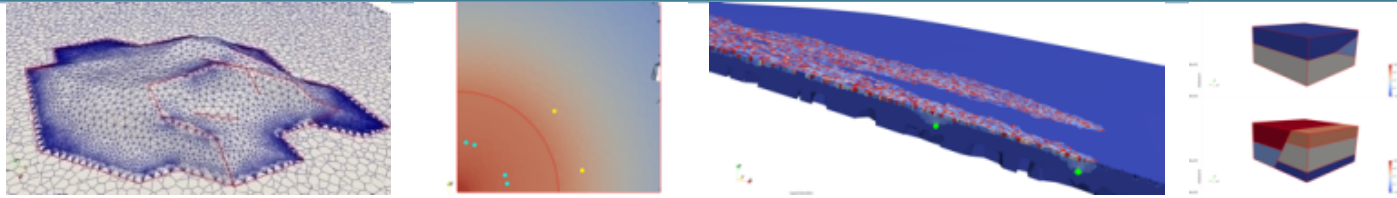




# Voronoi meshing to accurately capture geology in subsurface simulations



Tara LaForce<sup>1</sup>, Mohamed Ebeida<sup>1</sup>, Spencer Jordan, Terry Miller<sup>2</sup>, Phillip H. Stauffer<sup>2</sup>, Heeho Park<sup>1</sup>, Rosie Leone<sup>1</sup>

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# Outline



Why Voronoi meshes? (and what are they?)

The 'usual issues' researchers face when using Voronoi meshes

Analytical benchmark

Simulation on four test structures

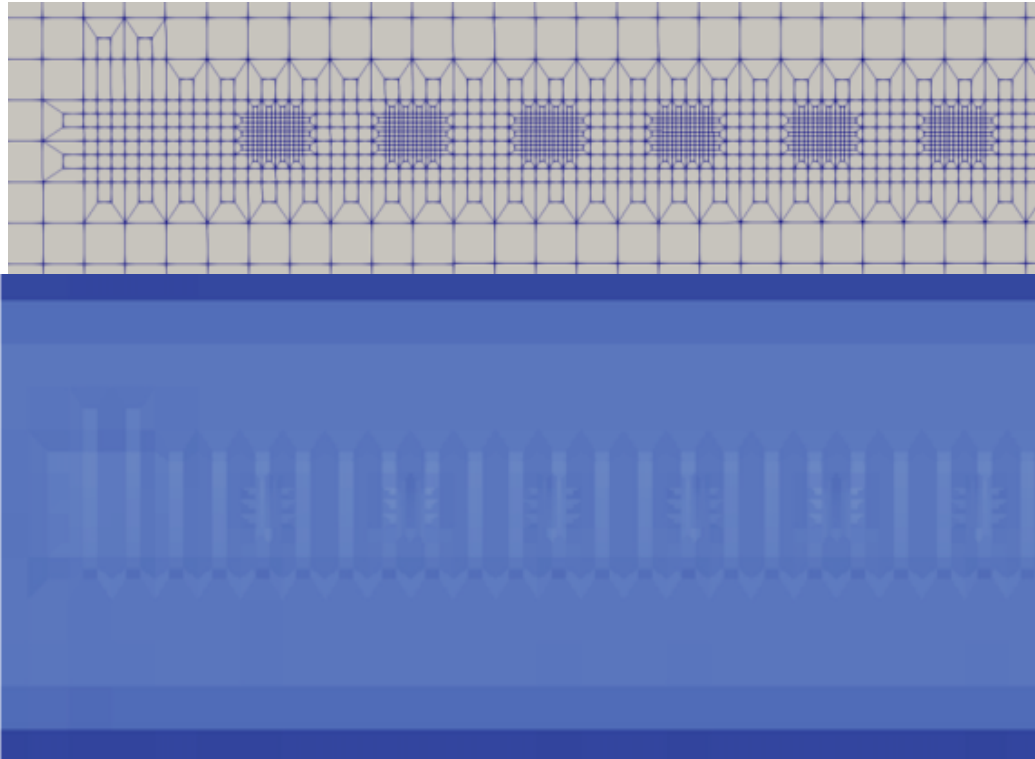
CO<sub>2</sub> storage in a geological model of the Rock Springs Uplift

Conclusions and future work

# Why Voronoi meshes?

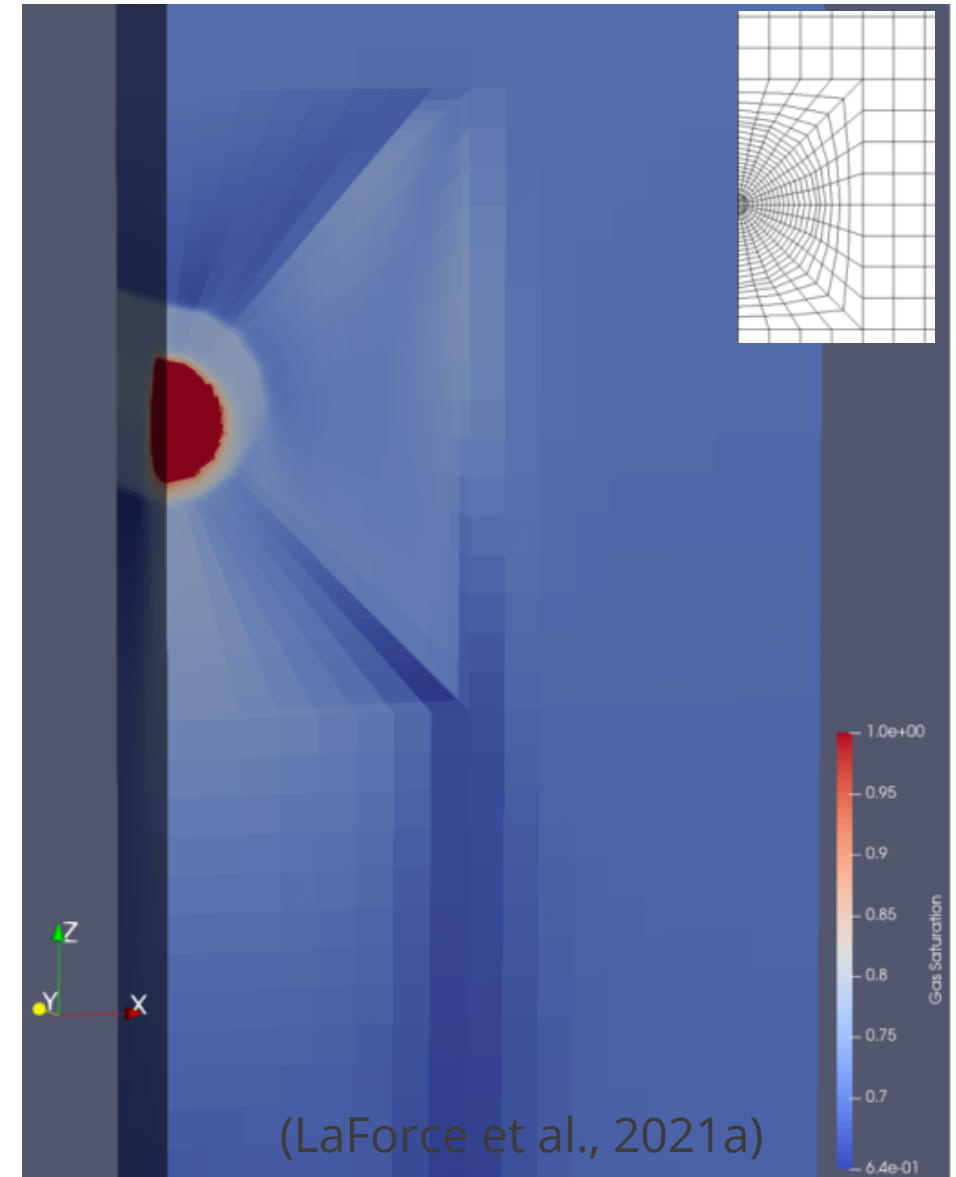
They rigorously honor complex geometries...

...without introducing non-orthogonal fluxes in simulations



Equilibration of an unsaturated heterogeneous model with infiltration using a refined hexahedral mesh.

Gas saturation around a heat source in an unsaturated model using a flexed hexahedral mesh.



(LaForce et al., 2021a)

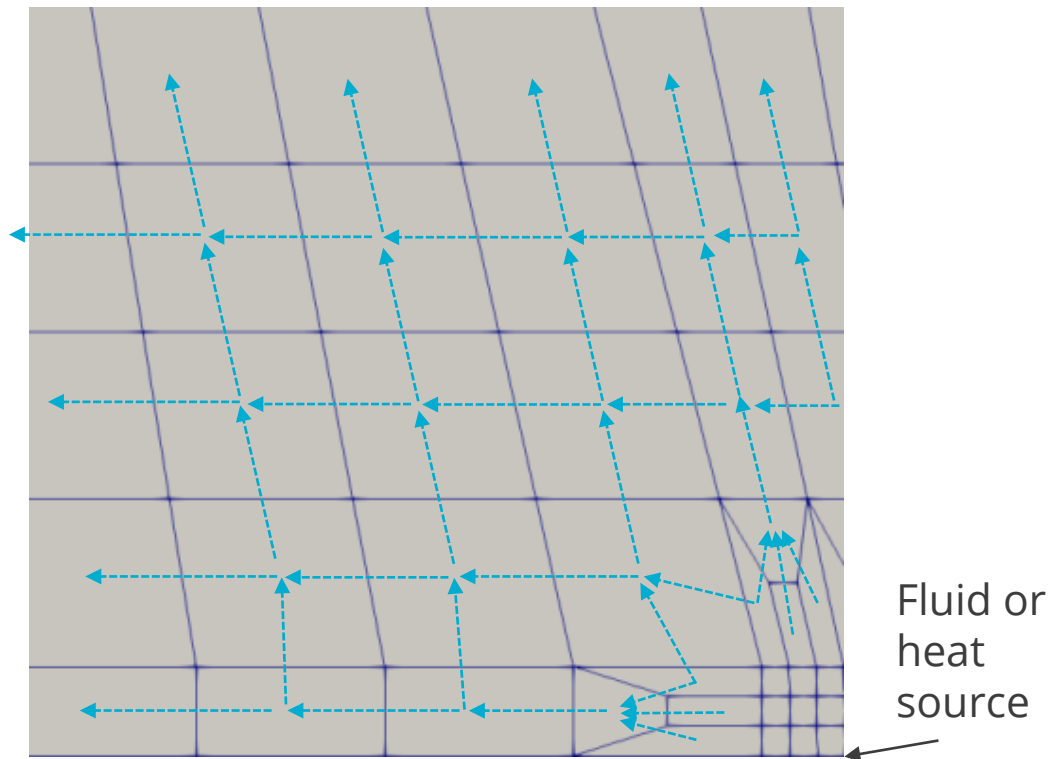


# Why Voronoi meshes? (and what are they?)



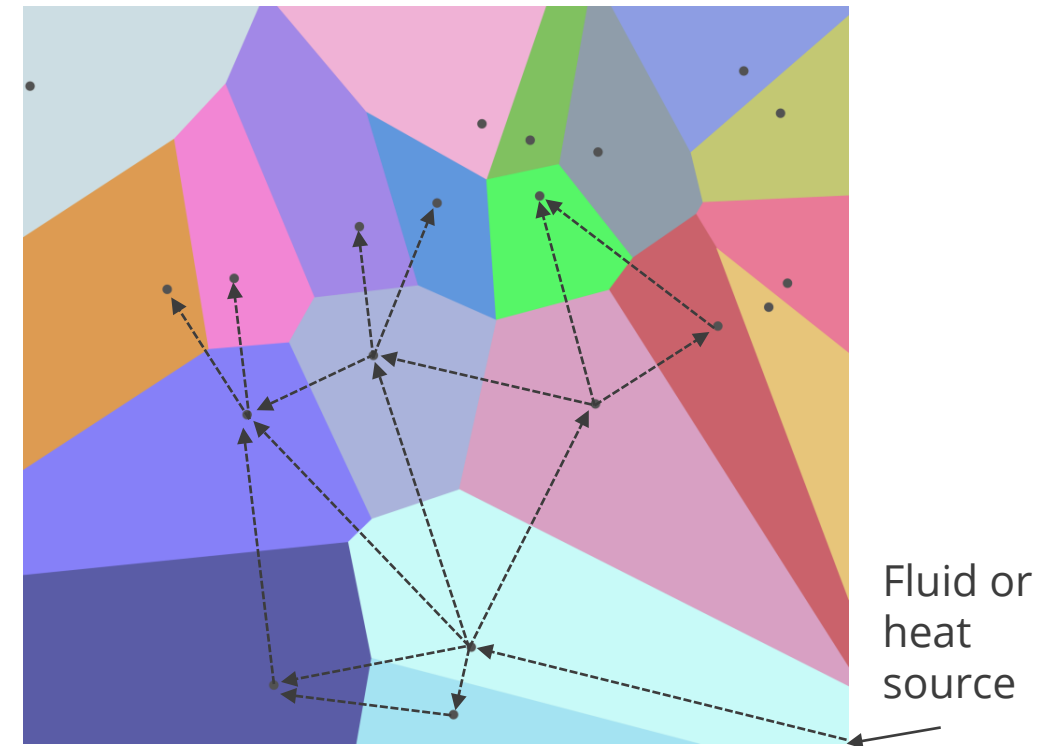
Grid refinement or flexing can bias flow directions

Non-orthogonal fluxes cause errors in SPU/TPFA



Fluxes are perpendicular to grid cell faces using Voronoi polyhedral cells

Solvers using two point flux approximation (TOUGH2/PFLOTRAN/FEHM) get accurate results



By Balu Ertl - Own work, CC BY-SA 4.0,  
<https://commons.wikimedia.org/w/index.php?curid=38534275>

# The 'usual issues' with Voronoi meshes

Creating a Voronoi mesh is hard to do

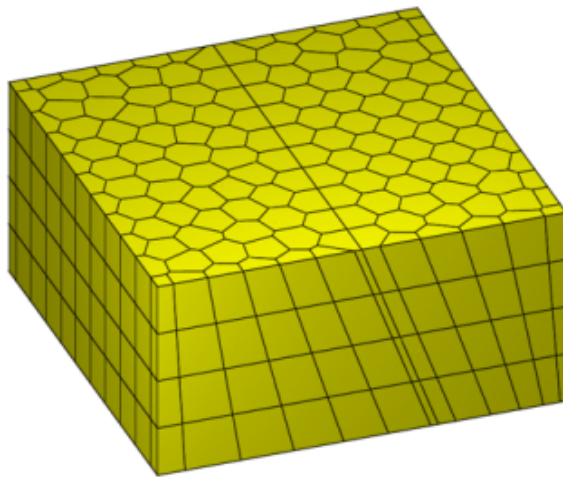


Figure 4.14: A 2.5D grid aligned with an inclined fault.

Many PEBI meshes in the literature are not Voronoi in 3D. (Berge, 2016)

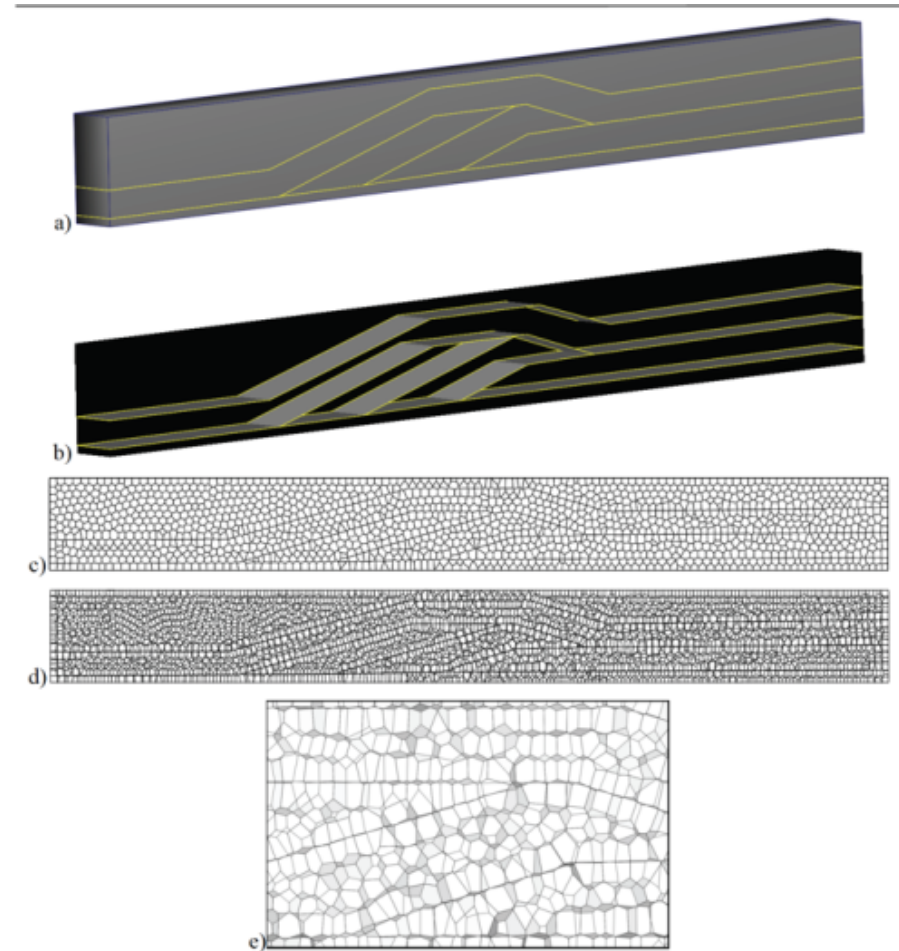


Figure 6: Duplex synthetic case. (a) outer view. (b) inner view. (c-e) optimization using an objective function measuring the outer volume ( $\alpha=0$ ,  $\beta=1$ ). (c) outer view of the grid. (d) slice along the y axis. (e) zoom of the slice along the y axis.

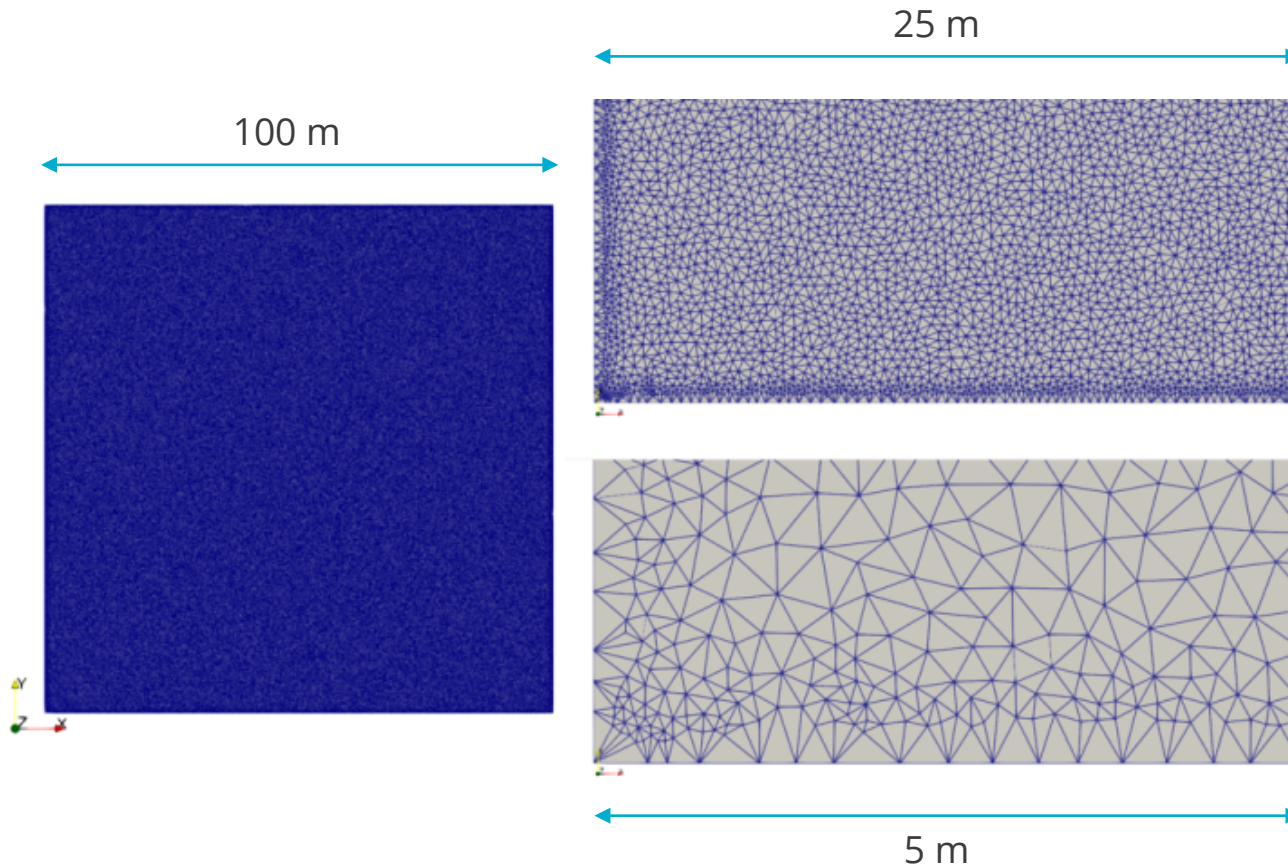
Voronoi, but only approximates interior surfaces (Merland et al, 2011)



# The 'usual issues' with Voronoi meshes



Too many grid cells



Too time-consuming for both humans and computers (after Freeman et al, 2014)

Voronoi meshes should be used when:

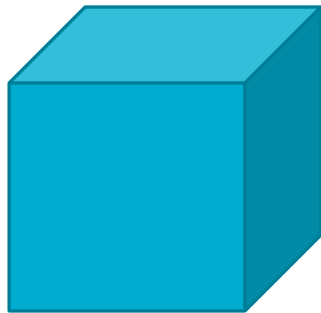
- They can represent geometries that cannot be efficiently meshed in other ways
- Decreased numerical performance is acceptable as there is no viable alternative

Voronoi meshes should only be used where they are suited to the demands of the problem

# The 'usual issues' with Voronoi meshes



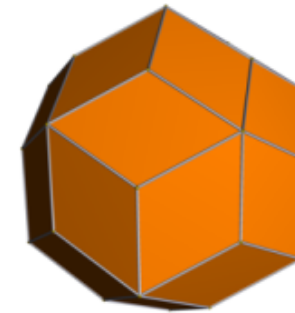
Additional computational overhead in polyhedral/Voronoi meshes



Hexahedral  
6 connections



Tetrahedral  
4 connections



n-sided polyhedral  
n connections

$$\begin{bmatrix} x & x & 0 & & x & 0 & 0 \\ x & x & x & \cdots & 0 & x & 0 \\ 0 & x & x & & 0 & 0 & x \\ & \vdots & & \ddots & & \vdots & \\ x & 0 & 0 & & x & x & 0 \\ 0 & x & 0 & \cdots & x & x & x \\ 0 & 0 & x & & 0 & x & x \end{bmatrix}$$

*Sparse, with just 4  
off – diagonal  
entries but  
not banded*

$$\begin{bmatrix} ? & \cdots & ? \\ \vdots & \ddots & \vdots \\ ? & \cdots & ? \end{bmatrix}$$

# Progress on the 'usual issues'



Meshing improvements: “The VoroCrust algorithm is the first provably correct algorithm for conforming polyhedral Voronoi meshing for non-convex and non-manifold domains with guarantees on the quality of both surface and volume elements.” Abdelkader et al, 2020

In other words, VoroCrust:

- Produces genuinely Voronoi meshes
- Guaranteed to produce a mesh that rigorously honors piecewise linear faceted input surfaces that create closed volumes

Also allows for local refinement near areas of interest and random generation of meshes

PFLOTRAN's (<http://www.pflotran.org>) parallel architecture makes extra computational time less of an issue

Still working on:

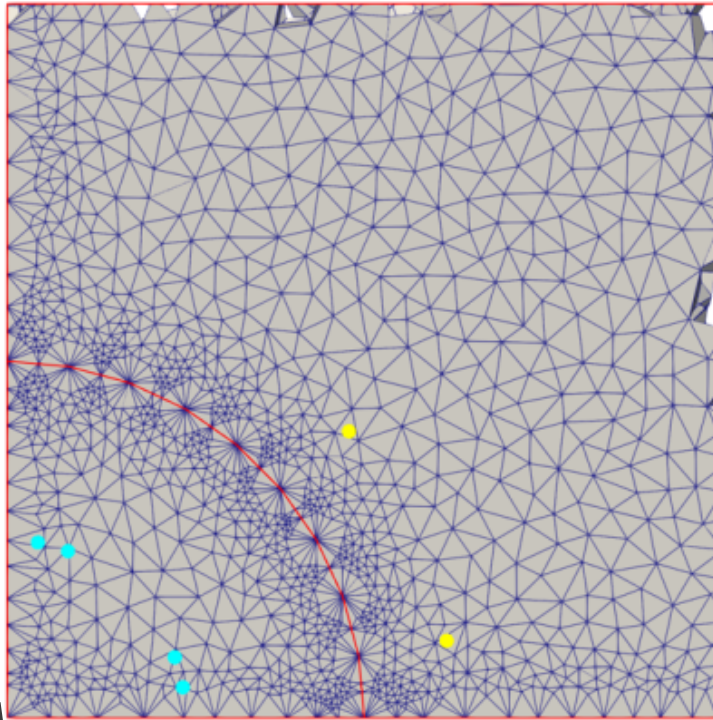
- Too many grid cells
- Meshing very narrow regions
- Need to consistently retain monitoring points



# Analytical benchmark: Two domain heating

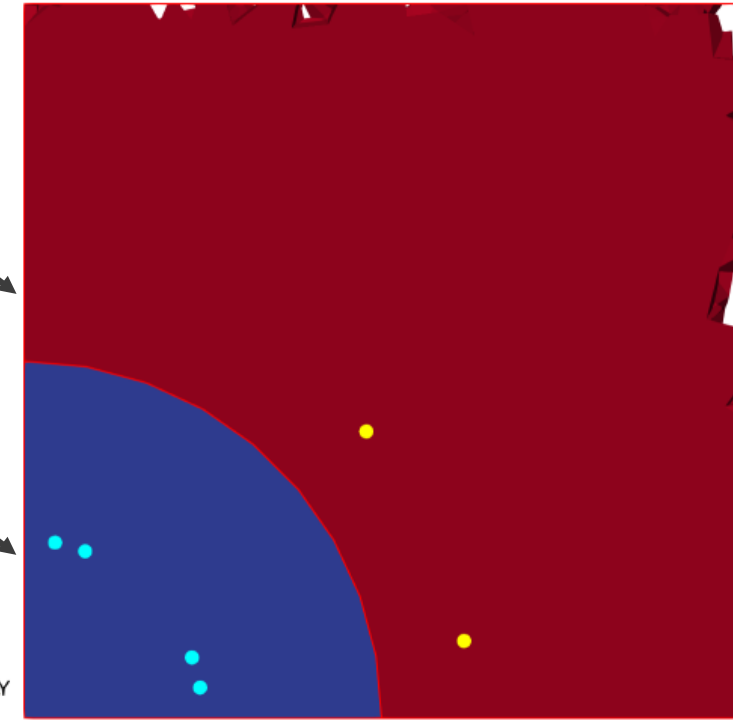


Heat source

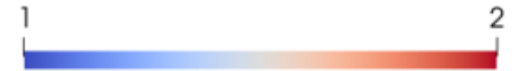


Low Thermal Conductivity

High Thermal Conductivity



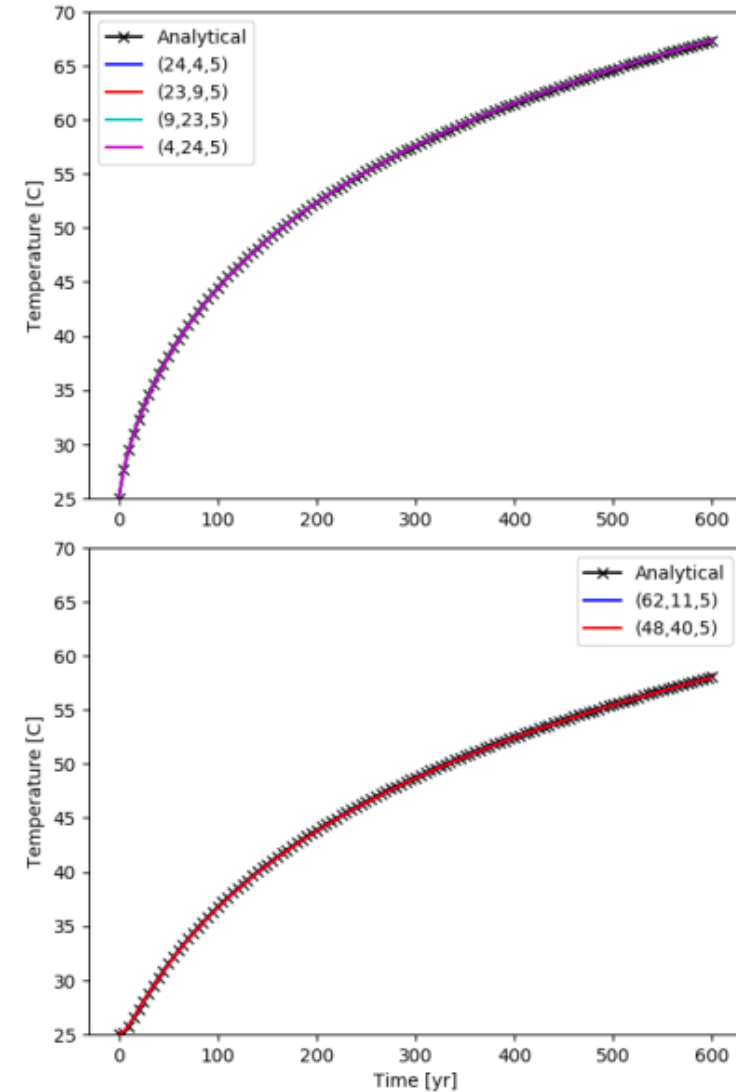
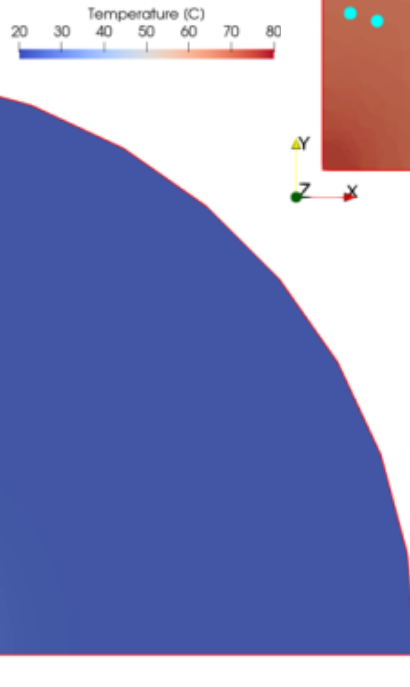
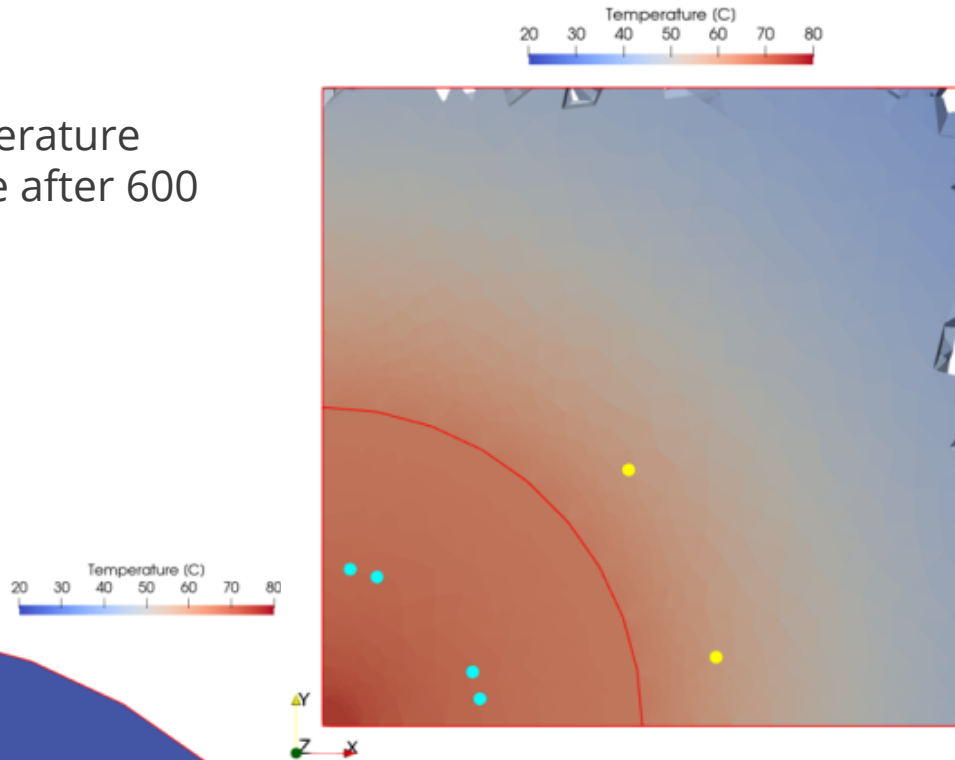
Material ID



# Analytical benchmark: Two domain heating



Temperature  
profile after 600  
years



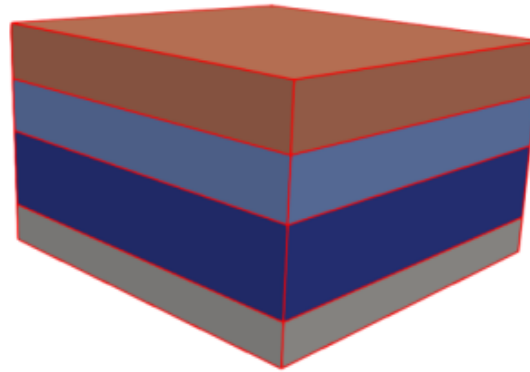
Simulated and analytical temperature at  $r = 25$  m (top) and  $r = 62.5$  m (bottom) for two-domain heating analytical benchmark. Error < 0.2%

# Four test case geometries (Gross et al. 2019)

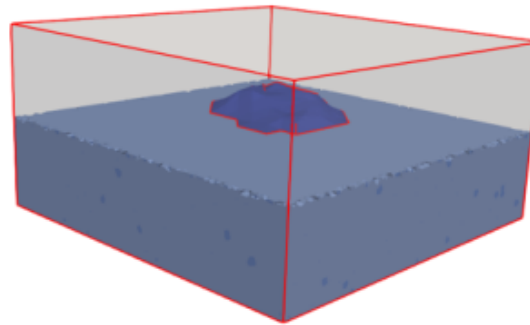
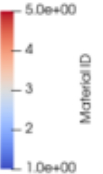
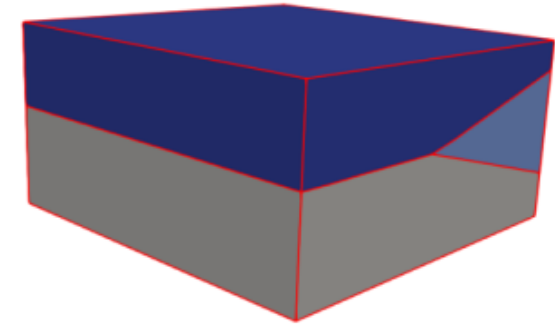


- 4 simulations on each model geometry
- 1.4-4.4 Heterogeneous, two phase (Richard's) downward flow
  - Constant flux at top boundary
  - Constant saturation and pressure at bottom boundary
  - Side boundaries are closed

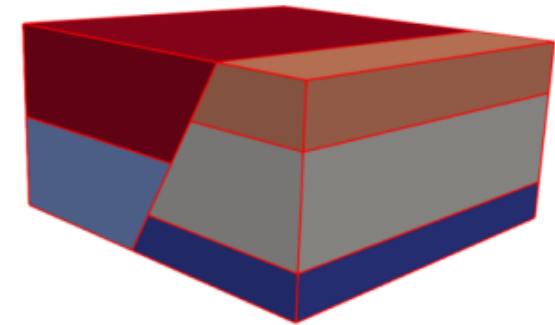
4 horizontal layers



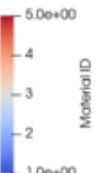
Pinch-out



Interior lens

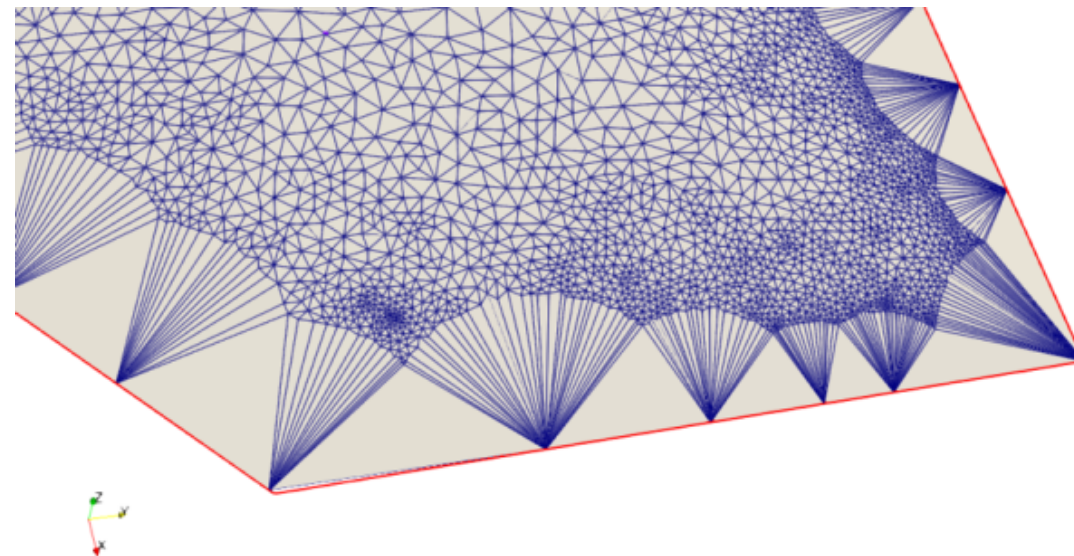
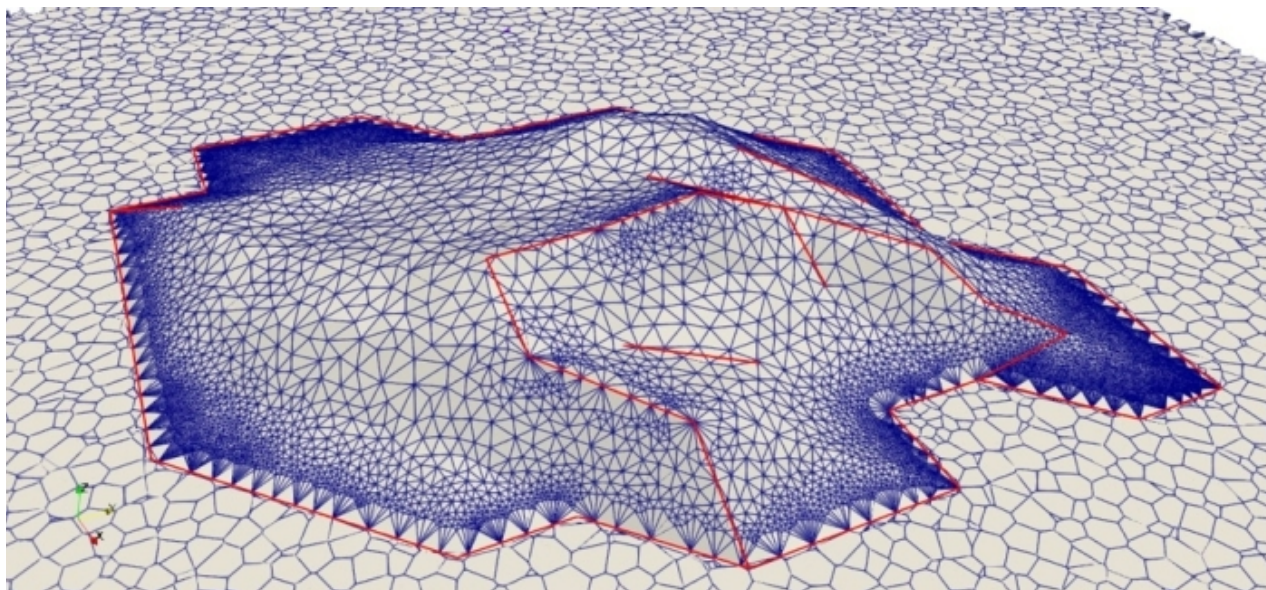
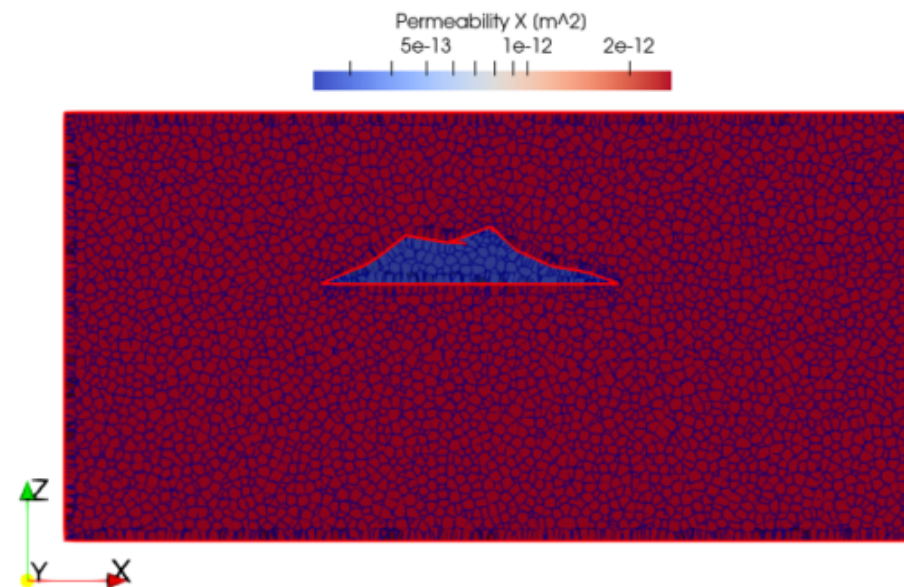
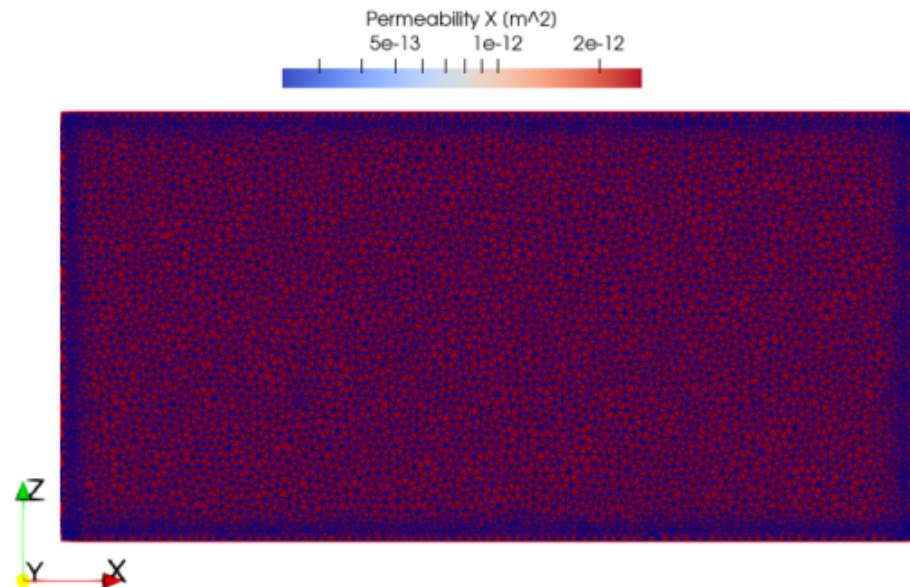


Offset fault





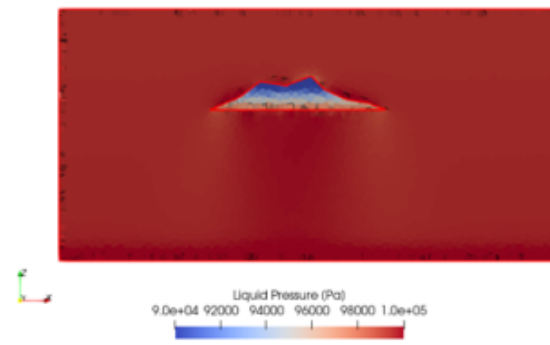
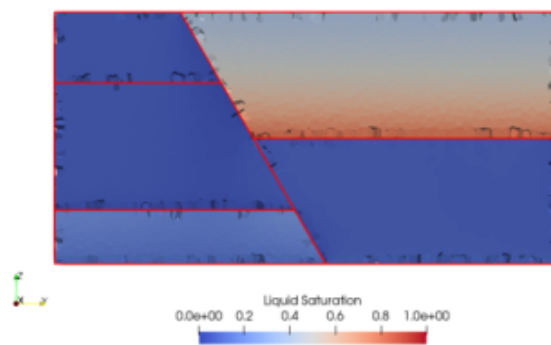
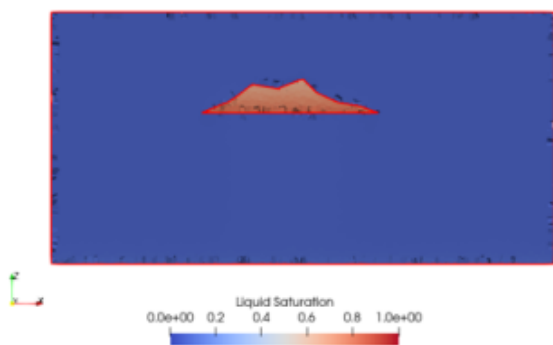
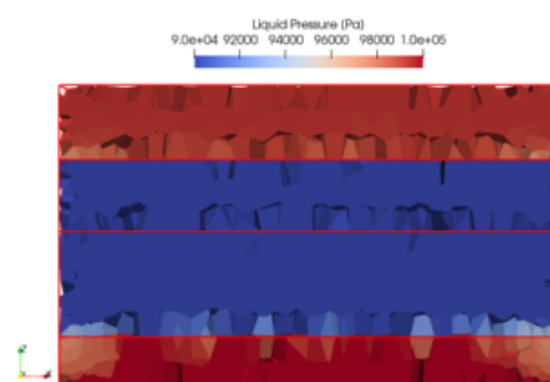
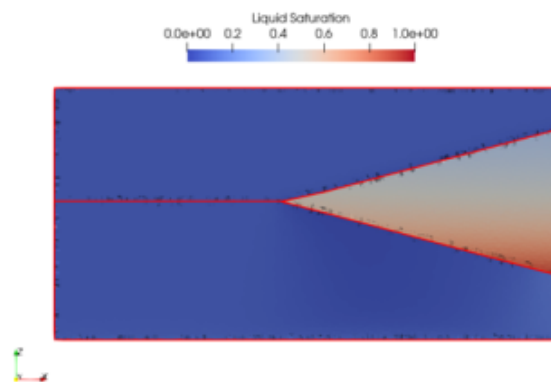
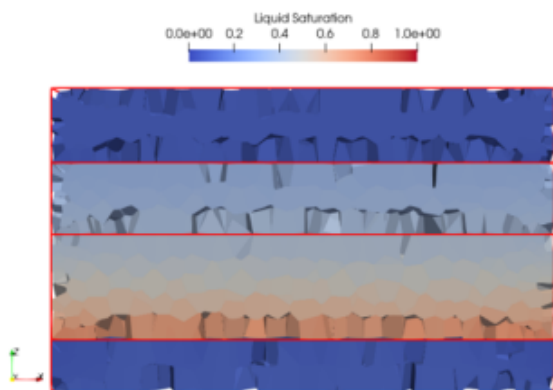
# Test structure 3 mesh



# Test case 1.4-4.4 results

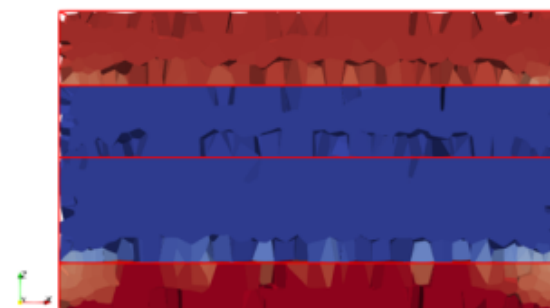


Steady-state liquid saturation

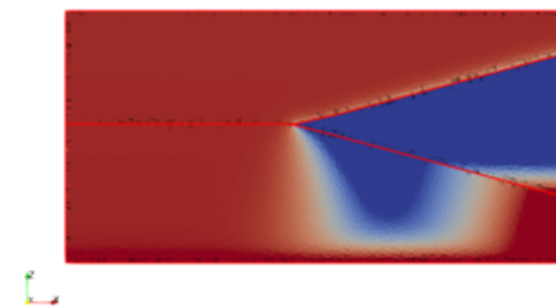


Steady-state liquid pressure

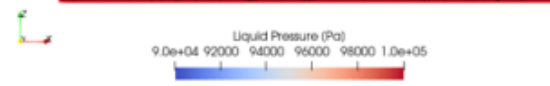
Liquid Pressure (Pa)



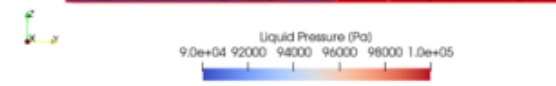
Liquid Pressure (Pa)



Liquid Pressure (Pa)



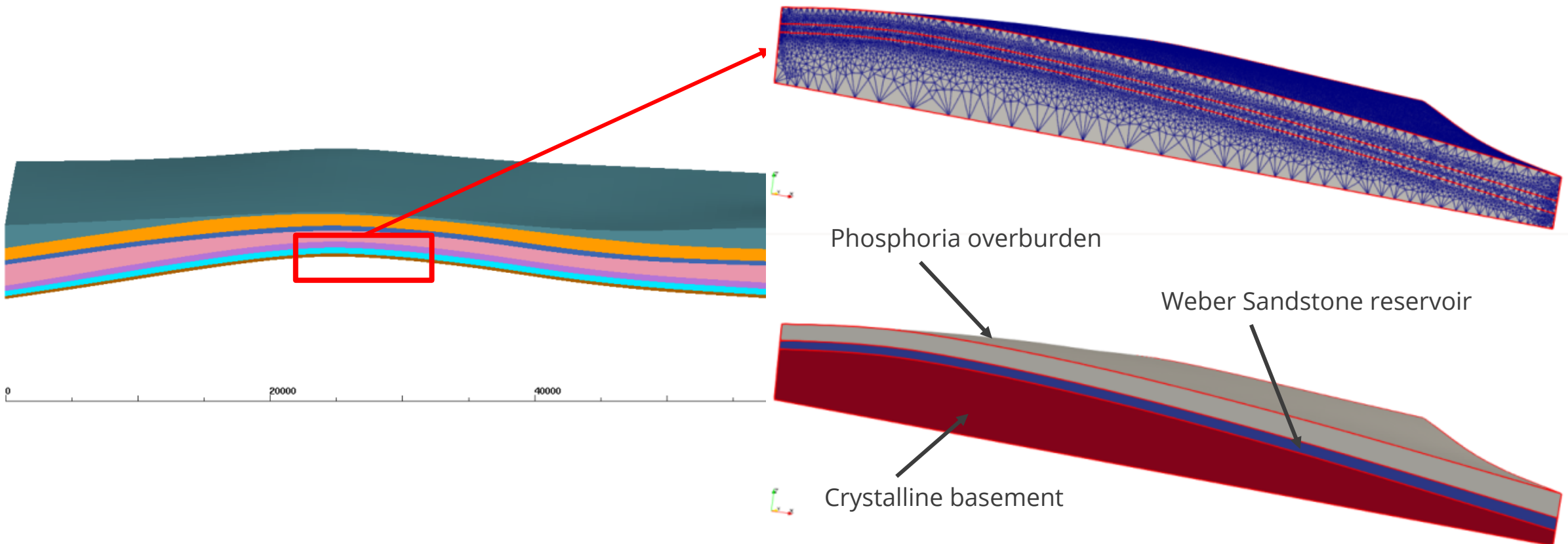
Liquid Pressure (Pa)





# Rock Springs uplift

(Stauffer et al. 2009, Deng et al. 2012 and Harp et al. 2017)



(LaForce et al., 2021b)

# Rock Springs uplift mesh



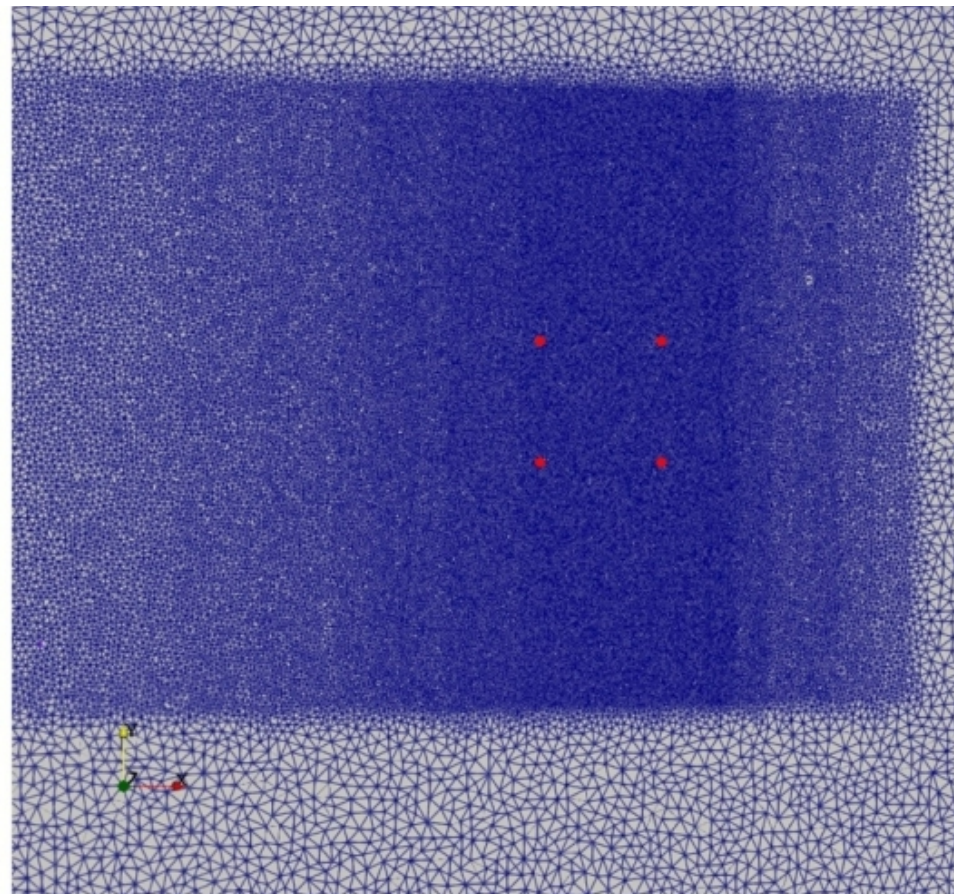
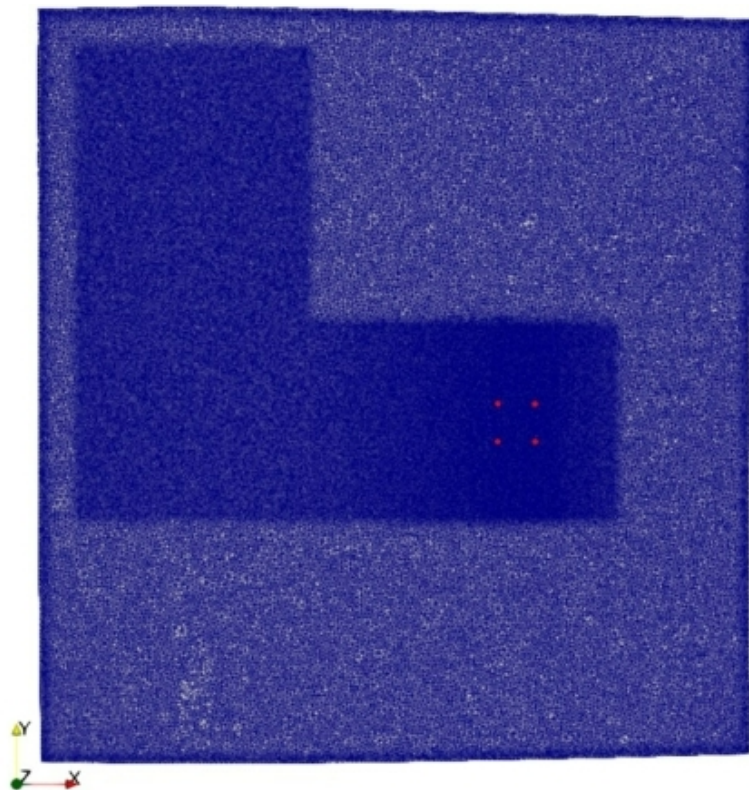
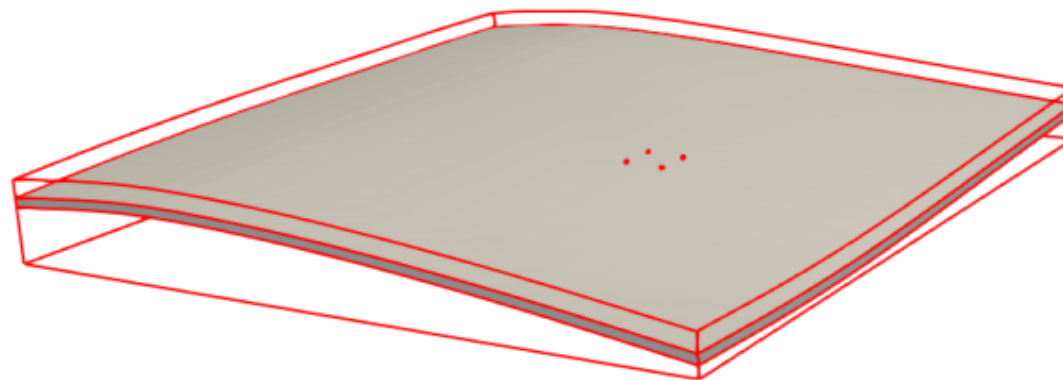
Using Los Alamos open-source software LaGriT excess layers are eliminated and mesh clipped to the region of interest.

- 4 surfaces are preserved to represent formation of interest, overburden and underburden
- Real underburden layer is eliminated because it was too thin and a flat base is used
- Model is clipped to 20 x 20 km square encompassing one side of uplift and the top structure

Using VoroCrust mesh refinement capability

- Volume near the 4 injection wells is refined to a maximum cell radius of 20 m
- Weber Sandstone updip and downdip of the wells is refined to maximum cell radius of 50 m
- Grid cell sizes in the rest of the mesh are automatically adapted to be the largest allowable for the geometry.

# Top Weber Sandstone mesh





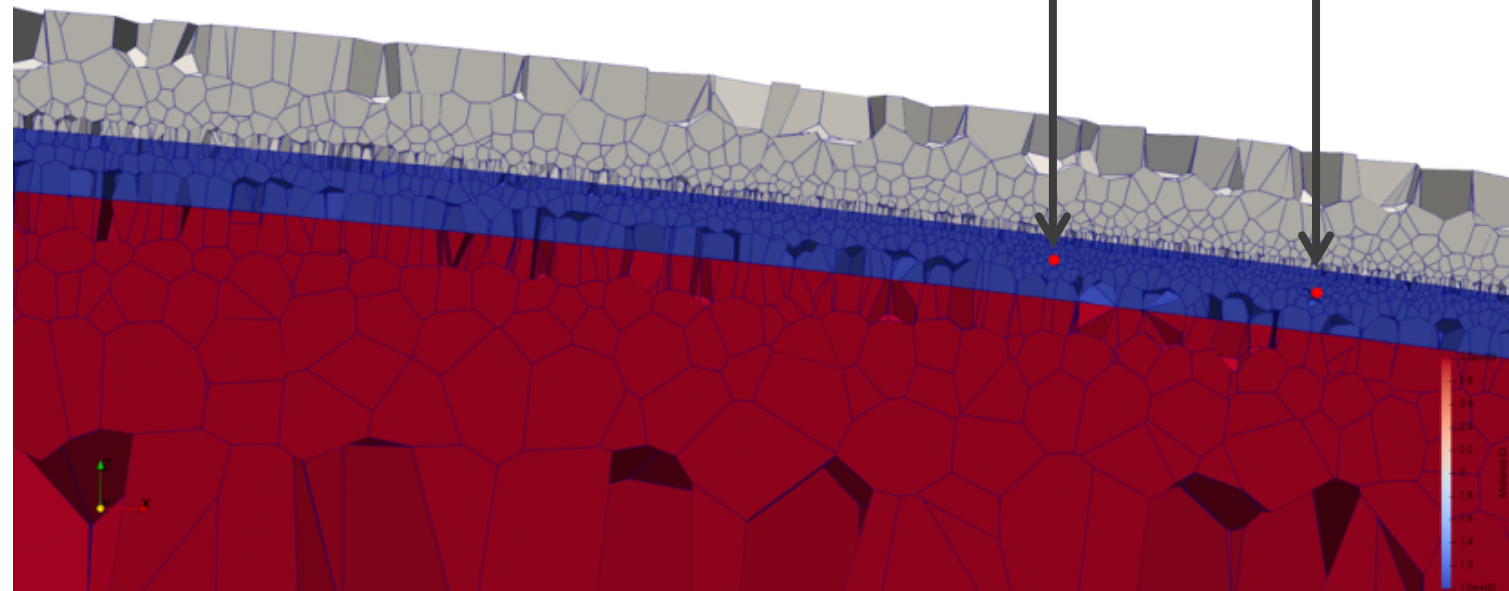
# Rock Springs uplift simulation



Realization	mesh 1	mesh 2	mesh 3
Grid cells	763,607	763,769	762,763
Maximum connections	36	36	37
Average connections	11	11	11
Minimum connections	4	4	4
Injector 1 (x,y,z)	(18500, 8500, -1390)	(18500, 8550, -1390)	(18500, 8500, -1390)
Injector 2 (x,y,z)	(18500, 9500, -1390)	(18500, 9550, -1390)	(18500, 9500, -1390)
Injector 3 (x,y,z)	(19500, 8500, -1515)	(19500, 8550, -1515)	(19500, 8500, -1515)
Injector 4 (x,y,z)	(19500, 9500, -1515)	(19500, 9550, -1515)	(19500, 9500, -1515)
Mesh generation time (hr)	1.87	1.40	1.44
Simulation time (hr)	24.7	25.1	28.2

Injection for 100 years at  
1 million tons per year

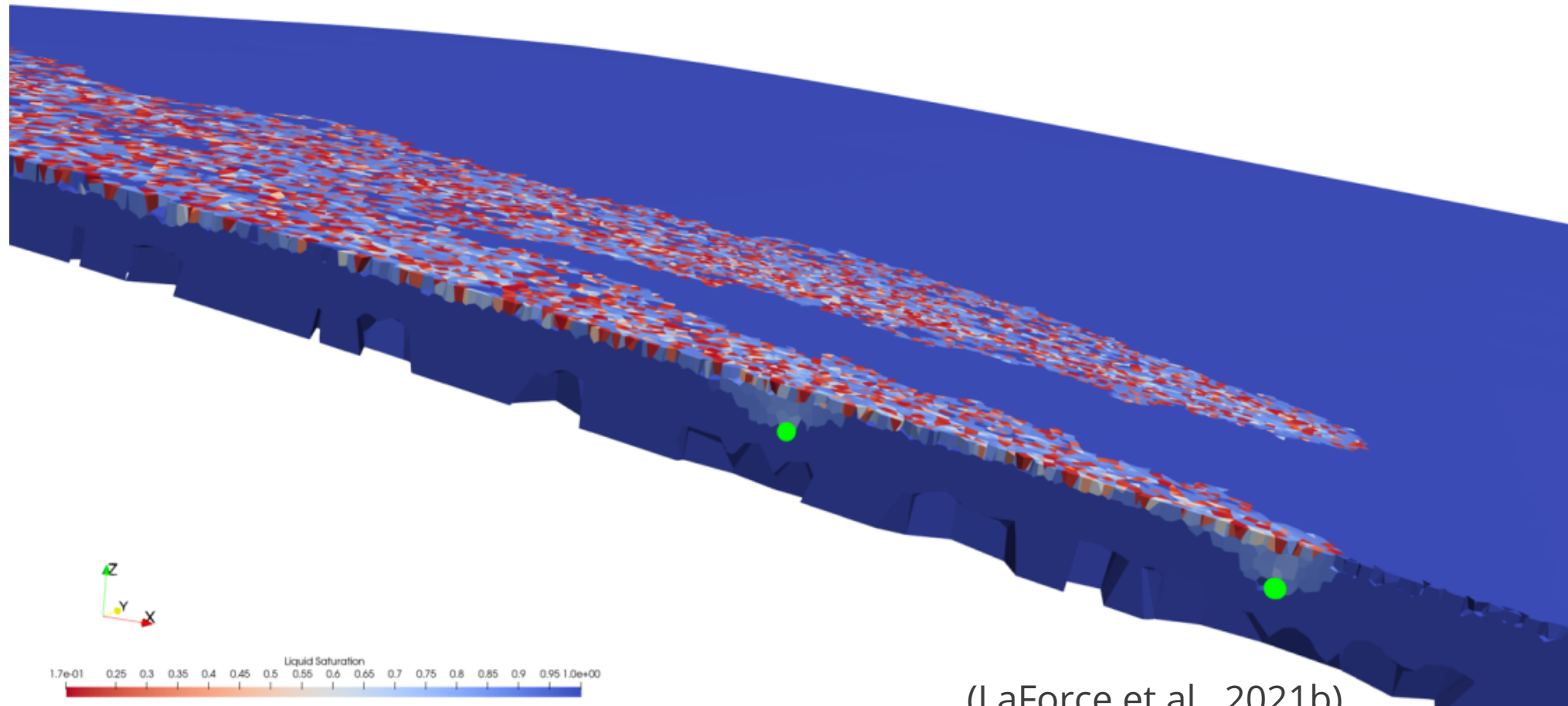
Slice through two of  
the wells at  $y = 9500$  m.



# Rock Springs uplift



Weber sandstone slice through two of the wells at  $y = 8500$  m. Time = 10 yr



(LaForce et al., 2021b)



# Rock Springs uplift: CO<sub>2</sub> at top of Weber Sandstone



2.5 yr

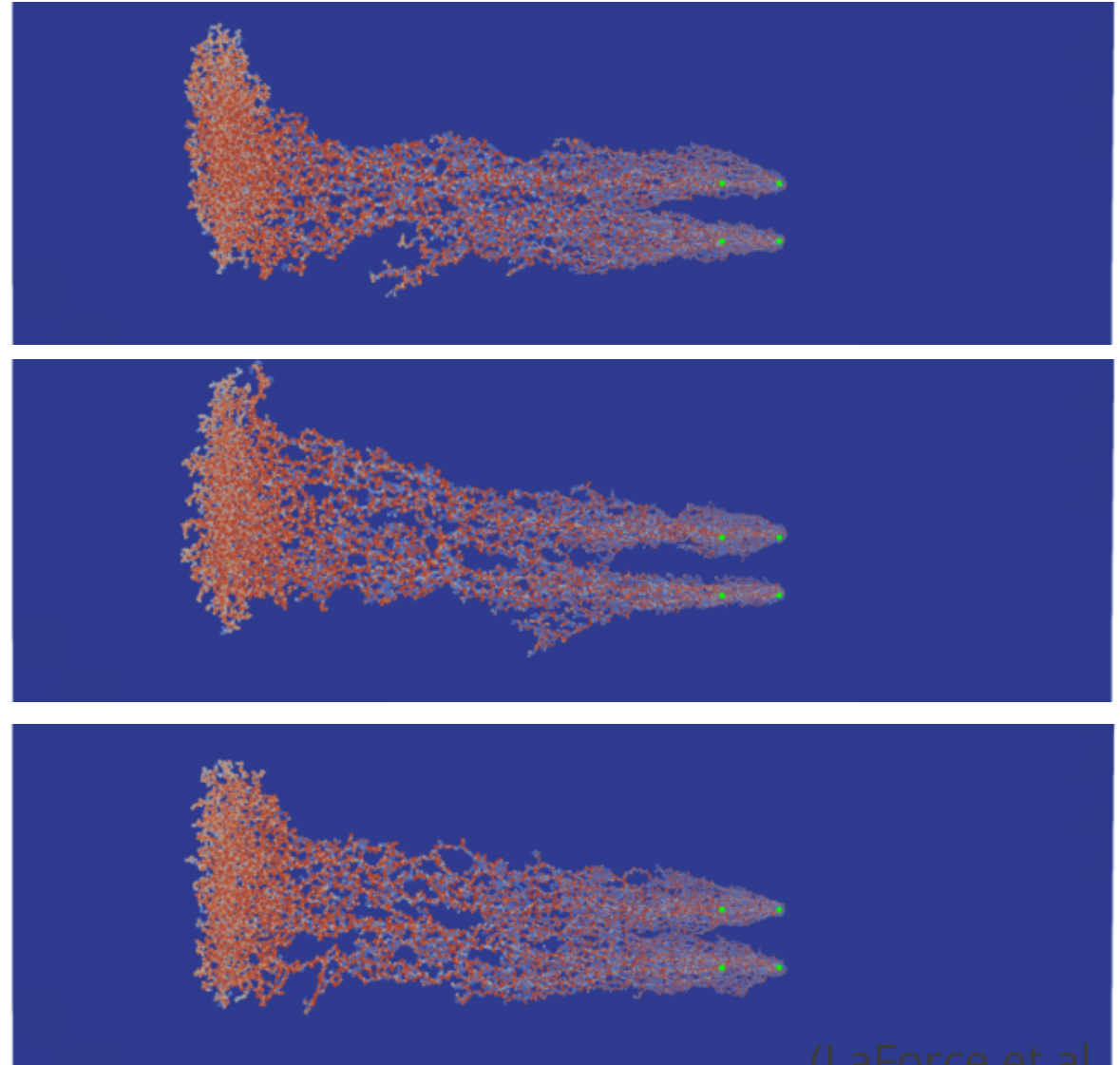
R1

R2

R3



10 yr

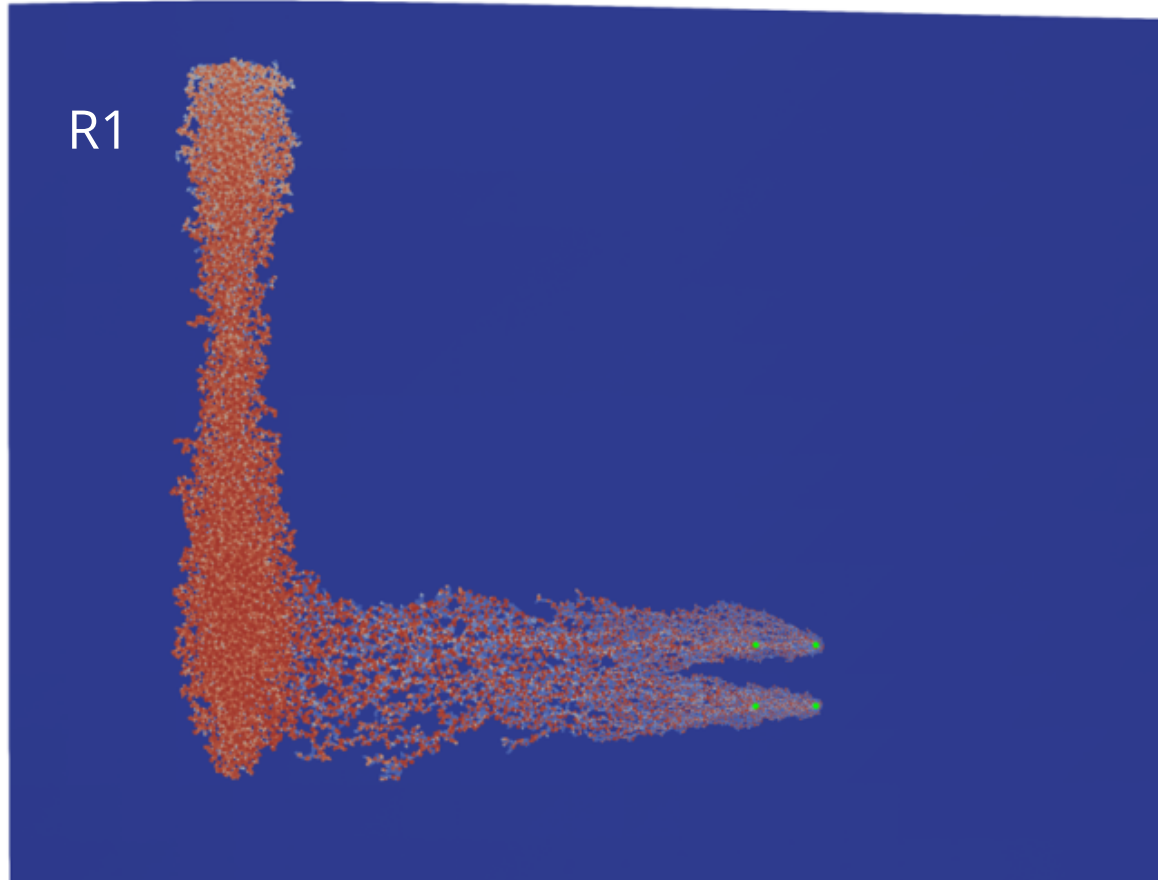


(LaForce et al., 2021b)

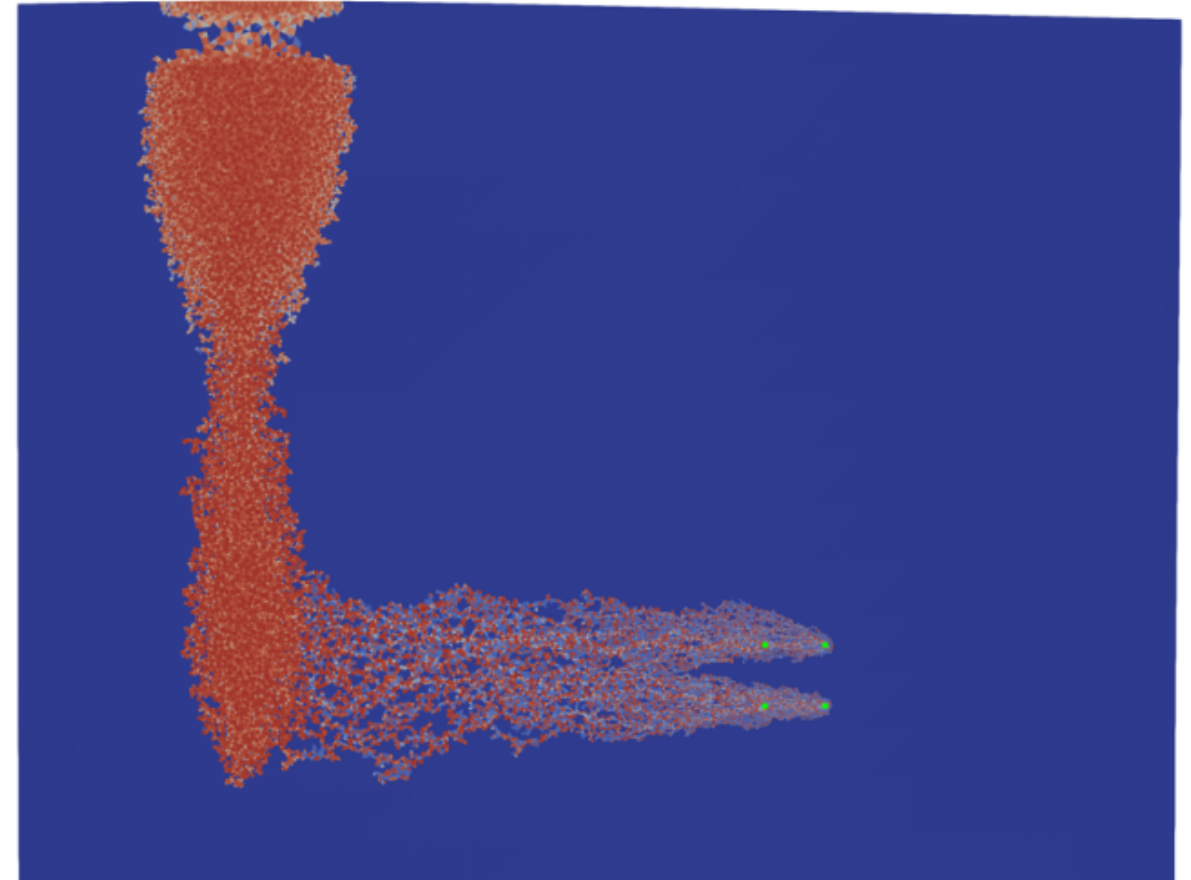
# Rock Springs uplift: CO<sub>2</sub> at top of Weber Sandstone



20 yr



30 yr



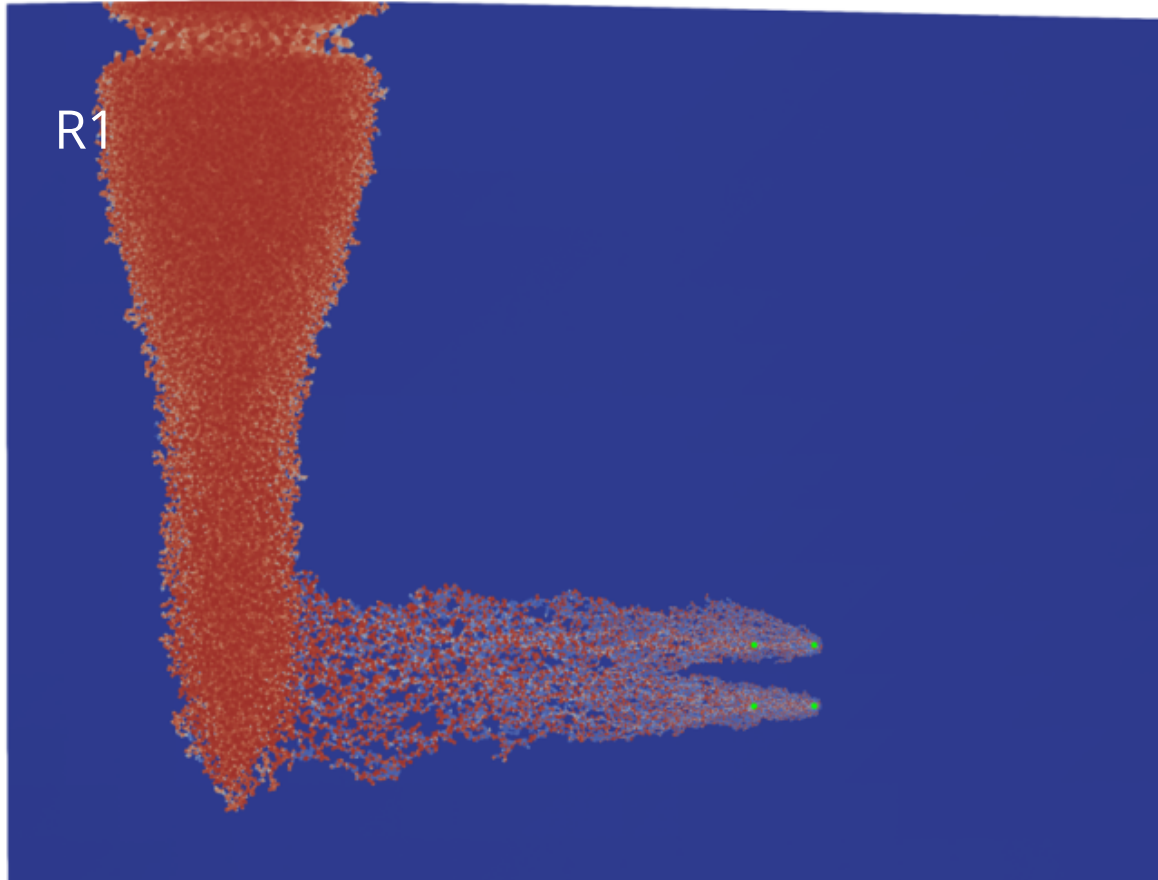
(LaForce et al., 2021b)



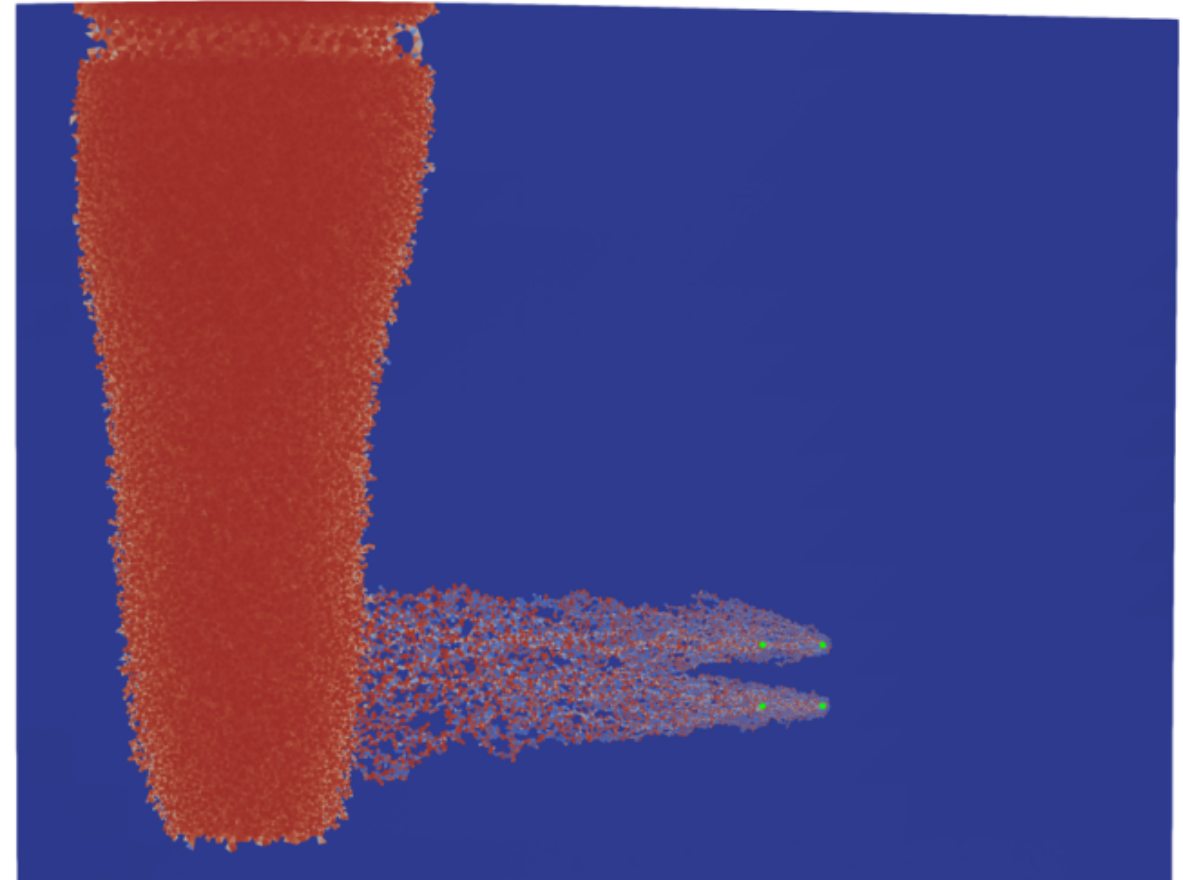
# Rock Springs uplift: CO<sub>2</sub> at top of Weber Sandstone



50 yr



100 yr



(LaForce et al., 2021b)



# Conclusions



Automated meshing allows us to overcome many of the 'usual issues' with Voronoi meshing

- Meshes are genuinely Voronoi and honor arbitrary interior surfaces
- Meshing is automated and requires little human or computer time
- Easy to change refinement locally or globally
- Easy to generate a new realization of the mesh

Benchmark simulation on Voronoi mesh is accurate against analytical solution and not prohibitively slow

Generating meshes and running simulations on the four test structures was successful and simulations are accurate

Field-scale CO<sub>2</sub> storage simulation of gas flow on multiple realizations of the mesh

# Future work

## Immediate future:

- Investigate Voronoi meshes for simulations with known grid orientation effects

## Medium term:

- Open-source version of the meshing software
- Add to uncertainty quantification and sensitivity analysis:
  - Impact of mesh realization
  - Introduce geological uncertainty

## Longer term:

- Mesh faults that terminate within the model
- Anisotropic meshing to reduce element numbers

Geology A



Geology B

Geology C





**LaForce T, Basurto E, Chang K W, Jayne R S, Leone R C, Nole M, Perry F, Stein E (2021a) GDSA Repository Systems Analysis investigations in FY2021. Technical report, Sandia National Lab.(SNLNM), Albuquerque, NM**

**LaForce T, Ebeida M, Jordan S, Miller T, Stauffer P H, Park H, Leone R, Hammond G (2021b) Voronoi meshing to accurately capture geology in subsurface simulations *submitted to Mathematical Geoscience***

Berge R L (2016) Unstructured PEBI-grids Adapting to Geological Features in Subsurface Reservoirs. Master's thesis, NTNU

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Freeman C M, Boyle K L, Reagan M, Johnson J, Rycroft C, Moridis G J (2014) MeshVoro: A three-dimensional Voronoi mesh building tool for the TOUGH family of codes. Computers & Geosciences 70:26–34

Abdelkader A, Bajaj C L, Ebeida M S, Mahmoud A H, Mitchell S A, Owens J D, Rushdi A A (2020) VoroCrust: Voronoi meshing without clipping. ACM Transactions on Graphics (TOG) 39(3):1–16

Gross M, Bussod G, Gable C, Kelley R, Lavadie-Bulnes A, Milazzo D, Miller E, Miller T, Roback R, Stauffer P, E S (2019) Progress report on the development of a geologic framework model capability to support GDSA. Technical Report LA-UR-19-27943, Los Alamos National Lab., Los Alamos, NM (United States)

Stauffer P H, Surdam R C, Jiao Z, Miller T A, Bentley R D (2009) Combining geologic data and numerical modeling to improve estimates of the CO<sub>2</sub> sequestration potential of the rock springs uplift, Wyoming. Energy Procedia 1(1):2717–2724

Deng H, Stauffer P H, Dai Z, Jiao Z, Surdam R C (2012) Simulation of industrial-scale CO<sub>2</sub> storage: Multiscale heterogeneity and its impacts on storage capacity, injectivity and leakage. International Journal of Greenhouse Gas Control 10:397–418

Harp D R, Stauffer P H, O'Malley D, Jiao Z, Egenolf E P, Miller T A, Martinez D, Hunter K A, Middleton R S, Bielicki J M, et al. (2017) Development of robust pressure management strategies for geologic CO<sub>2</sub> sequestration. International Journal of Greenhouse Gas Control 64:43–59