Task F – Salt PA Modeling Approach
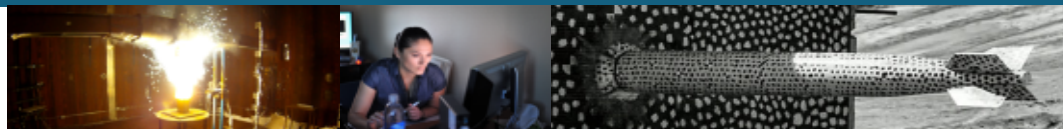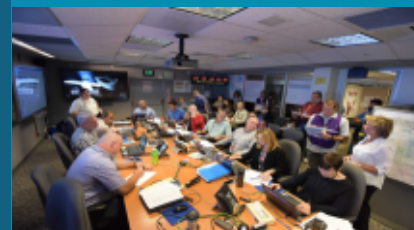
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Sandia National Laboratories

DECOVALEX Fall Meeting 2022

MODELING APPROACH - PFLOTRAN

General Mode

- Multiphase Flow
  - Computationally difficult
- Issues with convergence
  - Changed the rate at which grid cells grow
  - Made all relative permeability models the same
    - VG
  - All drifts and seals are $1E^{-17}m^2$ and 10% porosity
  - Starting liquid saturation = 20%
- Simulation time ~30 hours

Richards Mode

- Single phase unsaturated flow
- First iteration of simulations
  - Simulation time <20 min
  - Original simulations showed the repository at hydrostatic pressure within 25 – 50 years
- Second iteration
  - Changed initial pressure in repository to $-1.7E^6$ Pa to increase gas saturation
    - Negative liquid pressure is needed to impose ~20% liquid saturation
  - Simulation time ~24 hours
- How important is early time behavior of repository wetting up?

Cartesian Meshing

- Smaller model domain
- Larger number of grid cells
- Easier to add details without increased resolution
  - Shaft seal layers
  - Individual seals
  - Potentially individual waste packages if geometry is set up correctly
- Early time preliminary results only at this time
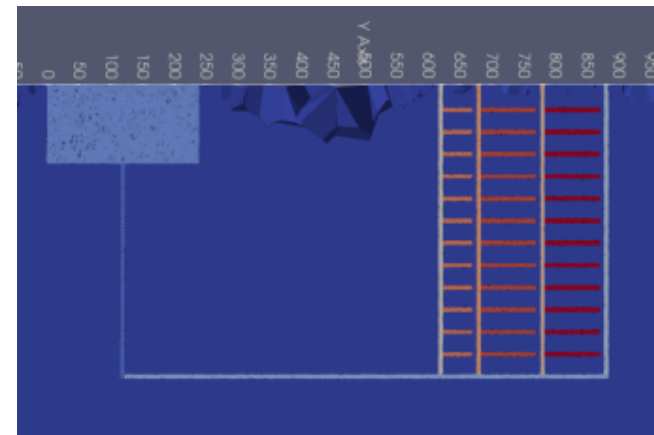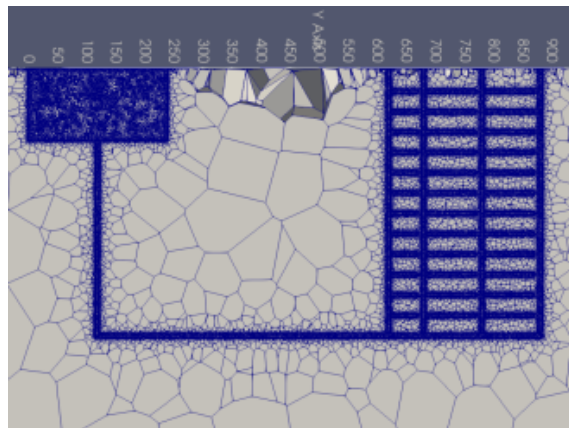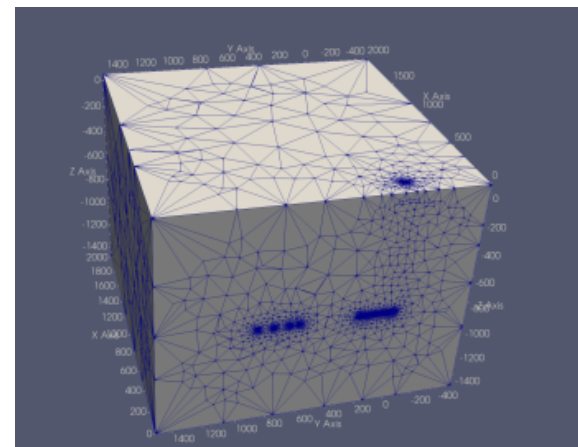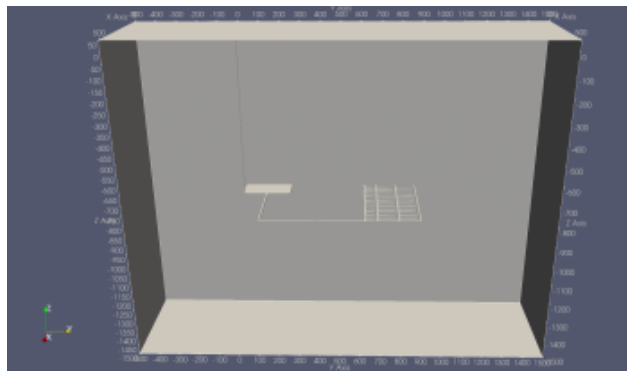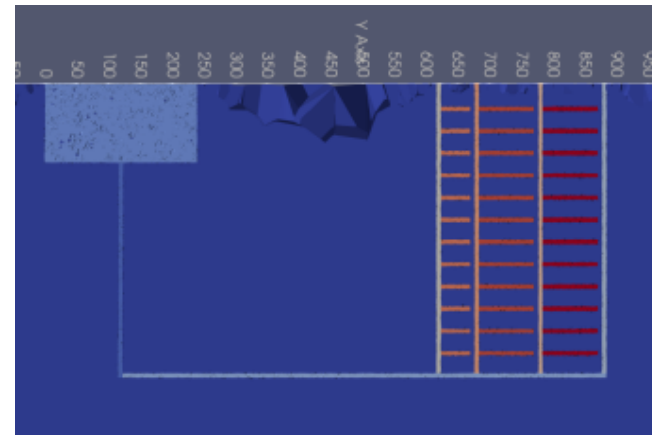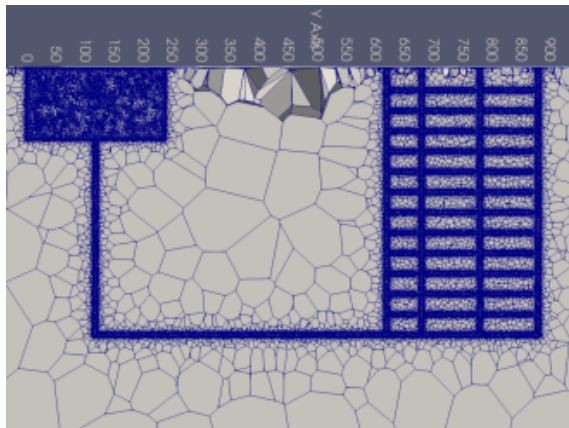
MESHING SCHEME - VOROCRUST

Create surfaces
◦ e.g. LaGrit

Vorocrust needs .obj format
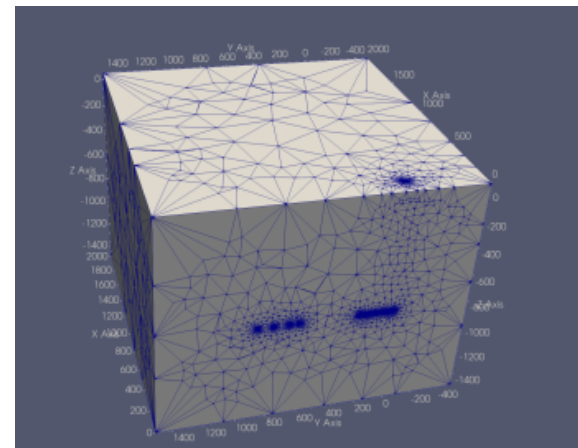
Few required parameters

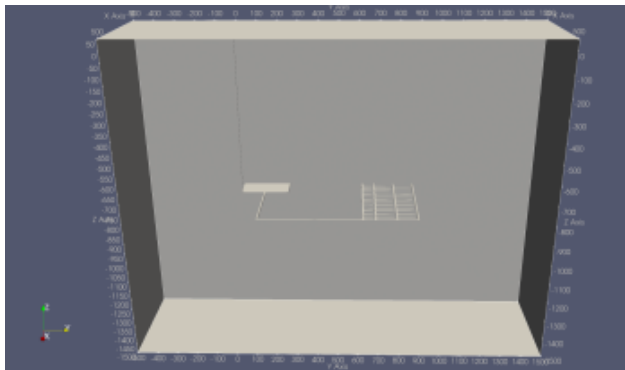Complex geometry with orthogonal discretization
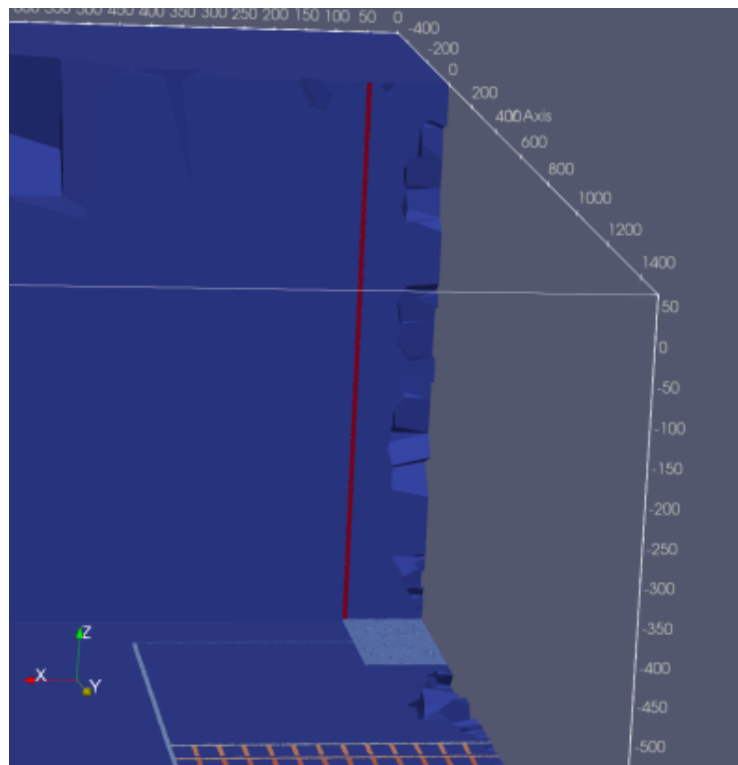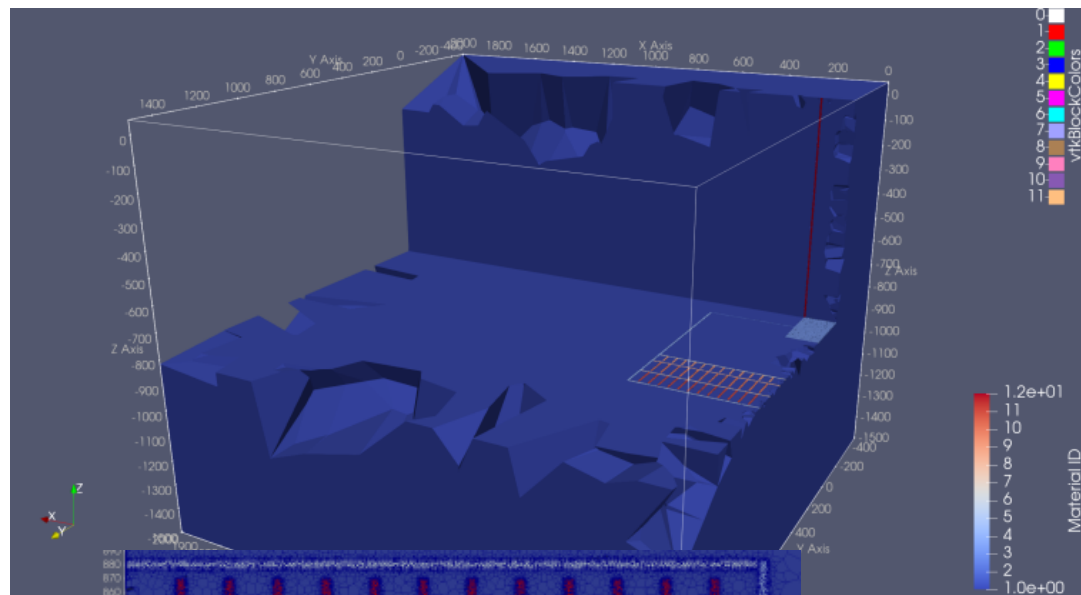
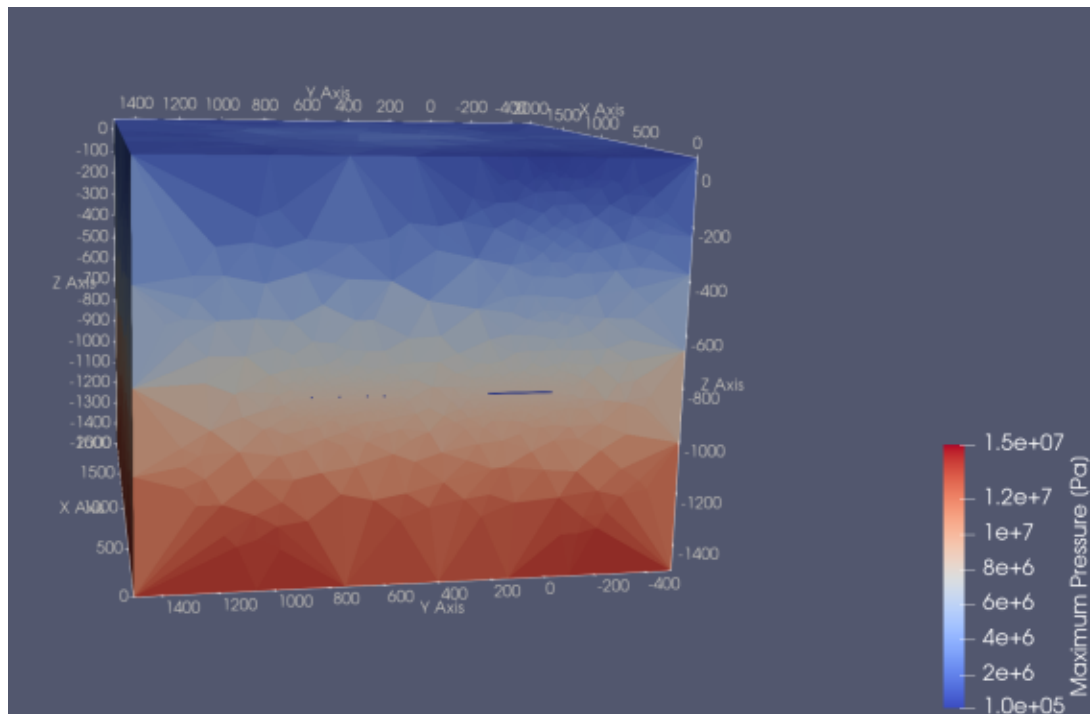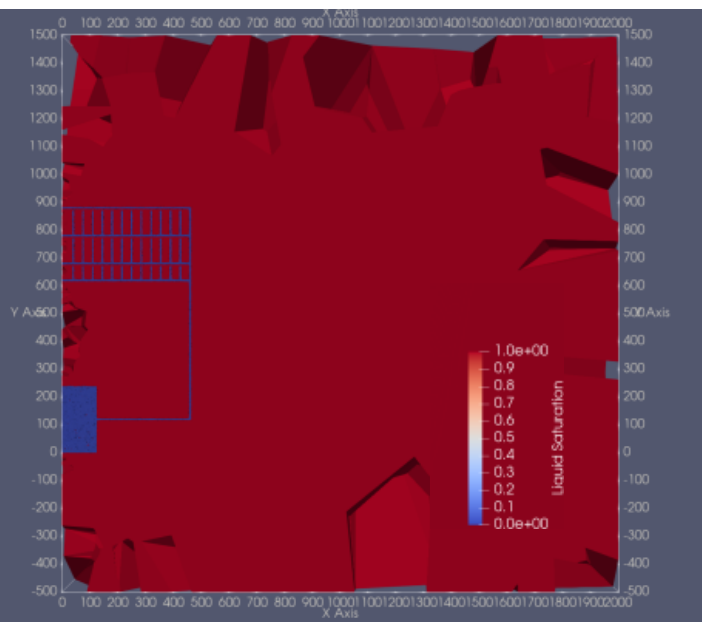# MESHING SCHEME - VOROCRUST

Current Mesh

- One geologic formation
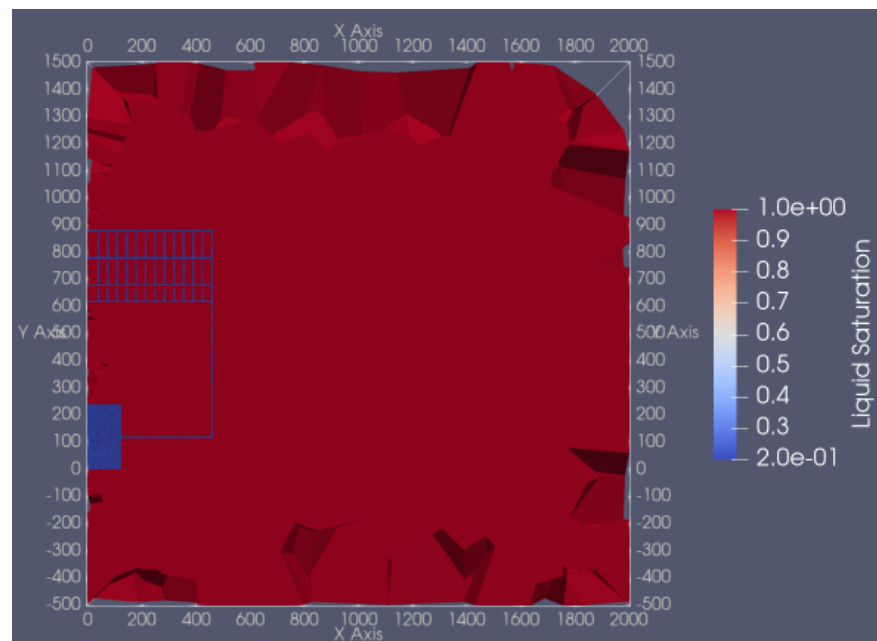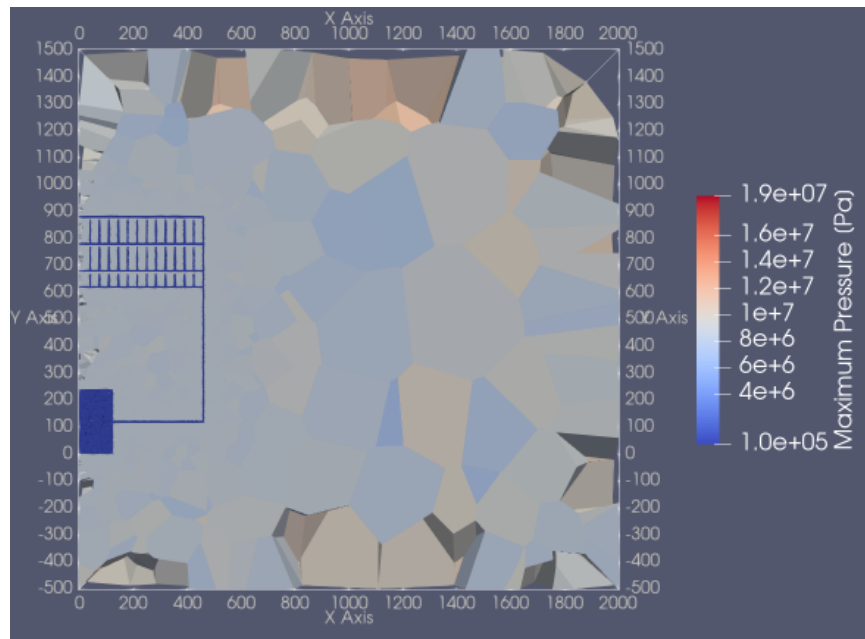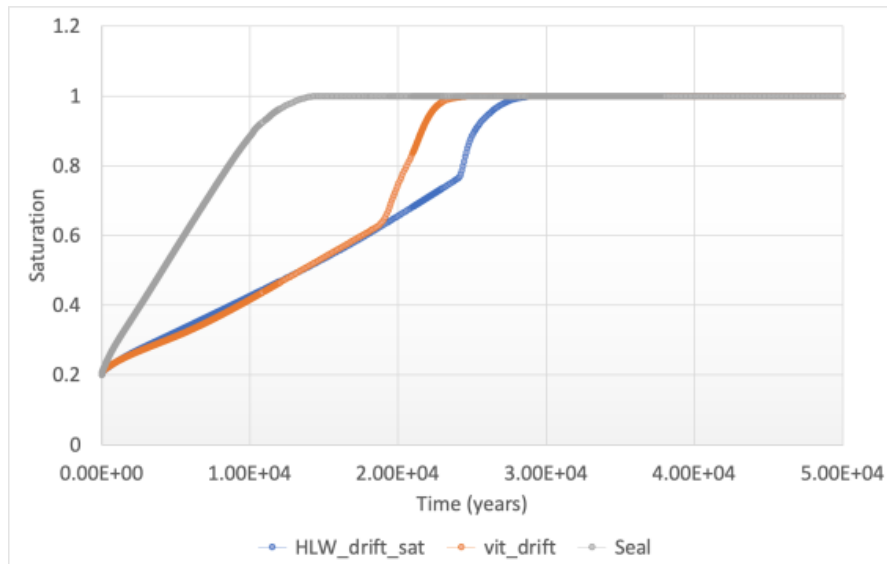 - Domal salt
- 2000 m x 2000 m x 1550 m
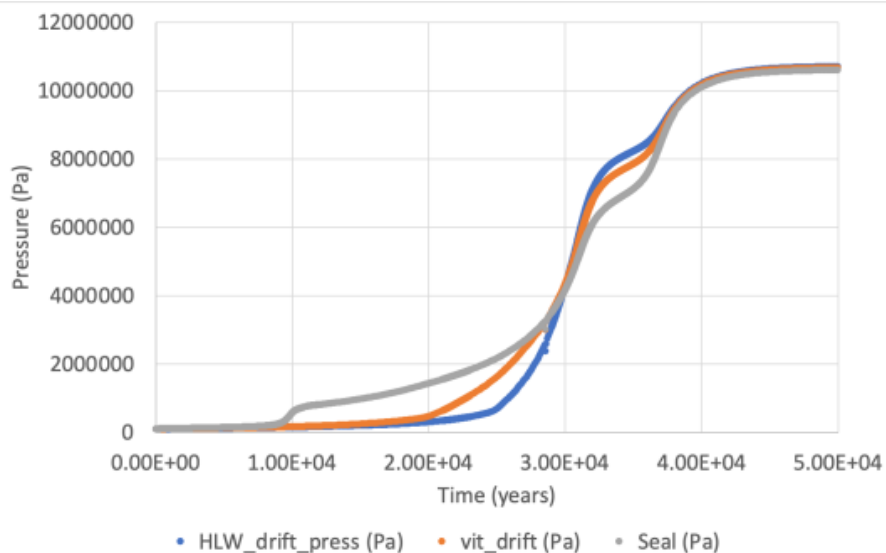- ~431,000 elements
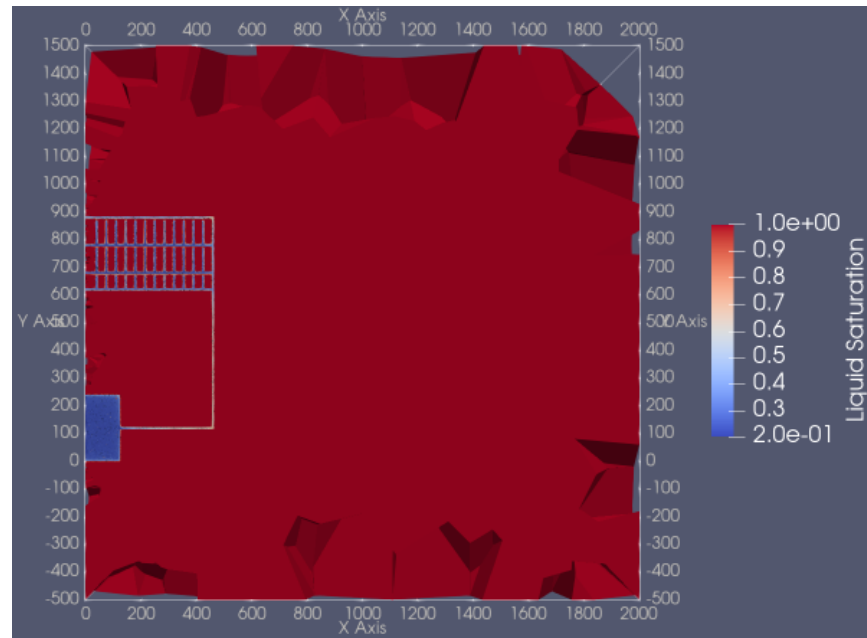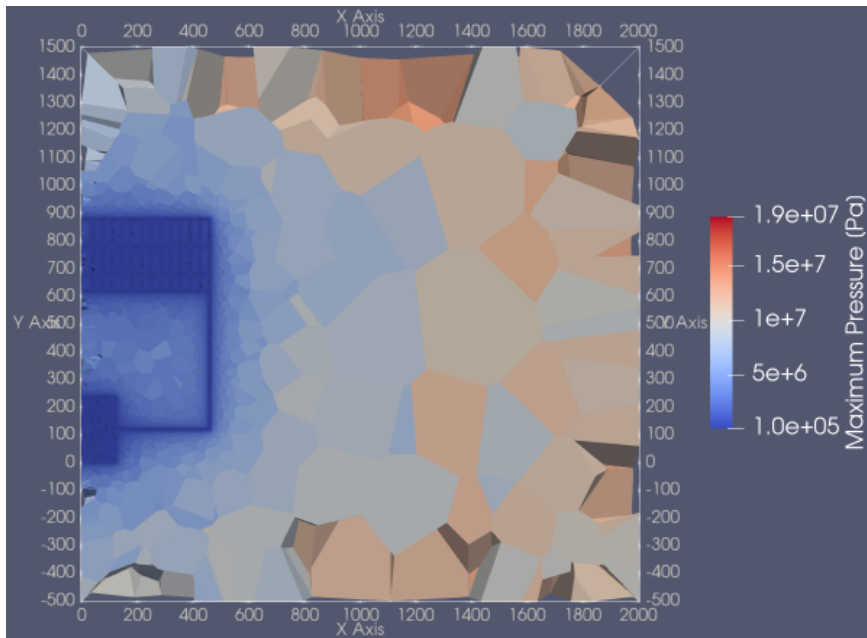
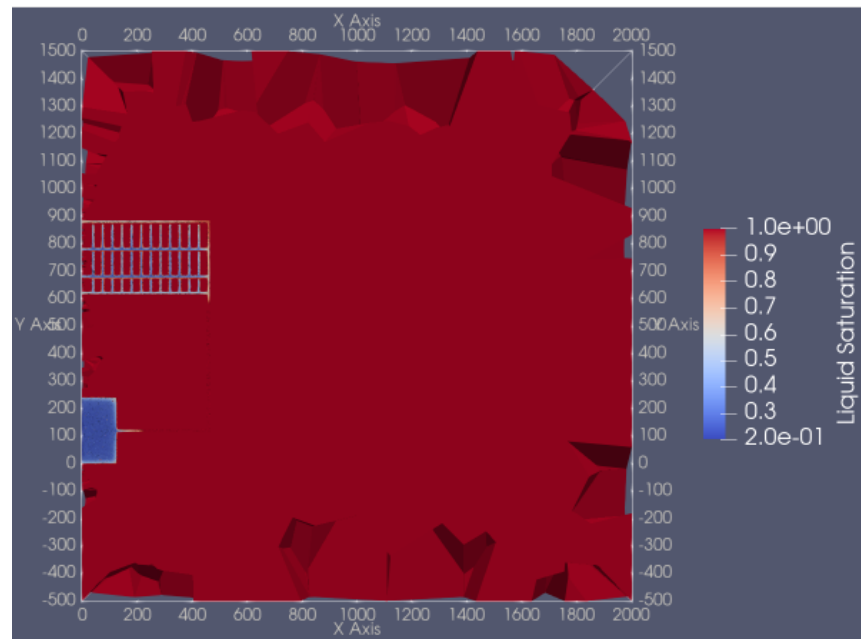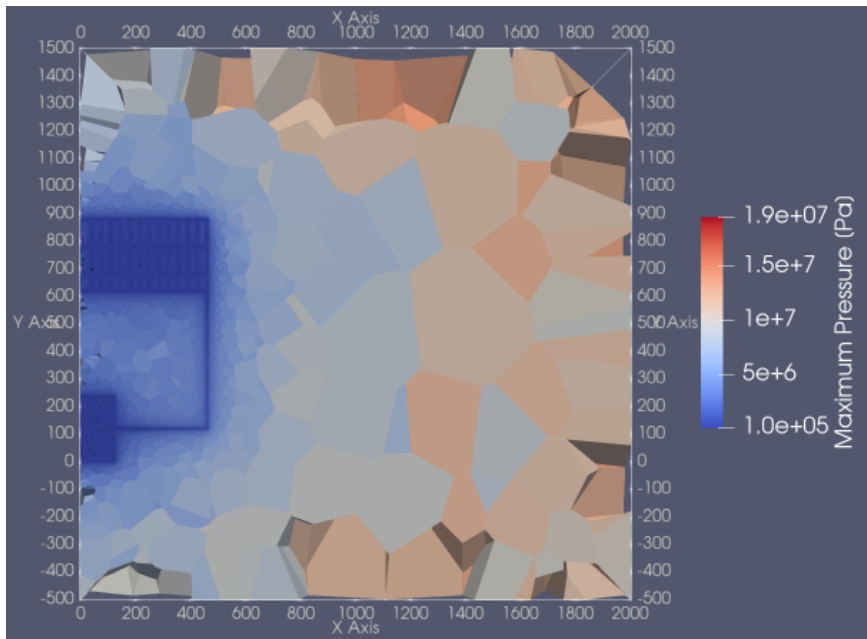# Meshing Scheme - Vorocrust

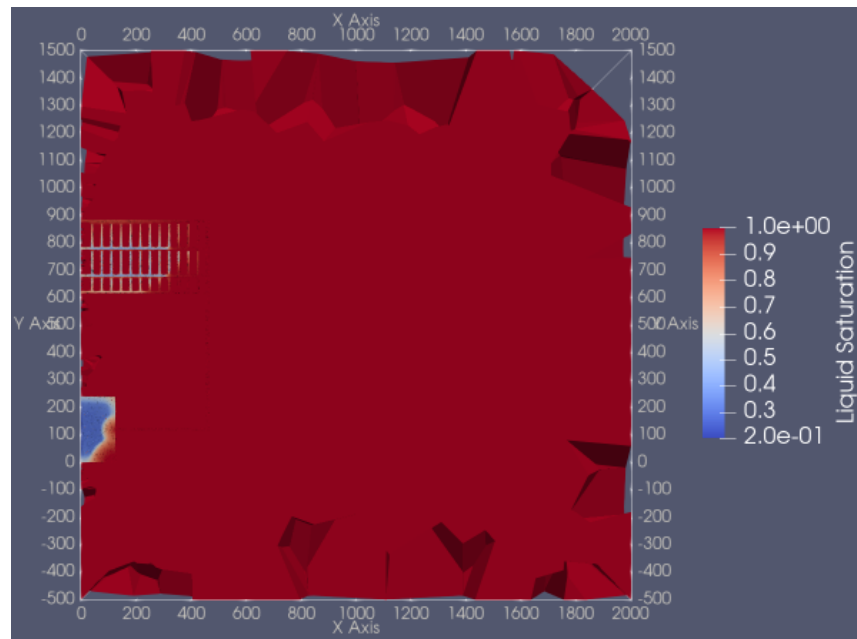# Initial Conditions
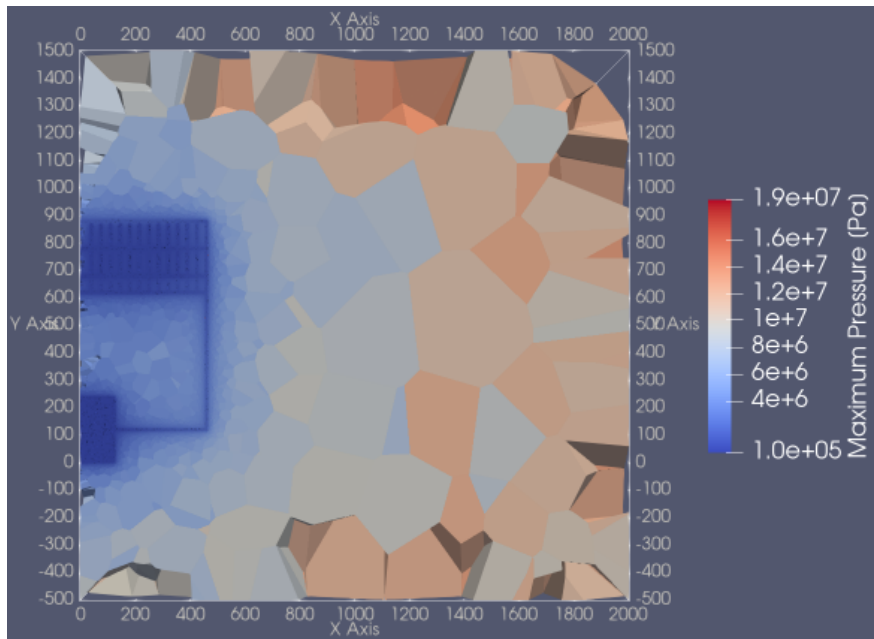
INITIAL CONDITIONS
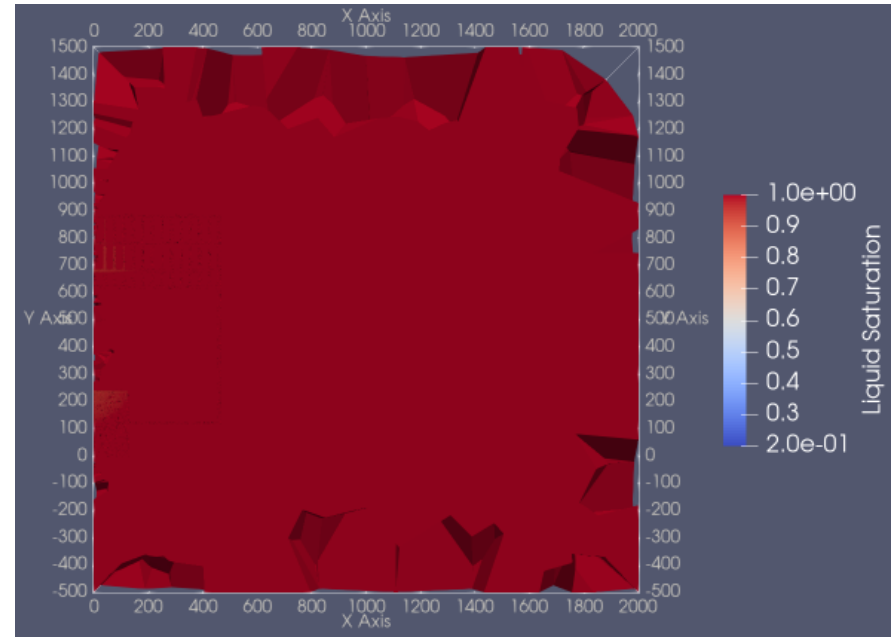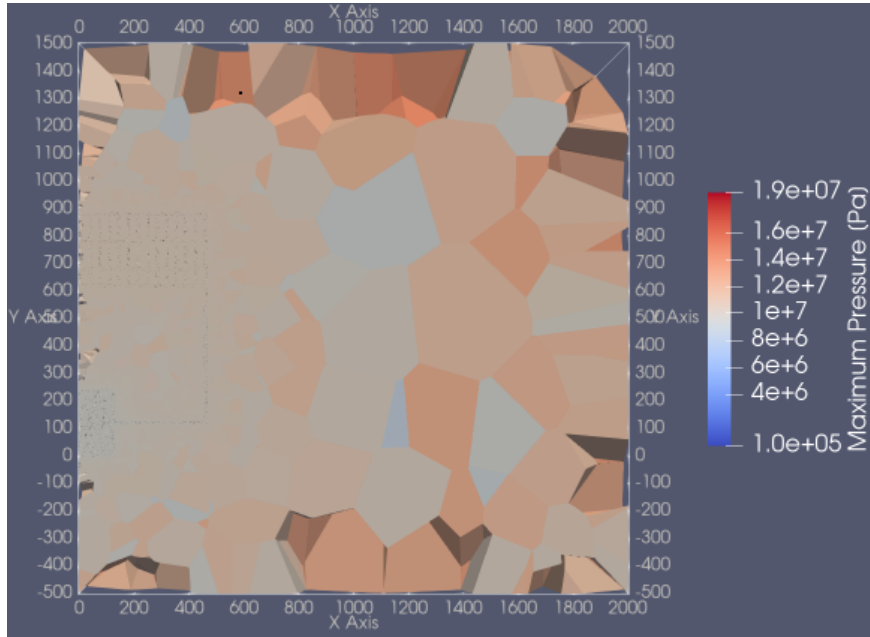
Summary of Results – General Mode
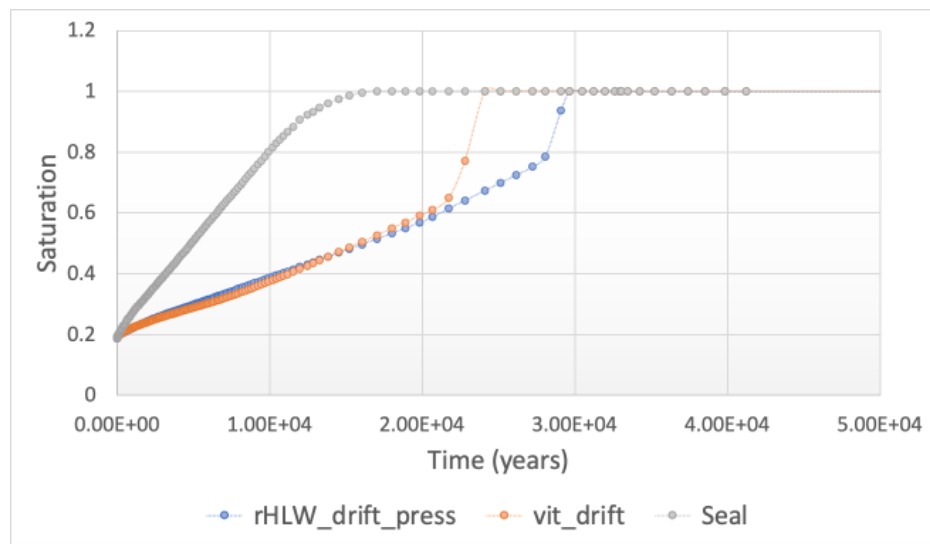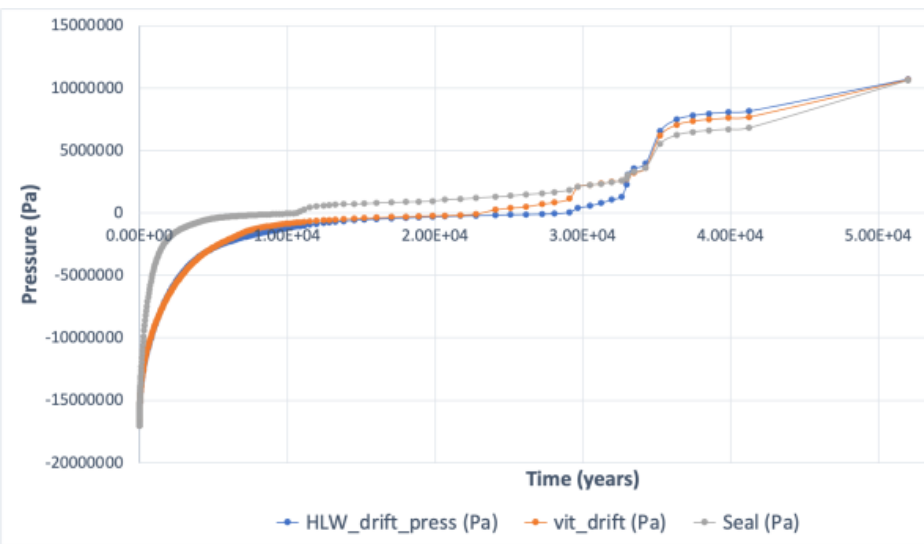
General Mode - 5,000 Years

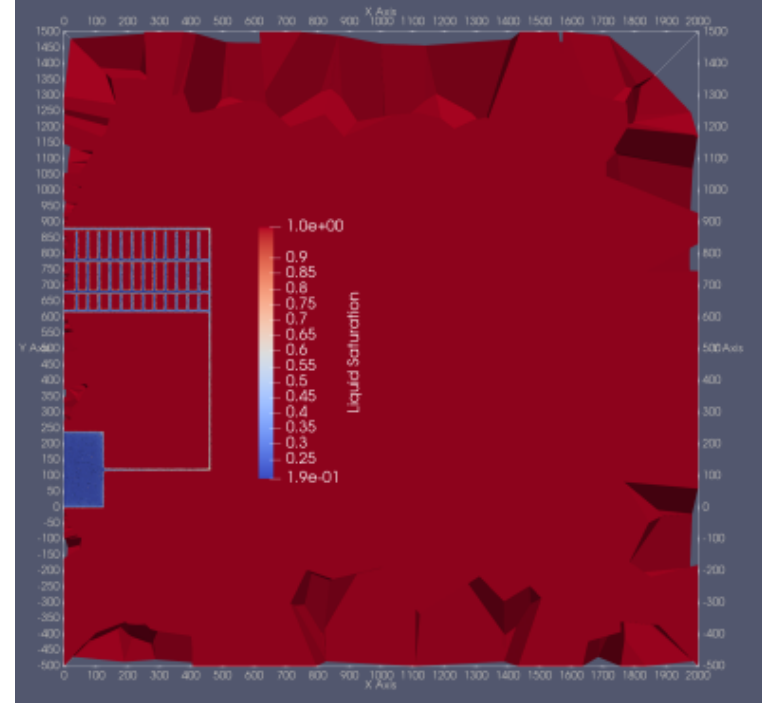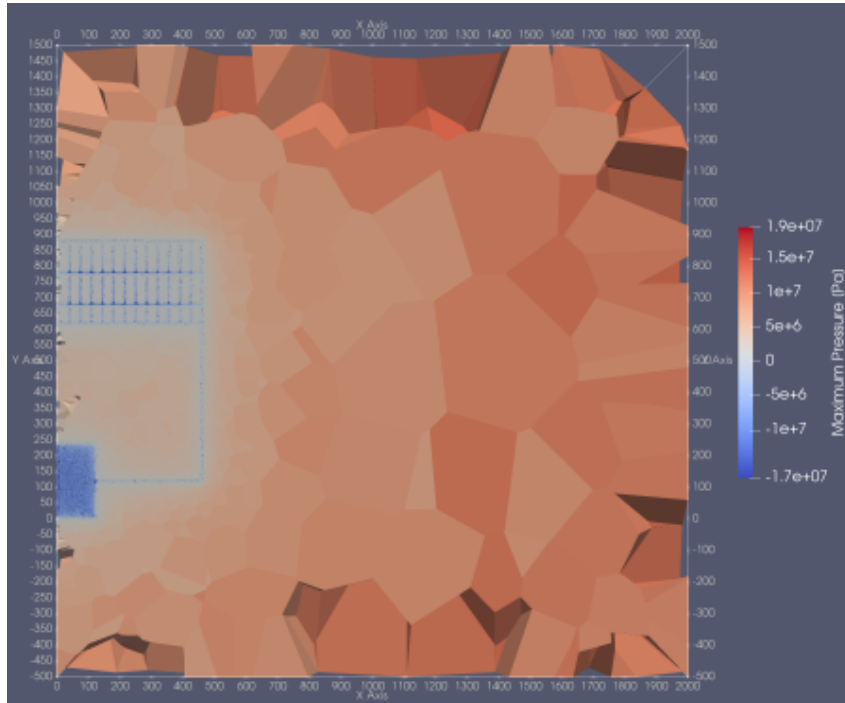# GENERAL MODE - 10,000 YEARS

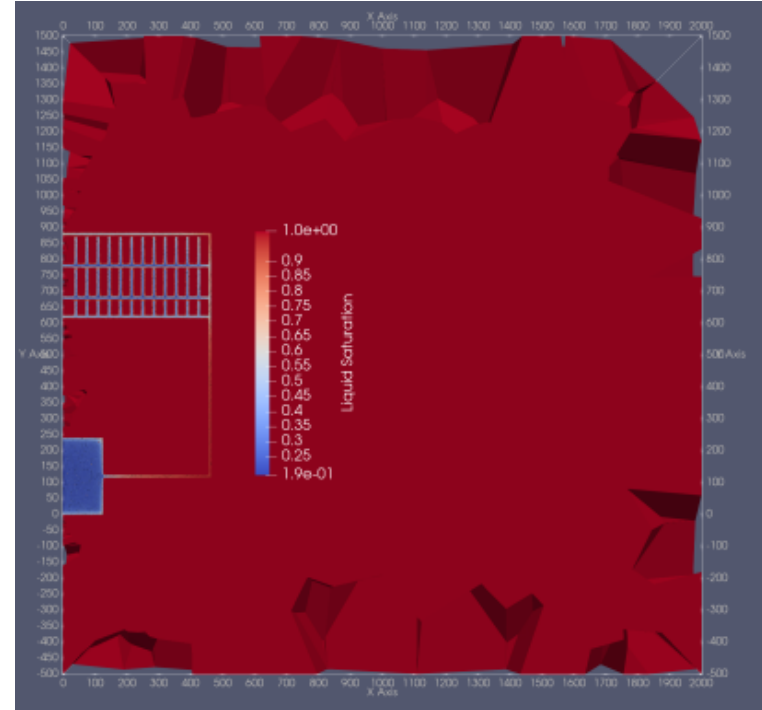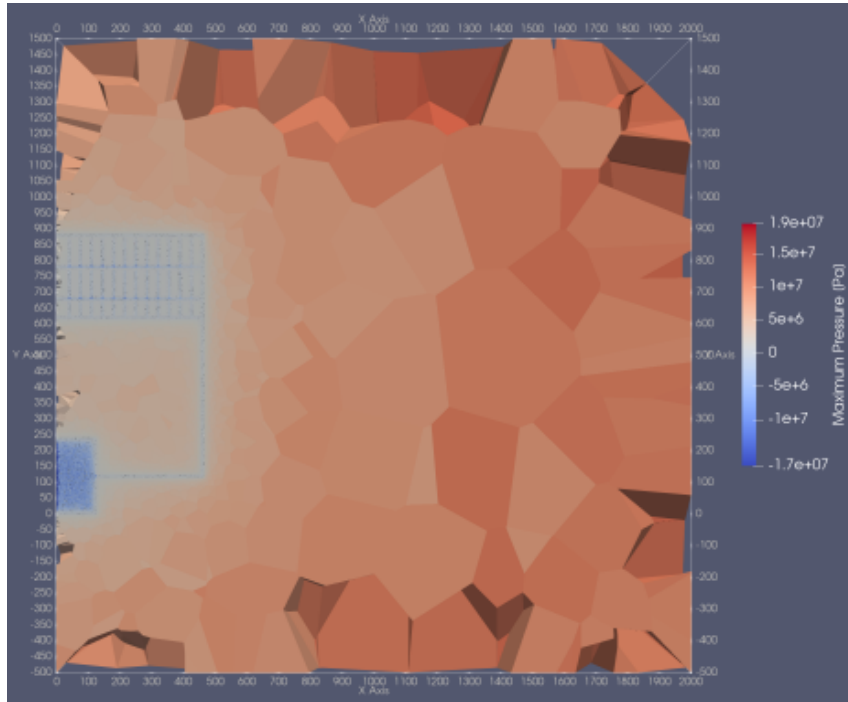# General Mode - 20,000 Years

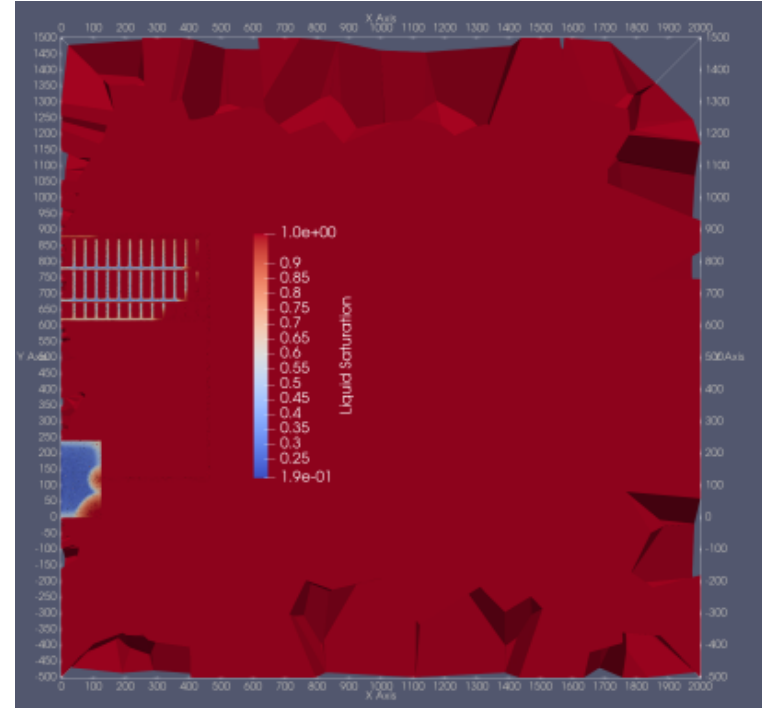# GENERAL MODE - 40,000 YEARS
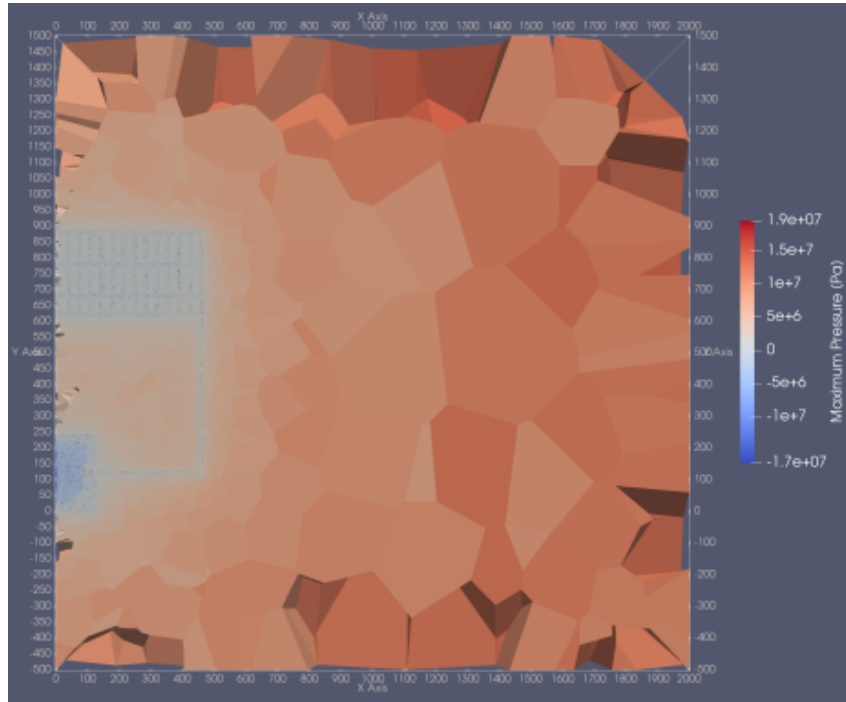
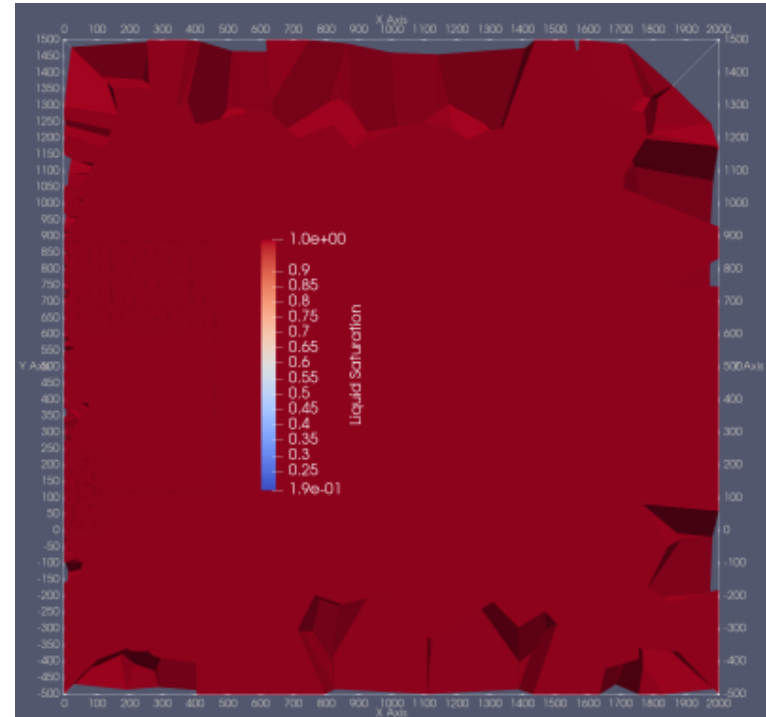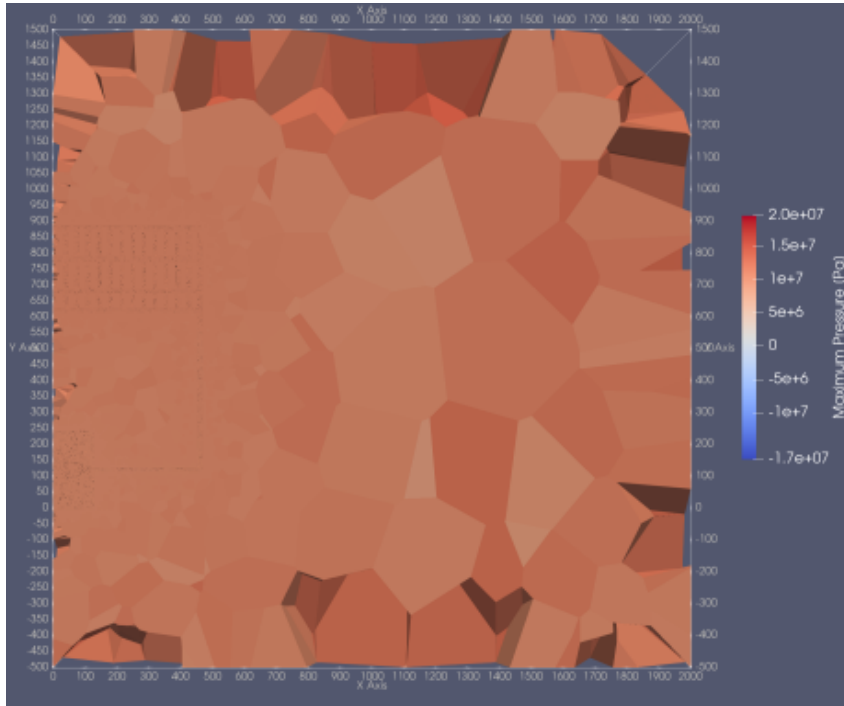# Summary of Results – Richards Mode

RICHARDS MODE – 5,000 YEARS

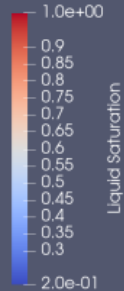# RICHARDS MODE – 10,000 YEARS

RICHARDS MODE – 20,000 YEARS

Richards Mode – 50,000 Years
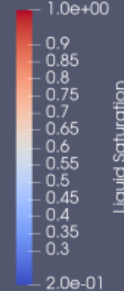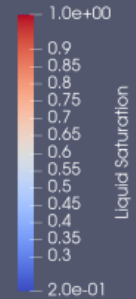
Shaft Saturation Results

5,000 years

10,000 years

15,000 years

CARTESIAN MESH – PRELIMINARY RESULTS
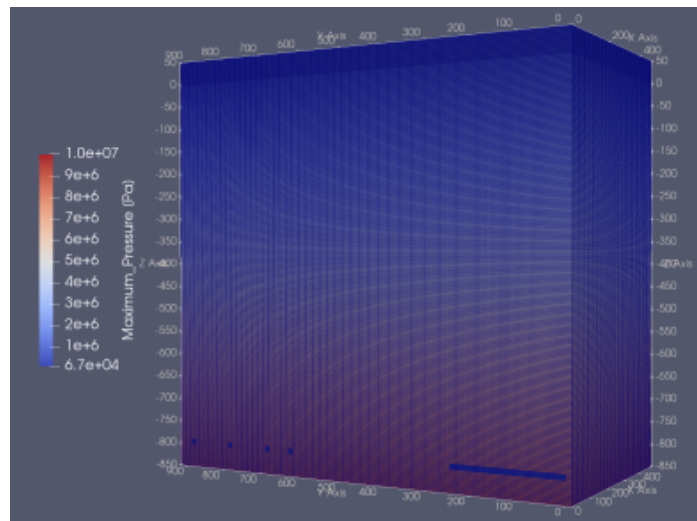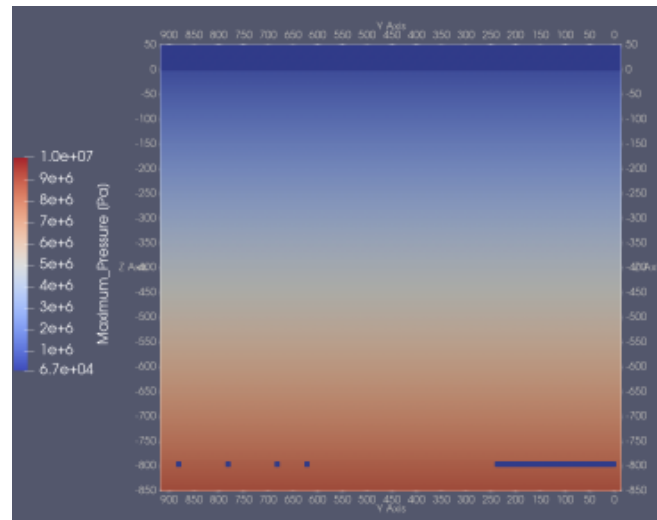
General Mode

◦ Multiphase Flow

◦ 4,000,000+ grid cells

  ◦ 483m x 932m x 900m

  ◦ 3.5m x 4.0m x 7.0m

◦ Includes overburden with aquifer
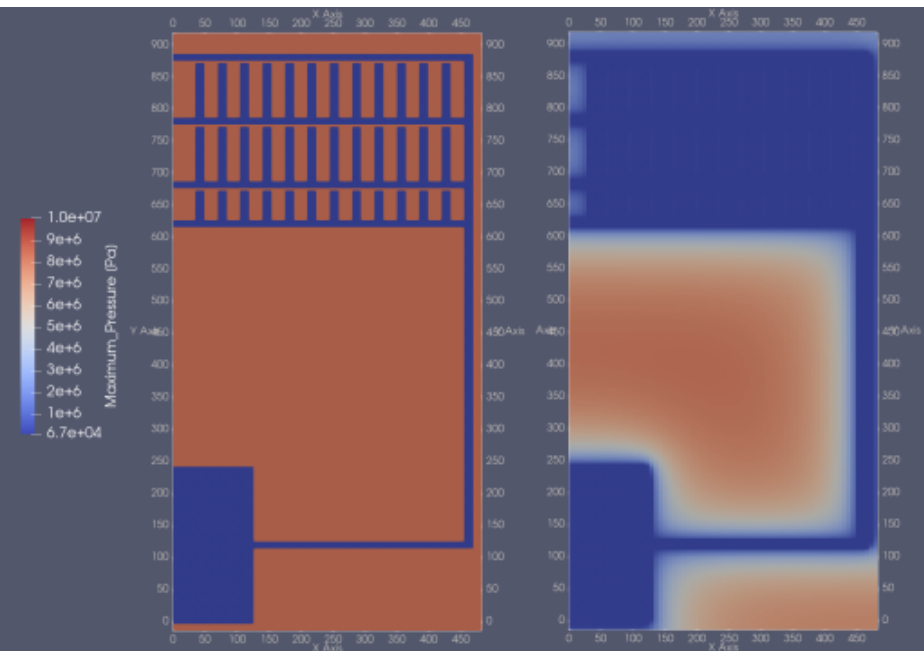
Potential Pros

◦ Can discretize more of the repository without increased resolution

  ◦ Shaft layers

  ◦ Individual seals

Cartesian Mesh – Preliminary Results
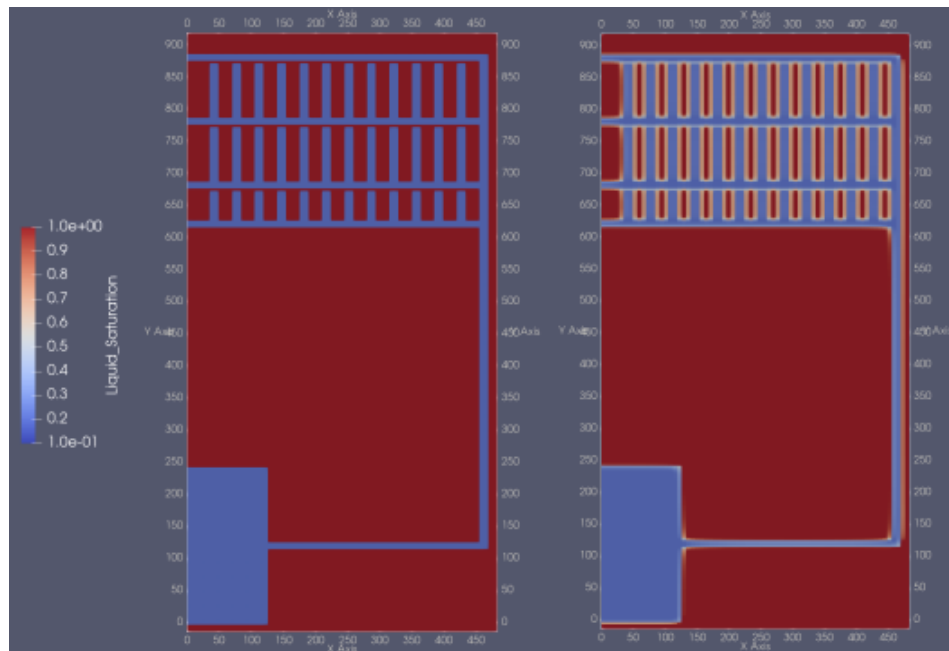
0 years   2500 years   0 years   2500 years

NEXT STEPS

Continue working with both General and Richards mode

Add transport – starting with tracers

Update material properties
◦ Different permeability and porosity between salt and seals, backfill, etc.

Simulate shaft seal failure
◦ Potentially discretize shaft seal (may have issues with convergence due to how small some grid cells may be) – most likely cartesian only

Geologic layers
◦ At minimum add high permeability overburden