



INCORPORATING GEOLOGICAL STRUCTURE INTO SENSITIVITY ANALYSIS OF CONTAMINANT TRANSPORT MODELING

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Motivation:

Simulating subsurface contaminant transport at the kilometer-scale often entails modeling reactive flow and transport within and through complex geological structures. These structures are difficult to mesh and as a result geologic structure is typically represented by one or a few deterministically generated meshes for uncertainty studies. Uncertainty in geologic structure can have a significant impact on contaminant transport and should be fully incorporated within uncertainty quantification (UQ) and sensitivity analysis (SA) for subsurface contaminant modeling.

Workflow:

- I. Single realization of a Pierre Shale Geological Framework Model (GFM) 69 x 83 km.
- II. Pseudo-uncertain models are generated by clipping 7 x 2.5 km sub-models from GFM.
- III. To focus on unknown subsurface, a single known top surface is used for all realizations.
- IV. Mesh and run simulation on models:

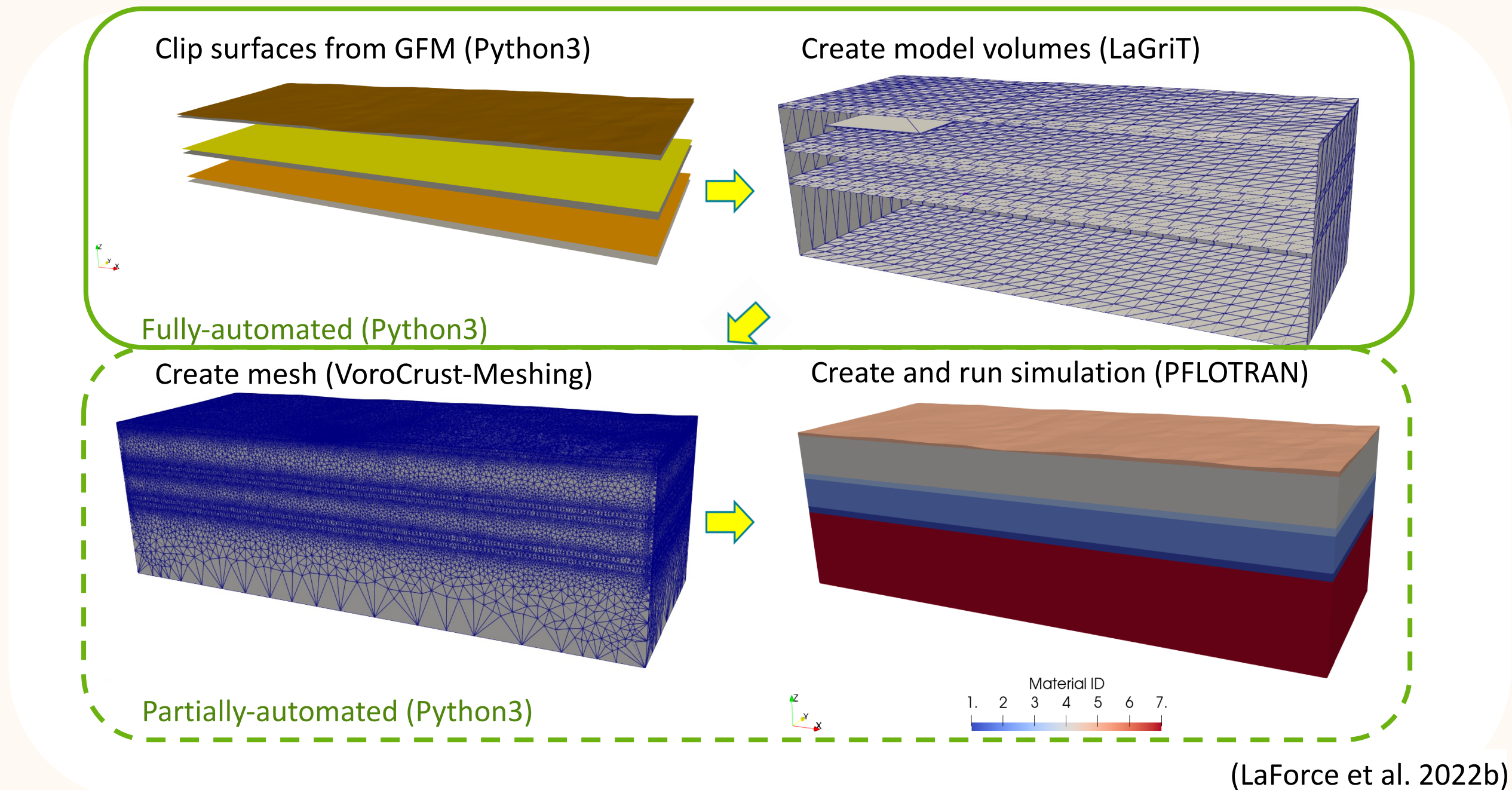


Figure 1: Depiction of the workflow used to create and mesh each realization.

Overview:

An open-source software modeling framework is used to perform a sensitivity analysis on transport of two tracers based on I-129 from a hypothetical radioactive waste repository in a shale host rock with uncertain geologic structure. Uncertain flow parameters are sampled in addition to realization of the geological structural model in a nested SA/UQ analysis. Concentration of the tracers at monitoring points downstream of the repository are used as the quantities of interest for determining model sensitivity to input parameters.

Geological model:

Each 7 x 2.5 x ~1.2 km model with hypothetical radioactive waste repository

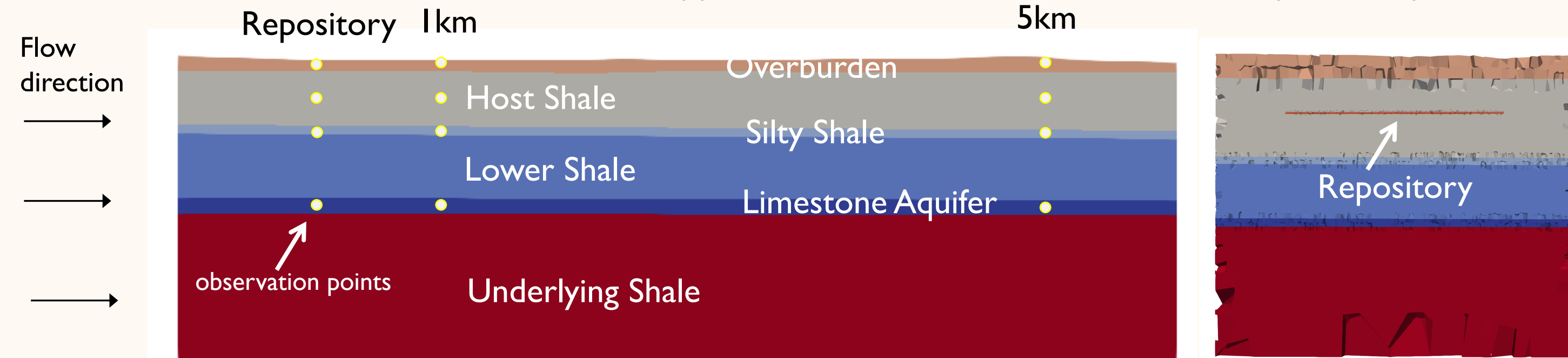


Figure 2: Side profile for realization 1 (left) and y-z plane slice through repository for realization 50 (right) are shown. The flow direction is indicated along with the locations of the monitoring points.

- 100 geological model realizations created, with 1, 50 & 100 chosen for this initial study.
- 30 samples of flow parameters on each realization via Dakota with Latin Hypercube Sampling (LHS) .
- Simulate in PFLOTRAN using a Dakota tool, the Next-Gen Workflow.

Parameter	Range	Units	Distribution
Overburden Permeability	10 ⁻¹⁵ -10 ⁻¹³	m ²	log uniform
Limestone Permeability	10 ⁻¹⁷ -10 ⁻¹⁴	m ²	log uniform
Silty Shale Permeability	10 ⁻¹⁷ -10 ⁻¹⁵	m ²	log uniform
Host Shale Porosity	0.1-0.25	-	uniform

Table 1: Sampled parameters and their distributions.

(LaForce et al. 2022b)

Results:

Final tracer 1 concentrations for all observation points.

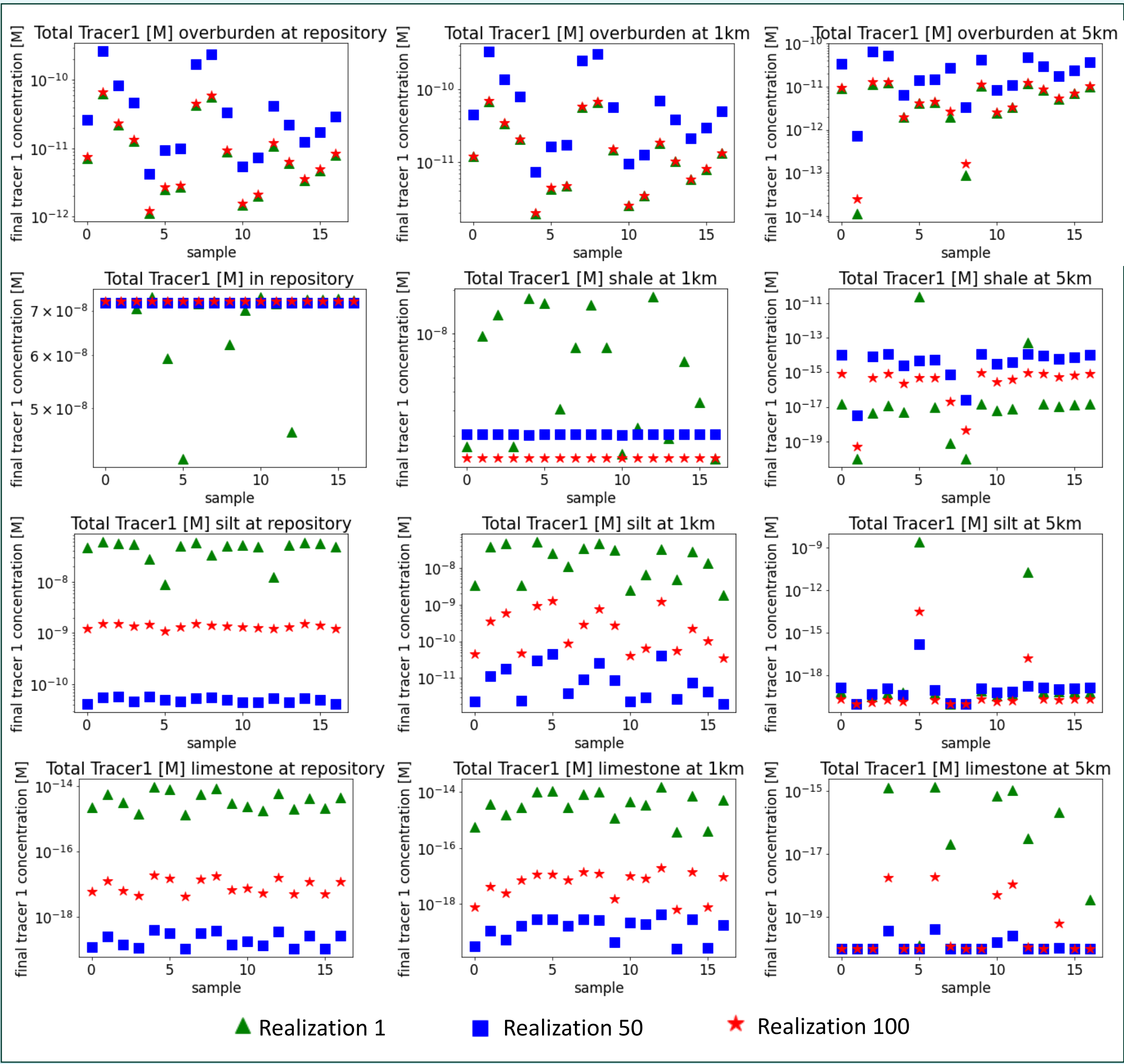


Figure 3: Semi-logarithmic plots of Tracer 1 concentration at final time, 10⁶ years, at all observation points for 17 samples.

Temperature at times 1000 & 10000 years.

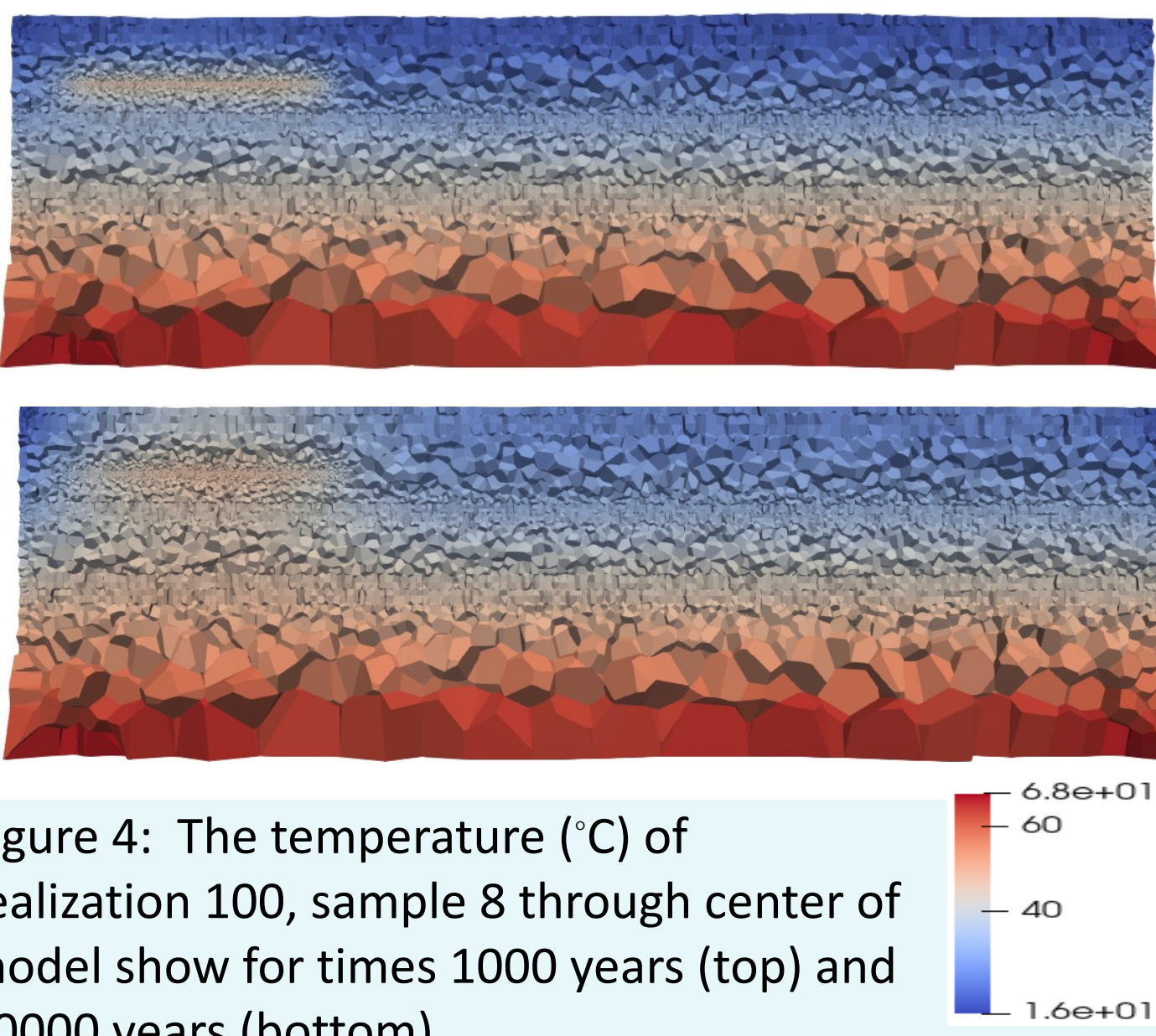


Figure 4: The temperature (°C) of realization 100, sample 8 through center of model show for times 1000 years (top) and 10000 years (bottom).

Summary:

- Overburden layer concentrations are sensitive to flow parameters, especially for realization 50.
- Tracer 1 concentration levels are more sensitive to variations in flow parameters for realization 1 than the other two realizations at observation points in the Silty Shale (silt), Host Shale (shale) and Limestone Aquifer (limestone).
- Further studies and analysis are planned.

Challenges

- Large unstructured meshes ~10⁶ cells.
- Statistically significant SA/UQ studies require a lot of time and computing power.

Future Work

- Statistical analysis of results
- Additional geologic realizations (already created) & geologic settings
- Improve flexibility and robustness of workflow

References

- I. LaForce T, Basurto E, Chang K W, Ebeida M, Eymold W, Faucett C, Jayne R S, Kuchinski N, Leone R C, Perry F (2022b) GDSA Repository Systems Analysis investigations in FY2022. Technical report, Sandia National Lab.(SNLNM), Albuquerque, NM
- II. Mariner, P. E., Stein, E. R., Frederick, J. M., Sevougian, S. D., and Hammond, G. E. (2017). *Advances in Geologic Disposal System Modeling and Shale Reference Cases*. SFWD-SFWST-2017-000044 / SAND2017-10304R. Sandia National Laboratories, Albuquerque, NM.

Resources

pflotran.org, vorocrust.sandia.gov, dakota.sandia.gov