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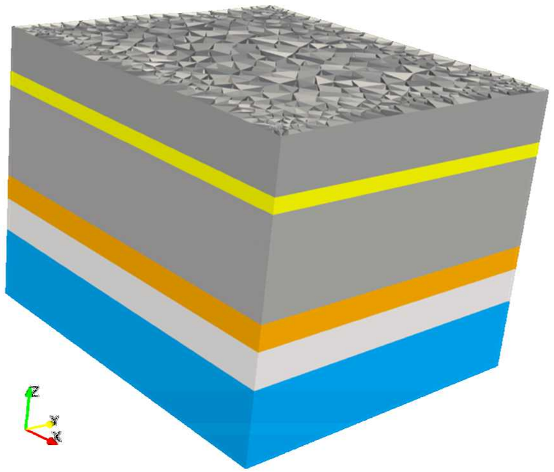
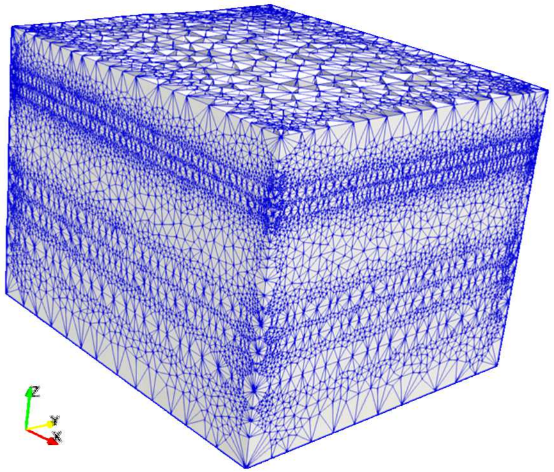
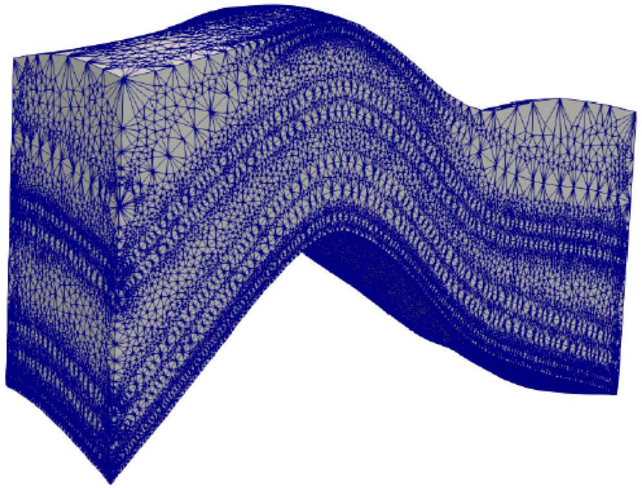






LANL/SANDIA/VOROCRUST EOFY 2020 meeting

Tara LaForce

SAND Number: SAND2020-XXXX

Agenda

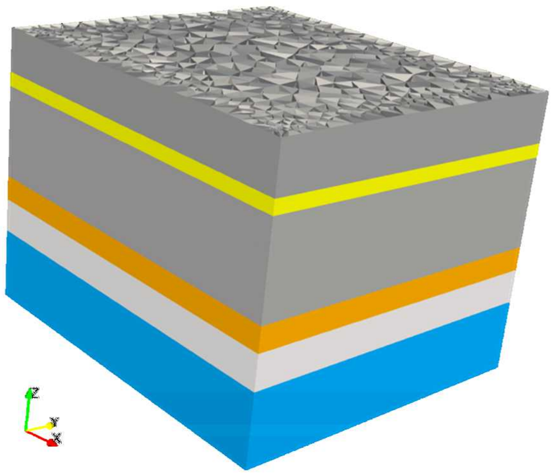
VOROCRUST (9-12)

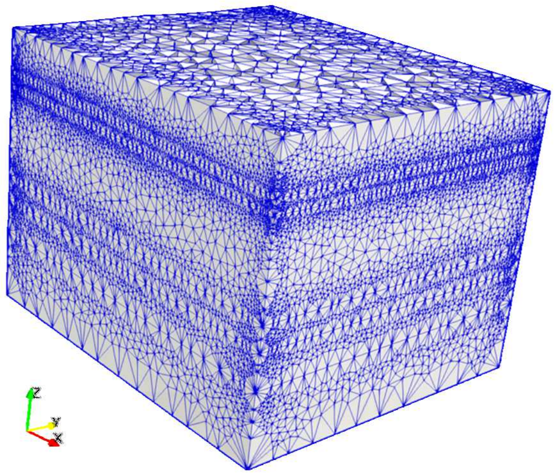
- 9-9:15 Tech set up and welcome
- 9:15-10:00 Mohamed Ebeida
- 10:00-10:20 Tara LaForce
- 10:20-10:50 Phil Stauffer
- 10:50-11:10 Terry Miller
- 11:10-12:00 Discussion and planning for next FY

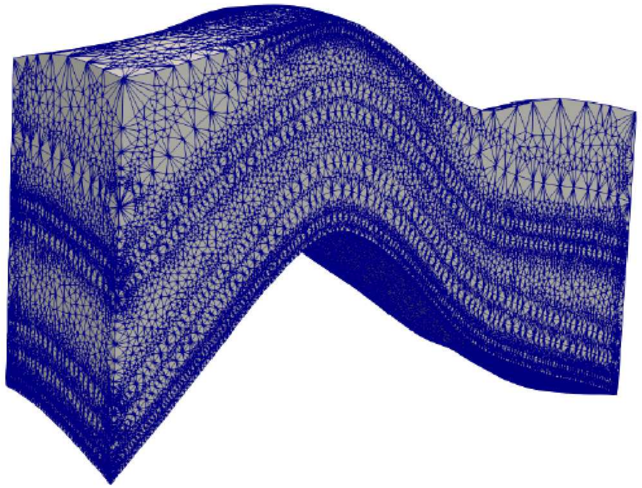
- Lunch (12-13:30)

Geology (13:30-16:30)

- 13:30-13:50 Michael Gross -Overview
- 13:50-14:10 Liz Miller
- 14:10-14:30 Erika Swanson
- 14:30-14:50 Damien Milazzo
- 14:50-15:20 Frank Perry
- 15:20-15:50 Tessica Oldemeyer and Glenn Russell
- 15:50-16:30 Discussion and planning for next FY







PFLOTRAN simulations on VOROCRUST meshes

Tara LaForce, Spencer Jordan, Mohamed Ebeida, William Mclendon

SAND Number: SAND2020-XXXX

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Workflow

LaGriT

- Create volumes or read in GFM software surfaces
- Generate surface mesh
- Export as .stl file

ParaView

- Import .stl file
- Export as .obj file

- Visualize output

Vc

- Import .obj file
- Create Voronoi mesh(s)
- Export .vcg file containing all the grid information needed by PFLOTRAN

python™

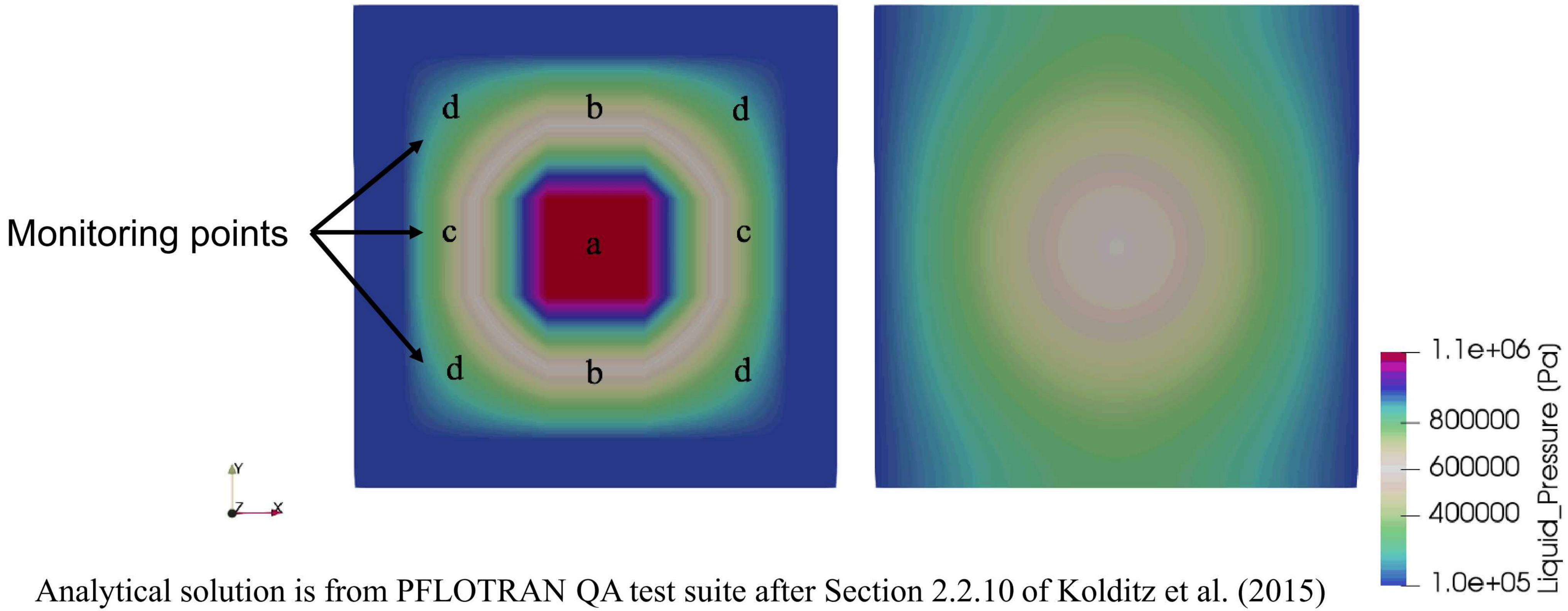
- Read .vcg file and export PFLOTRAN:
    - mesh.uge file
    - Boundary .ex files (aligned to axes only)
    - Material ID file

PFLOTRAN

- Import mesh.uge, boundary.ex, and MatID.h5 files
- Run simulation

Benchmark 1: Single-Phase Pressure

Figure 6-7 Pressure on the plane z=0.5 for the Richards Equation test problem on a 380x380x3 cell structured domain. Left: Initial pressure condition. Right: Pressure at t=0.1 days.

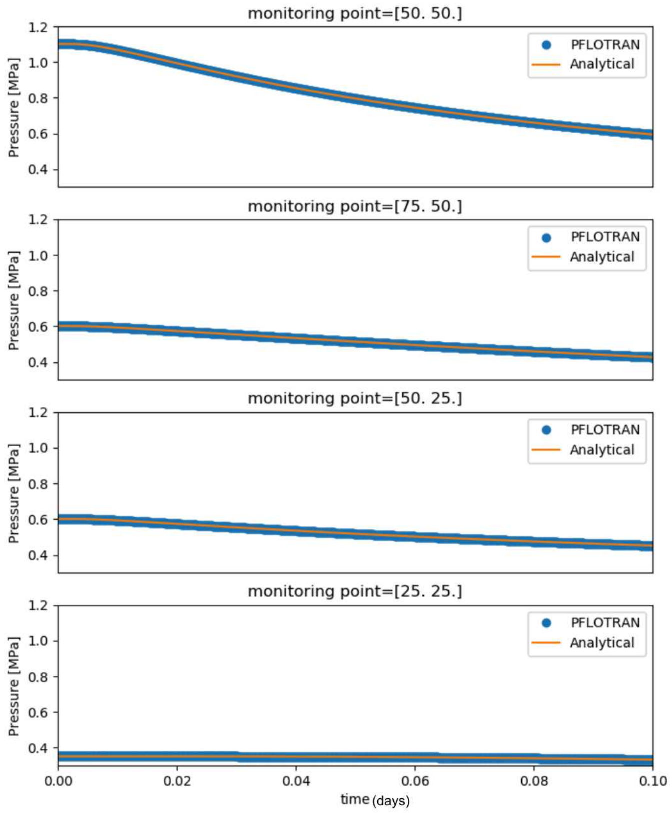


Analytical solution is from PFLOTRAN QA test suite after Section 2.2.10 of Kolditz et al. (2015)

Kolditz, O., Shao, H., Wang, W., and Bauer, S., 2015. *Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media: Modelling and Benchmarking Closed-Form Solutions* (O. Kolditz, H. Shao, W. Wang, & S. Bauer Eds.). Switzerland: Springer International Publishing.

Benchmark 1: Single-Phase Pressure

- Five realizations of the Voronoi meshes are created
- Hexagonal mesh of similar size is used as benchmark

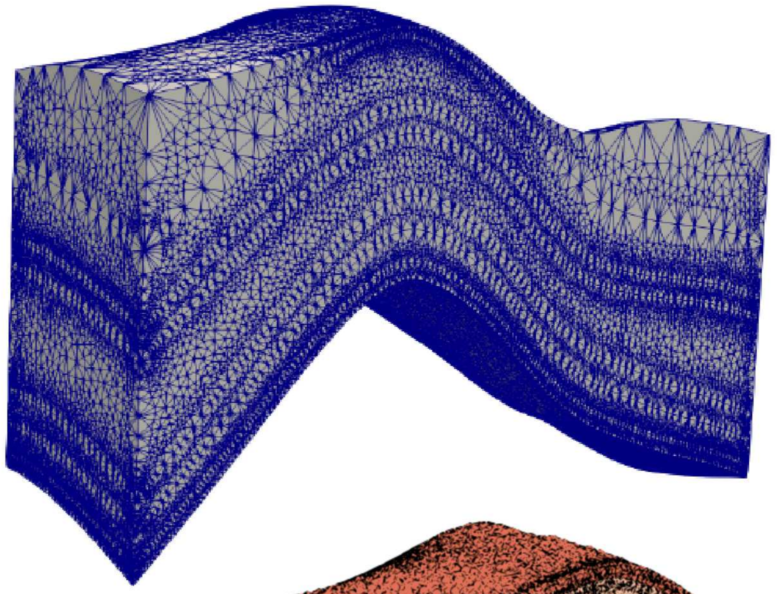


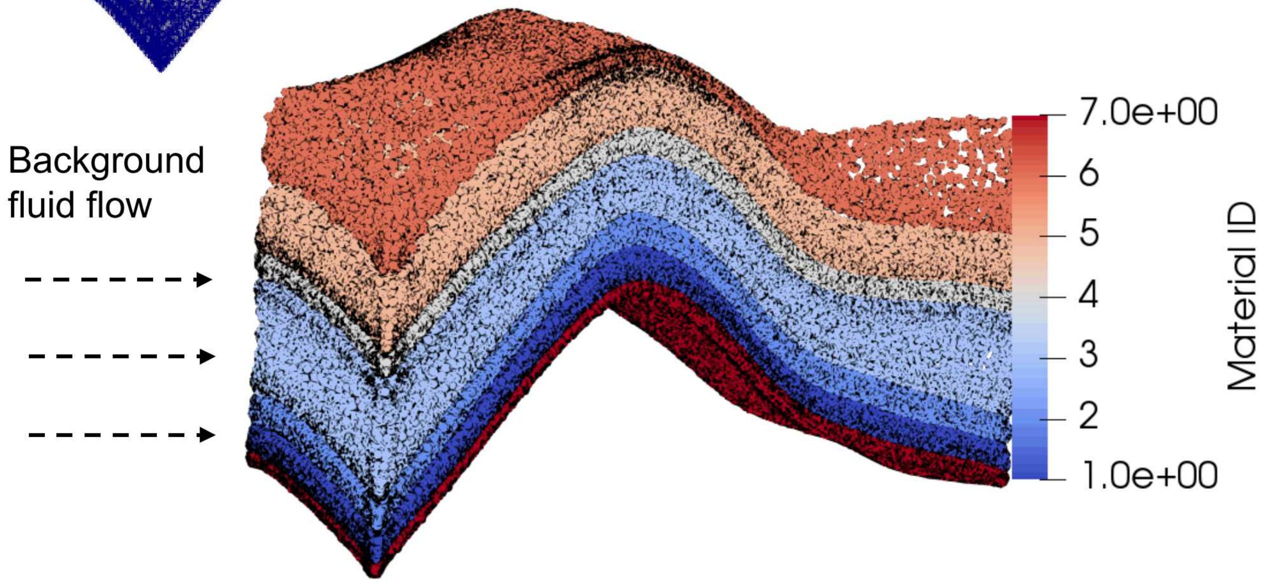
Mesh name	Number of cells	Monitoring points	Max error	Simulation time (min)
Structured	433,200	a (50.132, 50.132, 0.5), b (50.132, 75.132, 0.5), c (75.132, 50.132, 0.5), d (75.132, 75.132, 0.5)	0.045%	8.49
Voro2	432,941	b (50, 25, 0.5), d (25, 25, 0.5)	0.025%	20.8
Voro3	432,486	a (50, 50, 0.5), b (50, 25, 0.5), c (75, 50, 0.5), d (25, 25, 0.5)	0.043%	19.6
Voro4	432,102	a (50, 50, 0.5), b (50, 75, 0.5), d (75, 75, 0.5)	0.040%	22.2
Voro5	432,259	b (50, 25, 0.5), c (75, 50, 0.5), d (75, 75, 0.5)	0.043%	21.6
Voro6	431,656	a (50, 50, 0.5), d (75, 75, 0.5)	0.041%	21.3

New Wyoming Uplift Simulation

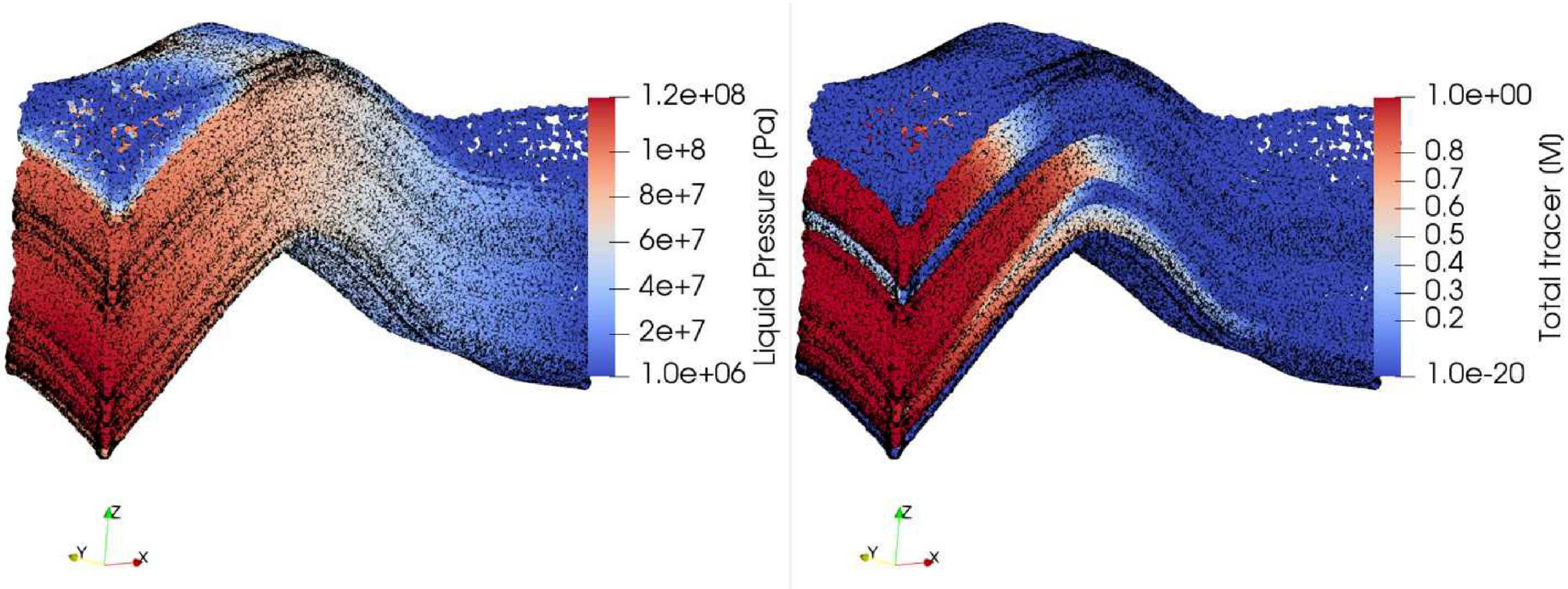
- Surfaces used are from: https://github.com/lanl/VoroCrust/tree/master/examples/Slope_Tests/uplift_slopes/7layers_6x
- 6x vertical exaggeration
- 204,965 cells
- Tracer flow from left to right

Layer Number	Permeability [m^2]	Porosity
1	$1x10^{-12}$	0.1
2	$1x10^{-13}$	0.15
3	$1x10^{-12}$	0.2
4	$1x10^{-14}$	0.15
5	$1x10^{-12}$	0.3
6	$1x10^{-18}$	0.01
7	$1x10^{-18}$	0.01





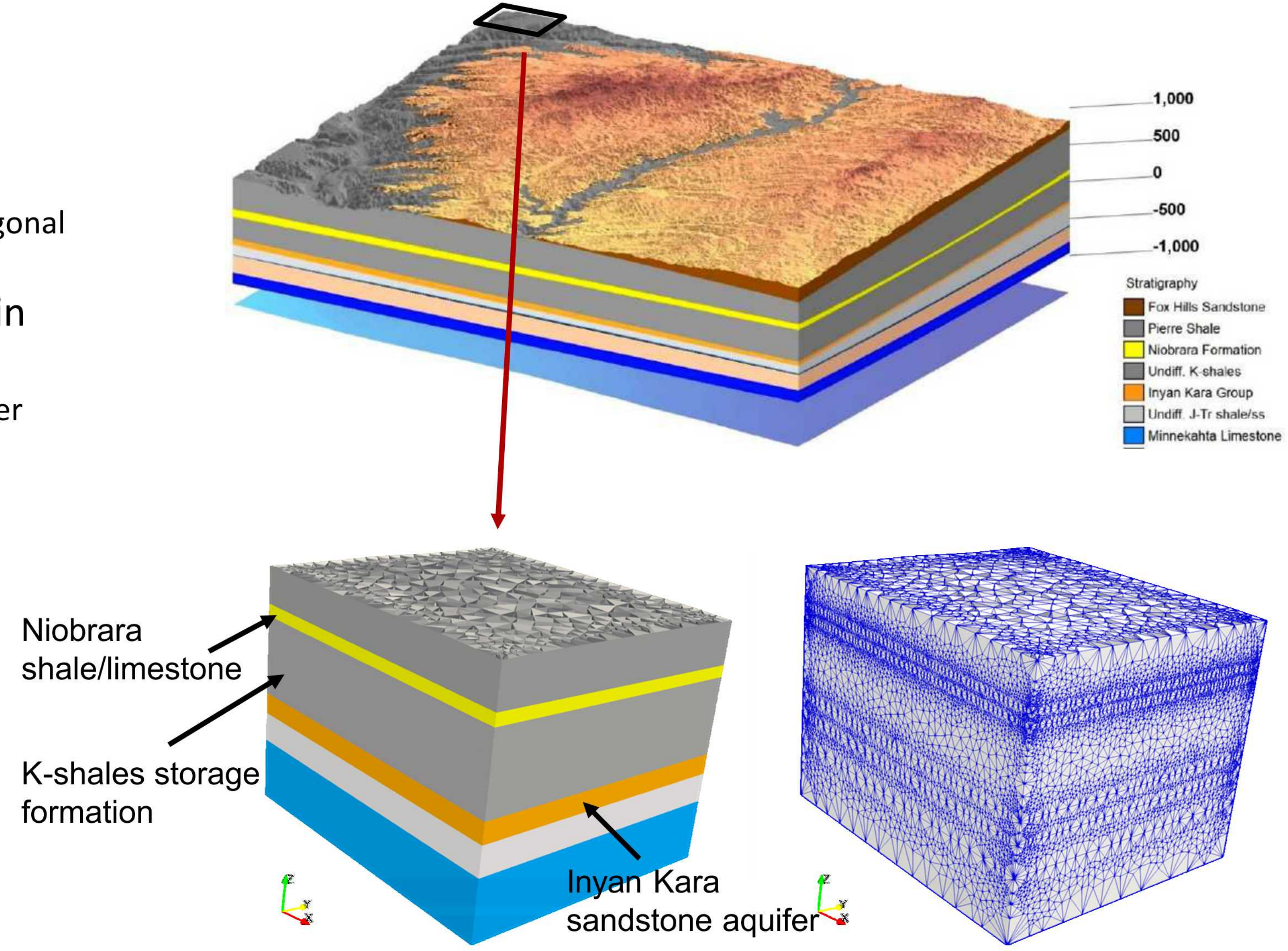
Wyoming Uplift Simulation



Shale Geological Framework Model Simulation

- In Sevougian et al. (2019)
  - Shale GFM was presented
  - An attempt was made to mesh it using hexagonal meshing software
- A simplified sector model was meshed in VOROCRUST
  - 1.75x2.0 km rectangle of southwestern corner
  - 101,319 cells
- Simulations of a tracer release from an underground source were conducted

Formation	Permeability [m^2]	Porosity
Pierre	1×10^{-19}	0.2
Niobrara	1×10^{-14}	0.4
K-Shales	1×10^{-20}	0.2
Inyan Kara	1×10^{-13}	0.2
J/T Shales	1×10^{-20}	0.2
Minnekahta/base	1×10^{-12}	0.1

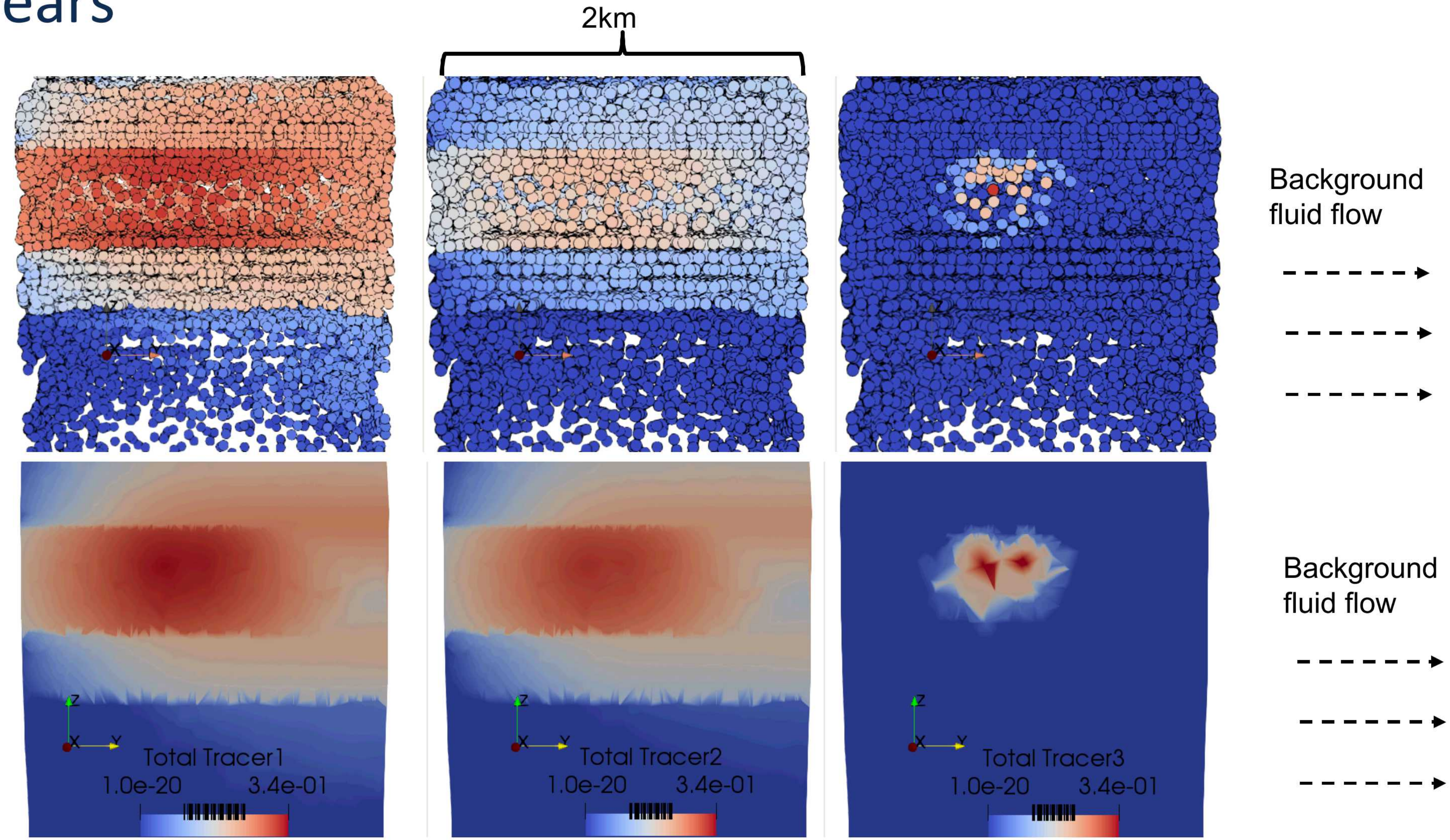


Sevougian, S. D., Stein, E. R., LaForce, T., Perry, F. V., Nole, M., Haukwa, C. B., and Chang, K. W., 2019b. *GDSA Repository Systems Analysis FY19 Update*. SAND2019-11942R. Sandia National Laboratories, Albuquerque, New Mexico, Sept 27, 2019.

Shale GFM Simulation: slice through the source after 100,000 years

Visualized as dots

Visualized using Paraview DELAUNAY 3D tessellation



Inert tracer

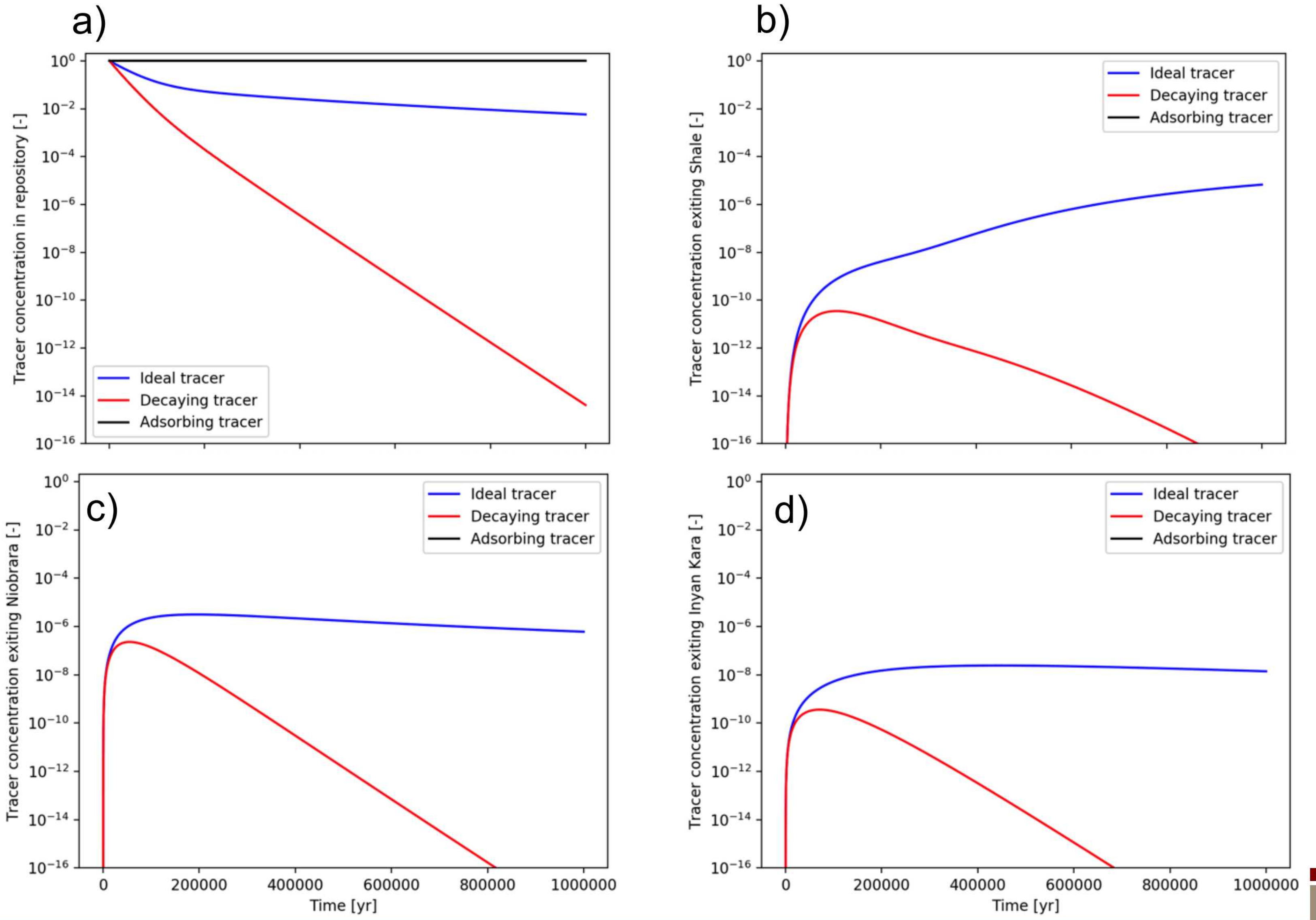
Tracer with decay rate of Pu239

Tracer with adsorption of U in shale

Shale GFM Simulation: Monitoring Points

a) In repository
b) In shale downstream
c) In Niobrara downstream
d) In Inyan Kara downstream

Figure 6-23 Tracer concentrations as a function of time at four monitoring points in the shale GFM sector model. Top Left: In the K-shale at the tracer source. Top Right: In the K-shale at the model boundary immediately downstream of the tracer source. Bottom Left: In the Niobrara aquifer at the model boundary immediately downstream of the tracer source. Bottom Left: In the Inyan Kara aquifer at the model boundary immediately downstream of the tracer source. Notice that the x-scale is logarithmic.



Observations and Conclusions

- Simulations on VOROCRUST meshes:
  - High quality as PFLOTRAN simulations rigorously converge to analytical models
  - Reproducible with similar errors for many realizations
- Possible to mesh and run simulations on GFM models

Future Work

- Need Exodus output for visualization
- Need to be able to mesh interior volumes (e.g. a thousand waste packages) without generating large numbers of grid cells
- Issues with meshing poor-aspect ratio regions remain

- Paper in progress that is focused on simulations using Voronoi meshes
  - Revisit two of the test cases from FY19 reports
  - Revisit two-domain heating benchmark from FY20 RSA report
  - One of:
    - Natural gas storage in Wyoming uplift (it's the easiest 2-phase problem I could think of)
    - Revisit high permeability CO_2 storage from Stauffer et al. (2009) (more interesting but harder in PFLOTRAN)
  - Shale GFM model done correctly with repository region as source for radionuclides

Stauffer, P.H., Surdam, R.C., Jiao, Z., Miller, T.A. and Bentley, R.D., 2009. Combining geologic data and numerical modeling to improve estimates of the CO2 sequestration potential of the Rock Springs Uplift, Wyoming. *Energy Procedia*, *1*(1), pp.2717-2724.