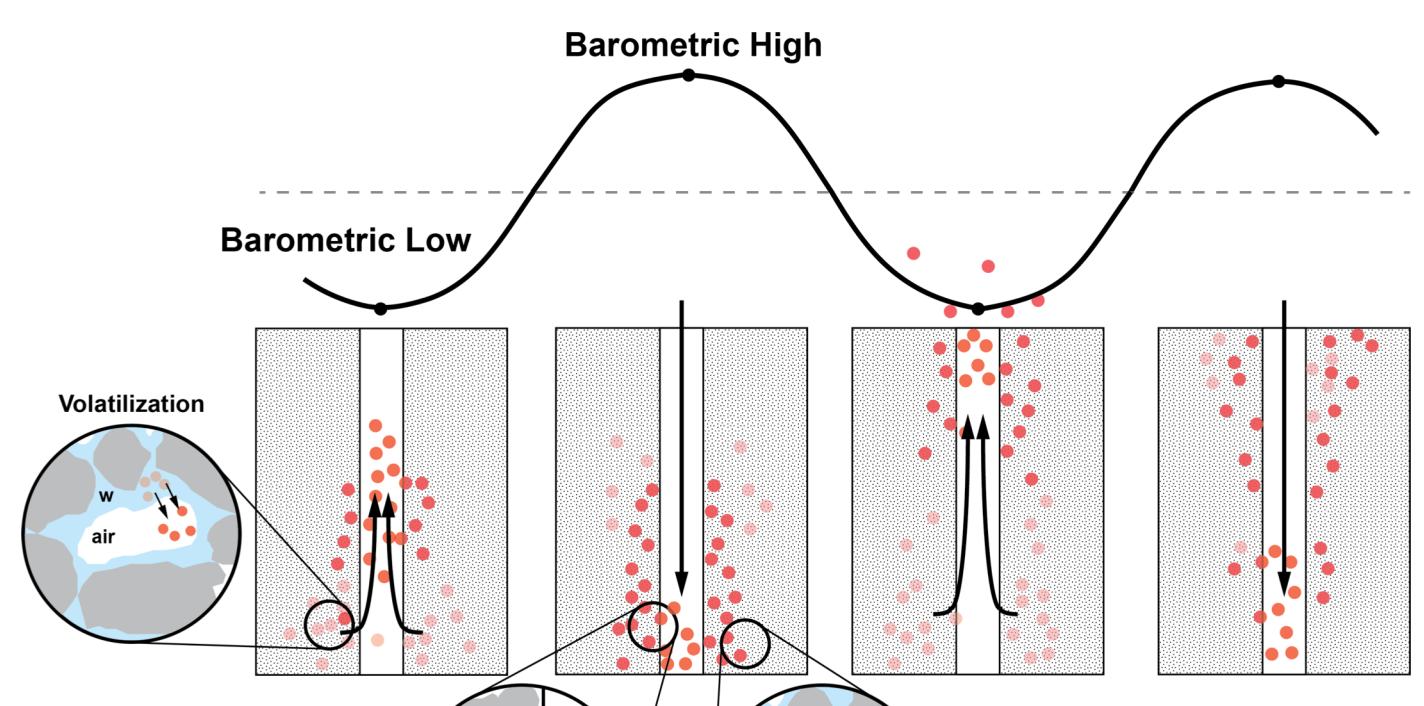


## Abstract

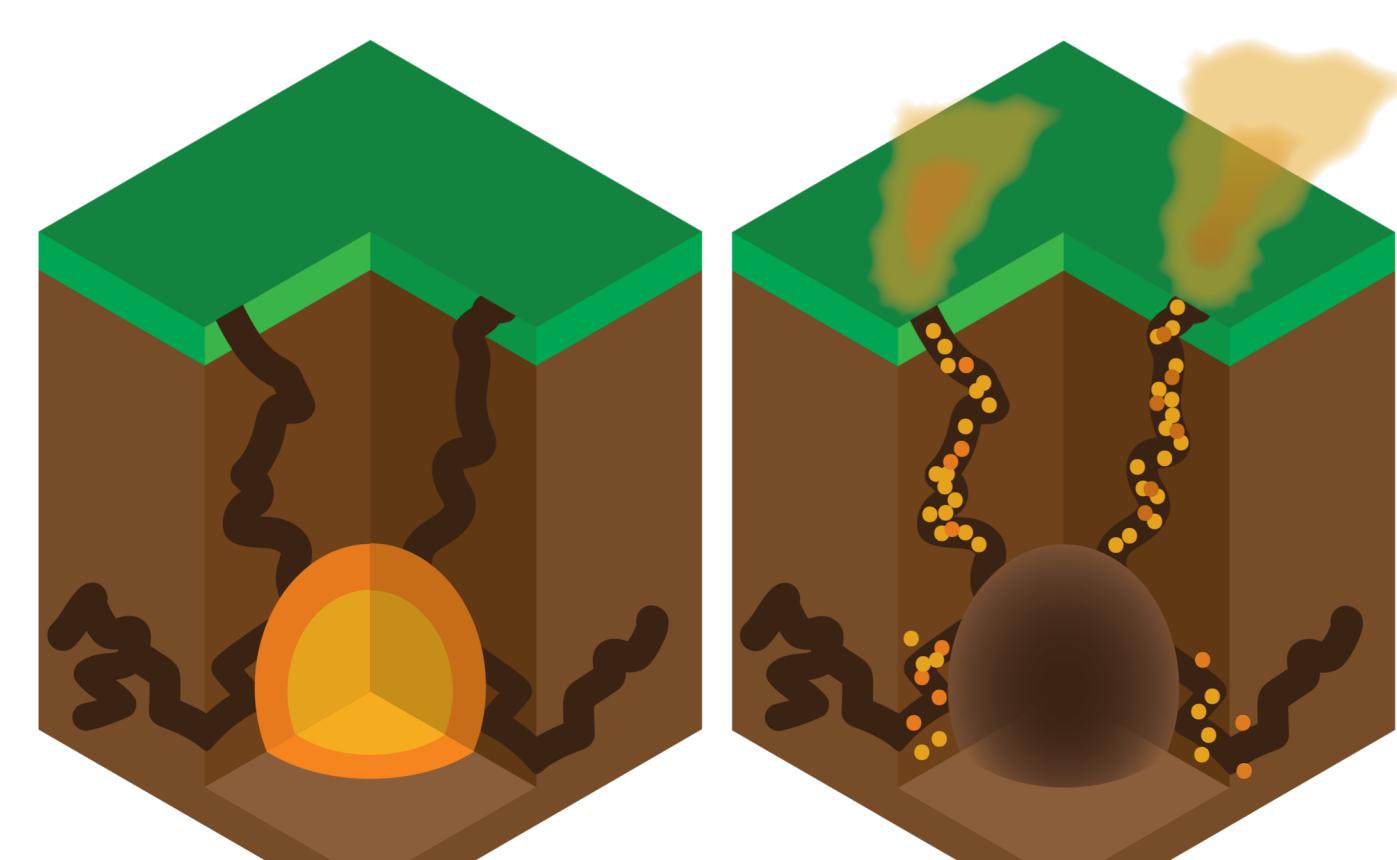
Driven primarily by barometric pumping, the time scale of relevant gas transport in fractured geologic media can vary from years to the order of days depending on the strength of the barometric signal and a variety of hydrogeologic parameters, including: rock type, fracture aperture, matrix permeability, porosity, and saturation. Although discrete fracture networks (DFNs) improve representations of preferential flow along fractures, they have limitations in transport applications where molecular and pressure diffusion into the rock matrix cannot be ignored. We will present numerical simulations that combine a single discrete fracture with an explicitly meshed 3D cavity zone. We employ a dual-porosity formulation to represent the matrix attached to the fracture in order to accurately model barometric pumping. Such simulations highlight the relative importance of different macro- and micro-scale processes in fractured flow and transport models while also promising to reduce computation time of multiphase simulations.

## Barometric pumping

Simulations of subsurface flow and transport in fractured media can be useful in tracking radionuclide gas migration from underground nuclear explosions (UNEs) for Comprehensive Nuclear Test-Ban Treaty (CTBT) verification. Under certain conditions in the presence of fractures, barometric pumping enhances gas transport by effectively “ratcheting” the contaminant upwards over multiple atmospheric fluctuation cycles (Harp *et al.*, 2018).



**Fig. 1:** Conceptual diagram of the barometric pumping mechanism “ratcheting” contaminants upwards over time via advection and multiple micro-scale processes that aid temporary storage.



**Fig. 2:** Over time, barometric pumping in fractured media can bring gaseous subsurface contaminants to the surface.

**Goal:** To combine discrete fractures with 3D continuum meshes for increased computational efficiency.

## Challenges

- DFNs are relatively untested in transient applications
- Explicit representation of fractures using continuum meshes require very high node counts for grids to “telescope” to fracture resolution
- Computationally difficult to calculate transient flow through a very small fracture (aperture  $\leq 1$  mm) into a large cavity volume
- Because of pressure attenuation in matrix, dissolution/exsolution, and diffusion, we cannot ignore the rock matrix in our simulations (must still be accounted for)

Discrete fracture networks (DFNs) overcome many of the limitations of continuum mesh approaches in simulations of flow and transport in fractured rock. Unlike continuum methods that use effective parameters to account for the influence of the fractures on flow, DFNs create a network of fractures in which the geometry and properties of individual fractures are explicitly represented as intersecting planar polygons in three dimensions.

However, DFNs are not perfect for all applications, such as subsurface flow/transport in a fracture connected to a large, contaminated cavity volume. DFNs are also relatively untested in transient simulations. We aim to develop these capabilities to strike a balance between high-efficiency discrete fracture meshes and computationally expensive continuum meshes.

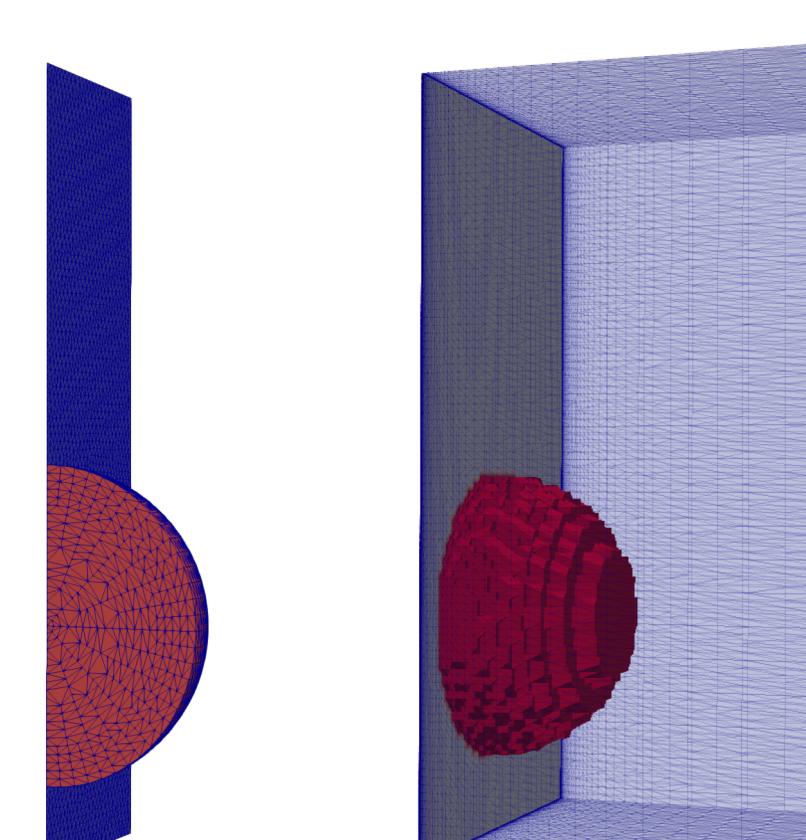
## Verification

We perform a suite of verification simulations using the multiphase flow and transport code FEHM (Finite-Element Heat and Mass).

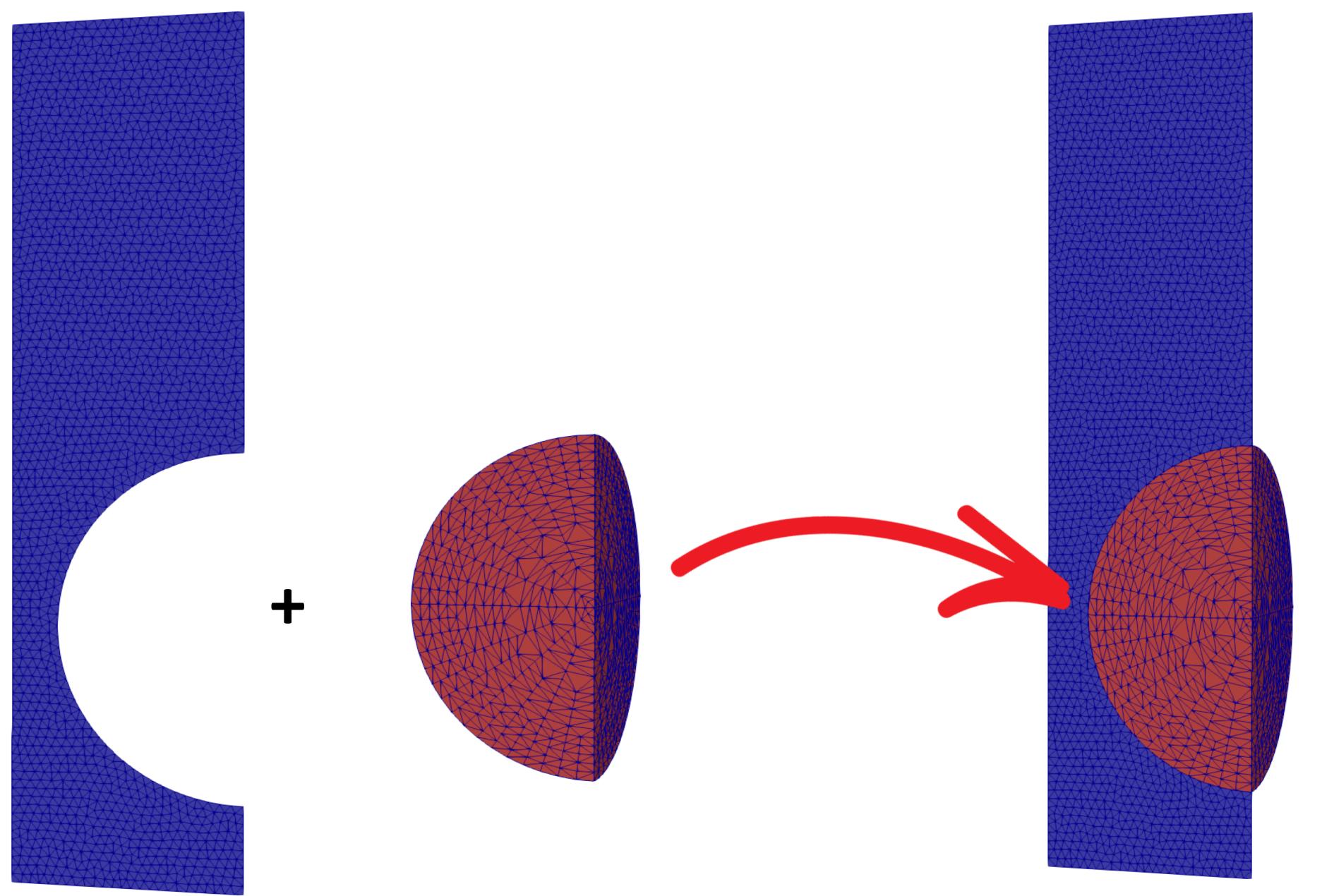
For flow verification, we compare subsurface pressures with those collected in an analogous simulation using a 3D continuum mesh driven by a sinusoidal pressure signal at the surface.

Transport verification was done in a similar manner, measuring breakthrough concentrations following the initial release of vapor contaminant in the cavity driven by the same pressure signal.

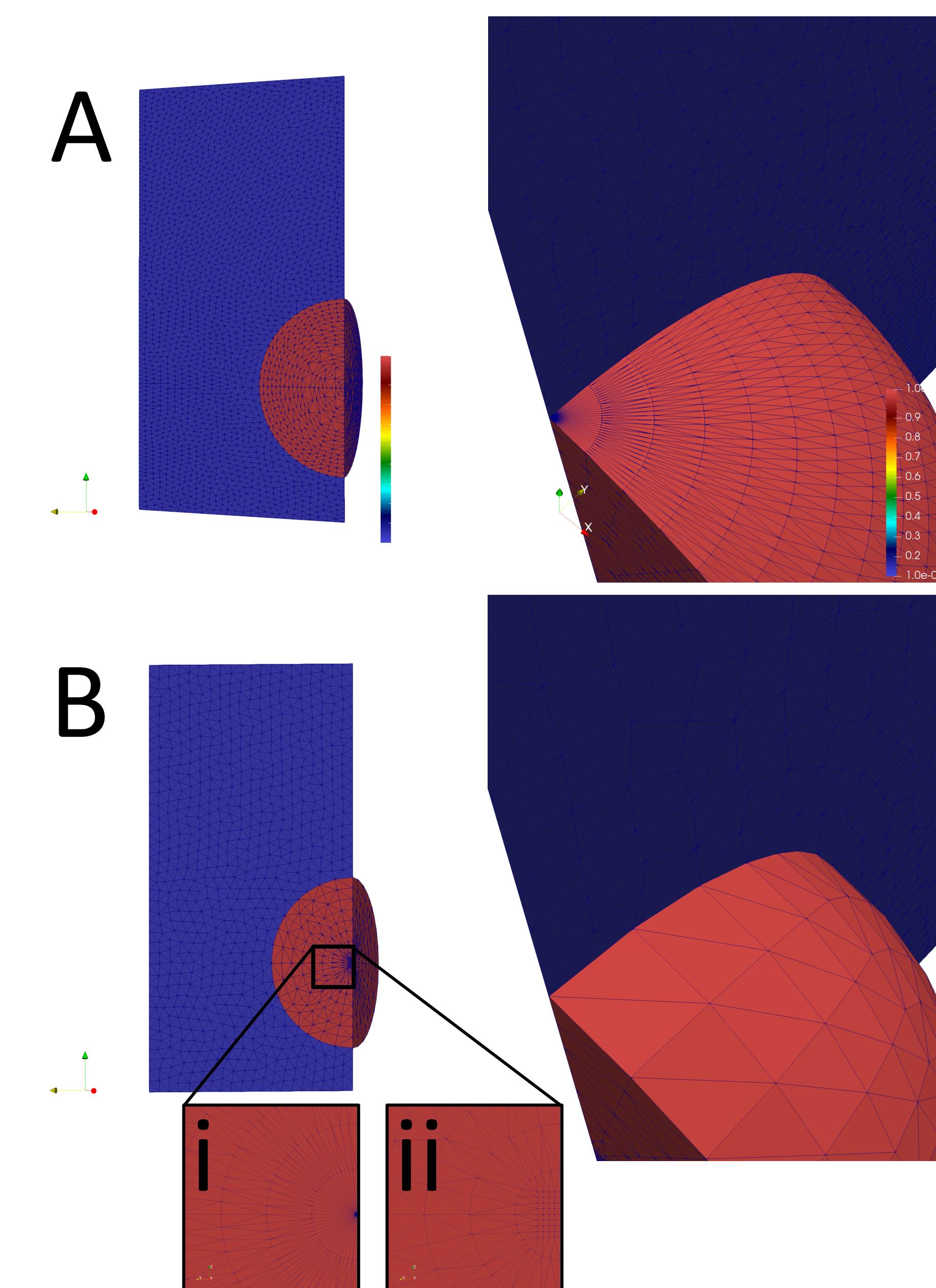
**Fig. 3:** (left) the combined DFN-continuum mesh, (right) 3D continuum mesh.



## Workflow development



**Fig. 4:** General workflow from left to right: generating 2D fracture plane, generating 3D continuum cavity with perimeter nodes collocated with those on the fracture plane, and merging the two mesh objects and geometric storage coefficients.



**Fig. 5:** Considerations given to mesh geometries. Cavity generated with spherical coordinates (A) created numerical issues at the poles because of too many nodal connections to a single point. This was rectified by projecting point distributions from a cube onto a sphere (B) and by replacing a radial point distribution at the cavity center (i) with a cubic one (ii).

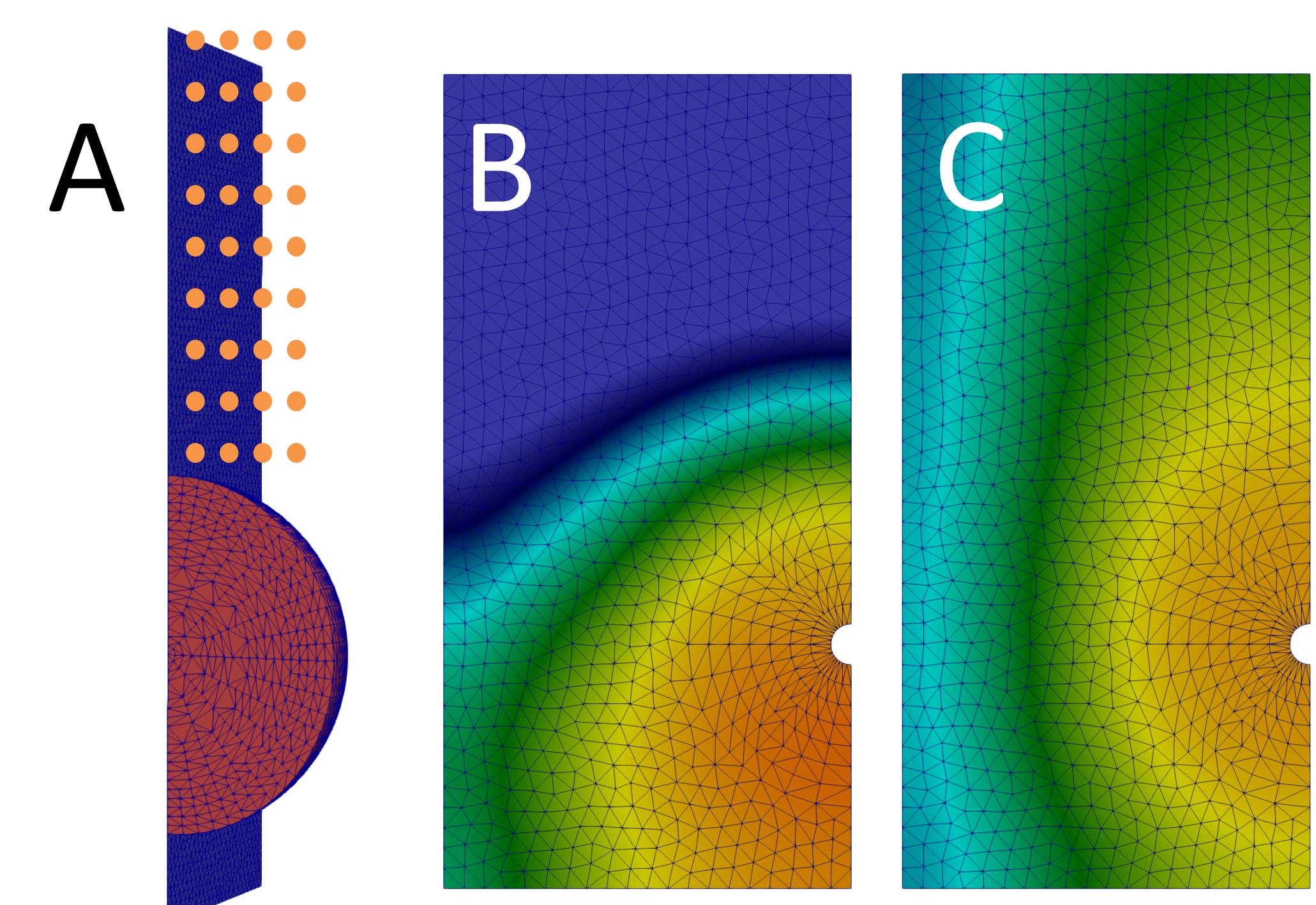
## Contact information

**John P. Ortiz**  
Post-Master's Researcher  
[jportiz@lanl.gov](mailto:jportiz@lanl.gov)  
(+1) 505-665-5901



## Ongoing work

Early transport simulations point to some challenges associated with how the FEHM simulator handles the merged 2D plane and 3D continuum mesh objects. Nodes collocated between the fracture and cavity do not seem to allow for the dissolution and volatilization of vapor contaminants.



**Fig. 6:** (A) Future work using dual-porosity nodes (orange) on the hybrid mesh to account for matrix diffusion, pressure attenuation, and storage. Preliminary results of gas transport (B) and (C) using 2D mesh slices with dual-porosity nodes during a barometric high and low, respectively. Note that these meshes remove the central ring of cavity nodes in an attempt to reduce suboptimal element shapes.

Simple verification tests currently ignore the rock matrix to ensure the accuracy of flow and transport physics for the fracture and cavity. Ongoing work uses dual-porosity nodes perpendicular to the fracture plane as a computationally efficient method to account for the matrix pressure attenuation, diffusion, and storage that contribute to the upward “ratcheting” of contaminants over many barometric pressure cycles.

## References

Harp, D.R., Ortiz, J.P., Pandey, S., Karra, S., Anderson, D., Bradley, C., Viswanathan, H. and Stauffer, P.H., 2018. Immobile Pore-Water Storage Enhancement and Retardation of Gas Transport in Fractured Rock. *Transport in Porous Media*, 124(2), pp.369-394.