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INCORPORATING GEOLOGICAL STRUCTURE INTO SENSITIVITY ANALYSIS OF CONTAMINANT TRANSPORT MODELING

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Motivation:

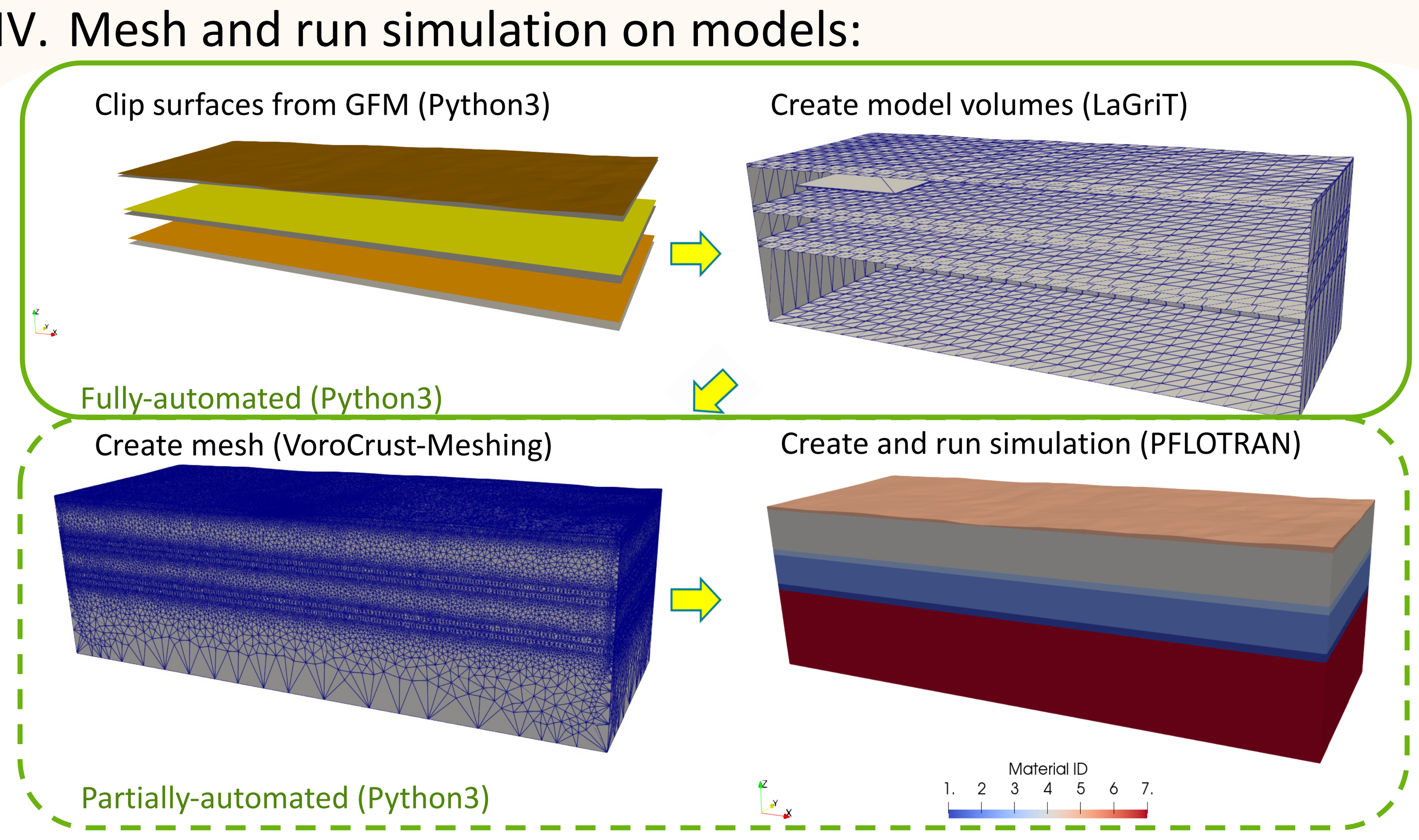
Simulating subsurface contaminant transport at the kilometer-scale often entails modeling reactive flow and transport within and through complex geological structures. These structures are difficult to mesh and as a result geologic structure is typically represented by one or a few deterministically 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.

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.

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 × 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:



(LaForce et al. 2022b)

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

Geological model:

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

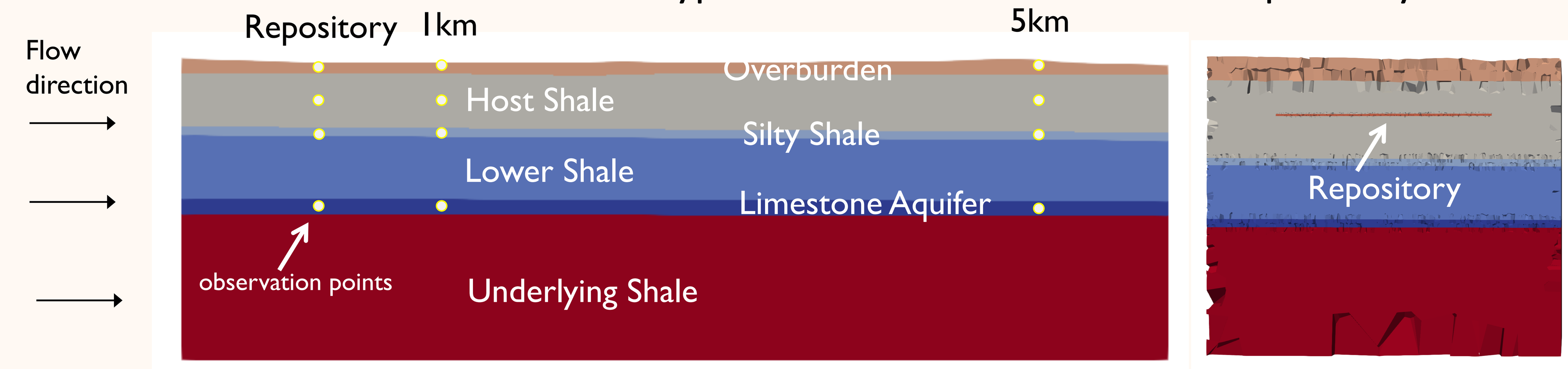


Figure 2: Side profile for realization 1 (left) and y-z plane slice through repository for realization 50 (right) are shown. The flow direction is indicated along with the locations of the monitoring points.

- 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.

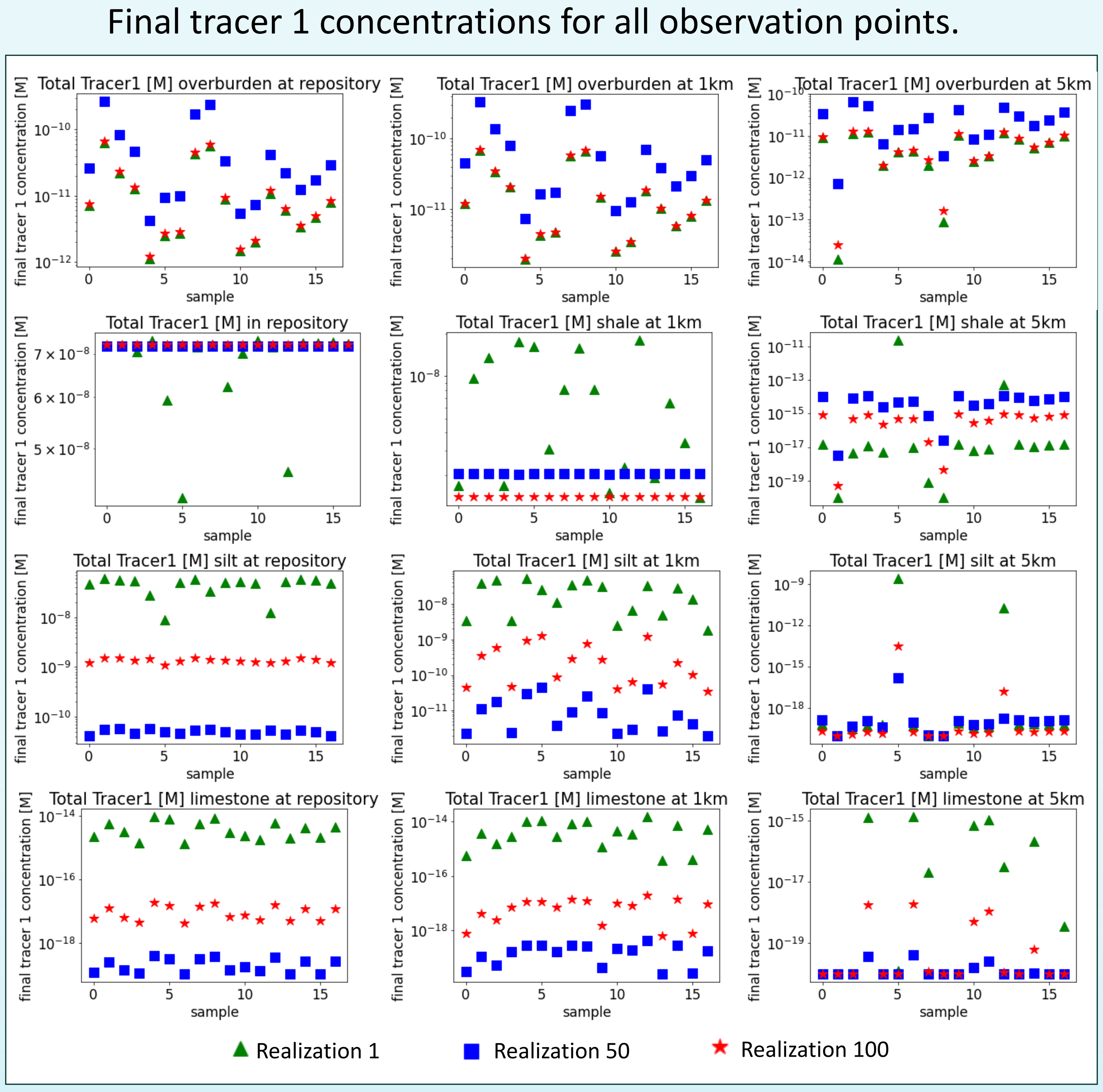


Figure 3: Semi-logarithmic plots of Tracer 1 concentration at final time, 10^6 years, at all observation points for 17 samples.

Temperature at times 1000 & 10000 years.

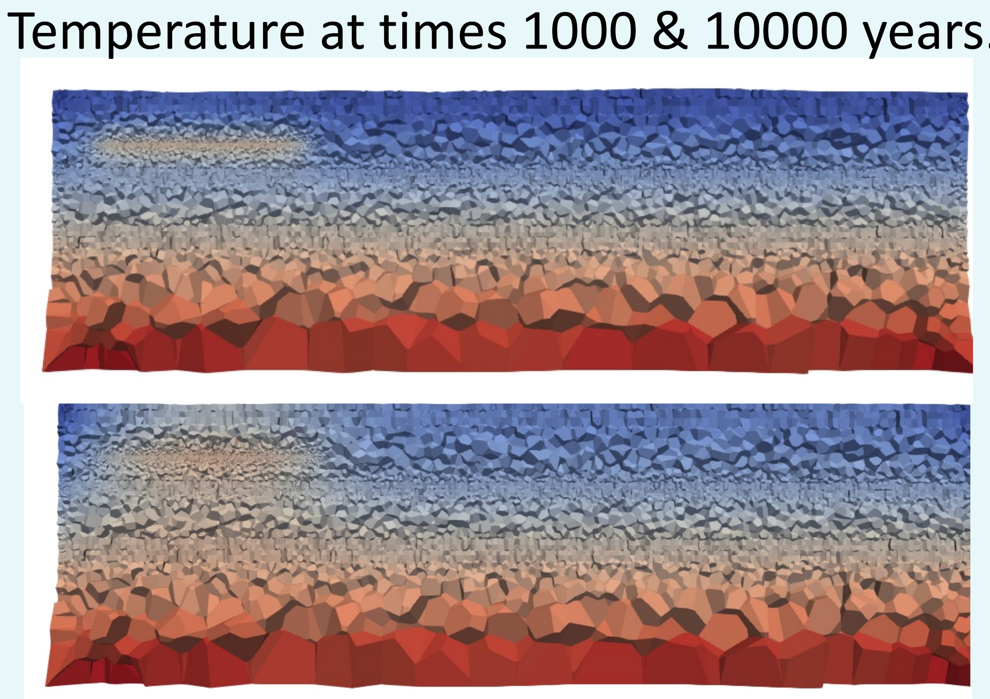


Figure 4: The temperature (°C) of realization 100, sample 8 through center of model show for times 1000 years (top) and 10000 years (bottom).

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 ~10^6 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

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SAND2023-04997C

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