SAND2022-15558C

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Newton Trust Region Methods for Nuclear Waste Repository Porous Media Simulations

ANS 2022 Winter Meeting - IHLWRM

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Disposal IV

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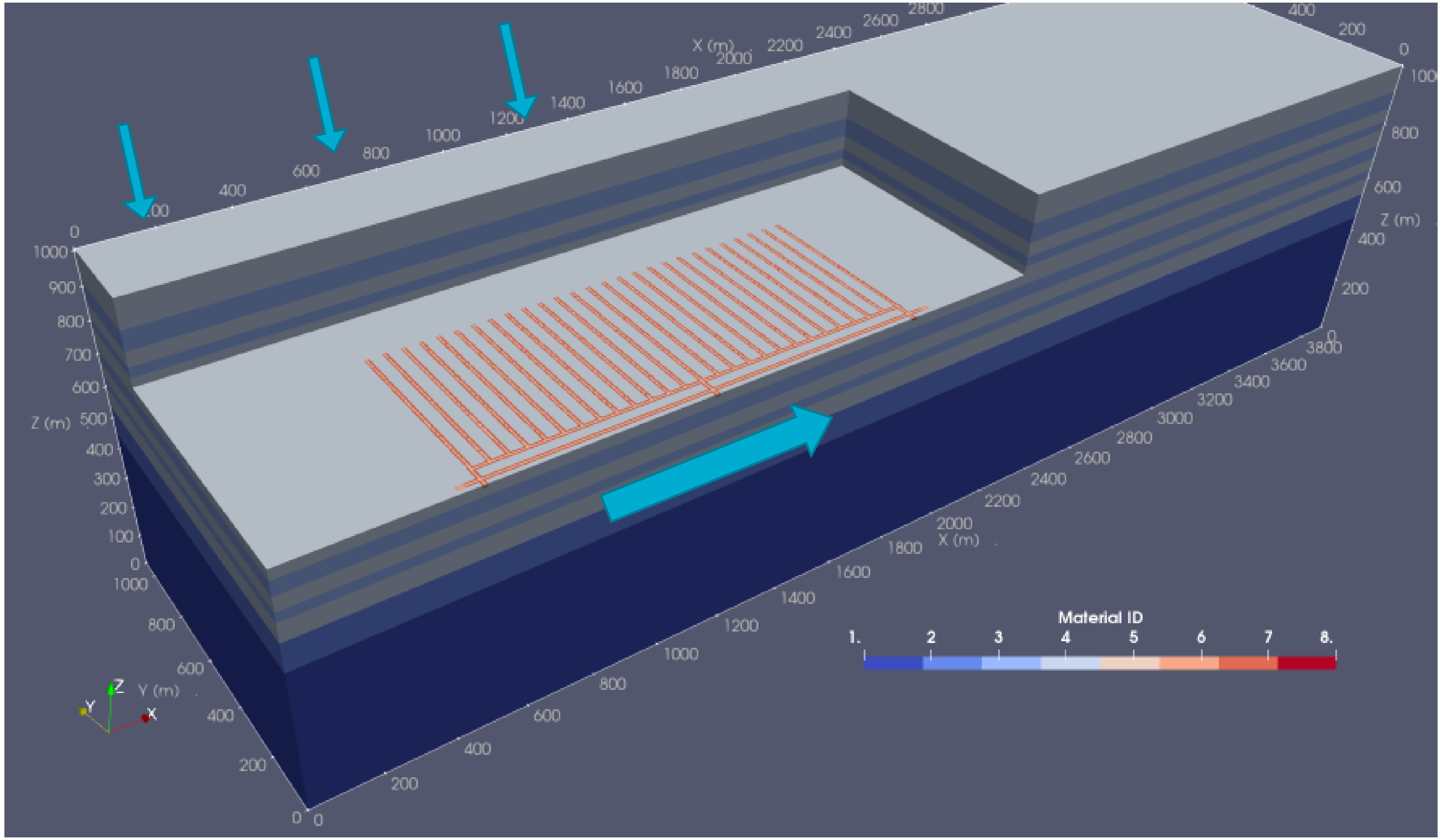
Introduction – large scale engineered subsurface systems

- Radioactive waste geologic disposal system
- Heterogenous geologic features, infiltration, and regional flow



Cropped view of the symmetric simulation domain of hypothetical Alluvial unsaturated zone radioactive waste repository.

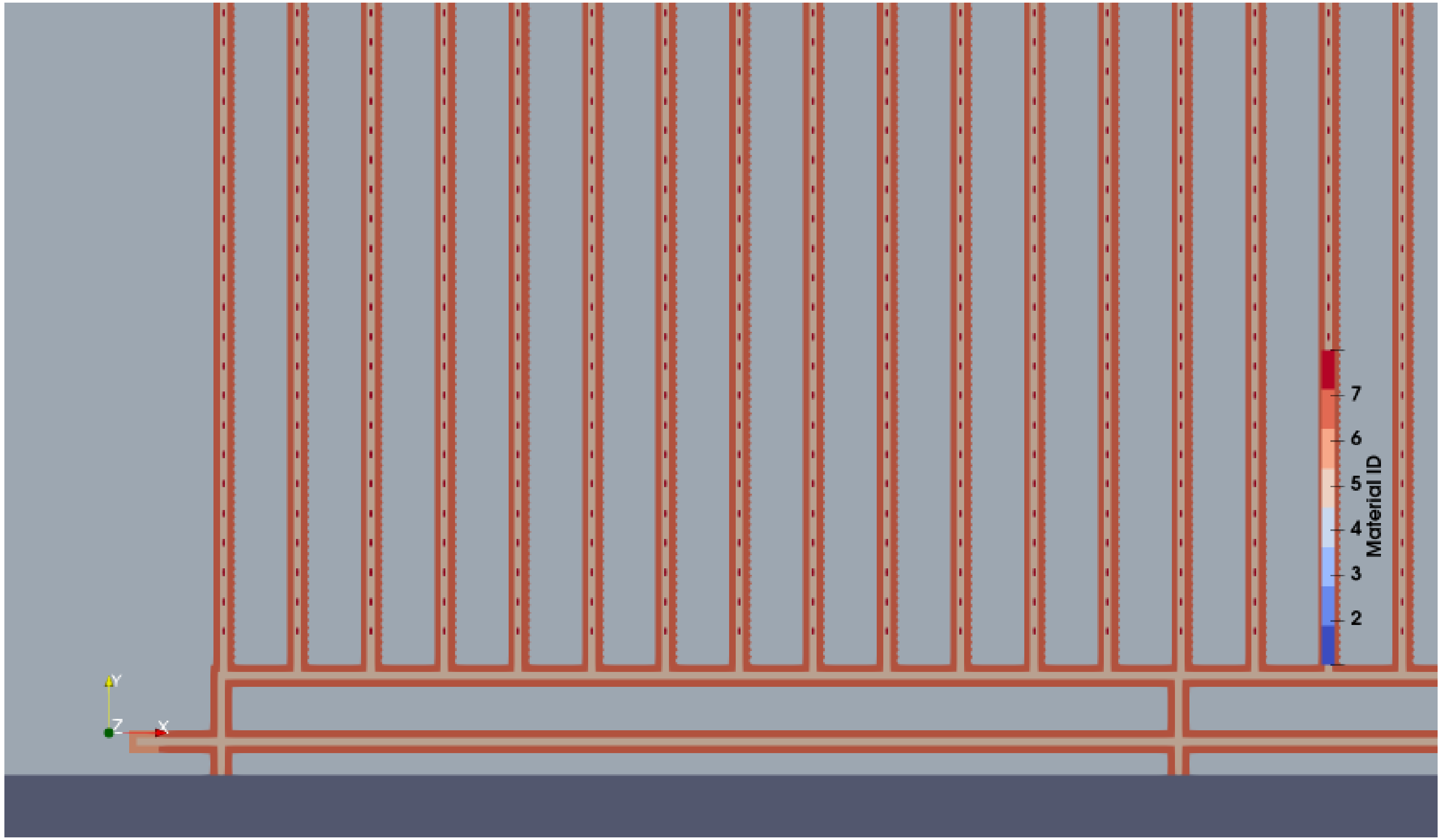
2.4M grid cells
7.2M unknowns

Meshed by: Emily Stein

Material ID
1: Lower basin
2: Aquifer
3: Upper basin (low k)
4: Upper basin (high k)
5: Backfill
6: UB DRZ (low k)
7: UB disturbed rock zone
8: Waste package

Introduction – the numerical challenges

- Small discrete features like shafts, tunnels, waste packages, and backfills
- Discrete and large contrasts in porosity and permeability



Top view of the waste repository

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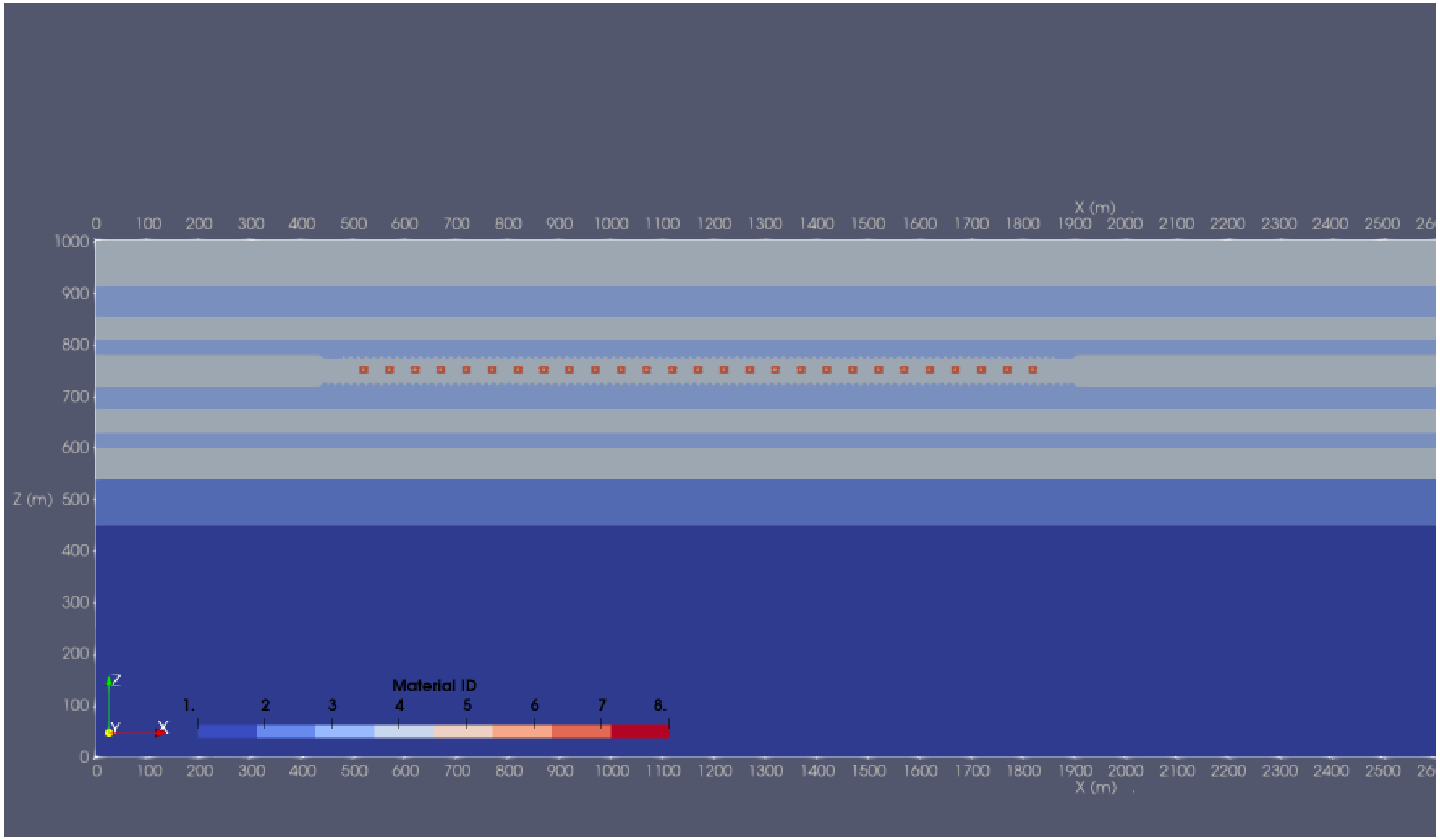

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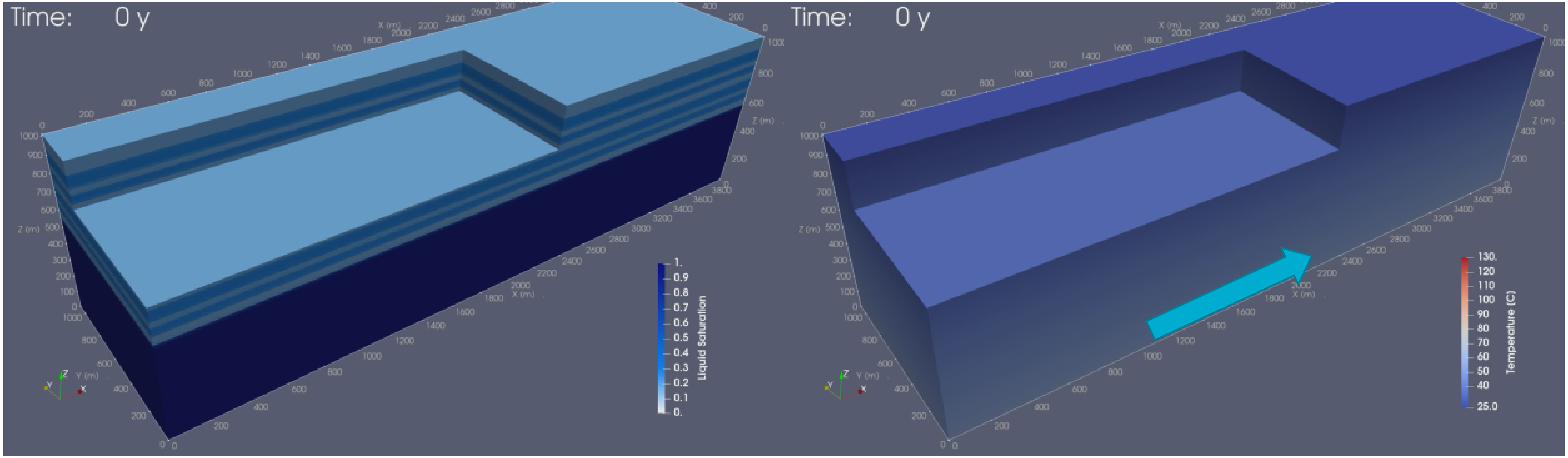
Introduction – the numerical challenges

- High decay temperatures from waste packages
- Heat-forced dry-out and re-saturation by natural forces

Saturation

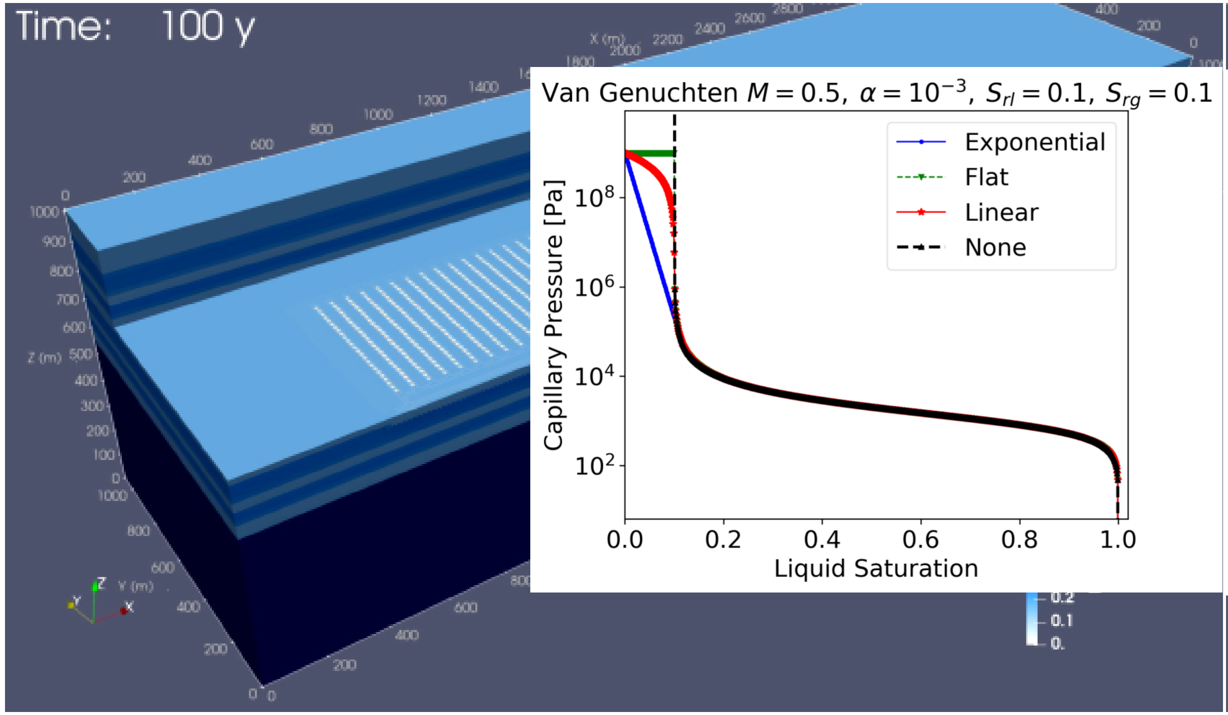
Temperature



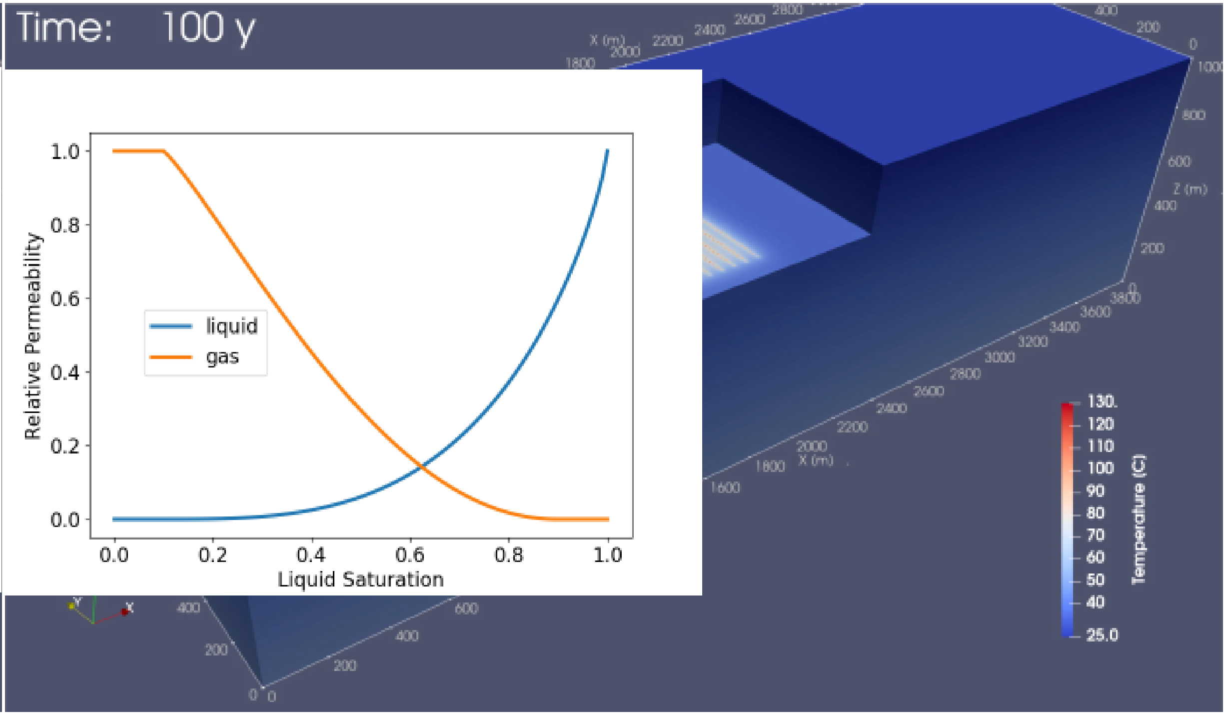
Introduction – the numerical challenges

- Testing extreme nonlinearities on both ends of the capillary pressure and relative permeability curve

Saturation



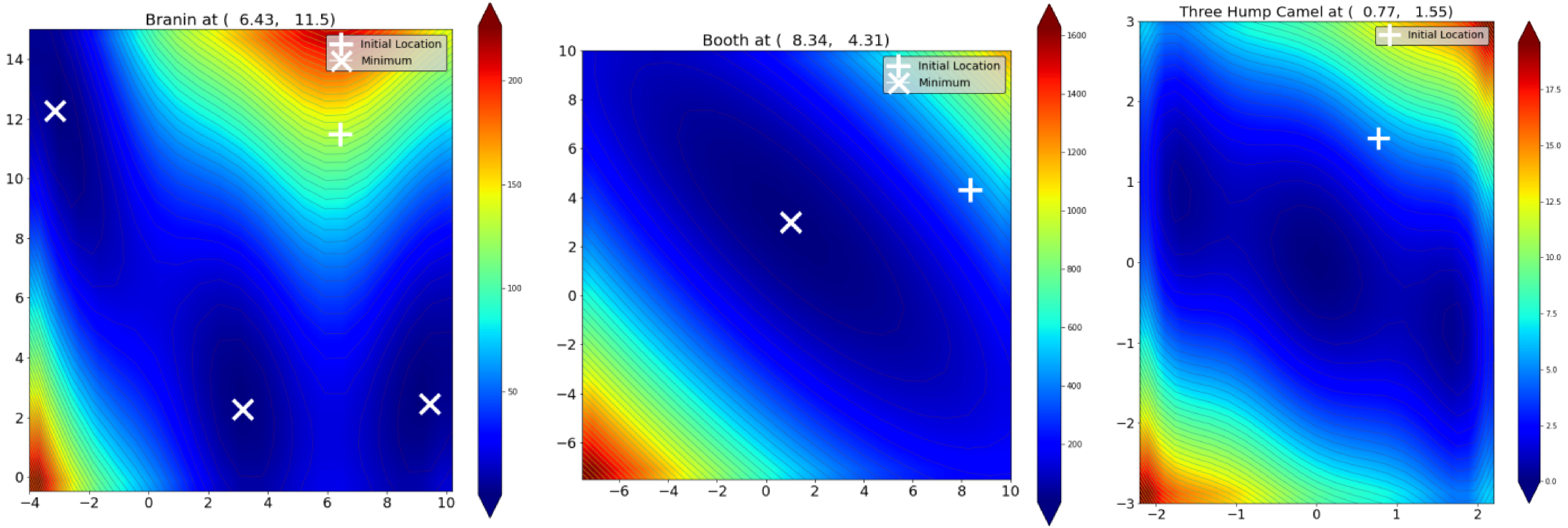
Temperature



Park H., et al. (2022), Newton trust-region methods with primary variable switching for simulating high temperature multiphase porous media flow, Advances in Water Resources, DOI: 10.1016/j.advwatres.2022.104285

Optimization problem

- Imagine a residual space for each grid cell
- the solver must optimize the solution of quantity in x and y to reach the minimum residual

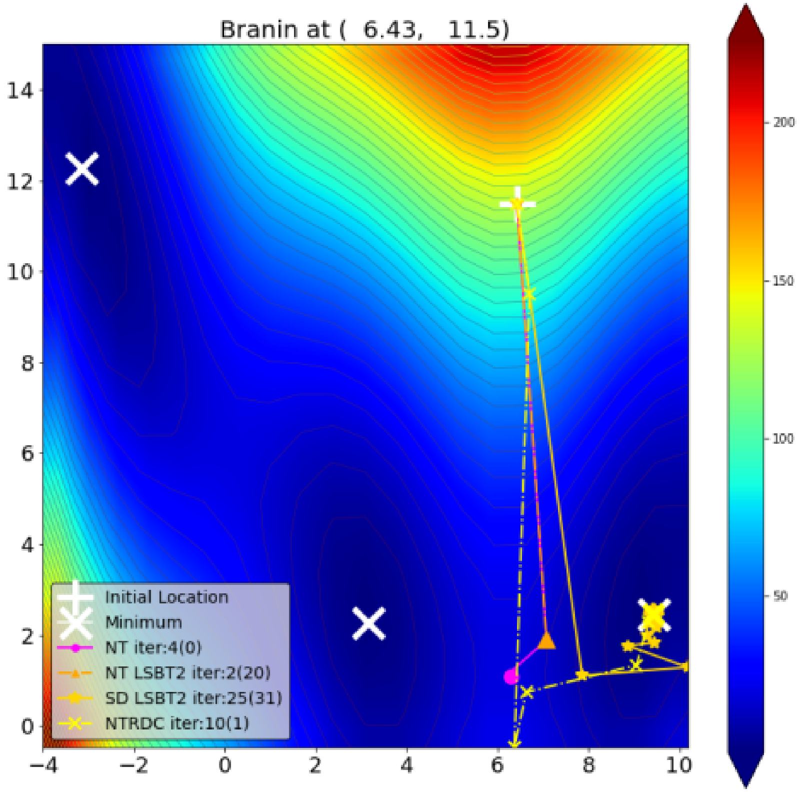


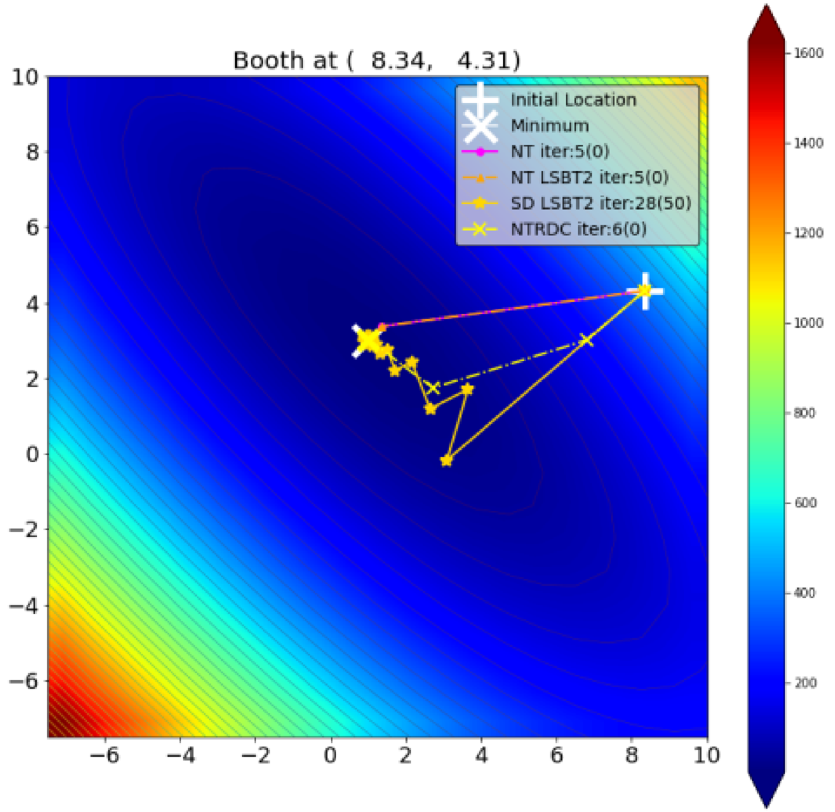
Red contour is high and blue contour is low representing residual space. '+' is the initial guess and 'x' is the solution.

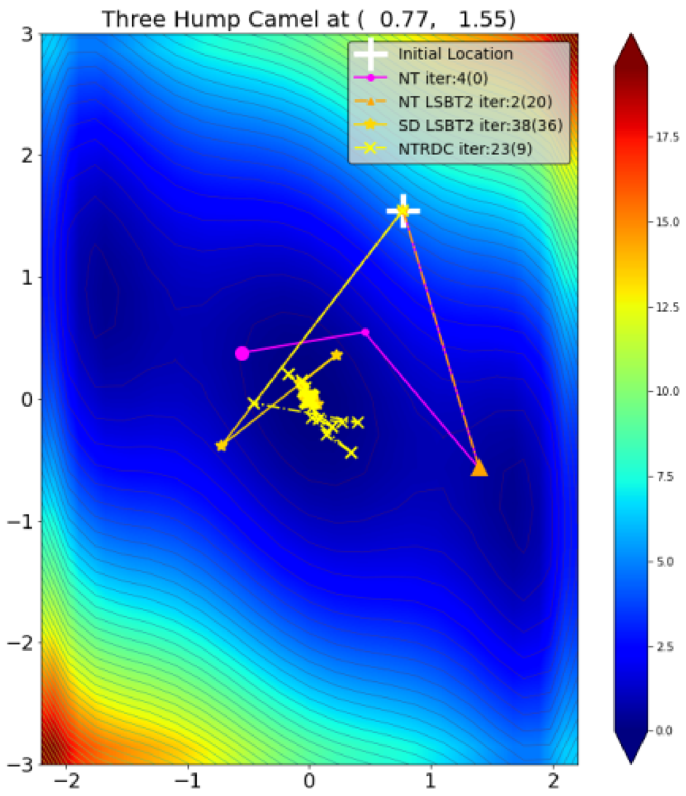
Optimization problem

- NT: Newton
- NT LSBT2: Newton Linesearch Quadratic Backtracking
- SD LSBT2: Cauchy Linesearch Quadratic Backtracking
- NTRDC: Newton Trust-region Dogleg Cauchy

Method	Test runs	Correct sol'n	Outer iter.	Inner iter.
NT	385	42.3%	8.03	---
NT LSBT2	385	63.3%	12.1	13.2
SD LSBT2	385	85.3%	30.8	56
NTRDC	385	85.3%	16.4	2.16







Python script available: bitbucket.org:iamhaho/optimization-py.git

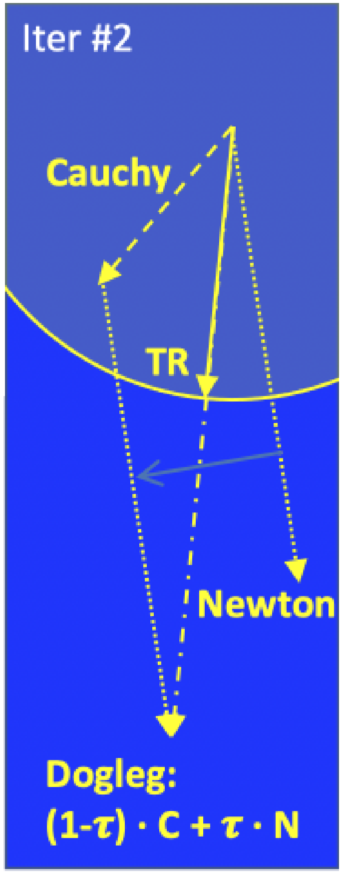
Newton Trust region Dogleg Cauchy

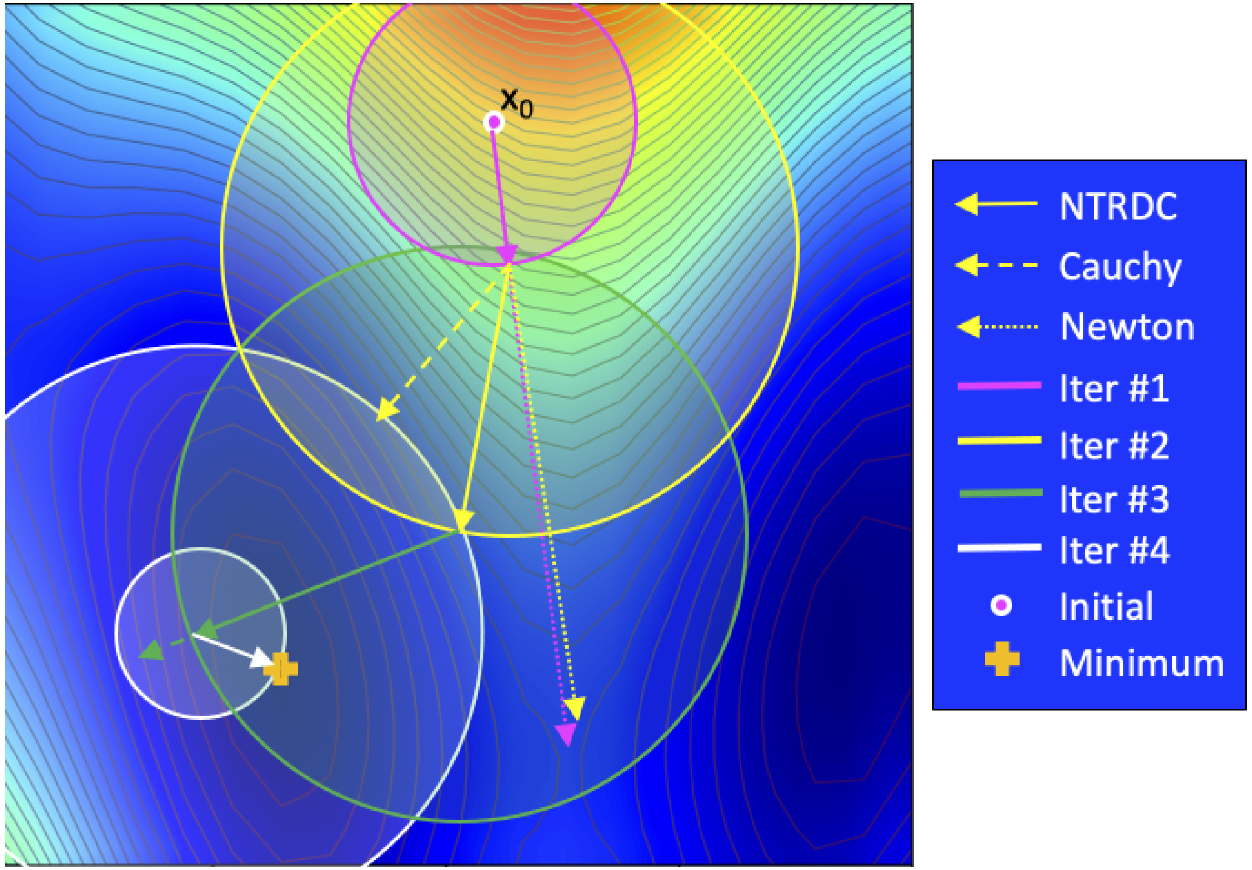
NTRDC works in a way that first define a region around the current best solution in which a quadratic model can, to some extent, approximate the original objective function.

$$f(u) := \frac{1}{2}||F(u)||_2^2 : \mathbb{R}^n \to \mathbb{R}.$$

$F(u)$: original objective function
$f(u)$: 2-norm

We want to find a solution $\vec{p}$ that is within the step size of Δ that minimizes the quadratic model m.





$$m_k(\vec{p}) = f_k + g_k^T\vec{p} + \frac{1}{2}\vec{p}^T B_k \vec{p} \;\; s.t. \;\; ||\vec{p}|| <= \Delta_k$$

Governing equations and the Jacobian matrix

Newton-Raphson Iteration

$$J_F(x_n)\delta x = -F(x_n) \text{ and } x_{n+1} = x_n + \delta x$$

System of Nonlinear Algebraic Equations

$$F_a(-,-,-) = 0$$

$$F_w(-,-,-) = 0$$

$$F_E(-,-,-) = 0$$

Definitions

J_F: Jacobian matrix

$\boldsymbol{\delta}$x: solution update or unknowns

n: iteration number

F: residuals

Liquid-phase state

$$\begin{bmatrix} \frac{\partial F_w}{\partial p_l} & \frac{\partial F_w}{\partial x_a^l} & \frac{\partial F_w}{\partial T} \\ \frac{\partial F_a}{\partial p_l} & \frac{\partial F_a}{\partial x_a^l} & \frac{\partial F_a}{\partial T} \\ \frac{\partial F_E}{\partial p_l} & \frac{\partial F_E}{\partial x_a^l} & \frac{\partial F_E}{\partial T} \end{bmatrix}_p \begin{bmatrix} \delta p_l \\ \delta x_a^l \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_w \\ F_a \\ F_E \end{bmatrix}_p$$

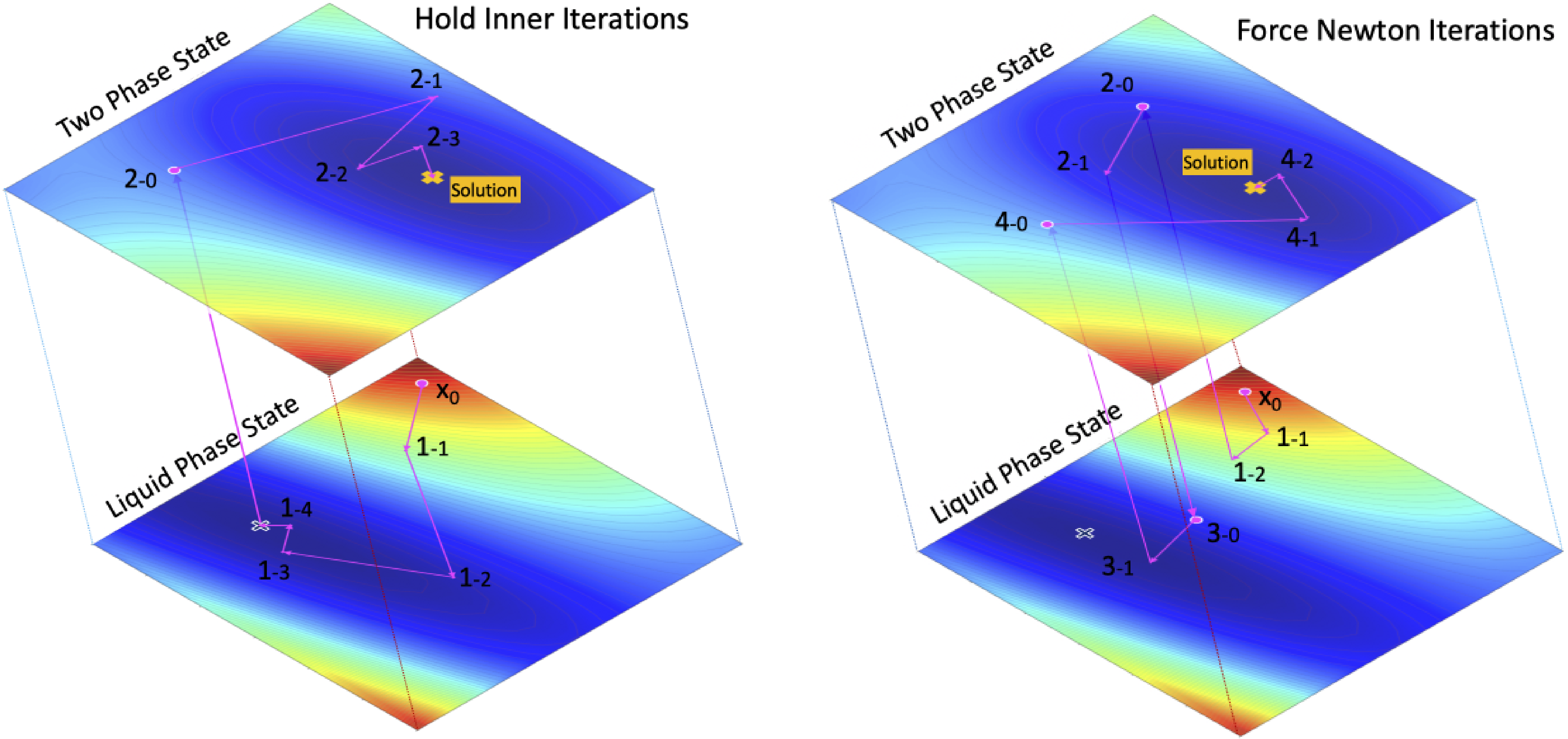
Two-phase state

$$\begin{bmatrix} \frac{\partial F_w}{\partial p_g} & \frac{\partial F_w}{\partial s_g} & \frac{\partial F_w}{\partial T} \\ \frac{\partial F_a}{\partial p_g} & \frac{\partial F_a}{\partial s_g} & \frac{\partial F_a}{\partial T} \\ \frac{\partial F_E}{\partial p_g} & \frac{\partial F_E}{\partial s_g} & \frac{\partial F_E}{\partial T} \end{bmatrix}_p \begin{bmatrix} \delta p_g \\ \delta s_g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_w \\ F_a \\ F_E \end{bmatrix}_p$$

Gas-phase state

$$\begin{bmatrix} \frac{\partial F_w}{\partial p_g} & \frac{\partial F_w}{\partial x_w^g} & \frac{\partial F_w}{\partial T} \\ \frac{\partial F_a}{\partial p_g} & \frac{\partial F_a}{\partial x_w^g} & \frac{\partial F_a}{\partial T} \\ \frac{\partial F_E}{\partial p_g} & \frac{\partial F_E}{\partial x_w^g} & \frac{\partial F_E}{\partial T} \end{bmatrix}_p \begin{bmatrix} \delta p_g \\ \delta x_w^g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_w \\ F_a \\ F_E \end{bmatrix}_p$$

Accommodating primary variable switching (PVS)



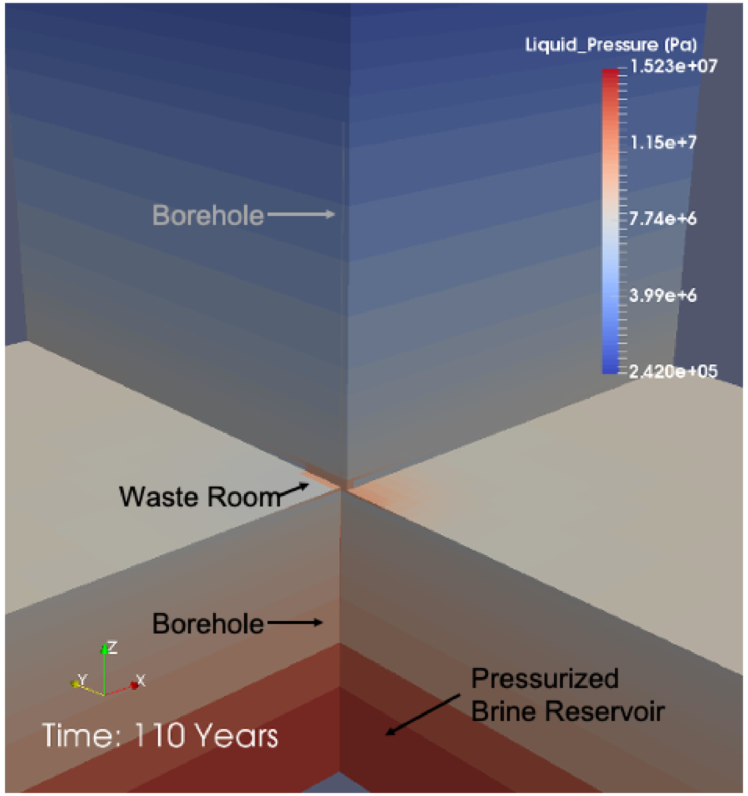
NTRDC in PETSc and PFLOTRAN

- Sandia develops the GDSA Framework tool for safety assessment of generic geologic disposal options
  - PFLOTRAN is the porous media flow and reactive transport code
  - PFLOTRAN parallel capability is based on PETSc parallel Framework

- NTRDC/NTR is implemented in PETSc v3.17 (March 2022)
  - Any PETSc-based code can use NTRDC out-of-the-box
- Official PFLOTRAN with NTRDC is available of FLOW and TRANSPORT (June 2022)
- NTRDC has seen up to 8x speedup or completed simulations that never finished (∞ speedup?)

Improvements in Richards flow

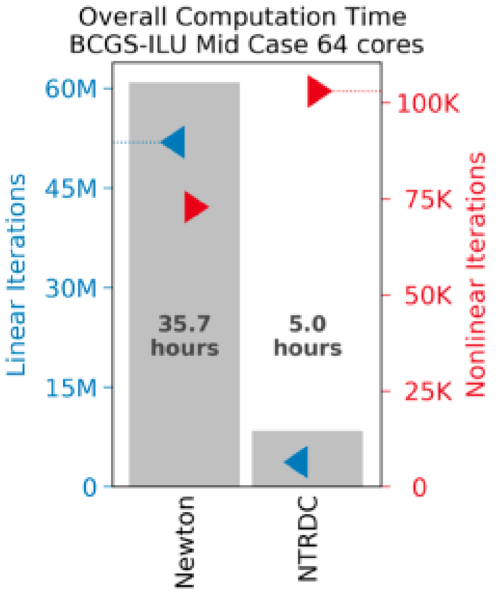
3D Model Test Cases	Compute Time [Min]	Nonlinear iter.	Linear iter.
Borehole in lithostatic reservoir			
Newton's method (NT)	68.6	8019	3026014
Trust Region Dogleg (NTRDC)	1.77	482	29975
Borehole in hydrostatic reservoir			
NT	32.2	1931	1363055
NTRDC	1.77	412	31386
Borehole in lithostatic reservoir 2			
NT	75.7	3457	3919579
NTRDC	3.42	621	60134
Borehole in hydrostatic reservoir 2			
NT	25.6	1812	1191325
NTRDC	2.85	510	51534

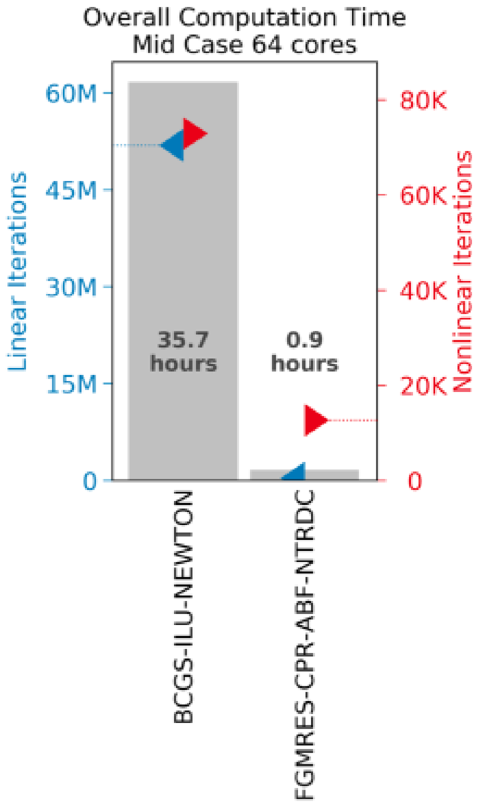


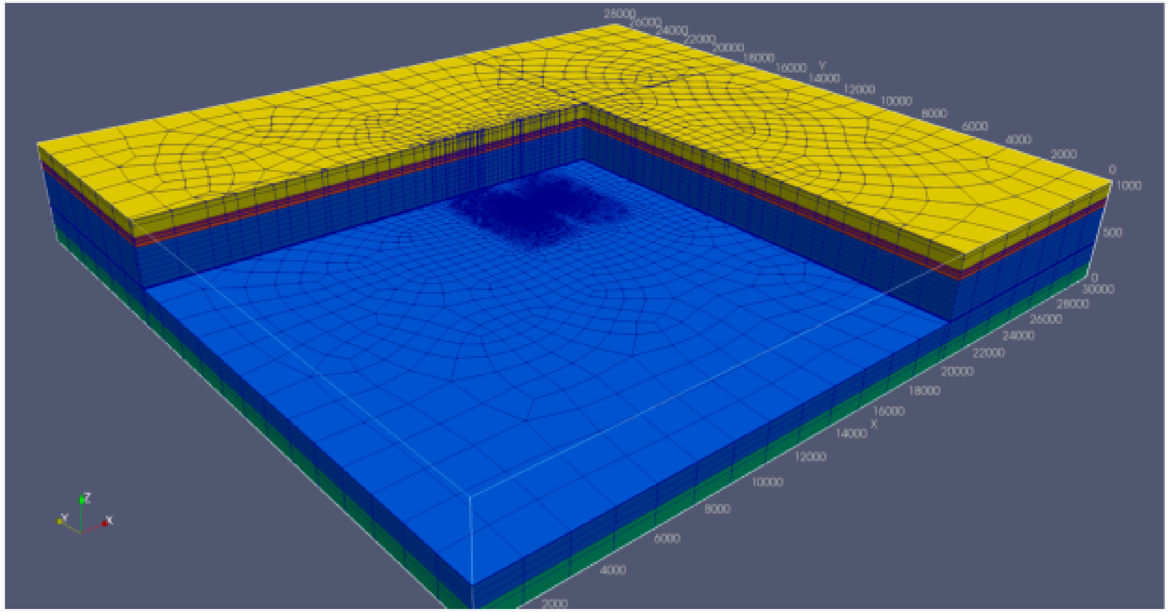
10,000-year sim. 1 core, 36k unknowns

Mariner,P.E., et al. (2020), Advances in GDSA Framework Development and Process Model Integration

Improvements in immiscible isothermal flow



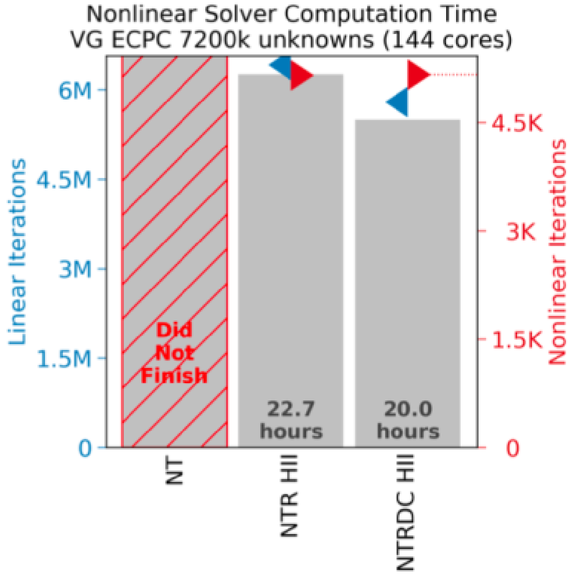


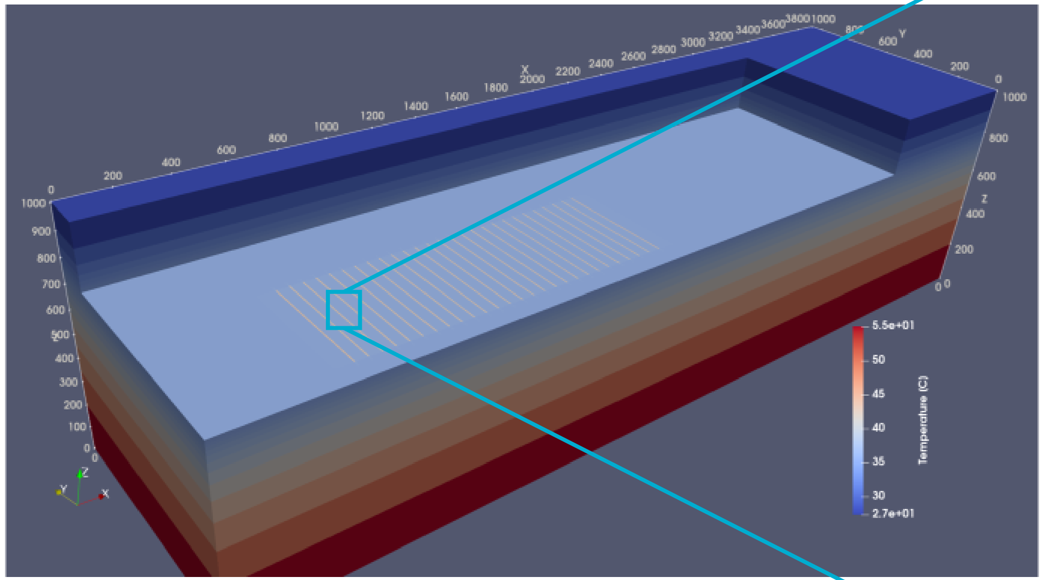


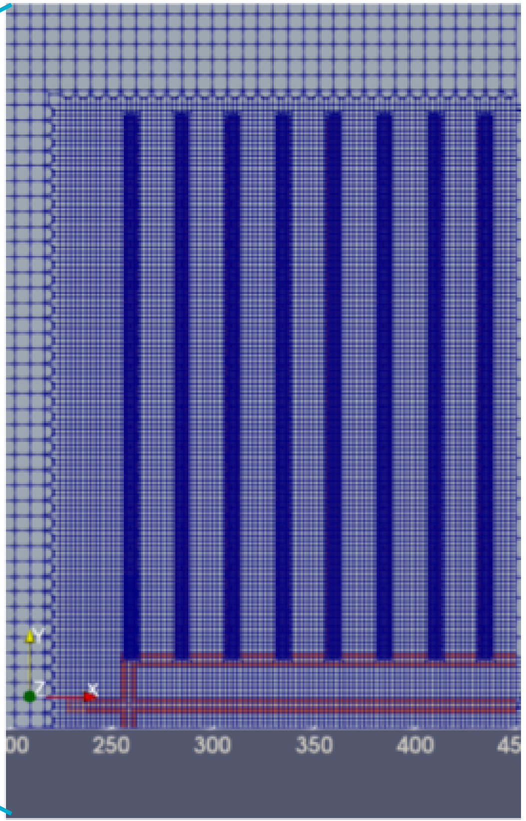
10,000-year sim. 64 cores, 920k unknowns, about 14,000 unknowns per core

Park H., et al. (2021), Linear and nonlinear solvers for simulating multiphase flow within large-scale engineered subsurface systems, Advances in Water Resources, DOI: 10.1016/j.advwatres.2021.104029

Improvements in miscible nonisothermal flow







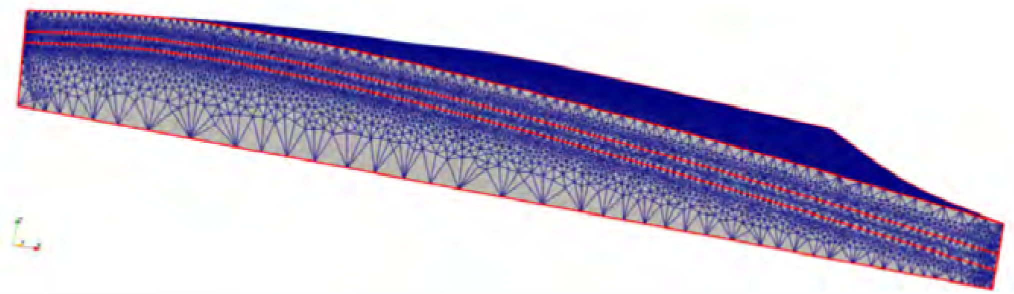
100,000-year sim. 144 cores, about 150,000 unknowns per core

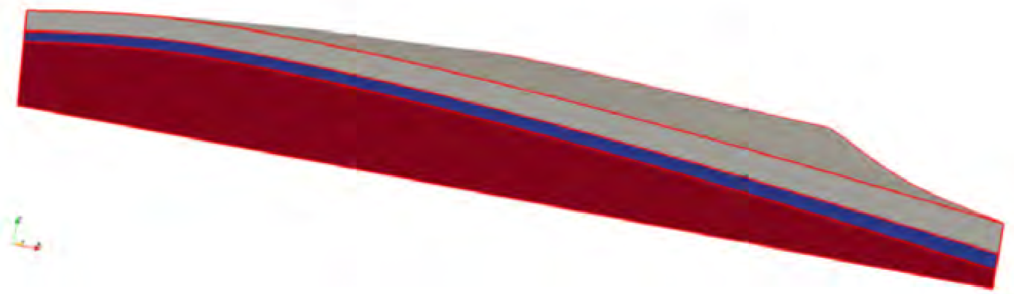
Park H., et al. (2022), Newton trust-region methods with primary variable switching for simulating high temperature multiphase porous media flow, Advances in Water Resources, DOI: 10.1016/j.advwatres.2022.104285

Improvements in multiphase flow (CO_2 injection)

Newton solver did not finish. NTRDC results in the table.

Realization	mesh 1	mesh 2	mesh 3
Grid cells	763,607	763,769	762,763
Simulation time (hr)	24.7	25.1	28.2

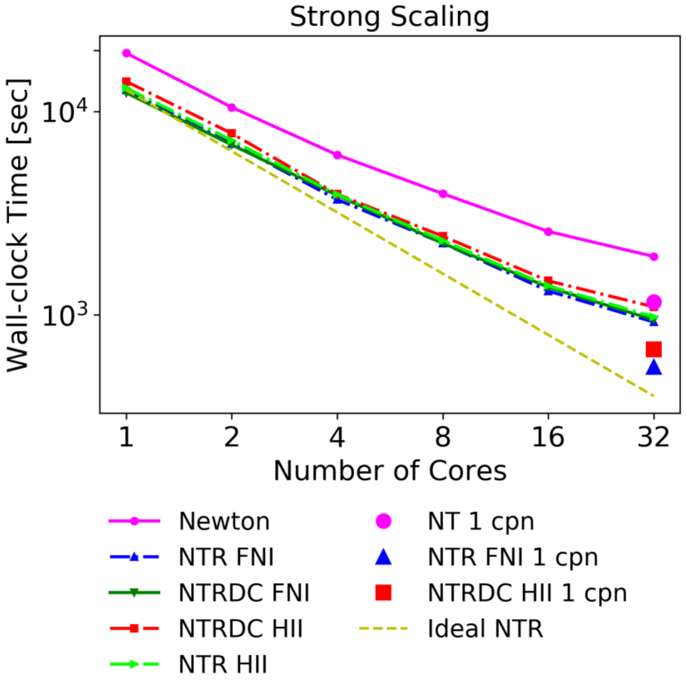


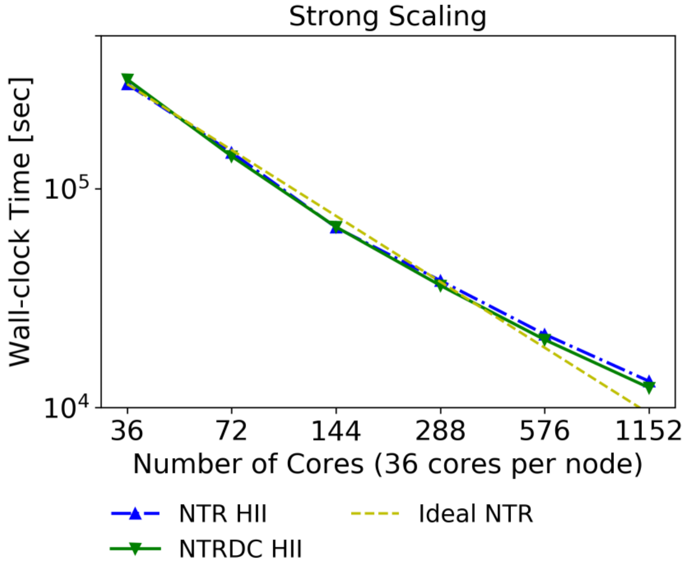


100-year sim. 144 cores, about 10,000 unknowns per core

LaForce, T., Ebeida, M., Jordan, S. et al. Voronoi Meshing to Accurately Capture Geological Structure in Subsurface Simulations. *Math Geosci* (2022). https://doi.org/10.1007/s11004-022-10025-x

Strong Scalability tests





- Parallel scalability is very important to run large-scale simulations
  - To consistently increase in speedup as you increase the number of cores
- In-node strong scaling effect (note 1cpn when memory channel bottleneck is avoided)
- Cross-node strong scaling effect

Questions?

Thanks for listening!