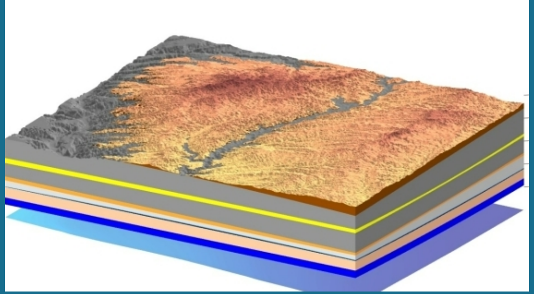
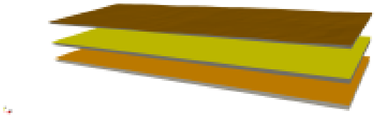
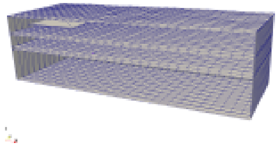
SAND2022-11113C

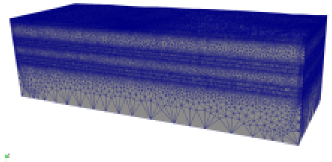
Sandia National Laboratories

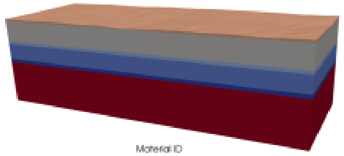
Automated Meshing for Simulations of Subsurface Contaminants











Tara LaForce and William Eymold

Sandia National Laboratories

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Nancy, France/Virtual
Sept 1, 2022

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Outline

Why is fully-automated meshing and simulation model building important?

Why Voronoi meshes (and what are they)?

A shale geological model

Tracer transport in the subsurface

Results of uncertainty simulations

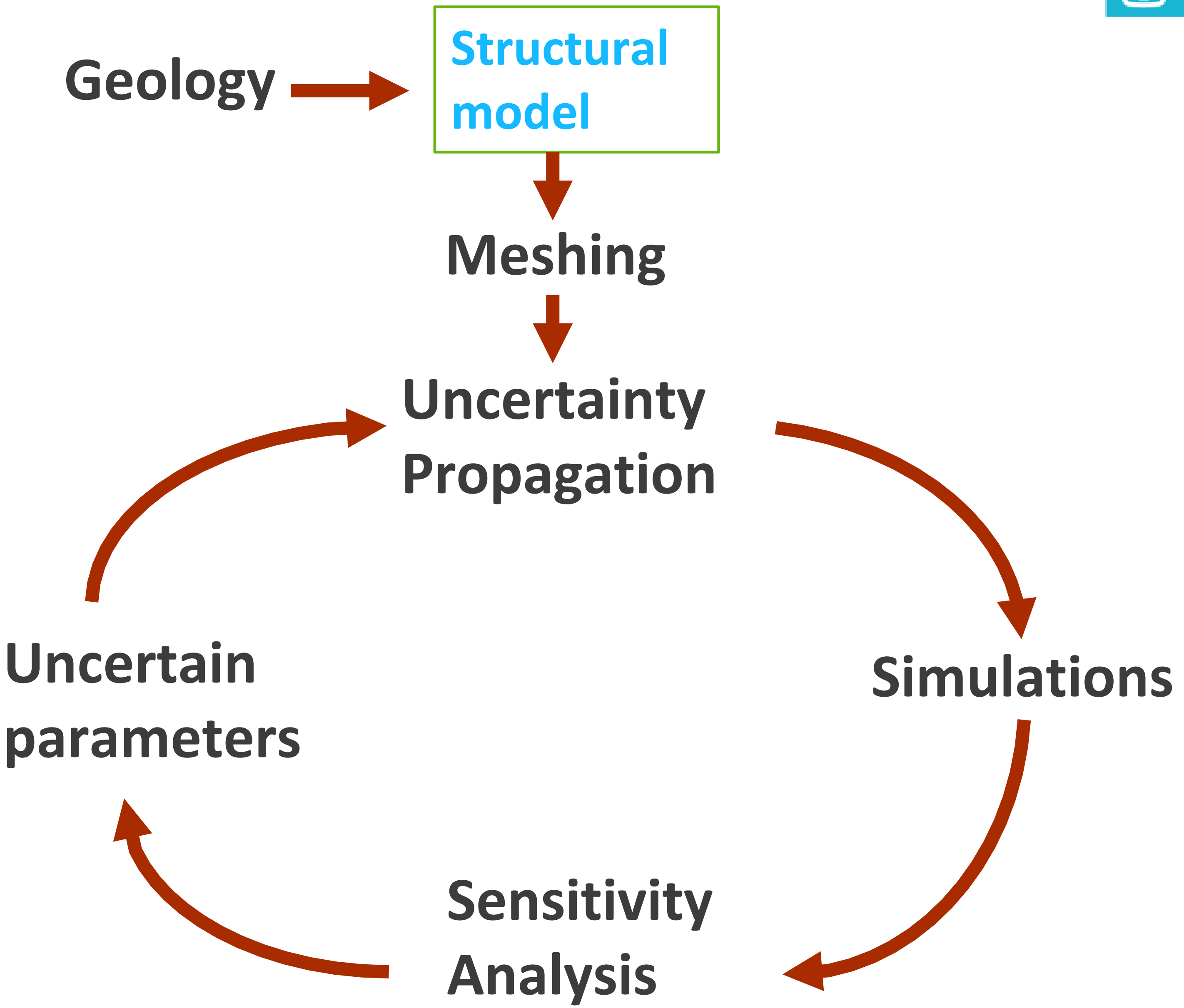
Conclusions and future work

Why Automate?

Sensitivity Analysis and Uncertainty Quantification (SA/UQ) can require hundreds or thousands of model iterations

Uncertainty in geological structure and numerical error introduced by the mesh are often neglected because model and mesh building are difficult and human-time intensive

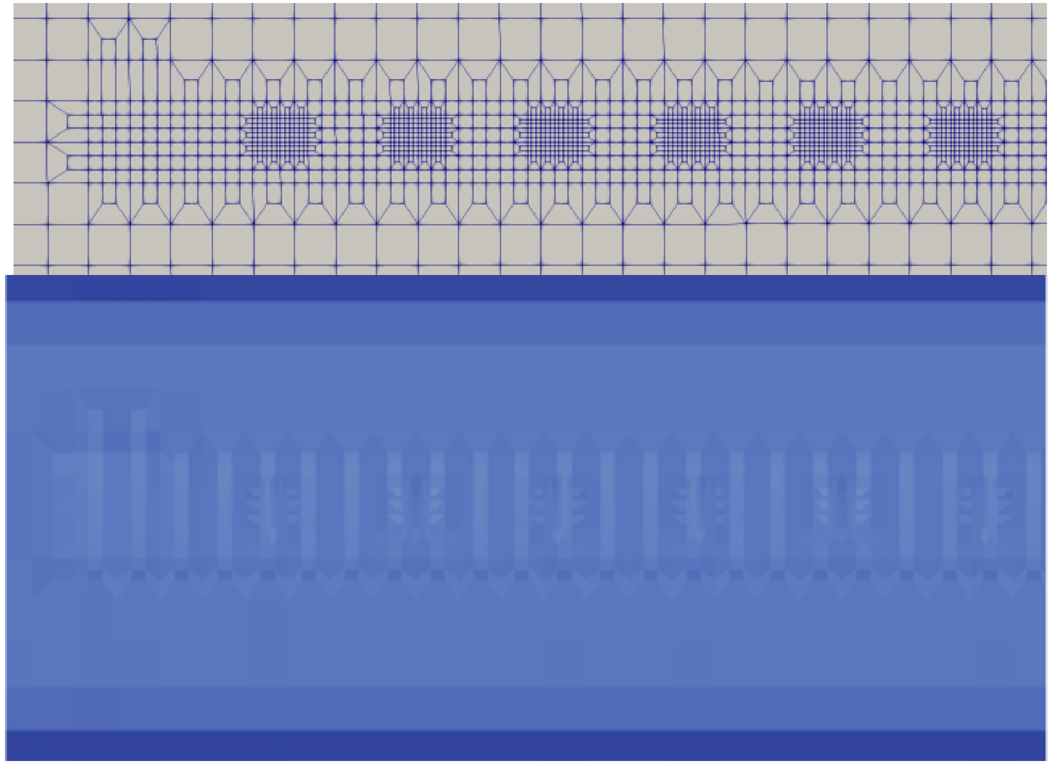
Yet geological structure can have a **first-order impact** on subsurface flow and transport processes



Why Voronoi meshes?

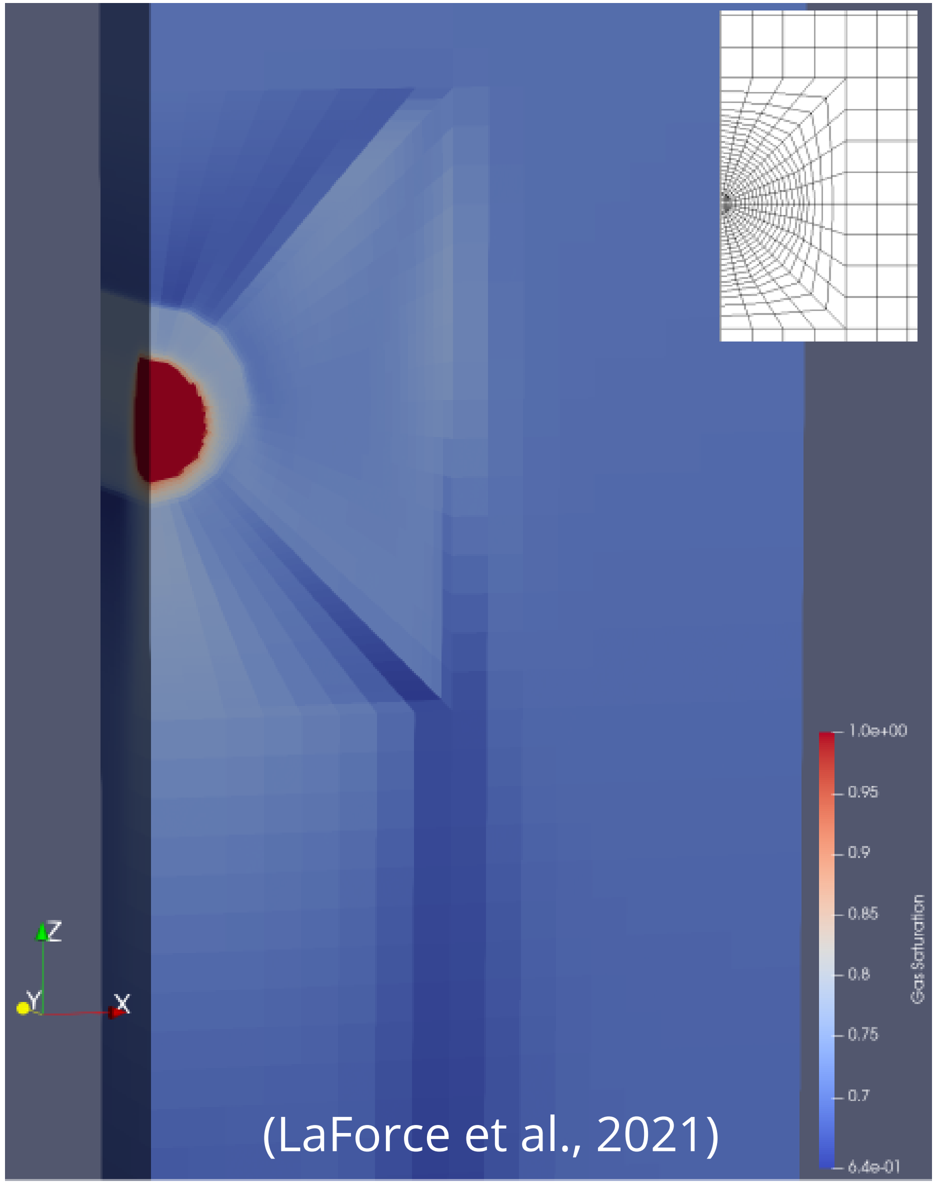
They rigorously honor complex geometries…

…without introducing non-orthogonal fluxes in simulations



Equilibration of an unsaturated heterogeneous model with infiltration using a refined hexahedral mesh.

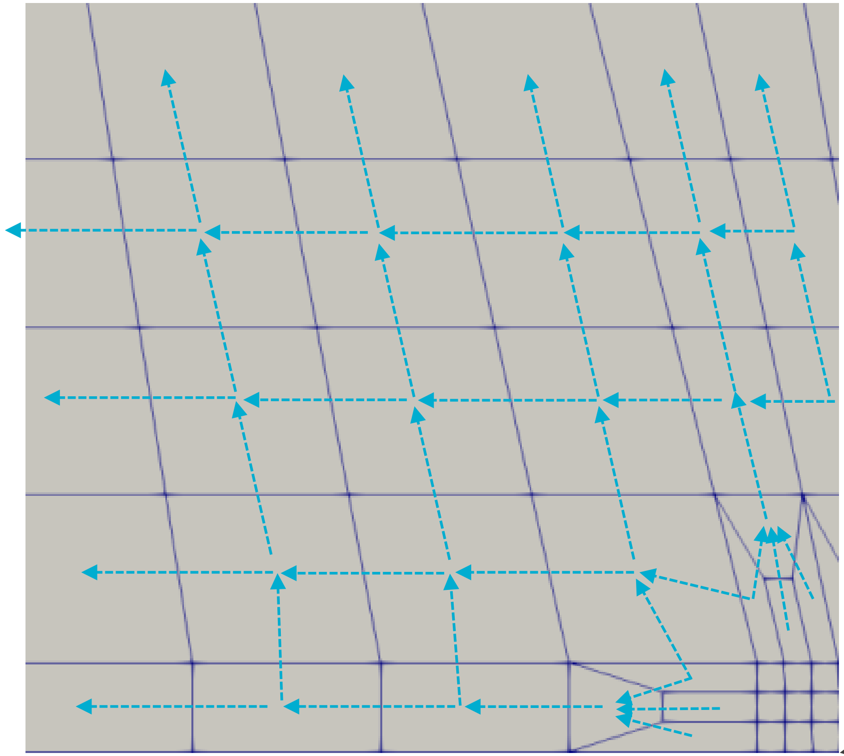
Gas saturation around a heat source in an unsaturated model using a flexed hexahedral mesh.



Why Voronoi meshes?

Grid refinement or flexing can bias flow directions

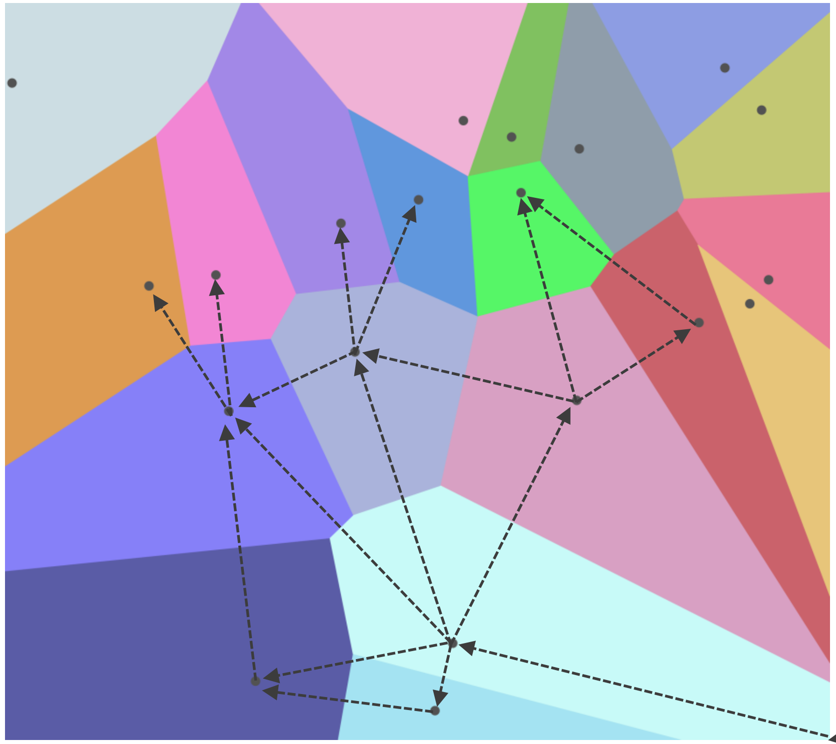
Non-orthogonal fluxes cause errors in two point flux approximation simulations



Fluid or heat source

Fluxes are perpendicular to grid cell faces using Voronoi polyhedral cells

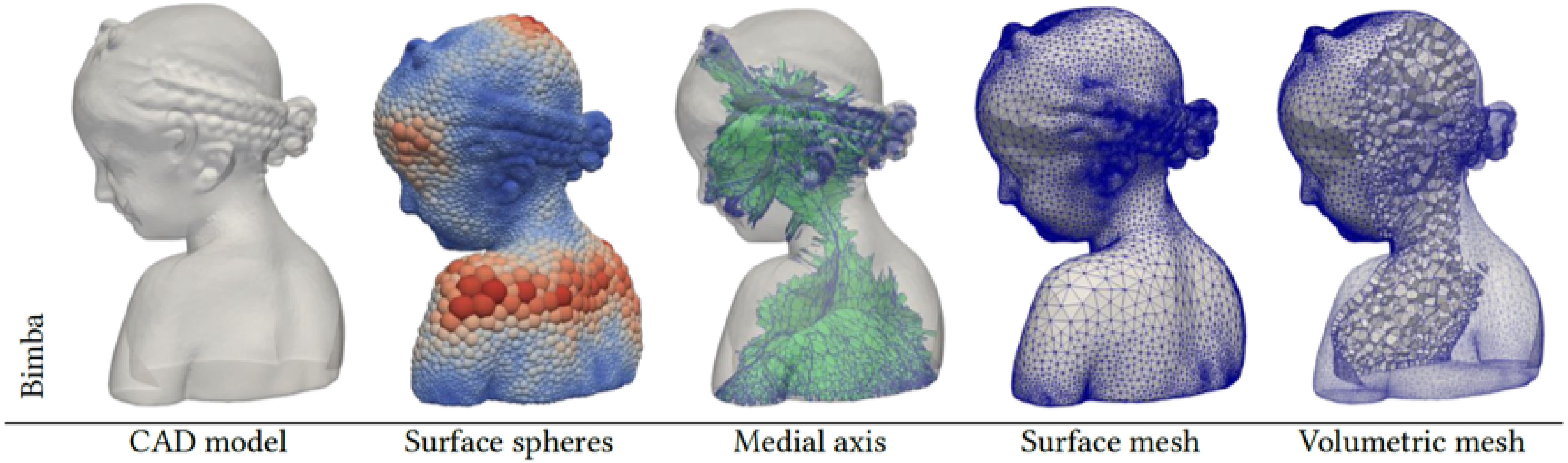
Solvers using two point flux approximation (TOUGH2/PFLOTRAN/FEHM) get accurate results



Fluid or heat source

VoroCrust-Meshing Voronoi Meshes

- Accepts as input
  - Any water-tight set of volumes
  - Desired monitoring points
  - Mesh refinement locations
- Fully automated mesh generation
- Surface mesh is triangular
- Interior elements are polyhedral
- Mesh is randomly generated so each VoroCrust run gives a new mesh

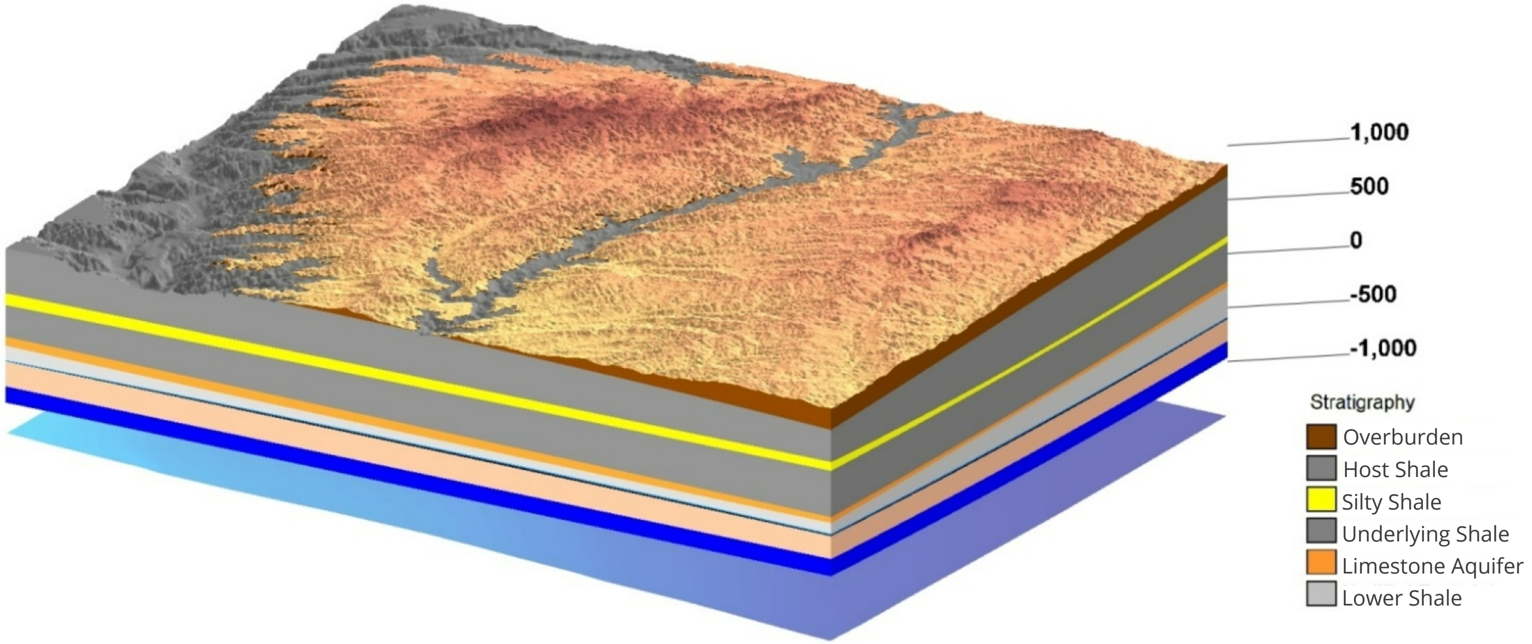


(LaForce et al. 2022a)

Shale Geological Framework Model

- Single realization of a Pierre Shale Geological Framework Model (GFM) 69 x 83 km
- Pseudo-uncertain models are generated by clipping 7 × 2.5 km sub-models from GFM
- All models must have:
  - At least 15 m dip downward in positive x-direction
  - Surface sediment present over entire model
- 87 prospective geological models created
- 10 models will be randomly sampled in Dakota and populated with parameters

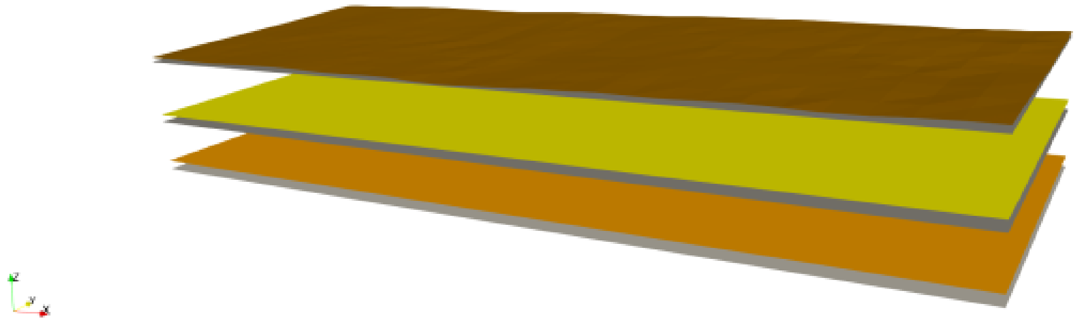
GFM at 10x vertical exaggeration



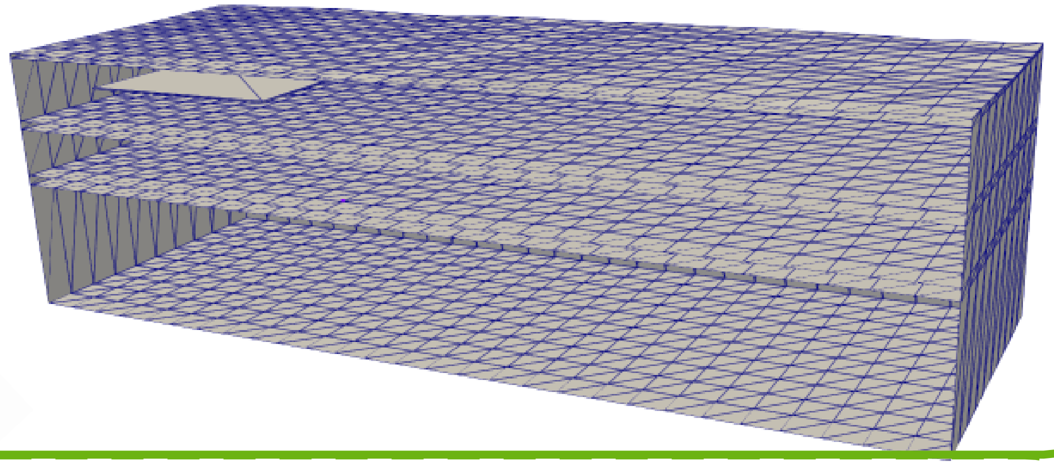
(Sevougian et al, 2019; LaForce et al. 2022b)

Meshing and Simulating Realization 1

Clip surfaces from GFM (Python3)

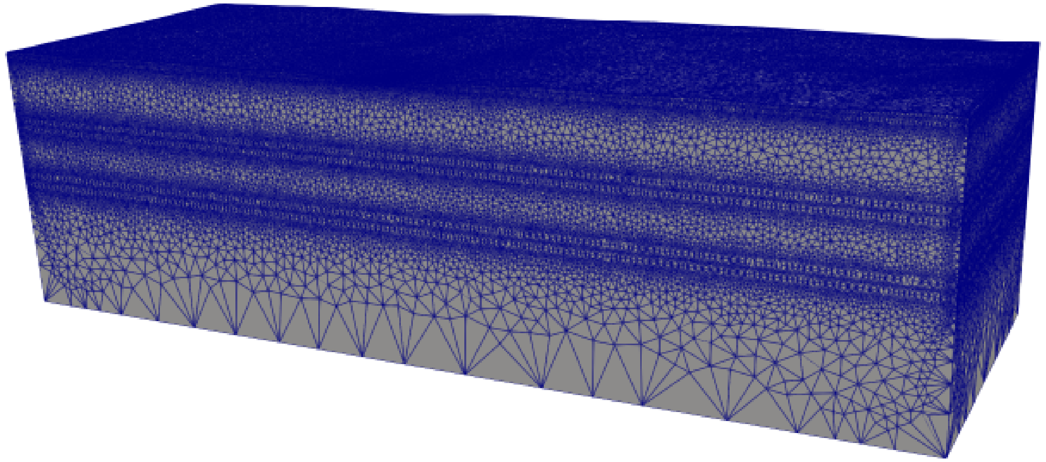


Create model volumes (LaGriT)

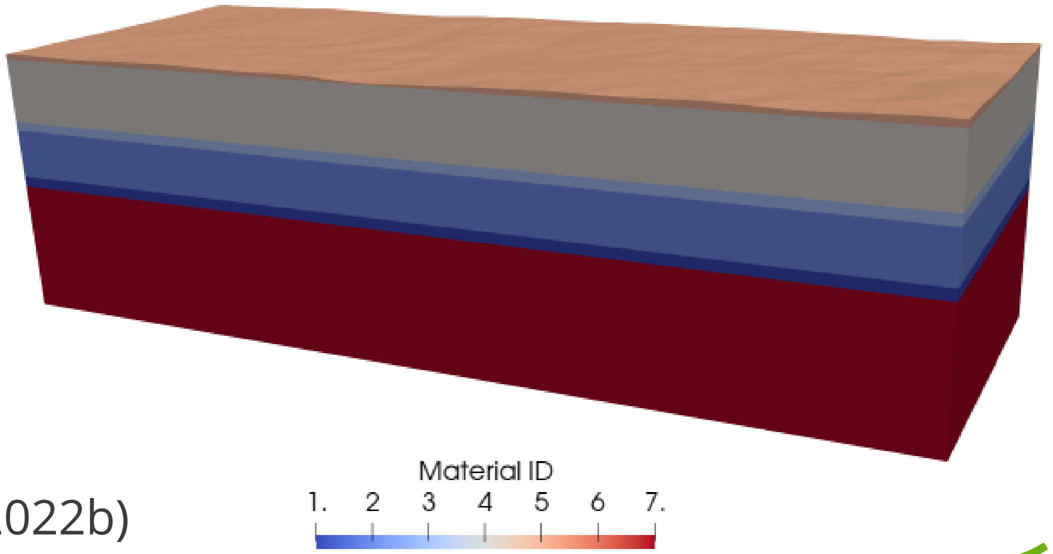


Fully-automated (Python3)

Create mesh (VoroCrust-Meshing)



Create and run simulation (PFLOTRAN)



Partially-automated (Python3)

(LaForce et al. 2022b)

Steps to Automate

- Convert
  - LaGriT stereolithography (.stl) output file to Wavefront object (.obj) file VoroCrust-Meshing input file
  - VoroCrust-Meshing output file (.vcg) to PFLOTRAN explicit unstructured mesh file (.uge) format
- Add monitoring points to PFLOTRAN simulation input file

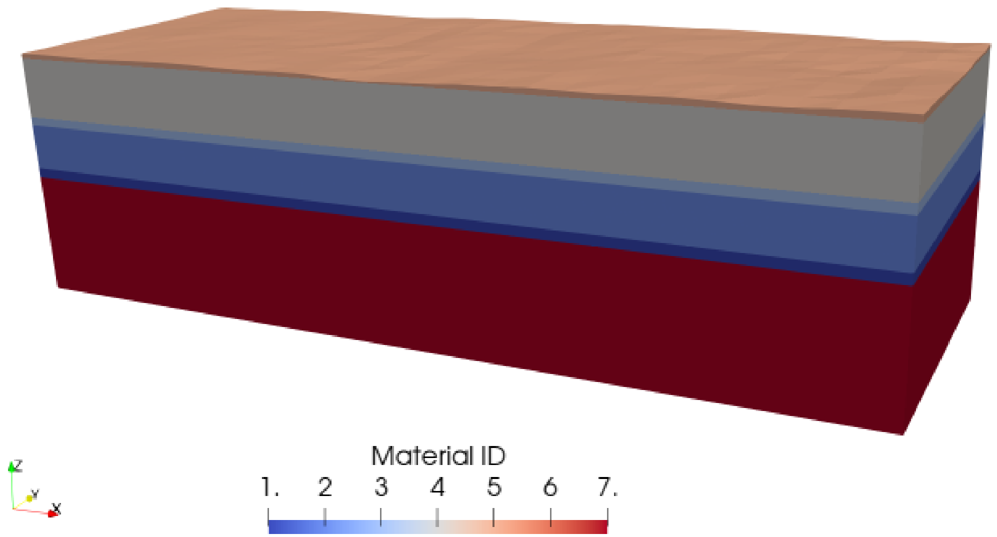
Trivial

- Running VoroCrust-Meshing and PFLOTRAN flow and transport simulations
  - Meshing took 3-15 hours on workstation
  - Simulations took 1-3 hours on super-computer

Requires queueing system for multiple realizations

Mesh 1 Statistics

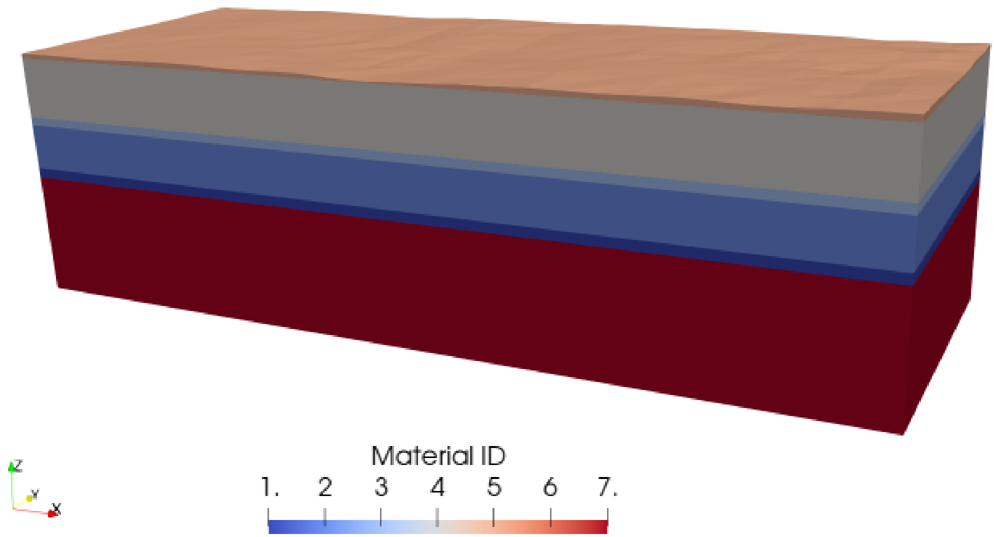
- Largest cell: 3.15×10^7 m^3 in Lower Shale
- Smallest cell: 0.478 m^3 in Overburden
- 1.5 million cells



Model Region	Input Volume (m^3)	Meshed Volume (m^3)	Relative difference $\frac{abs(V_{in}-V_m)}{V_{in}}$	Number of Grid Cells
Overburden (ID 5)	6.8390×10^8	6.8353×10^8	5.40×10^{-4}	**295,696**
Host Shale (ID 4)	8.2916×10^9	8.2912×10^9	4.28×10^{-5}	**642,293**
Silty Shale (ID 3)	1.2143×10^9	1.2142×10^9	9.88×10^{-5}	**94,481**
Underlying Shale (ID 2)	6.2624×10^9	6.2619×10^9	7.82×10^{-5}	**129,830**
Limestone (ID 1)	1.3601×10^9	1.3600×10^9	9.56×10^{-5}	**78,848**
Lower Shale (ID 7)	1.6878×10^{10}	1.6872×10^{10}	3.08×10^{-4}	**65,056**
Repository (ID 6)	3.7515×10^7	3.7509×10^7	1.65×10^{-4}	**221,284**
Full Model	3.4727×10^{10}	3.4721×10^{10}	1.92×10^{-4}	**1,527,491**

PFLOTRAN Simulation Model

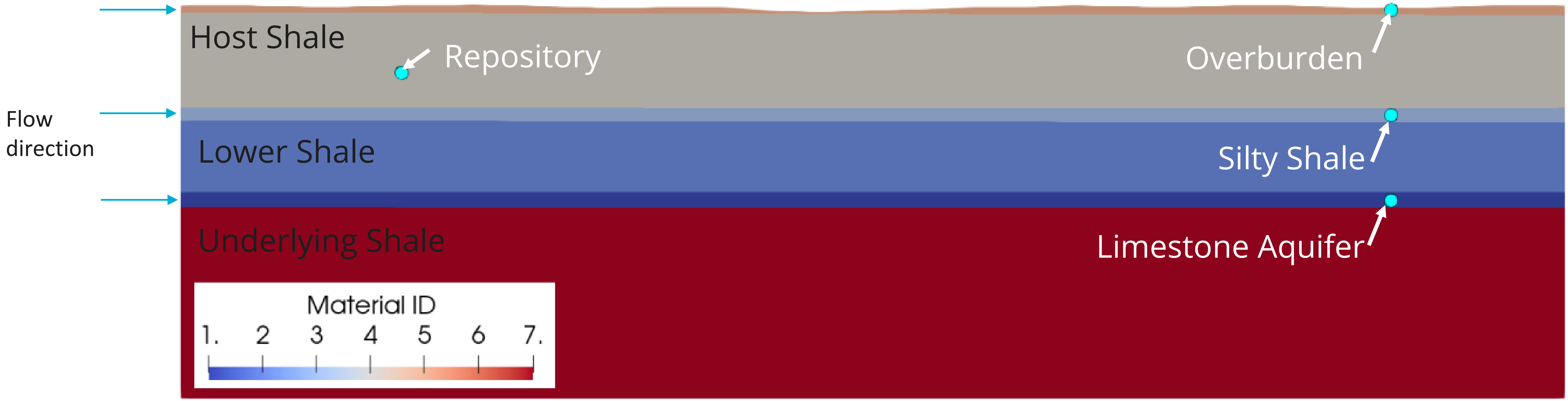
- 7,000 × 2,500 × ~1,200 m
- Geological realization ID: 72
- Four additional sampled parameters
- Tracer source is hypothetical waste repository
  - Dimensions are 1640 × 1525 × 15 m
  - Depth: 250 m to 400 m
- Tracer properties
  - Released at time t = 0 years
  - Properties representative of ^{129}I
  - Decay and adsorption neglected
- Simulations are fully saturated and isothermal (GENERAL MODE)



Model Region	Permeability (m^2)	Porosity
Overburden (ID 5)	1.65×10^{-15} *	0.20
Host Shale (ID 4) and Underlying Shale (ID 2)	1.00×10^{-19}	0.196 *
Silty Shale (ID 3)	1.56×10^{-17} *	0.20
Lower Shale (ID 7)	1.00×10^{-20}	0.10
Limestone (ID 1)	2.18×10^{-16} *	0.10
Repository (ID 6)	1.00×10^{-20}	0.35
*sampled		

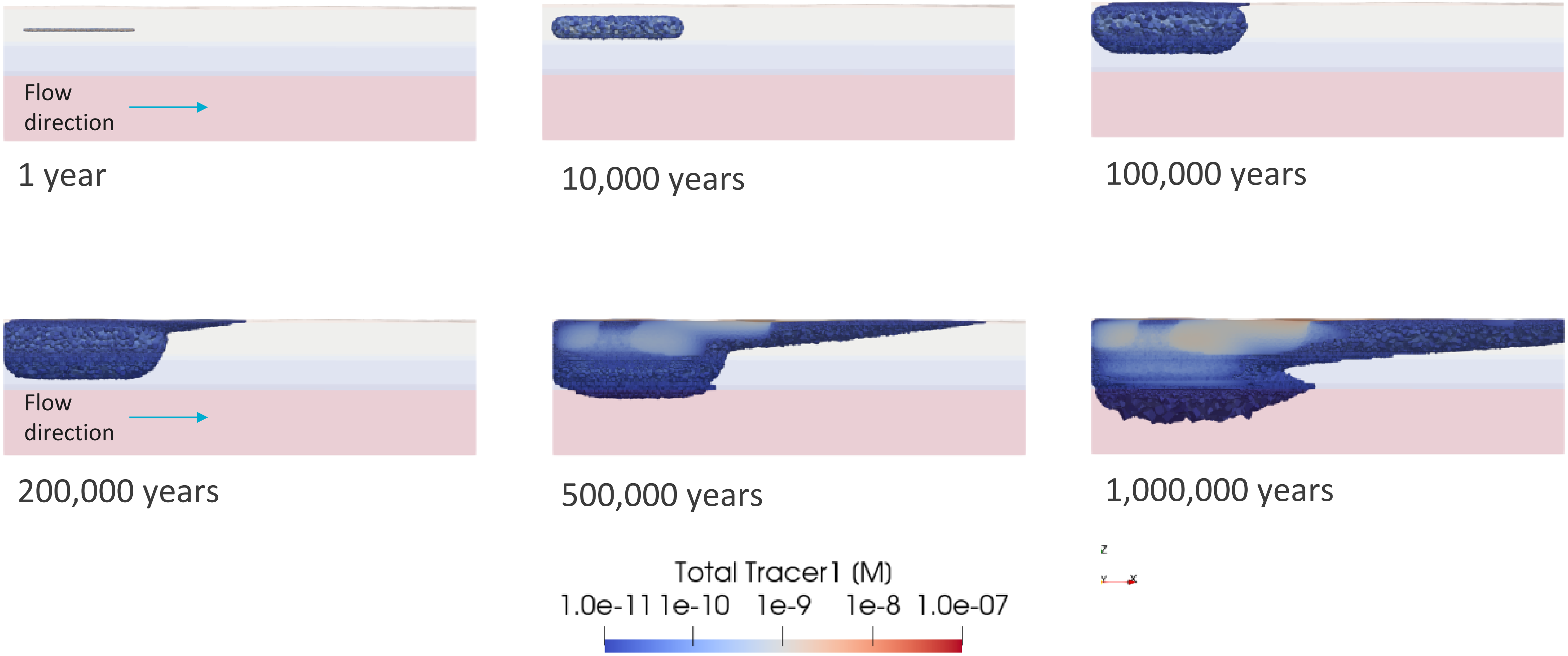
Monitoring Locations

- Groundwater flow in x-direction with head gradient 0.0021 m/m
- Tracer concentration is monitored at blue points shown
  - Three monitoring points 5 km downstream of the repository in potential flow intervals
  - One monitoring point is in the center of the repository
- Average tracer concentration in the repository volume is also monitored

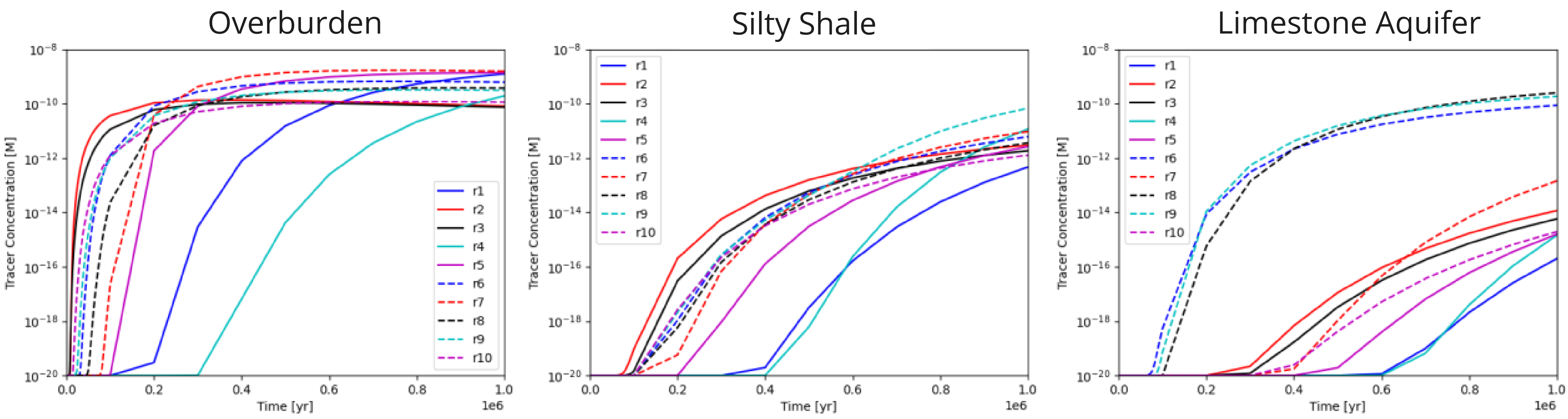


Mesh 1 Tracer Transport Results

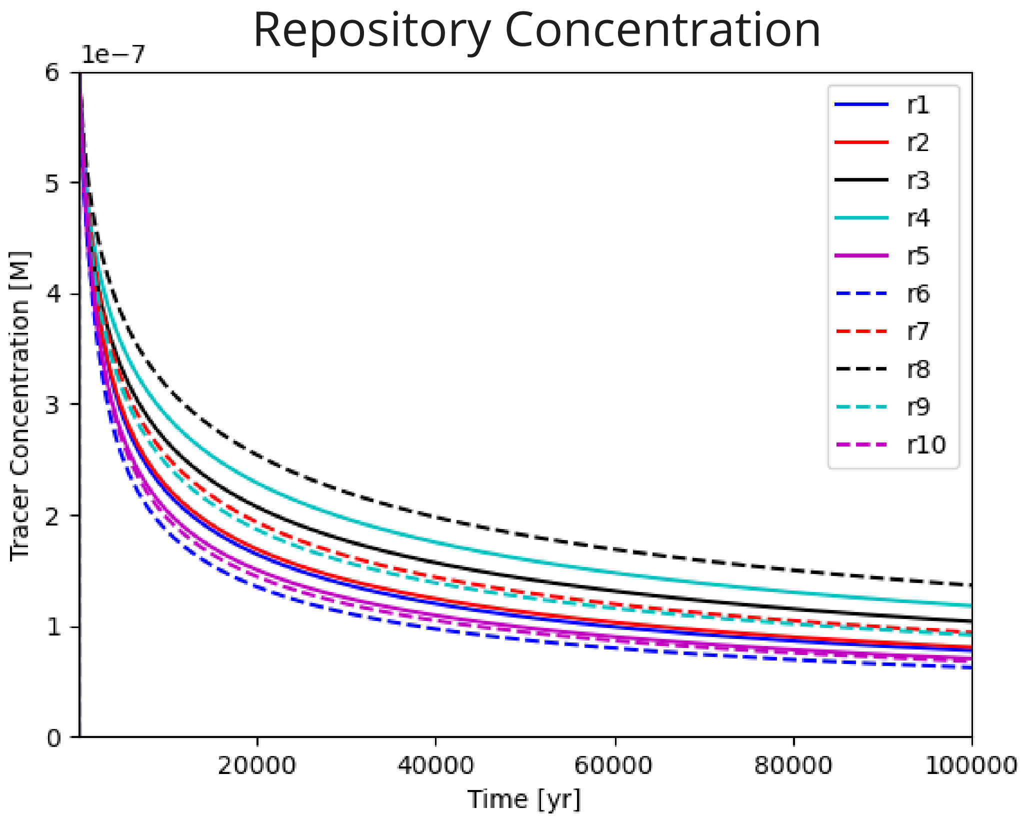
Tracer concentrations above 1×10^{-11} (M) are overlain on the full model colored according to Material ID

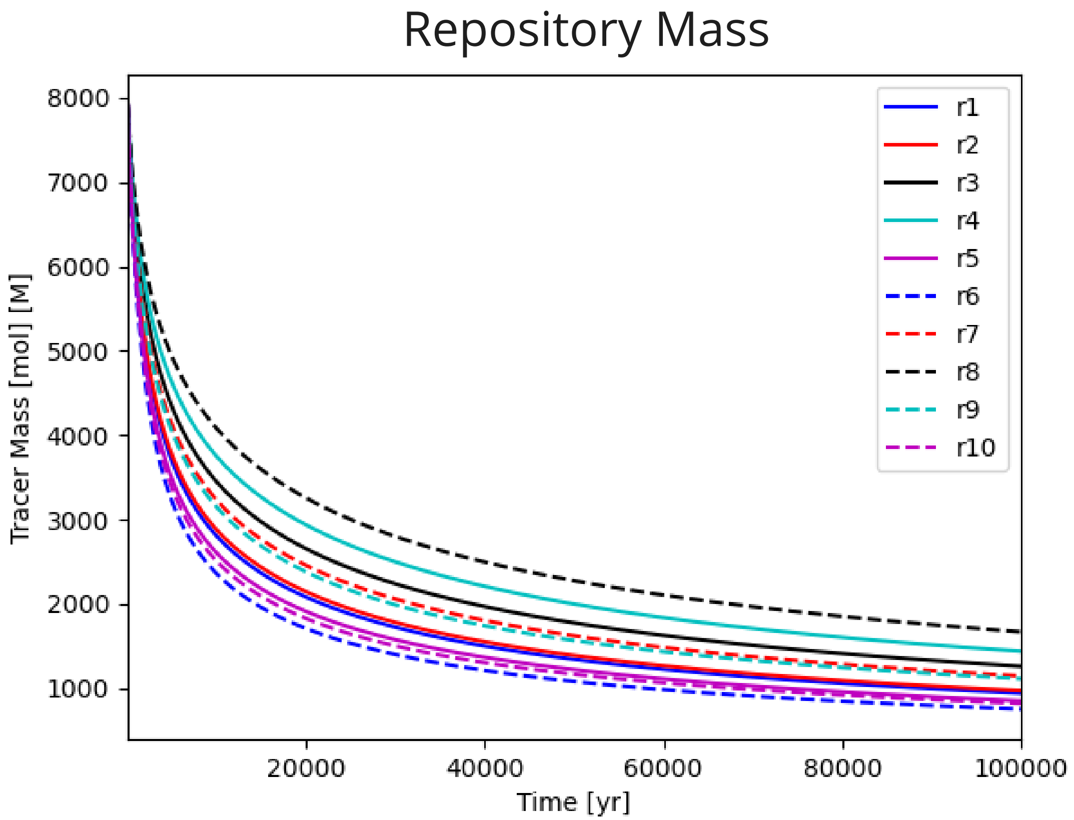


Probabilistic Results: Downstream



Probabilistic Results: In the Repository





Conclusions

- Meshes were generated and simulations run on 10 stochastically-generated realizations of a geological model for tracers released from a hypothetical waste repository
- Simulated tracer concentration downstream and in the repository is produced for all realizations
- Most of the process is automated:
  - Sampling realizations
  - Clipping geological surfaces to realization, building volumes to mesh
  - Creating simulation input decks for each mesh populated with 4 sampled flow parameters
  - Creating meshing input deck and creating mesh from input volumes
- Some pieces require additional work:
  - **Easy**: File conversions, adding monitoring points to simulation
  - **More Challenging**: queueing system for multiple realizations in parallel

Future work

Immediate future:

- Open-source version of the meshing software so entire workflow utilizes free and open-source software

Medium term:

- Full automation using Sandia's Next Generation Workflow
- Complete uncertainty quantification and sensitivity analysis including
  - Thermal and two-phase flow effects
  - Impact of mesh realization/discretization
  - Geological uncertainty

Longer term:

- Mesh repository features in detail
- Mesh faults that terminate within the model
- Anisotropic meshing to reduce element numbers

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