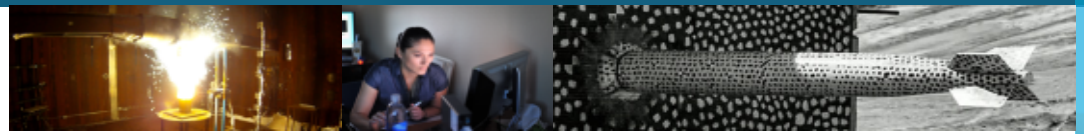
SAND2021-14106C

Sandia National Laboratories

Task F – Salt PA Modeling Approach



Rick Jayne
Sandia National Laboratories
Fall DECOVALEX Meeting 2021

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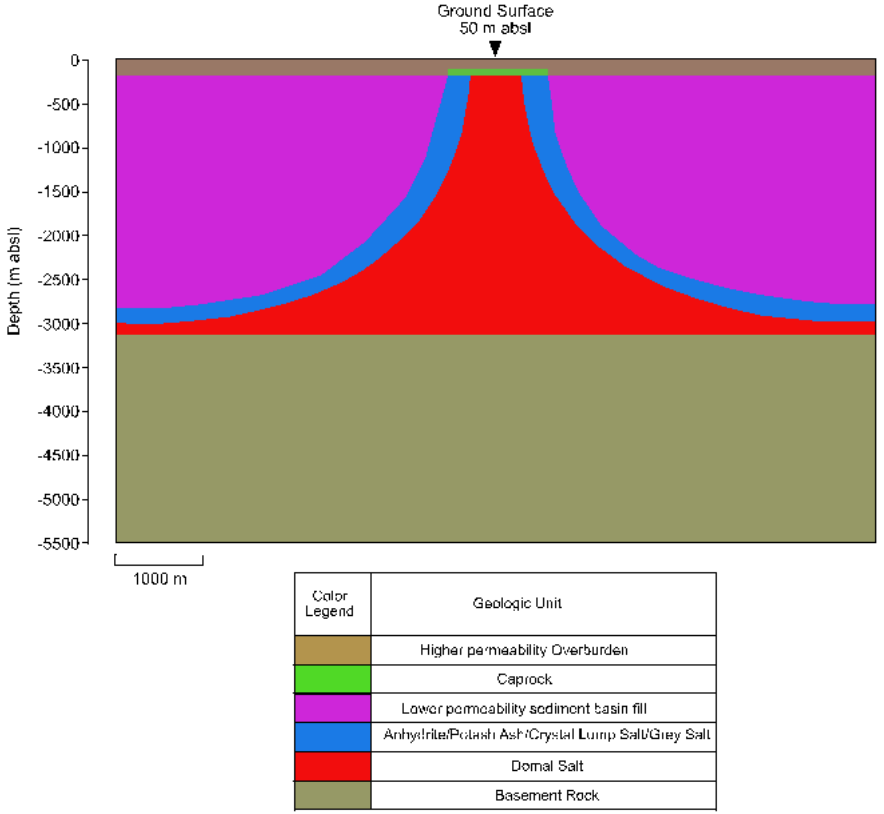
Overview

- Meshing Scheme
  - LaGrit
  - Vorocrust
- Material Properties
- Initial Conditions
- Preliminary Results
  - Pressure and Saturation @ 100 years



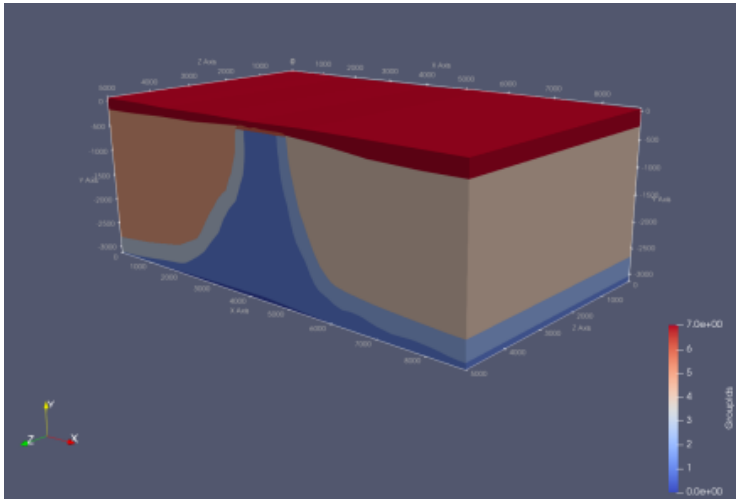
Modeling Approach

LaGrit

- Create surfaces for Vorocrust input

Vorocrust

- First provably correct algorithm for conforming Voronoi meshing of non-convex and non-manifold domains
- Smaller selection of output file types
- Outputs = Voronoi mesh for PFLOTRAN



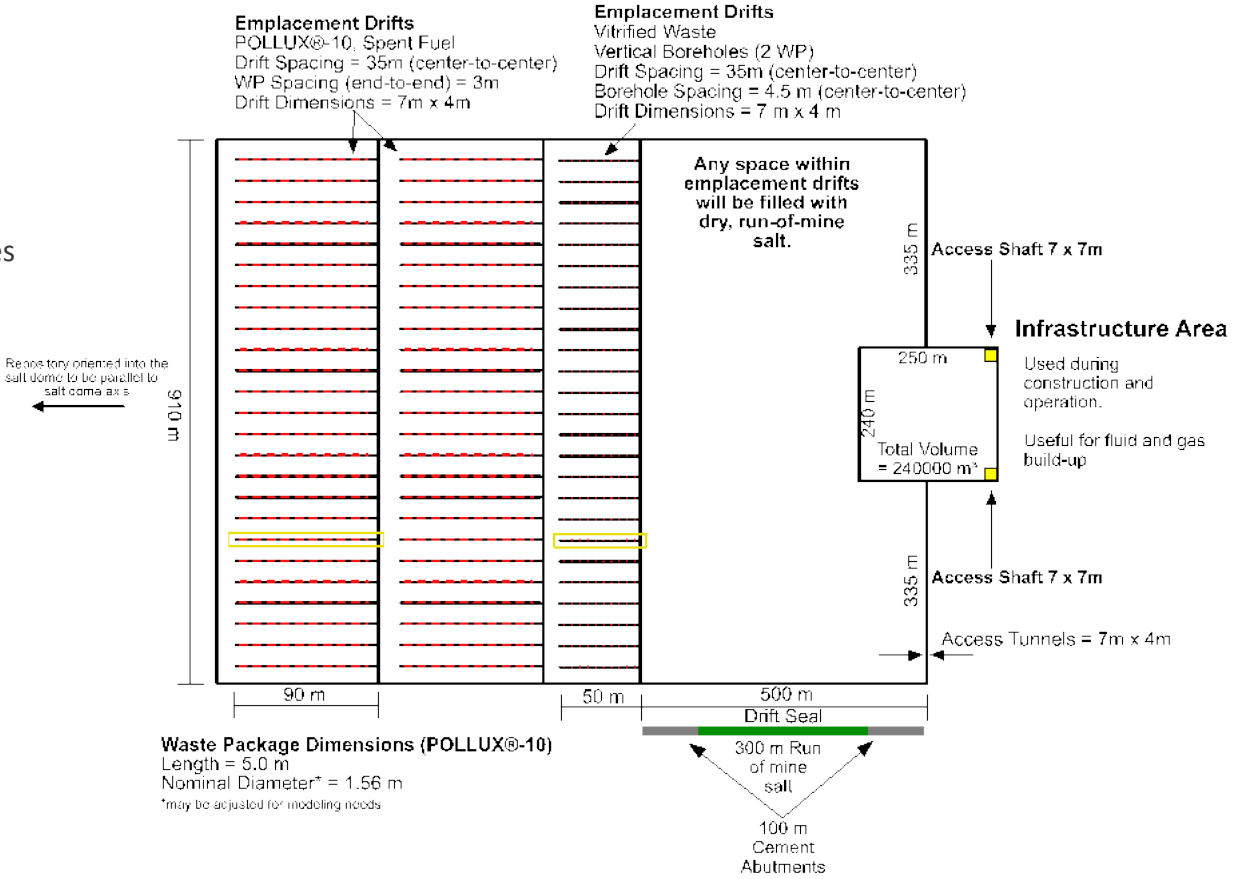
How to Include Proposed Layout?

Meshing

- Vorocrust
- Resolution?
  - Not yet individual waste packages

Vorocrust

- Improvements needed to discretize the repository



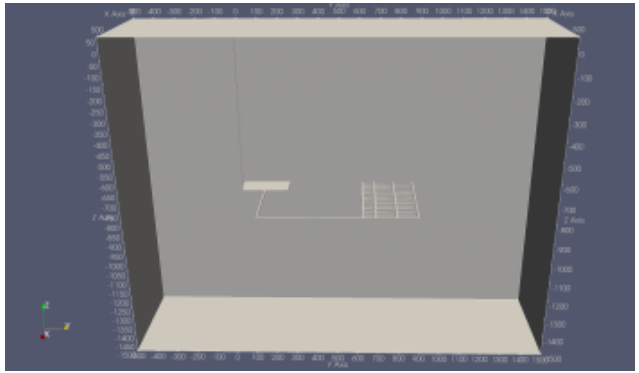
Meshing Scheme - Vorocrust

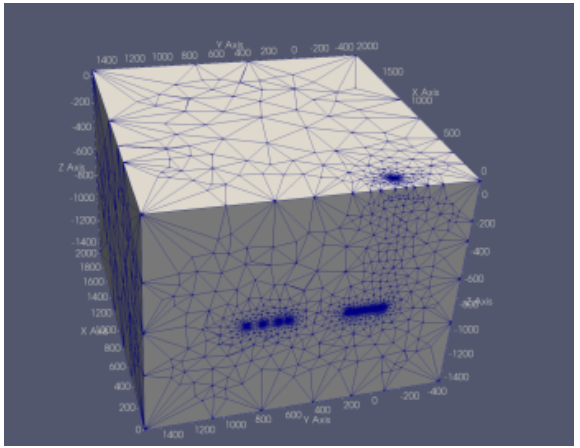
Create surfaces
- e.g. LaGrit

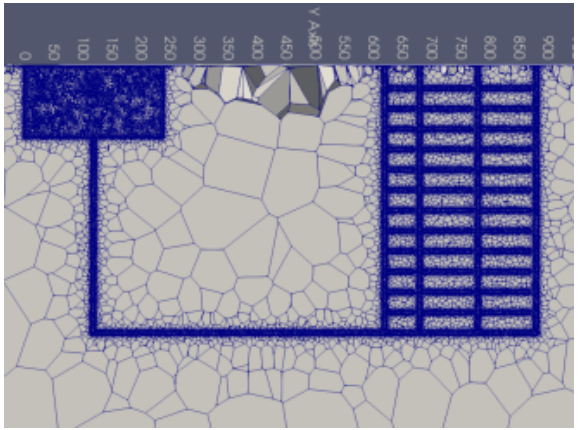
Vorocrust needs .obj format

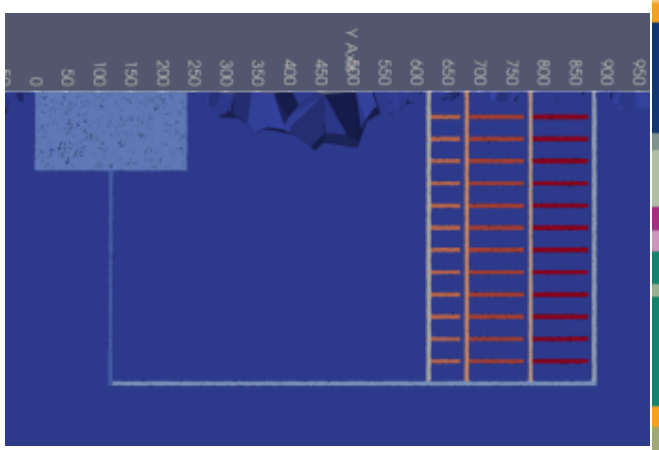
Few required parameters

Complex geometry with orthogonal discretization









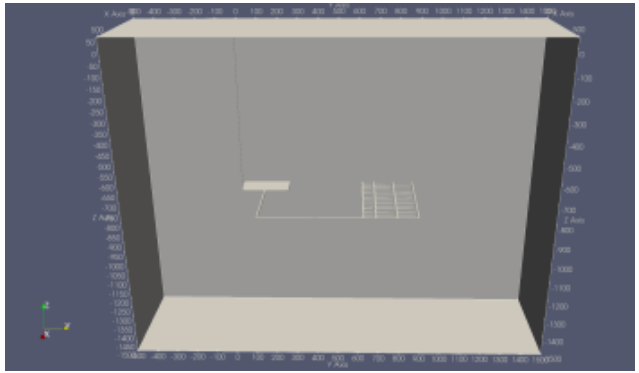
Meshing Scheme - Vorocrust

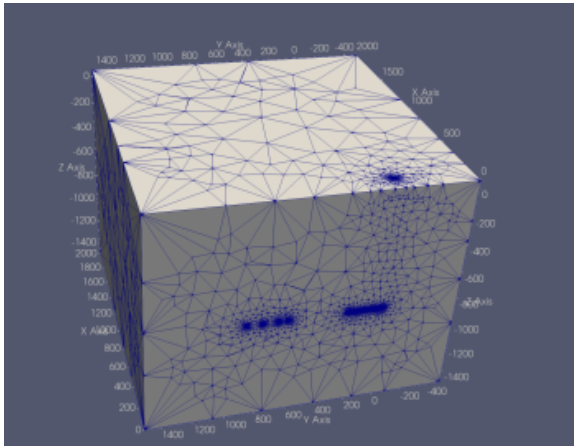
Current Mesh

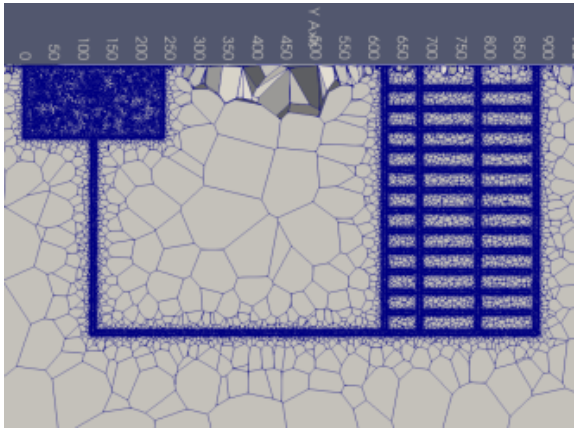
- No geologic layers
- 2000 m x 2000 m x 1550 m
- ~364,000 elements

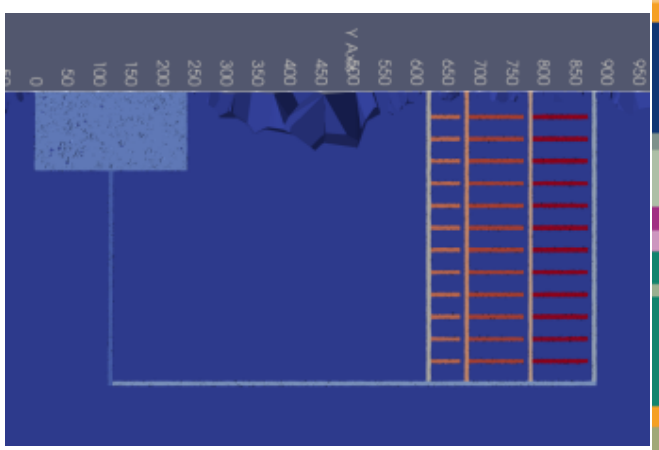
Improvements Needed

- Grid cells grow too quickly
- Add in geologic layers
- Break longer drifts and access shaft into sections to account for seals

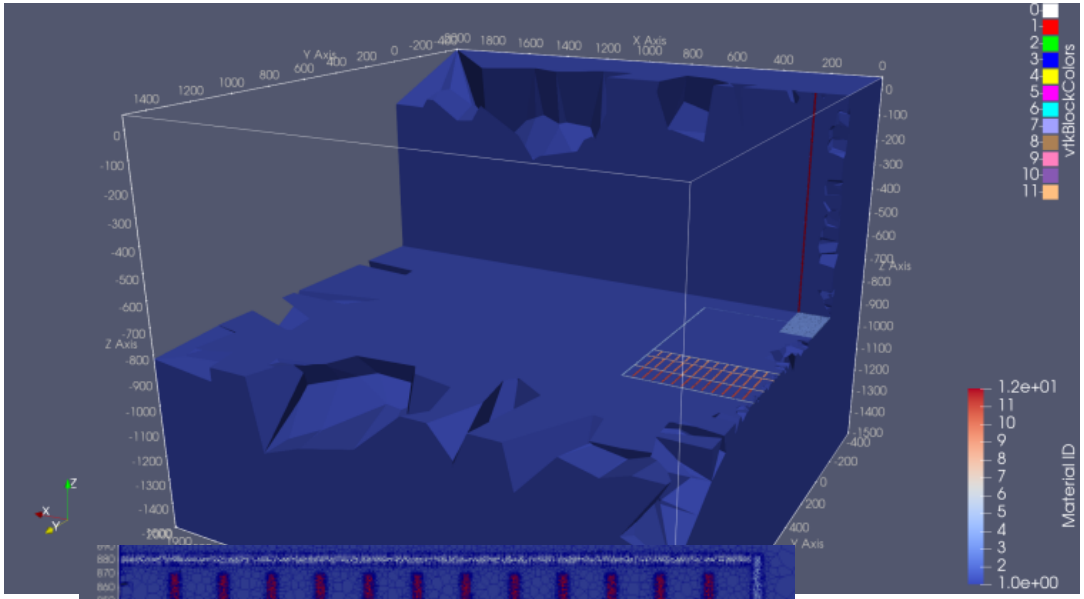


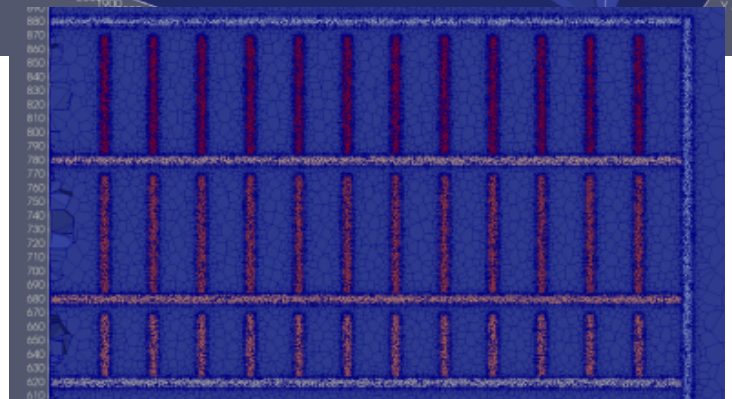


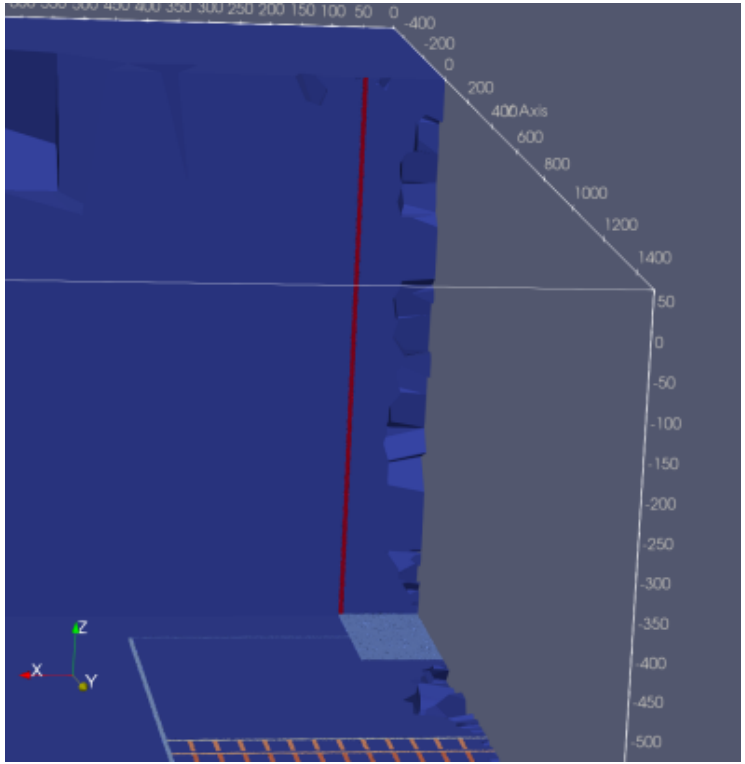




MESHING SCHEME - VOROCRUST







MATERIAL PROPERTIES – DIRECTLY FROM TASK S

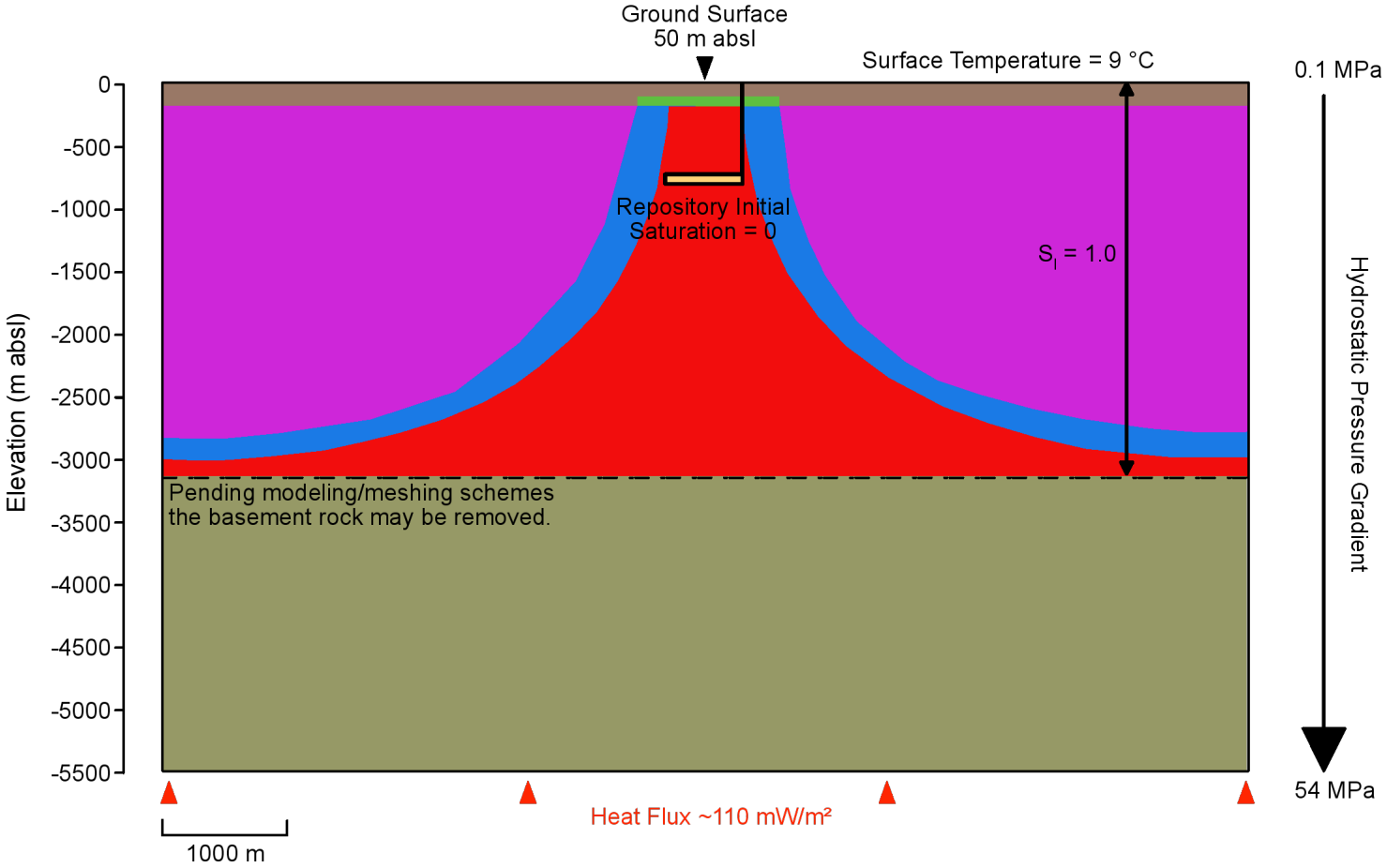
	Intrinsic Permeability (m^2)	Porosity	- Tortuosity (-)[b]	Effective Diffusion Coefficient (m^2/s)[c]	Compressibility (1/Pa)[d]	Grain Density (kg/m^3)	Heat Capacity (J/kg*K)	Thermal Conductivity (W/m²)[a]
Overburden	1.00E-15	0.2	0.2	9.2E-11	1.00E-08	2600	800	2.3
Caprock	1.00E-18	0.4	0.4	3.68E-10	1.00E-09	2200	950	2.2
Basin Fill	1.00E-17	0.25	0.25	1.44E-10	1.00E-08	2500	900	2.5
Anhydrite/Potash	1.00E-19	0.05	0.05	5.75E-12	1.00E-11	2700	750	2.6
Domal Salt	1.00E-22[a]	0.001[a]	0.0001	2.3E-15	1.00E-11	2200	880	5.5
Basement	1.00E-21[a]	0.01	0.01	2.3E-13	1.00E-12	3000	850	2.7

[a] from Bertrams et al., 2020
[b] Tortuosity (τ) set equal to porosity (ϕ). Order of magnitude estimates, subject to future improvement.
[c] Effective diffusion coefficient, $D_e = D_m \phi \tau$, where D_m, the molecular diffusion coefficient in free water, = 2.3E-09 m^2/s.
[d] Order of magnitude estimates, subject to future improvement.
All other parameters taken from general geologic property tables.

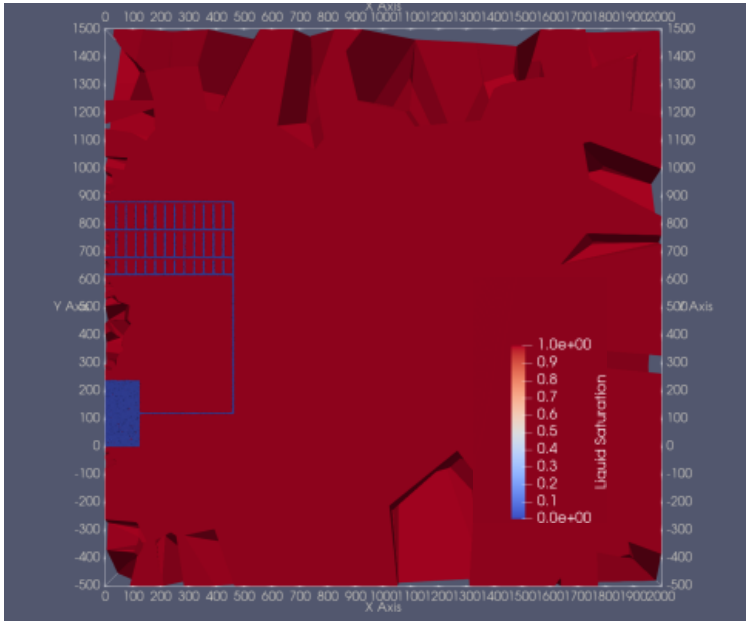
	Intact Salt[1]	Crushed Salt[1]	Shaft Seal[1]	Concrete[2]	Gravel[3]
Relative Permeability Function	Corey	Corey	Corey	Mualem - VG	VG
Residual Liquid Sat (S_{lr})	0.1	0.03	0.03	0.2	0.19
Residual Gas Sat (S_{gr})	0	0	0	0.1	0
Van Genuchten's	0.6	0.6	0.6	0.56	0.675
Van Genuchten's P_0 (MPa)	5.7	1.6	1.6	7.7	1.6
Van Genuchten's S_{lr}	0.01	0.02	0.02	0.0	0.0

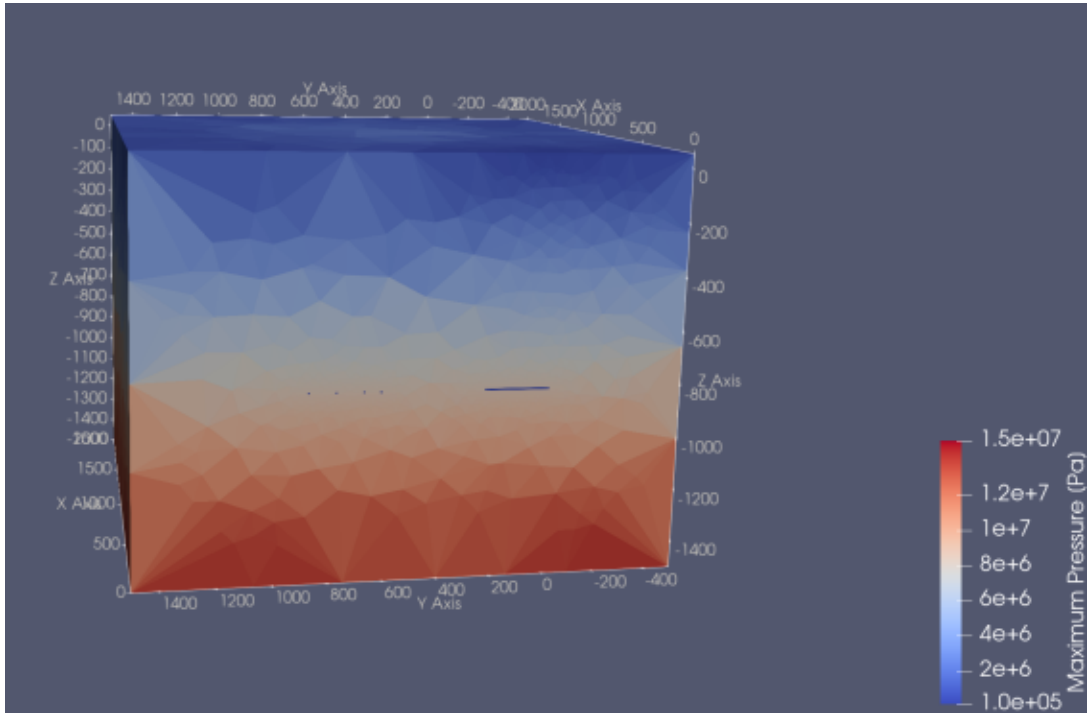
[1]Blanco-Martín et al. (2018)
[2]Ecay et al. (2020)
[3]Osselin et al. (2015)

Initial Conditions



Initial Conditions

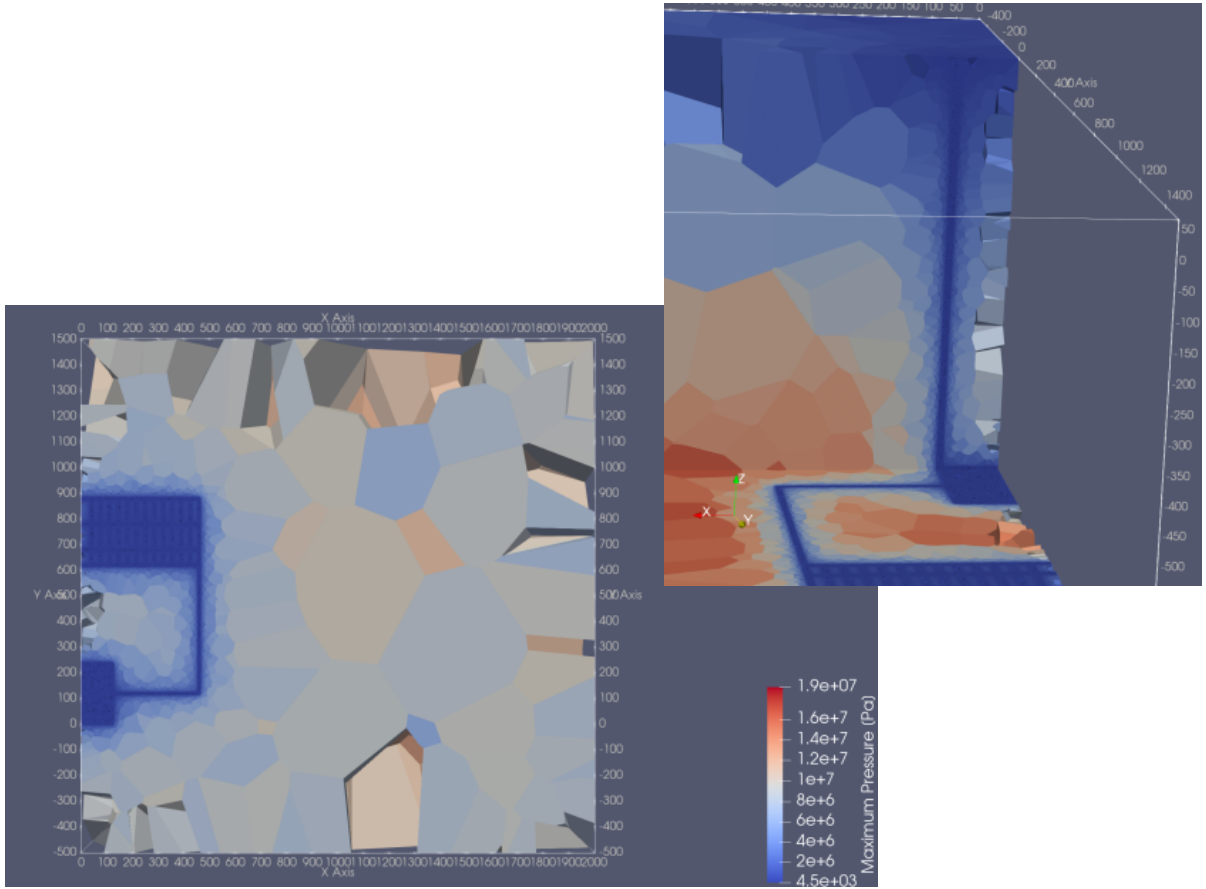




100 Years – Pressure & Saturation – No Radionuclides

Grid cells are colored based on pressure at center of the grid cell

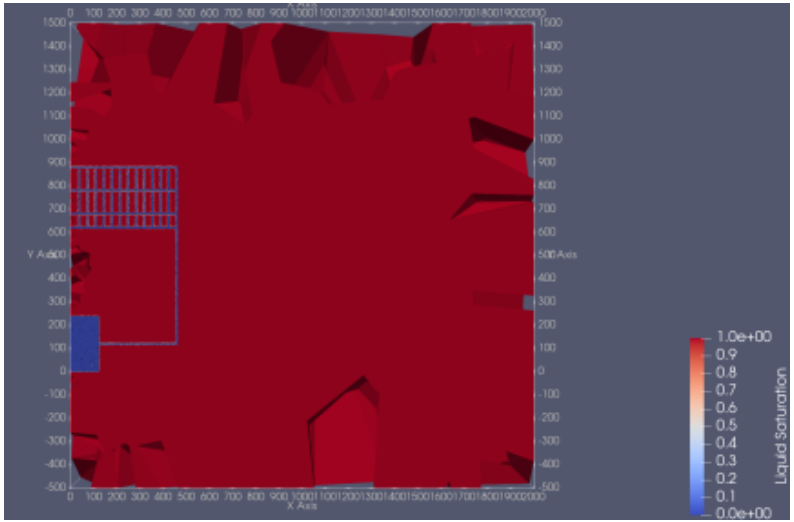
- Center of elements may be out-of-plane
- Higher resolution is most likely needed

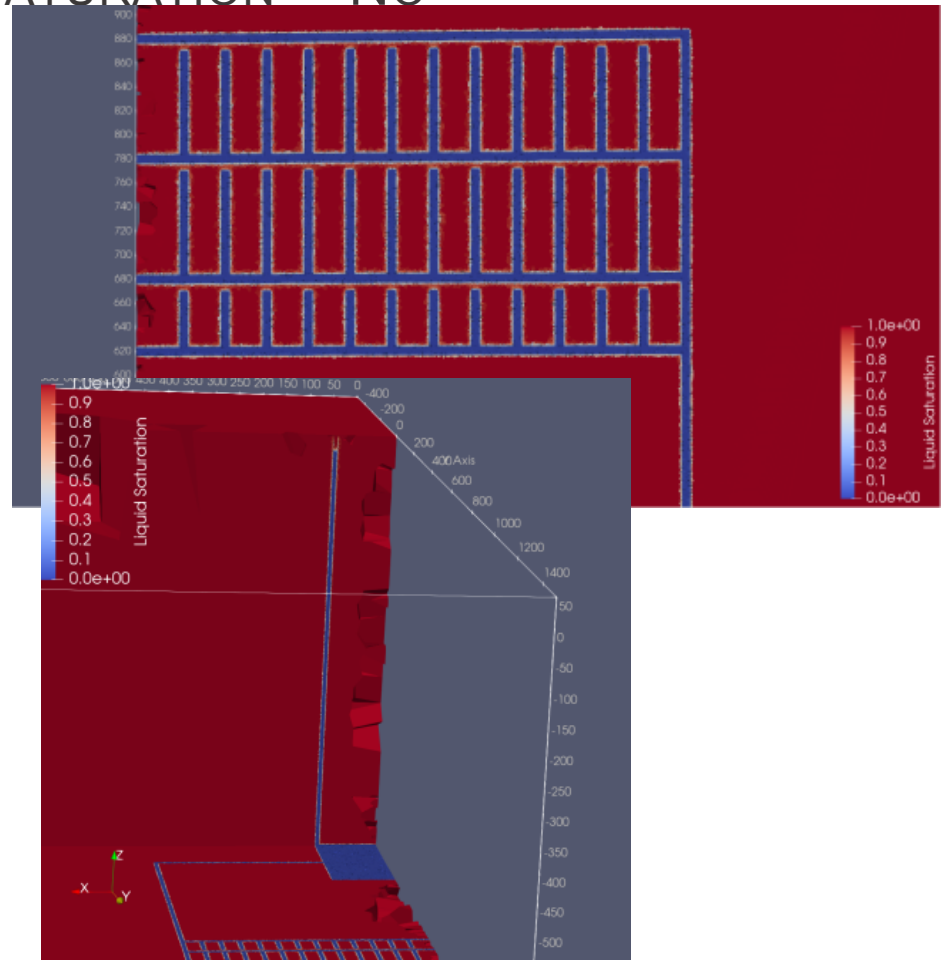


100 Years – Pressure & Saturation – No Radionuclide

Liquid Saturation does not have the same issues as pressure

Only 100 years simulated do to convergence issues





Next Steps

Additional functionality may be added to Vorocrust in the future

- Currently able to merge multiple obj files
  - Adding in geologic layers will be easier now, but how to handle areas of intersection?

Simulations currently running smoothly at small timesteps

- Wallclock time is high (>48 hrs for 150 years of simulation)
- Larger timesteps lead to instability
- Potentially allow timesteps to grow larger with different preconditioner settings
- Change boundary conditions (i.e. RH = 75% vs. S_l = 0.01)

Meshing

- Create larger, higher resolution mesh once this round of simulations complete
- Add in geologic layers

Radionuclides & Waste Package Heat

- Average over the entire drift since individual waste packages are not discretized

Can add monitoring points for comparisons