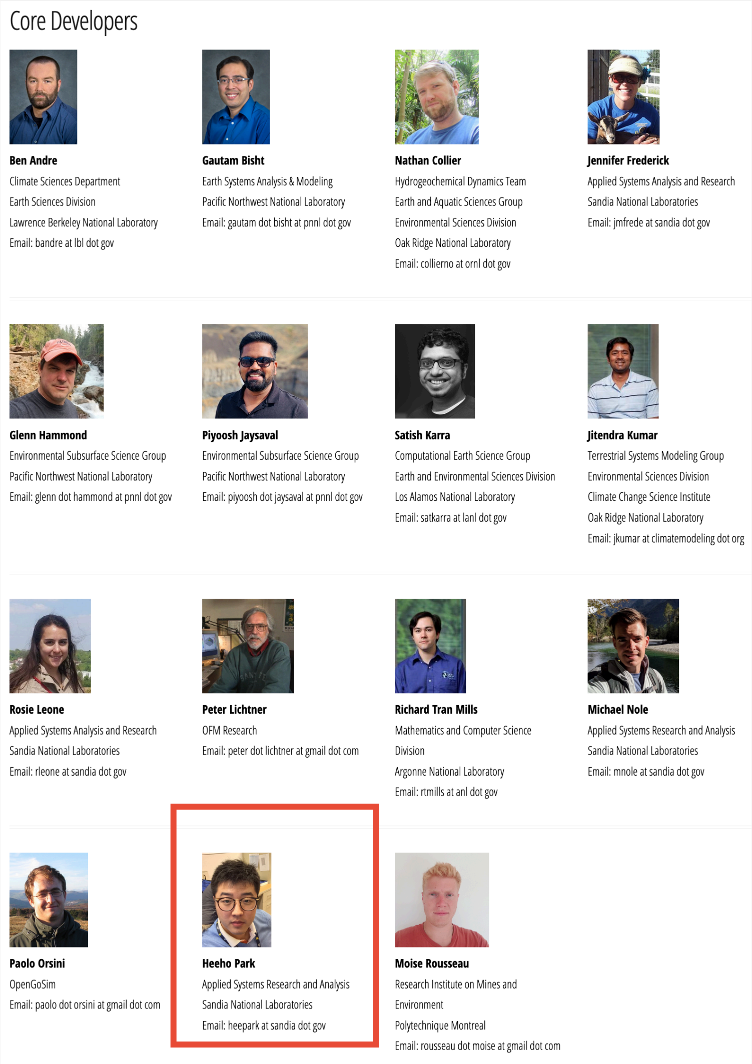
PETSc Newton Trust-Region for Simulating Large-scale Engineered Subsurface Systems with PFLOTRAN

Heeho D. Park

6/5/2023, PETSc Annual Meeting 2023, Chicago, IL

PFLOTRAN

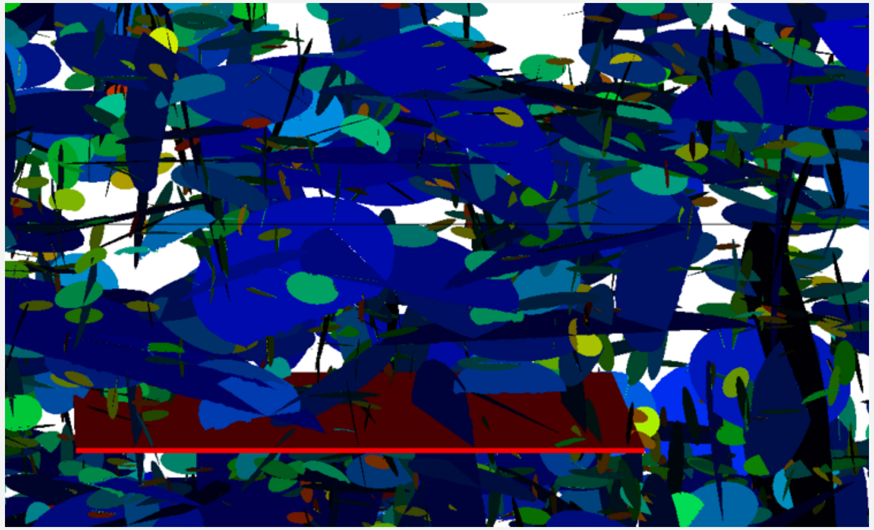


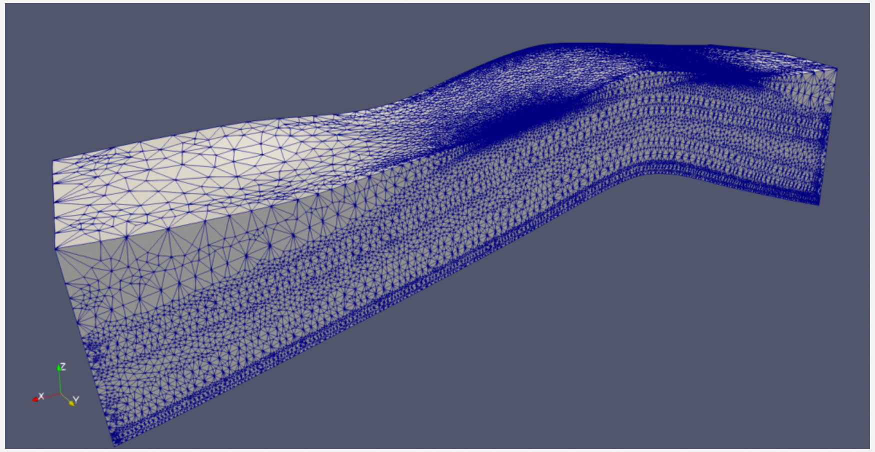
https://www.pflotran.org/developers.html

Flow and Reactive Transport code in porous media

- Funded by US DOE
- Open-source and community-driven code
- Written in modern Fortran; employs PETSc framework
  - Runs in HPC, workstations, and laptops
  - Jaguar at ORNL with 262k cores on 3.3B unknowns
- Numerical methods
  - Backward Euler temporal discretization
  - Finite volume spatial discretization
- Flow: multiphase, CO_2 two-phase, black-oil, Richards, thermal-hydrologic models
- Transport: multicomponent aqueous complexation, sorption, precipitation dissolution
- METIS/PARMETIS libraries for unstructured grids
- HDF5 and ASCII files for input and output

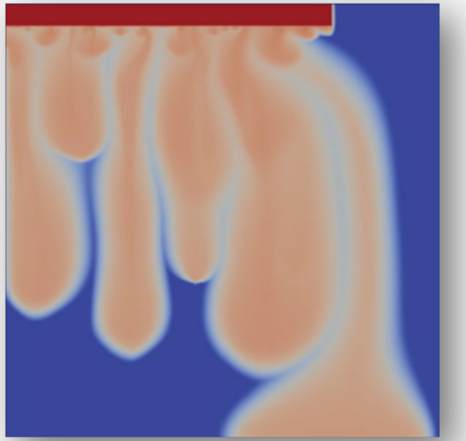
Geologic Disposal Safety Assessment (GDSA) Framework



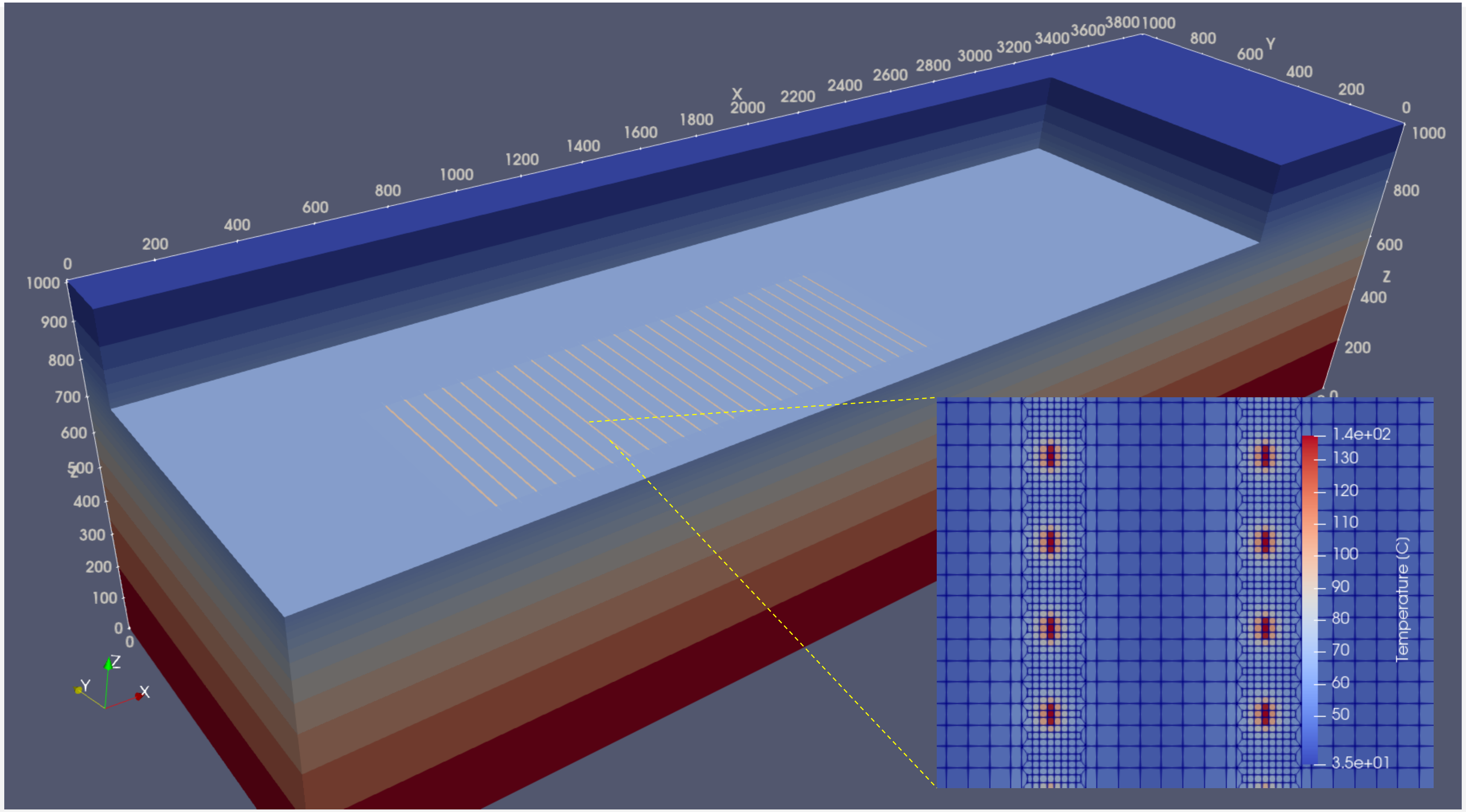


Background

- Purpose:
  - open-source software toolkit for probabilistic performance assessment of deep geologic repositories for nuclear waste
- Large-scale engineered system
  - Hypothetical Nuclear Waste repository in host rocks such as salt, argillite, crystalline, and alluvium.
  - Heat-generating high-level nuclear wastes
  - Possibly water-boiling peak temperature
  - 1 million-year simulations
  - Hypothetical domain spans in kilometers
  - Excavation, shaft access, ramp access, Engineered barriers (bentonite), Natural barriers, multiple soil types, and constitutive relations



Observation and Motivation



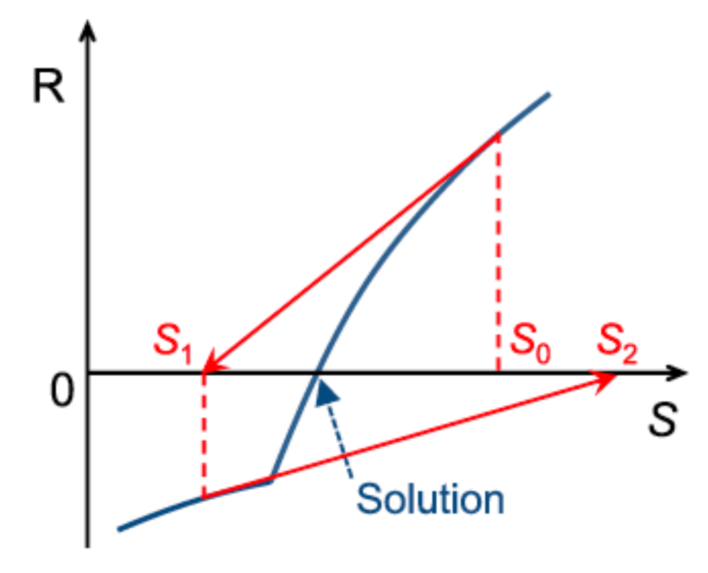
- GDSA Alluvial Unsaturated Zone (UZ) reference case
- 105k grid cells
- Miscible Nonisothermal
- Heat-generating spent nuclear waste packages

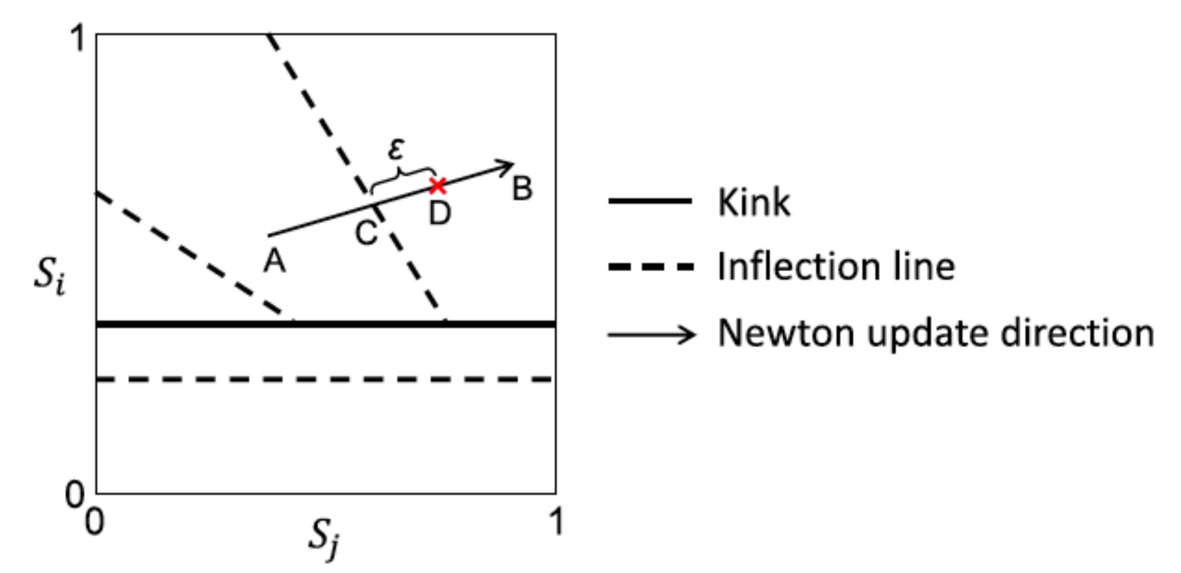
- Newton-Raphson (Newton)
- Simulations ended with non-convergence failure
- Higher peak temperature simulations failed sooner
- Cannot handle discontinuous phase state changes

A Potential Solution

Literature Search

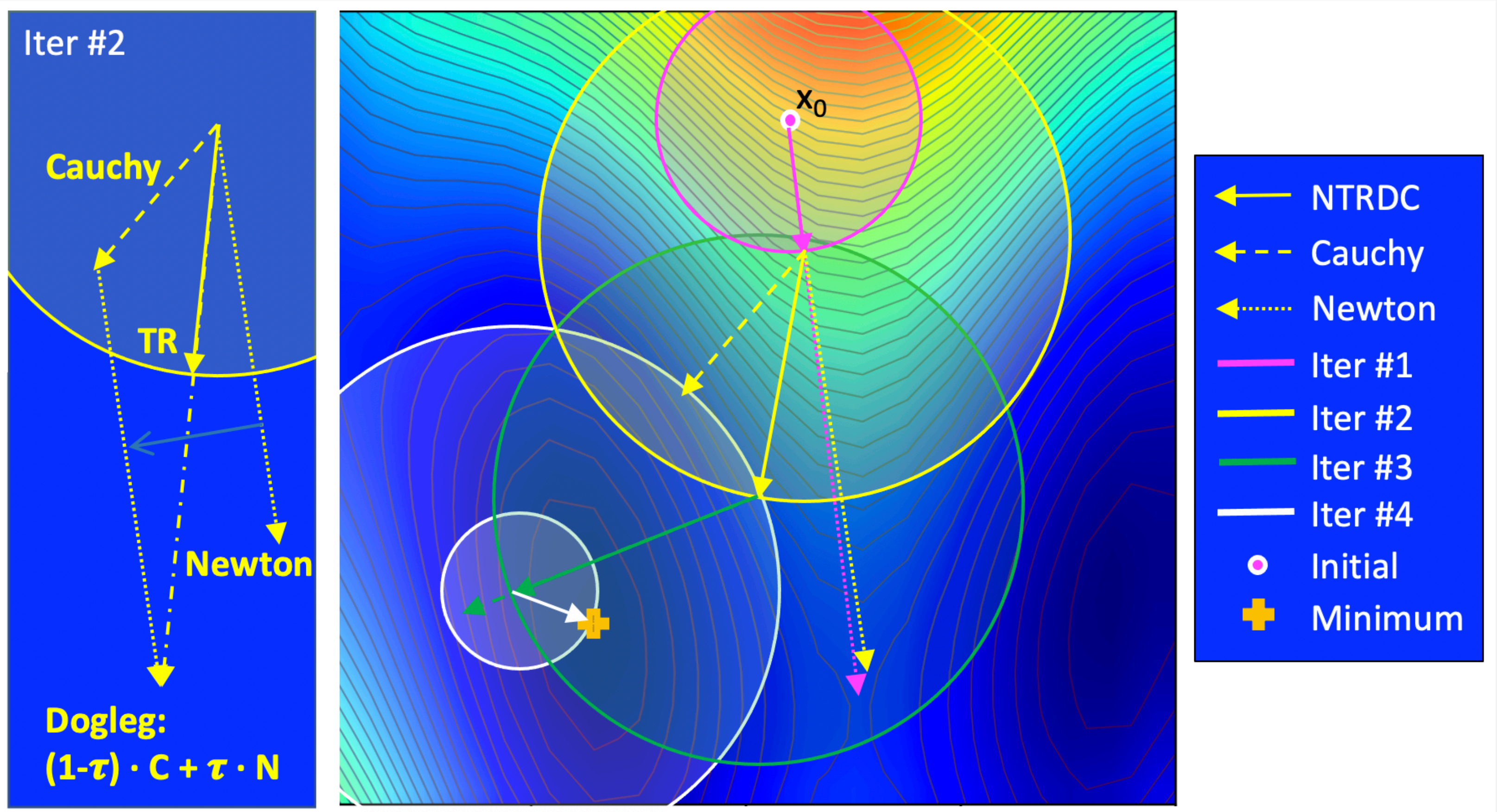
A successful numerical trust-region simulation by Li (2015) for specific capillary pressures with kinks and relative permeability functions in two-phase porous media model. Time step size 10 days (NT) vs 1M days (NTR)





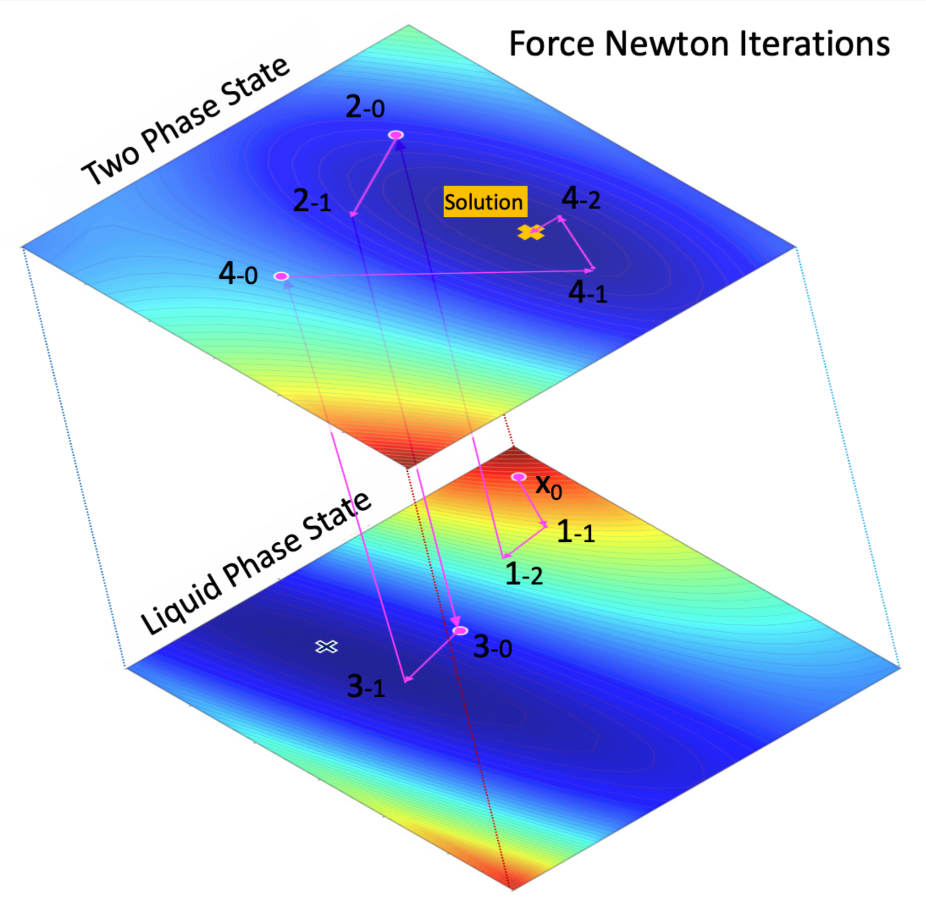
Li, B., Tchelepi, H.A., et al., 2015. *Nonlinear analysis of multiphase transport in porous media in the presence of viscous, buoyancy, and capillary forces,* Jour. of Comp. Phy. DOI:10.1016/j.jcp.2015.04.057

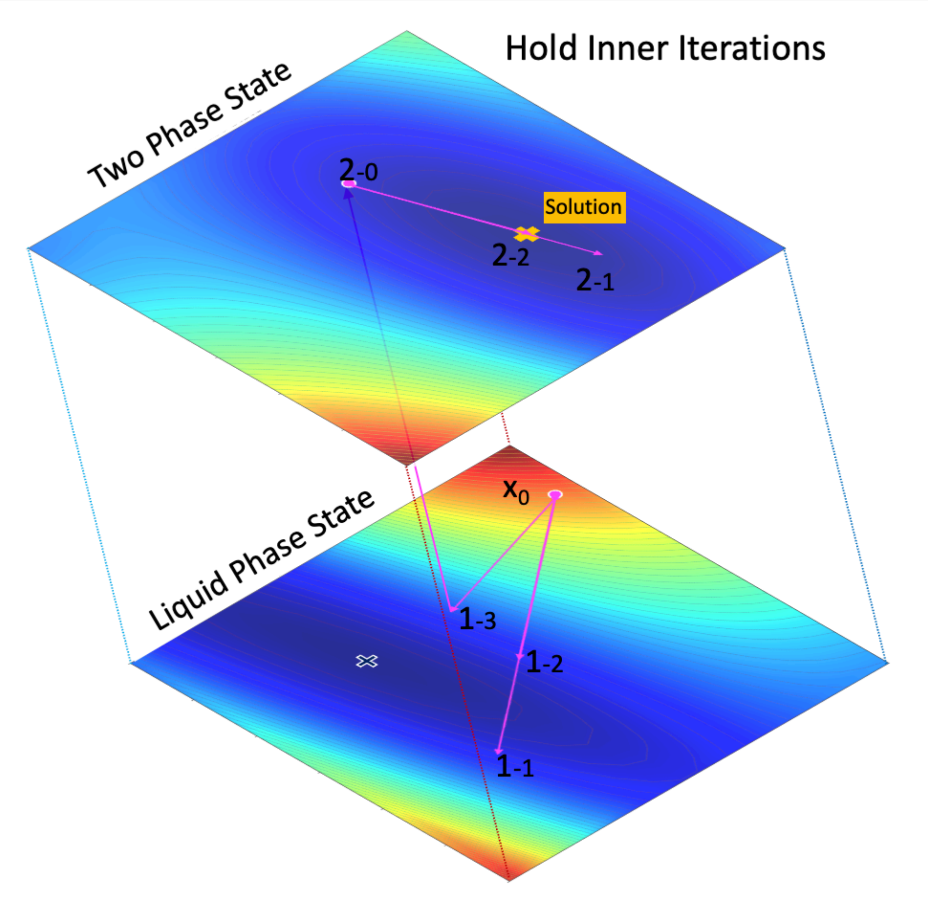
Newton trust-region dogleg Cauchy nonlinear solver



Red contour is high and blue contour is low representing residual space. x_0 is the initial guess and golden cross is the solution. Cauchy evaluates the solution in steepest descent direction.

Accommodating PVS in Advanced Nonlinear Solver



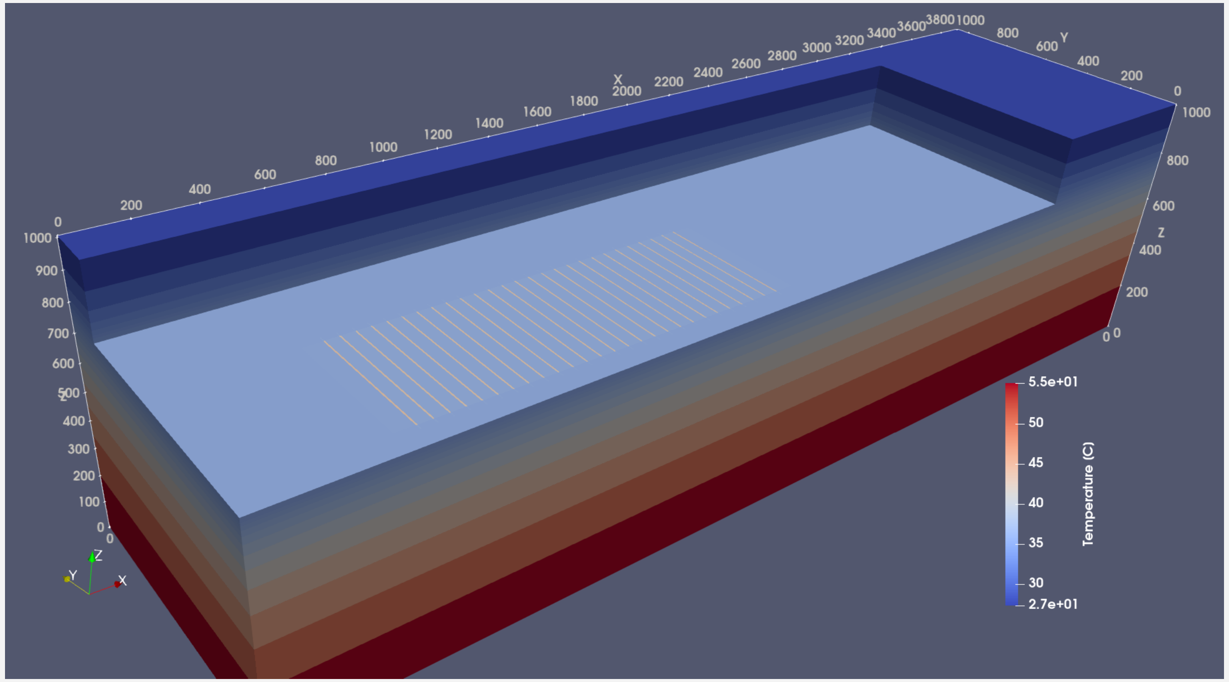


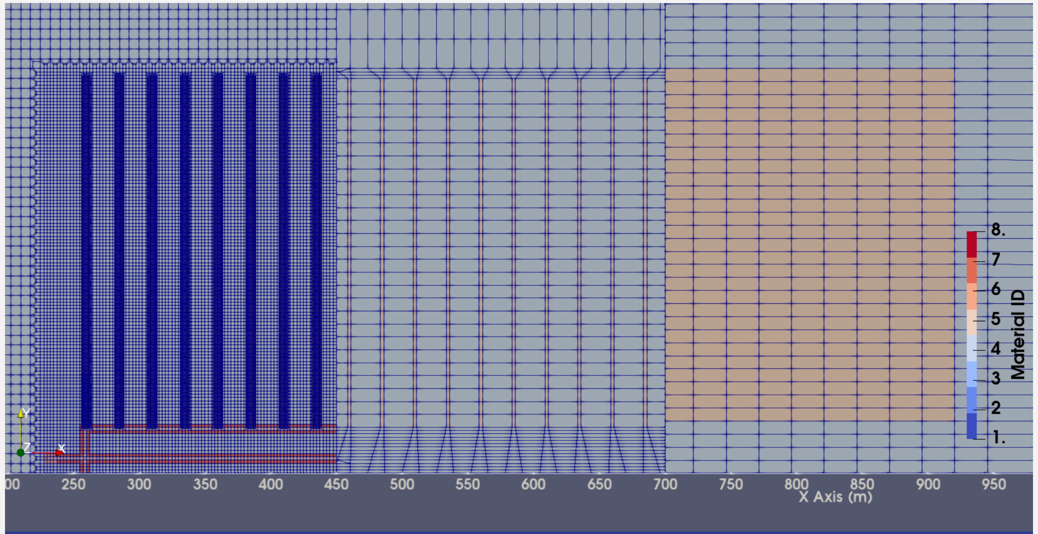
This is my original idea to accommodate PVS for trust-region. Same treatment is needed for any advanced nonlinear solvers. The first number is outer iteration and the second number is inner iteration.

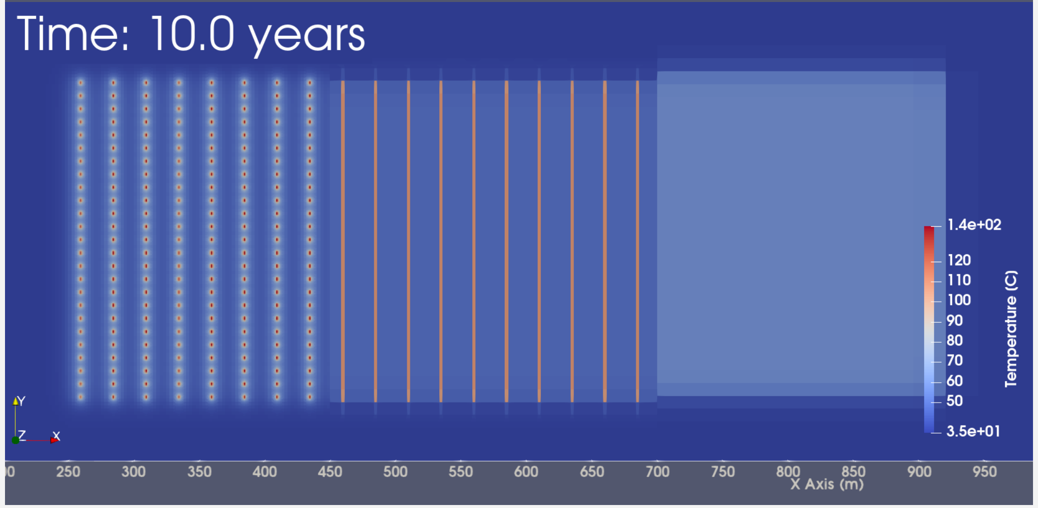
Numerical Experiment

Alluvium Unsaturated Zone Model

- Fully-refined (7.2M unknowns), refined (313k), uniform (190k) testing domains
- Refinement controls peak temperature of the domain
  - Same heat source different volumes



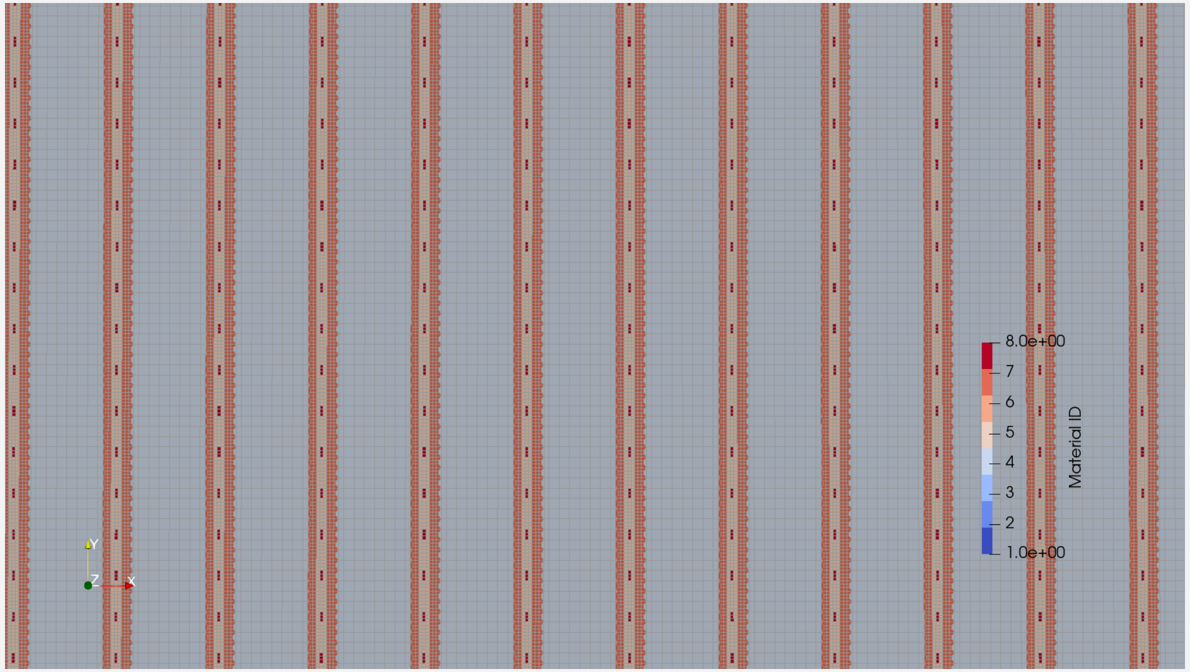


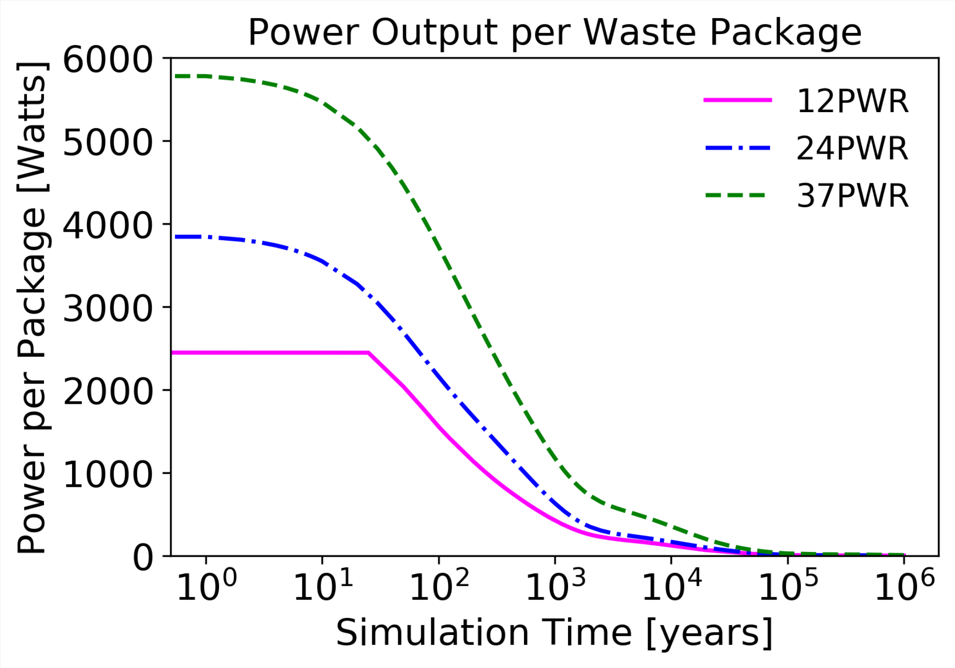


Numerical Experiment

Fully refined Model and heat source

- 5m long waste package, engineered barrier, damaged rock zone, host rock
- Number of fuel assemblies from pressurized water reactor (PWR)

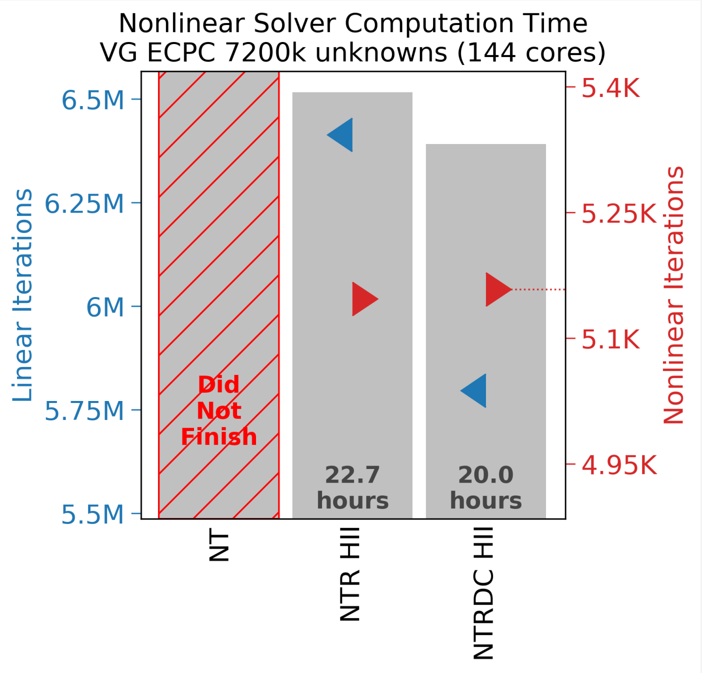




Results

Fully-refined Simulations

- Fully-Refined domain with 12PWR heat source
  - Reaches 140 C peak temperature in the domain
- 100,000-year simulation
  - Experiences 2.2M phase state changes
- Newton fails with nonconvergence
  - Fails with 24PWR and 37PWR as expected
- Trust-region methods (NTX) perform similarly
  - NTR and NTRDC with FNI and HII

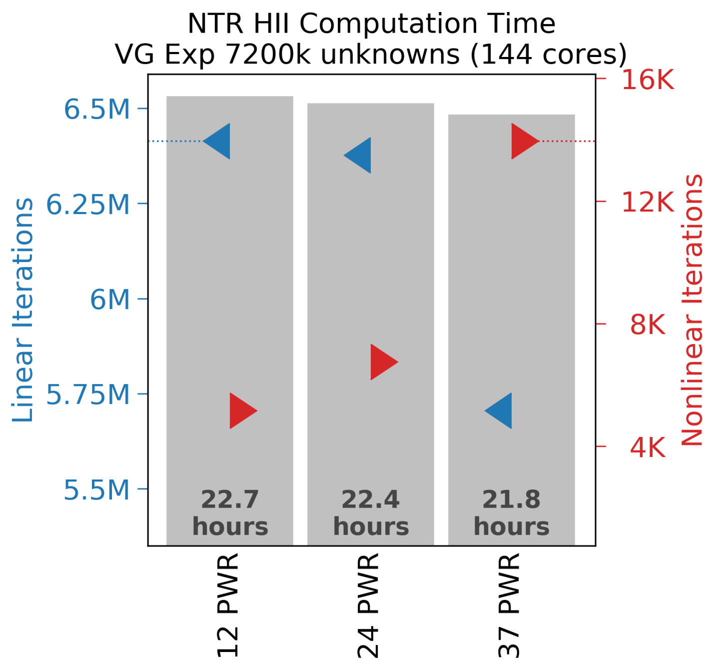


Park et al. (2022), Newton trust-region methods with primary variable switching for simulating high temperature multiphase flow, Advances in Water Resources, DOI:10.1016/j.advwatres.2022.104285

Results

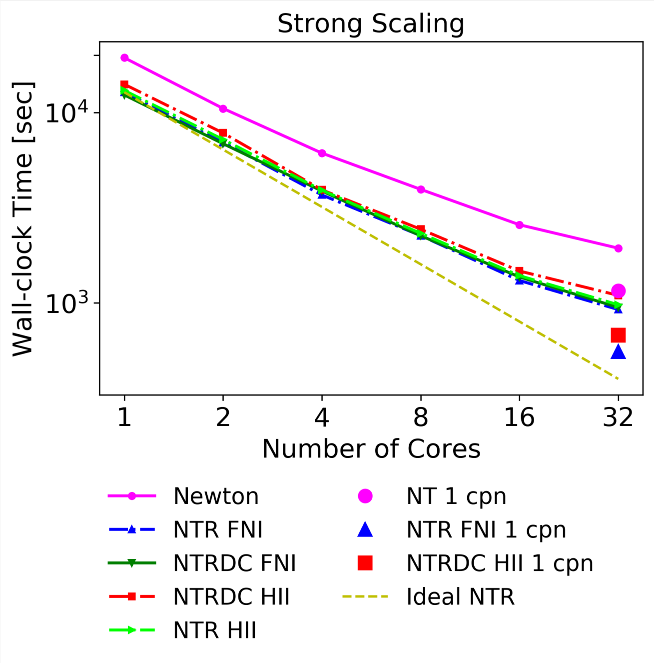
Fully-refined Simulations

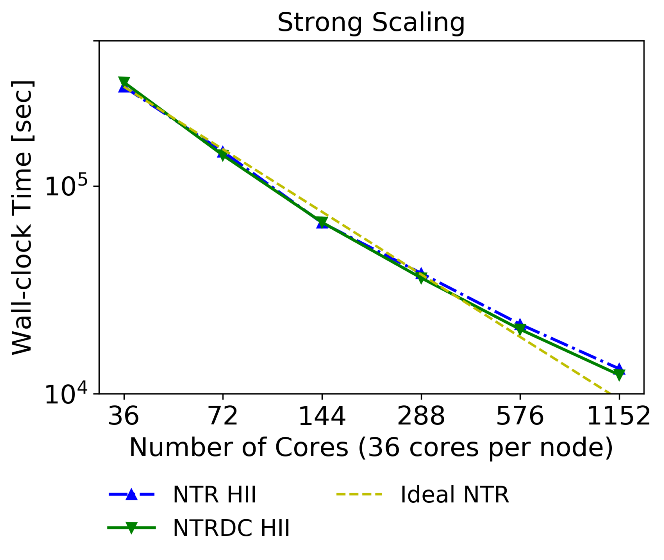
- 12PWR, 24PWR, 37PWR heat source
- 100,000-year simulation
  - Experiences 2.2M phase state changes for 12PWR
  - Experiences 4.3M phase state changes for 24PWR
  - Experiences 9.4M phase state changes for 37PWR
- More nonlinear iterations for 37PWR
  - Nonlinear iterations caused by phase state changes
- Shows the robustness of NTR solver



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

Strong Scalability



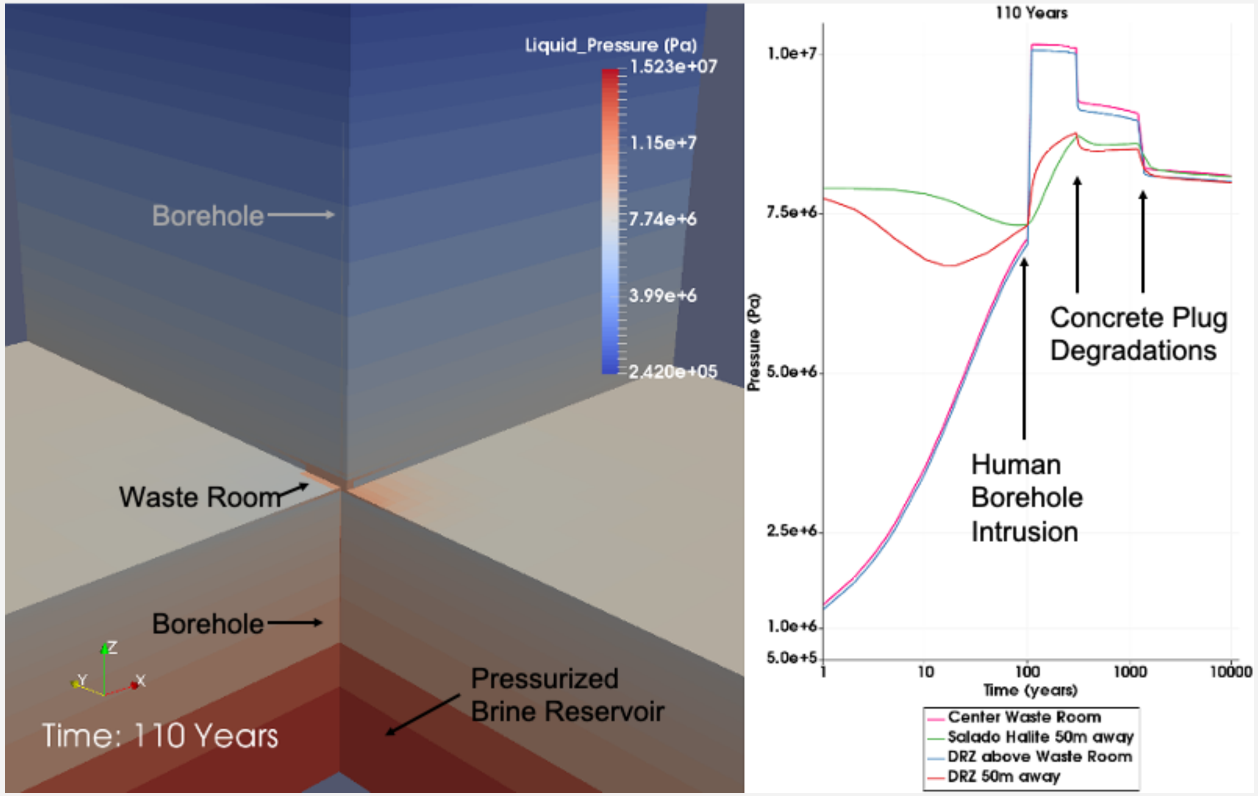


- Parallel scalability is very important to run large-scale simulations
  - Wall-clock time should decrease in proportion to the number of cores
- In-node strong scaling effect (note 1cpn when memory channel bottleneck is avoided)
- Cross-node strong scaling effect
- 36 cores with Intel Xeon Gold 6240 Processor 2.60 GHz, 24.75 MB cache in two sockets with 6 memory channels

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

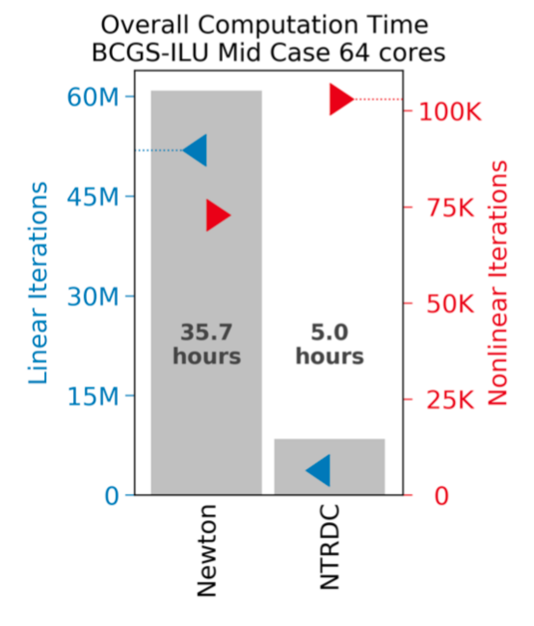
Richards unsaturated flow

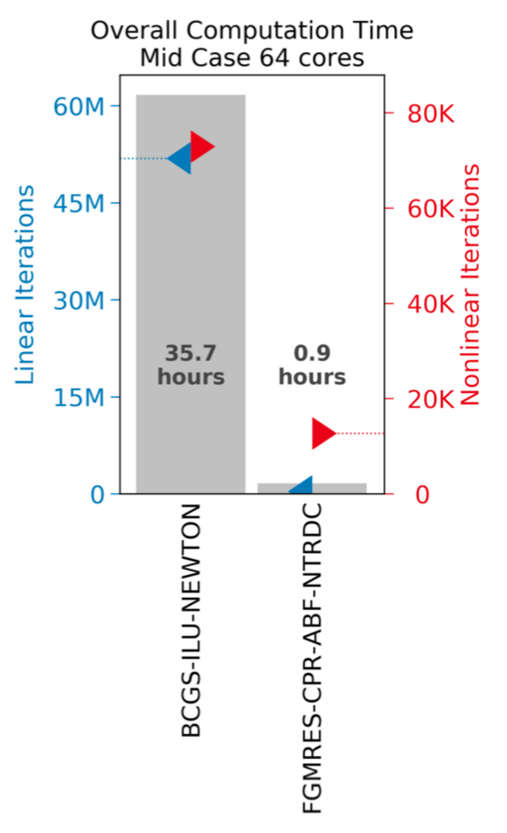
3D Model Test Cases	Compute Time [Min]	Nonlinear iter.	Linear iter.
100-year intrusion lithostatic			
Newton’s method (NT)	68.6	8019	3026014
Trust Region Dogleg (NTRDC)	1.77	482	29975
100-year intrusion hydrostatic			
NT	32.2	1931	1363055
NTRDC	1.77	412	31386
350-year intrusion lithostatic			
NT	75.7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



Mariner et al. (2020), Advances in GDSA framework development and process model integration, Spent fuel and waste disposition, M2SF-20SN010304042

Isothermal Immiscible Flow





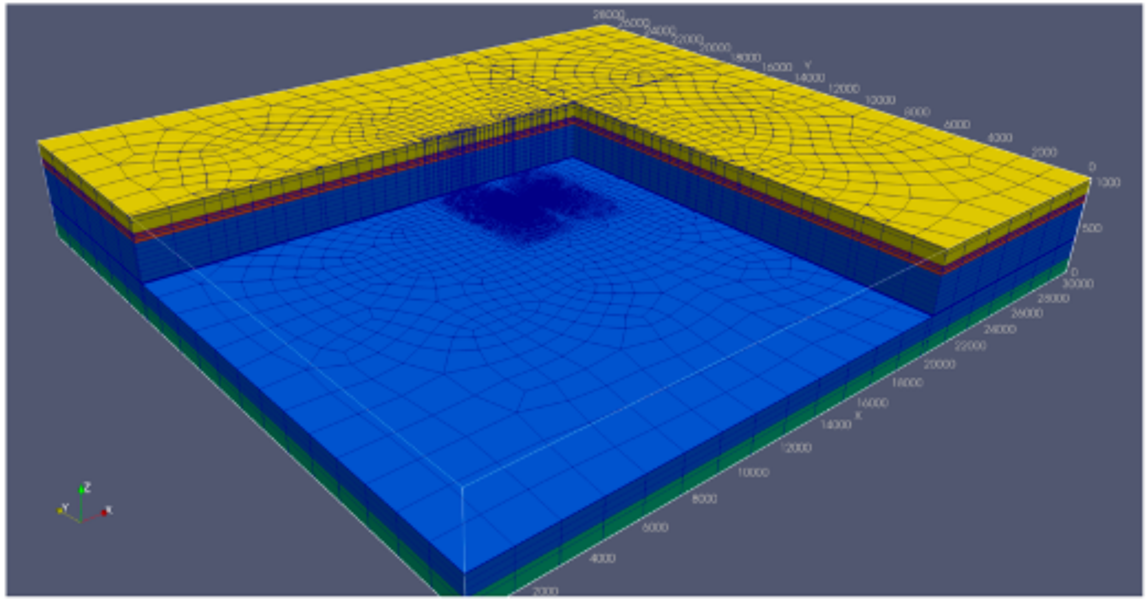


Figure 3.3: Far view of the cropped [ ] simulation model. The domain spans approximately 30 km in the x-, 28km in the y-, and 1km in the z-direction. The repository is the finely gridded region near the center of the model.

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

Park 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

Voronoi cell domain/CO_2 injection

100-year sim. 144 cores, about 10,000 unknowns per core (LaForce, 2022)
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

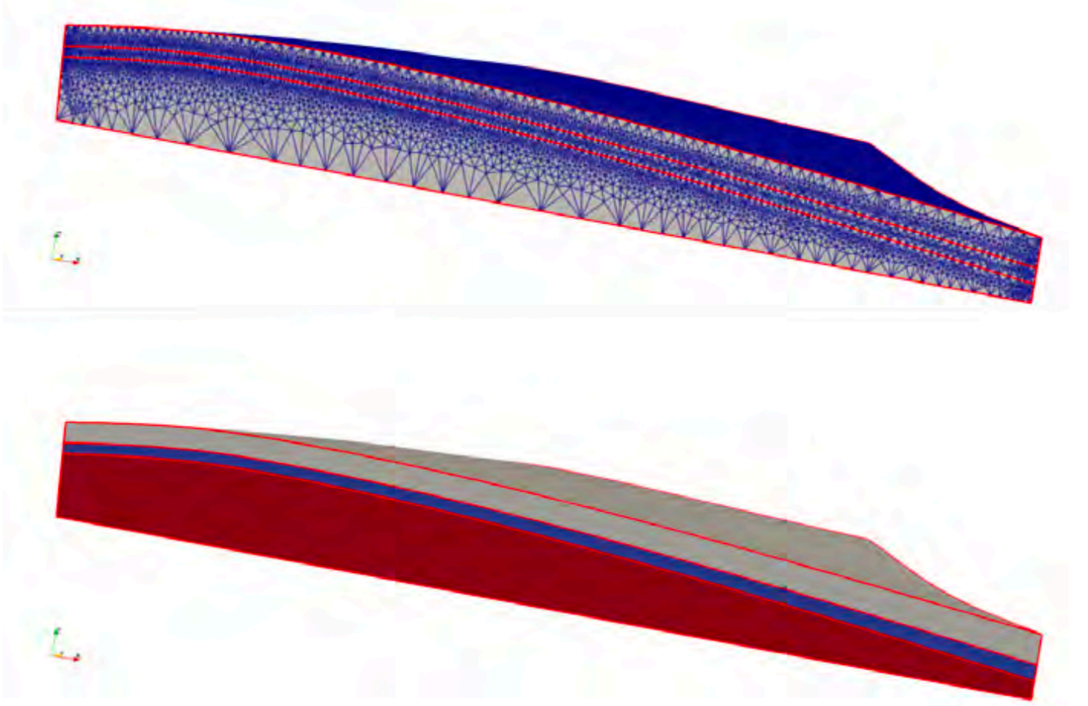


Fig. 19 Isometric view of mesh 3. Top: surface mesh of the model. Bottom: Reservoir volumes colored by the material IDs of each layer. The Phosphoria caprock is shown in gray, Weber Sandstone injection interval is blue and crystalline basement is red.

LaForce et al. (2022), Voronoi meshing to accurately capture geology in subsurface simulations, Mathematical Geoscience manuscript,
DOI: 10.1007/s11004-022-10025-x

Reactive Transport Simulation

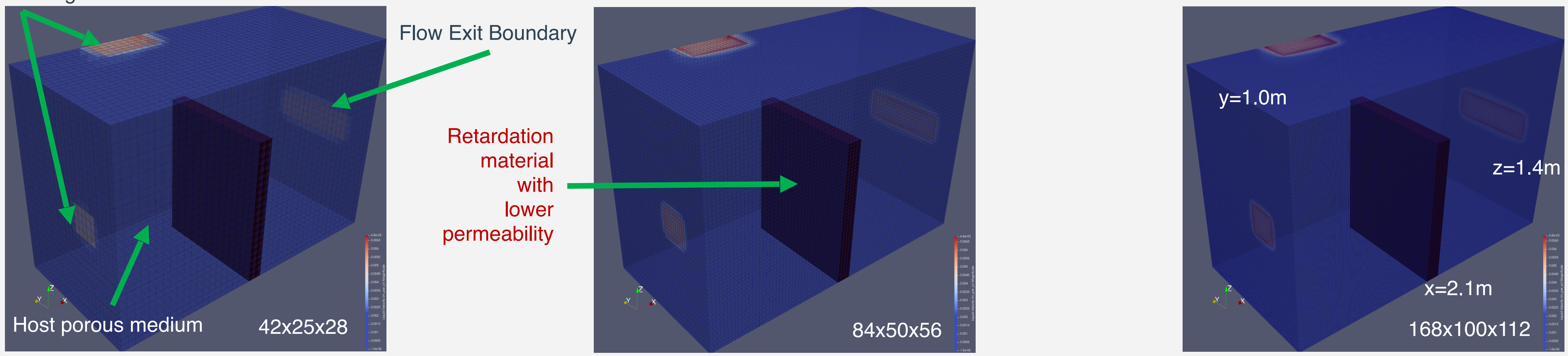


Table 1. Characteristics of the media		
	Host	Low perm.
Porosity θ	0.25	0.5
Hydraulic cond. K (m/yr)	1.0E-2	1.0E-5
Site (S) Conc. (mol/m³)	1.0	10.0
Dispersion αL (m)	1.0E-2	6.0E-2

Table 2. Chemical concentration of the initial and boundary cond.					
Total Conc.	T1*	T2	T3	T4	TS
Host	0.0	-2.0	0.0	2.0	1.0
Low perm.	0.0	-2.0	0.0	2.0	10.0
Injection @ 0yrs	0.3	0.3	0.3	0.0	
Leaching @ 1500y	0.0	-2.0	0.0	2.0	

secondary species (aqueous)

$C1 \rightleftharpoons -X2$

$K = 10^{-12}$

$C2 \rightleftharpoons X2 + X3$

$K = 1$

$C3 \rightleftharpoons -X2 + X4$

$K = 1$

$C4 \rightleftharpoons -4X2 + X3 + 3X4$

$K = 0.1$

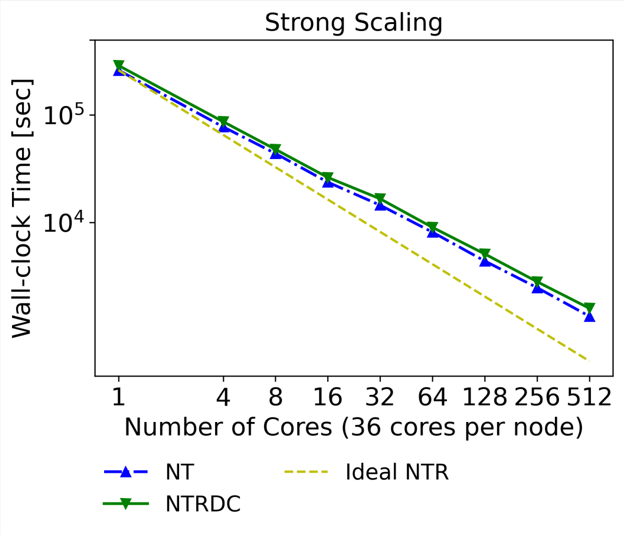
$C5 \rightleftharpoons 4X2 + 3X3 + X4$

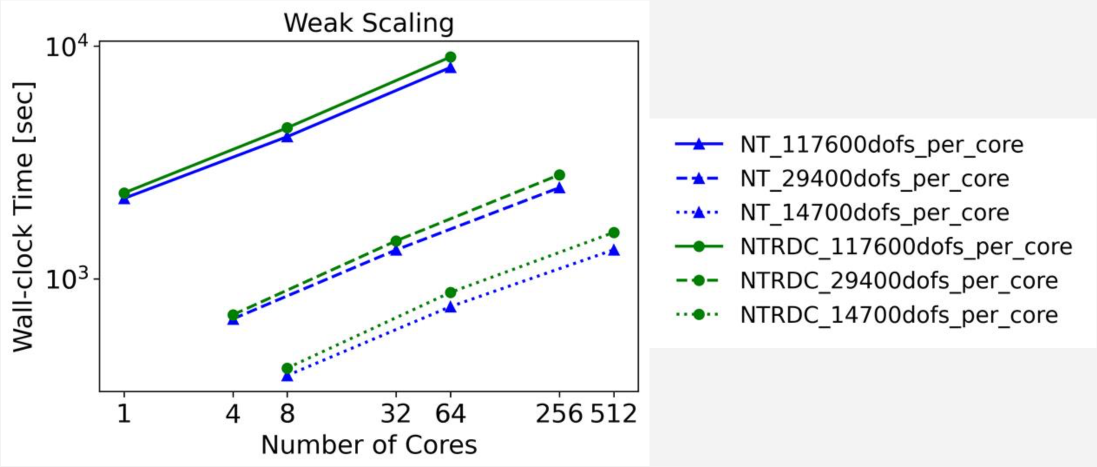
$K = 10^{35}$

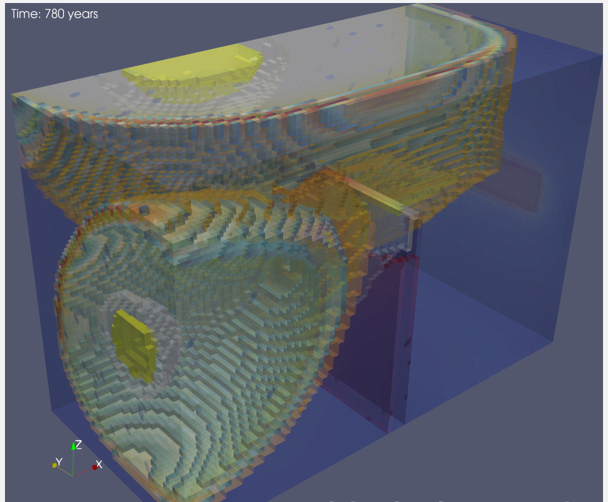
surface complexation (sorbed)

$CS1 \rightleftharpoons 3X2 + X3 + S$

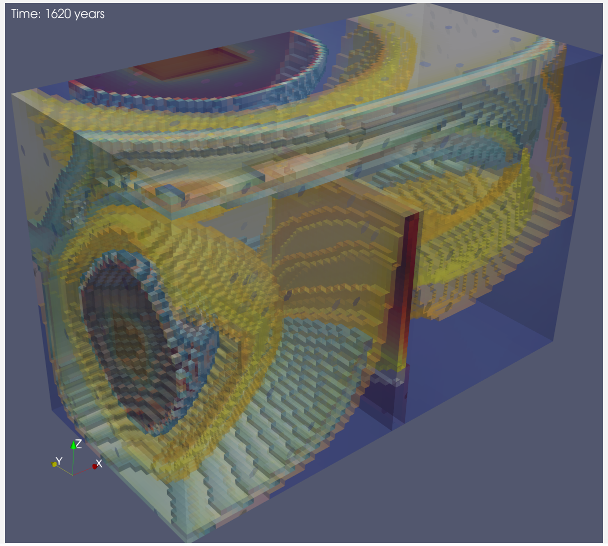
Results

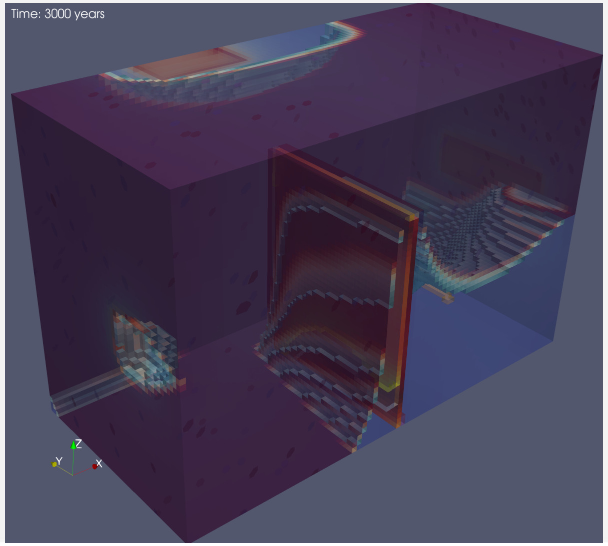






Reaction Plume of CS_1 C_4 C_5 X_2 X_1 SX_3





Questions?

Thank you for listening