A Unified Multiphase Compositional Flow Simulation Model in PorePy

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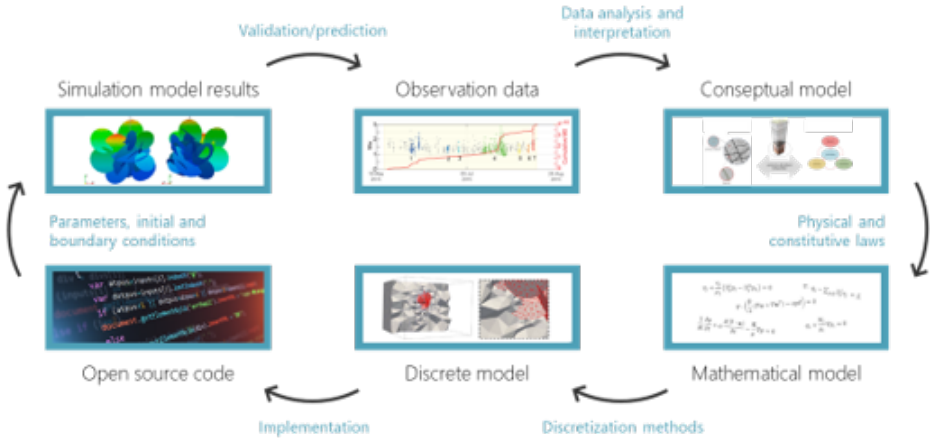
The Porous Media Group (PMG)

Key Information

- Dates back to 1985
- Leading international research group in applied and computational mathematics of porous media
- Strong interdisciplinary nature
- Applications: CO_2 storage, geothermal energy, and biomedicine
- Majority of publications within mathematics and geoscience
- Strong interdisciplinary and intersectoral collaboration within CO_2 storage and geothermal energy

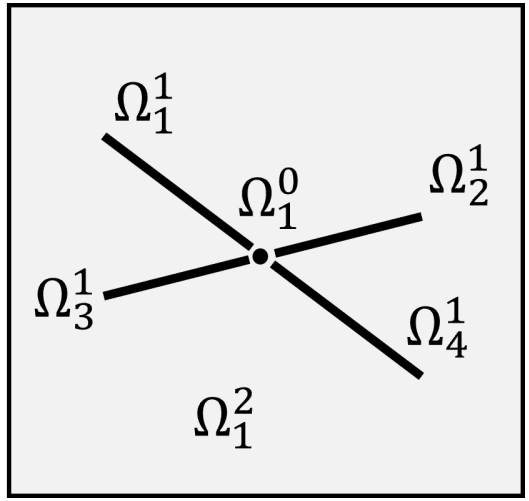
Team

- 5 professors (Berre, Dahle, Kumar, Nordbotten, Radu)
- 1 senior researcher 1183 (Keilegavlen)
- 2 researchers (Both, Stefansson)
- 14 PhD students (Jan 2025), 2 postdocs

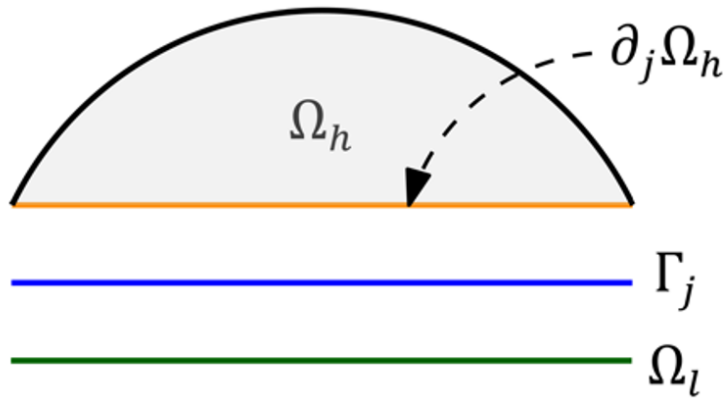


PorePy

- Open-source code developed at UiB
  github.com/pmgbergen/porepy
- Mixed-dimensional simulations using domain decomposition of rock, fractures and intersections
- Modeling physical processes using governing equations within subdomains
- Coupling across interfaces between subdomains with dimension gap 1
- Mixed-dimensional domain is a graph, with subdomains as nodes and interfaces as edges
- Meshing on individual subdomains and interfaces resembles that of a standard problem.
- Subdomain models resemble fixed-dimensional problems.
- Coupling manifests as BC or source terms



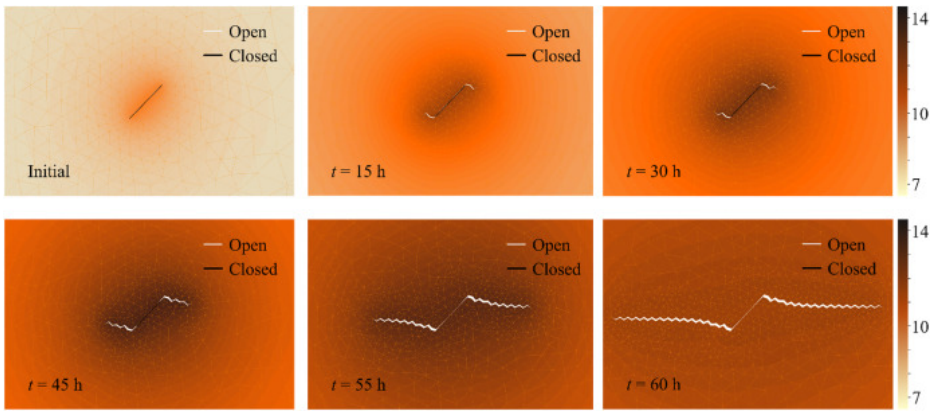
Schematic representation of rock (dim D), fractures (dim D-1) and intersections (dim D-2).



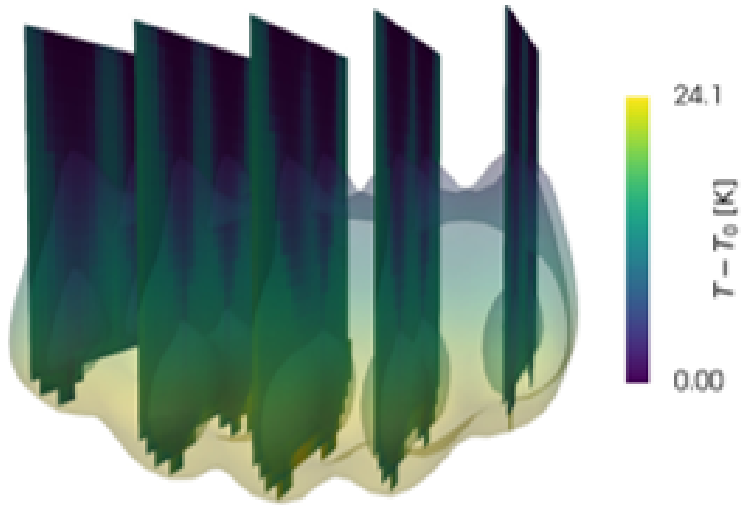
Higher-dimensional subdomain Ω_h coupled via interface Γ_j to lower-dimensional subdomain Ω_l.

PorePy

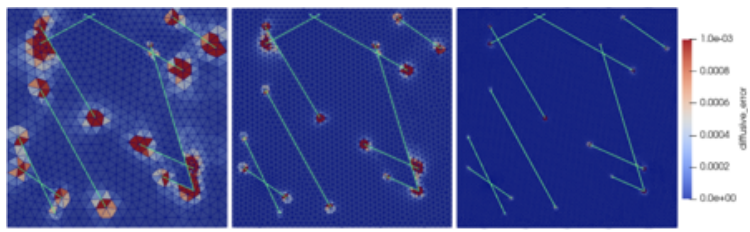
- Interface equations and discretizations make the difference from fixed-dimensional problems
- Finite-volume based modeling (MPFA, MPSA, Upwinding)
- Translation of general multiphysics model to numerical format using automatic differentiation adapted to mixed-dimensional setting



Dang et al. Two-level simulation of injection-induced fracture slip and wing-crack propagation in poroelastic media. IJRMMS 160, 105248 (2022).



Stefansson et al. Numerical Modelling of Convection-Driven Cooling, Deformation and Fracturing of Thermo-Poroelastic Media. TiPM 140, 371–394 (2021).



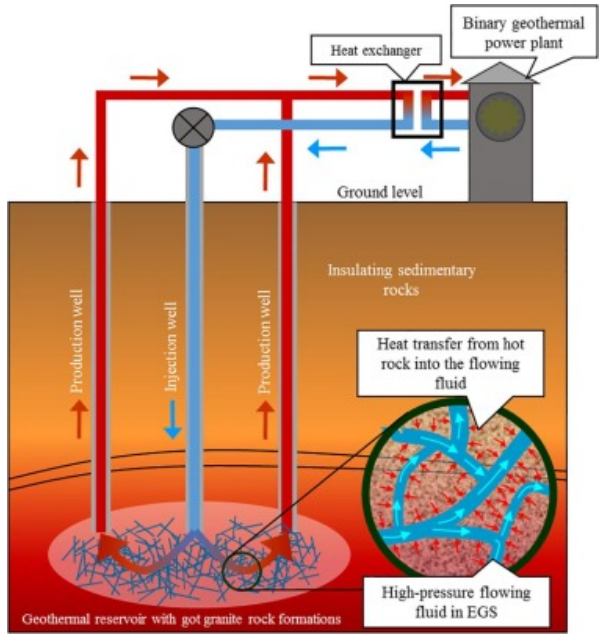
Varela et al. A posteriori error estimates for hierarchical mixed-dimensional elliptic equations. JNM 31 (4), 247-280 (2023).

Motivation

Geothermal System as a Compositional System

Geothermal reservoirs are complex, multiphase systems requiring a unified compositional approach for consistent modeling of fluid behavior.

- **Persistent Variables and Equations:** Describe system state across all phases
- **Flexible EOS:** Adaptable to simulate both high-and low-enthalpy geothermal conditions

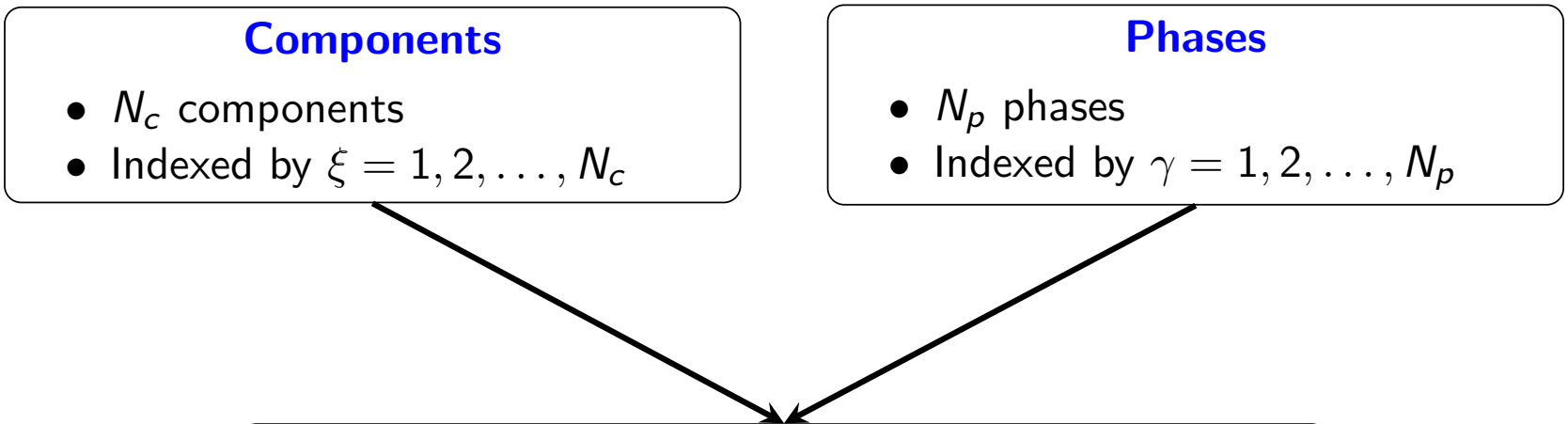


Schema of conceptual EGS [1].

[1] Isaka, B.A. et al. (2019). Super-critical CO_2 in geothermal systems. SETA, 36, 100547.

Non-Isothermal Compositional Flow Model

Describes the non-isothermal flow and transport of multiple fluid components in a continuum.



Primary Equations (PDEs)

Component Balance

$$\frac{\partial}{\partial t}(\phi \rho z_\xi) - \nabla \cdot (f_\xi \mathbf{D} \nabla p) = q_\xi$$

Pressure (Total Mass) Balance

$$\frac{\partial}{\partial t}(\phi \rho) - \nabla \cdot (\mathbf{D} \nabla p) = q$$

Energy Balance

$$\frac{\partial}{\partial t}(\phi[\rho h - p] + (1-\phi)\rho_s h_s) - \nabla \cdot \left(\sum_\gamma f_\gamma h_\gamma \mathbf{D} \nabla p + \mathbf{D}_h \nabla T \right) = q_e$$

Parameters:

ϕ: porosity [–]
ρ: bulk density [kg/m^3]
z_ξ: component overall fraction [–]
f_ξ: fractional flow [–]
$\mathbf{D} = \lambda \mathbf{K}$: diffusive tensor [m^2/Pa·s]
q_ξ: component source/sink term [kg/m^{3}s]
p: pressure [Pa]
h: fluid specific enthalpy [J/kg]
ρ_s: solid density [kg/m^3]
$\mathbf{D}_h$: thermal diffusivity tensor [W/m·K]
T: temperature [K]
q_e: energy source/sink term [J/m^3/s]
q : total mass source/ sink term [kg/m^{3}s]

Independent Variables

Assume that $N_p \geq 2$ and $N_c \geq 2$ and phase N_p and component N_c are references.

Primary Variables ($N_c + 1$):

$$\mathbf{x} = [p, h \text{ or } T, z_1, z_2, \ldots, z_{N_c-1}].$$

Reference component overall fraction (Closure relation 1):

$$z_{N_c} = 1 - \sum_{\xi=1}^{N_c-1} z_\xi$$

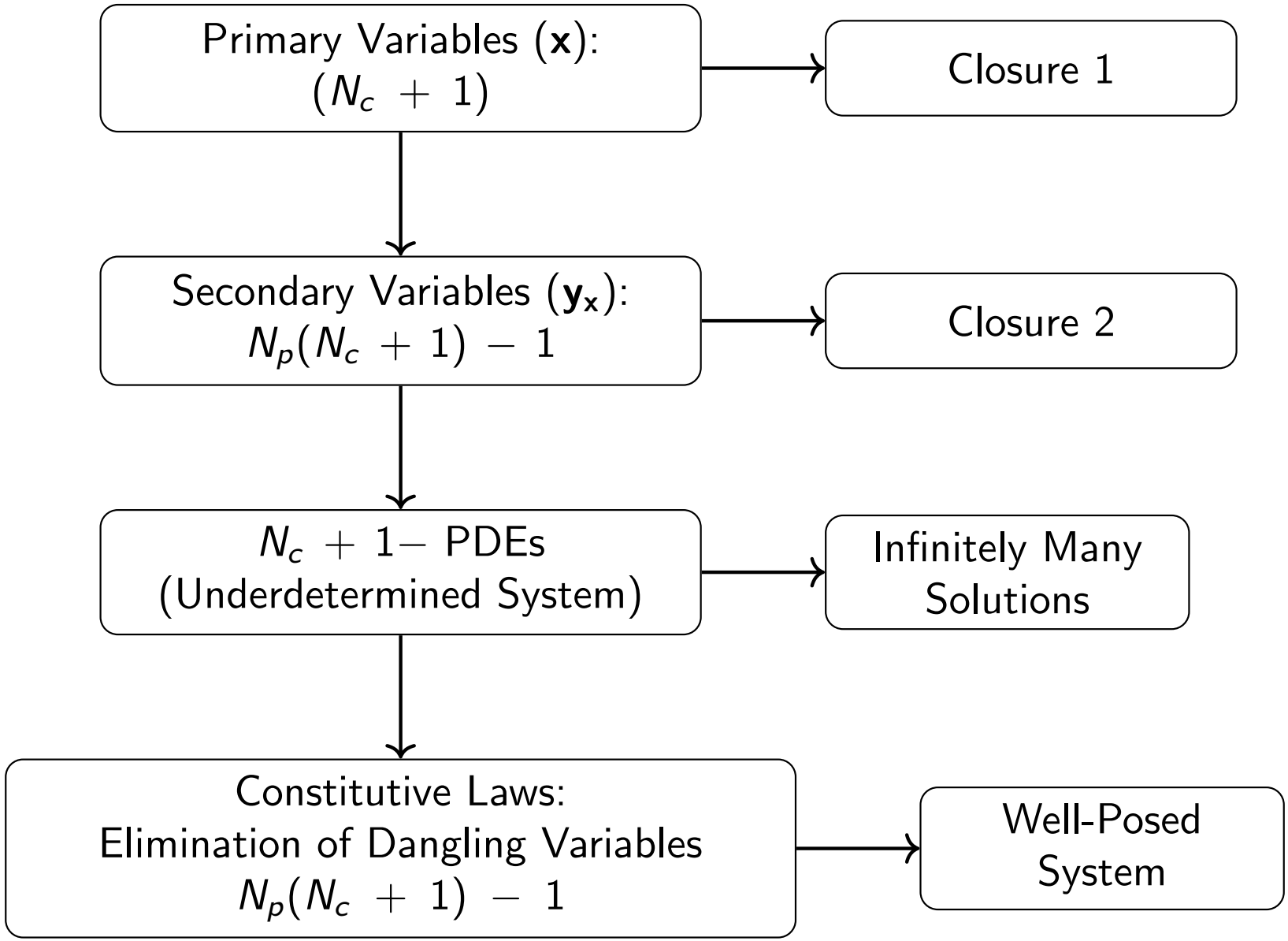
Secondary Variables ($N_p(N_c + 1) - 1$):

$$\mathbf{y_x} = \{T \text{ or } h\} \cup \{s_\gamma : \gamma = 1, \ldots, N_p - 1\} \cup \{y_\gamma : \gamma = 1, \ldots, N_p - 1\}$$
$$\cup \{\chi_{\xi\gamma} : \xi = 1, \ldots, N_c - 1,\ \gamma = 1, \ldots, N_p\}$$

Reference phase quantities (Closure relation 2):

$$\underbrace{s_{N_p} := 1 - \sum_{\gamma=1}^{N_p-1} s_\gamma}_{\text{Saturation}}, \quad \underbrace{y_{N_p} := 1 - \sum_{\gamma=1}^{N_p-1} y_\gamma}_{\text{Fraction}}, \quad \underbrace{\chi_{N_c\gamma} = 1 - \sum_{\xi=1}^{N_c-1} \chi_{\xi\gamma}}_{\text{N}_c\text{- component partial fraction}}$$

Model Variables and Well-Posedness



Secondary Equations (Non-PDEs)

Eliminate Secondary (Dangling) Variables

Secondary Equations (Non-PDEs) in PorePy

- **Local Equilibrium Equations** (Flash Calculations):
  - Solve phase equilibrium problem to determine phase compositions and transitions [2,3]
  - Additional system of non-linear equations (computationally intensive)
- **Correlation-Based Calculations:**
  - Use pre-computed flash results over a discretized space of primary variables
  - Rely on correlation formulas to approximate equilibrium properties, e.g., using NaCl-H_2O phase diagram [1]

[1] Driesner, T., & Heinrich, C. A. (2007). The system H2O–NaCl. Part I: Correlation formulae for phase relations in temperature–pressure–composition space from 0 to 1000°C, 0 to 5000 bar, and 0 to 1 XNaCl. Geochimica et Cosmochimica Acta, 71(20), 4880-4901.
[2] Gharbia, I. B., Haddou, M., Tran, Q. H., & Vu, D. T. S. (2021). An analysis of the unified formulation for the equilibrium problem of compositional multiphase mixtures. ESAIM: Mathematical Modelling and Numerical Analysis, 55(6), 2981-3016.
[3] Lauser, A., Hager, C., Helmig, R., & Wohlmuth, B. (2011). A new approach for phase transitions in miscible multi-phase flow in porous media. Advances in Water Resources, 34(8), 957-966.

Correlation Formulation of NaCl-H_2O System

Evaluation range

For each $\tau \in \mathbf{y_x}$, the correlation [1,2] is given as

$$\tilde{\tau} : \mathcal{D} \longrightarrow \mathbb{R}$$
$$\tilde{\mathbf{x}} \longmapsto \tau := \tilde{\tau}(\tilde{\mathbf{x}})$$

$$\tilde{\mathbf{x}} = (\mathrm{p},\ \mathrm{T},\ z_{\mathrm{NaCl}})$$
$$\mathbf{x} = (\mathrm{p},\ \mathrm{h},\ z_{\mathrm{NaCl}})$$

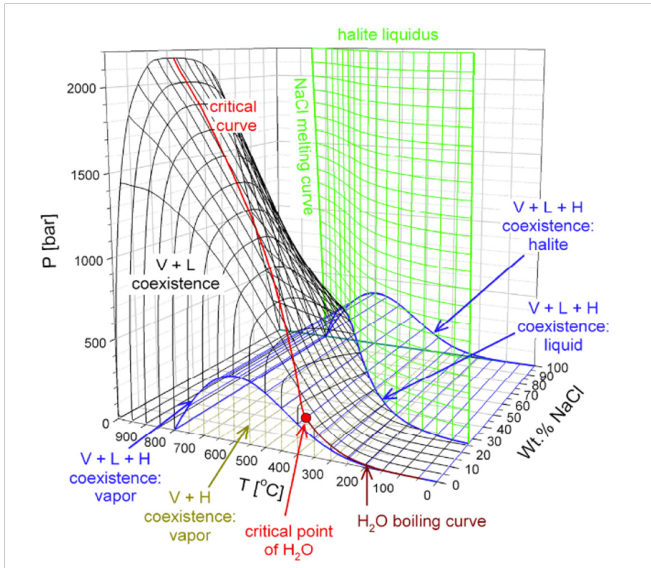
$\mathcal{D} = [0, 5000]\,\mathrm{bar} \times [0, 1000]^{\circ}\mathrm{C} \times [0, 1]$ (Use Regula-Falsi method to transform $\tilde{\mathbf{x}}$ to $\mathbf{x}$-space).

Offline

- Compute each τ over the pre-discretized domain of primary quantities with uniform or adaptive resolution
- Derive $\partial_{\mathbf{x}}\tau$ using finite difference method
- Save grid values and derivatives in VTK format

Online

- At any (p,h,z_{NaCl}), use VTK data to interpolate the values and derivatives as needed



Saltwater phase diagram [2].

[1] Guo, Z., et al. (2021). swEOS: Salt-water equation of state (1.7.0). Zenodo.
[2] Driesner, T., & Heinrich, C. A. (2007). Correlation formulae for H_2O–NaCl. *Geochimica et Cosmochimica Acta*, 71(20), 4880-4901.

Physical Quantities in Correlation-Based Formulation

- To determine other phase-specific physical quantities, such as density or viscosity, for each phase γ, we define the quantity θ_γ by solving the equation:

$$g_\gamma(\mathbf{x}, \mathbf{y}, \theta_\gamma) = 0$$

- Relationship is typically established using suitable equation of state (EoS) combined with appropriate mixture rules

Solution Strategy (Monolithic)

Overall Solution at Each Time Step:

Assume that full system of unknowns is:

$$\mathbf{X}^t = \begin{pmatrix} \mathbf{x}^t \\ \mathbf{y}^t \end{pmatrix}$$

- **Spatial Discretization**: Multipoint Flux Approximation (MPFA) method with an upwind scheme applied for advective terms
- **Temporal Discretization**: Implicit Euler method

Non-Linear System:

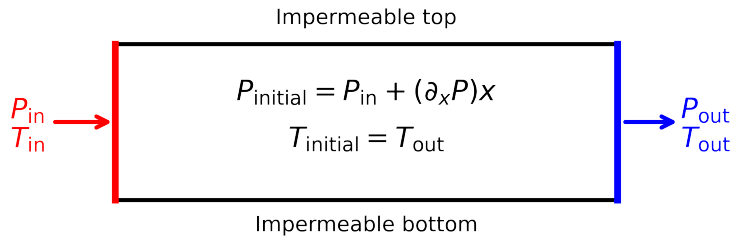
$$\mathbf{G}(\mathbf{X}^t) = \mathbf{0}$$

Newton Linearization:

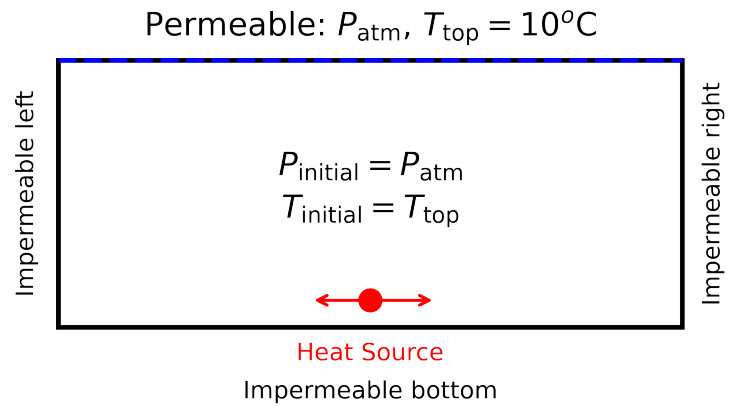
$$J(\mathbf{X}^{t,n})\,(\mathbf{X}^{t,n+1} - \mathbf{X}^{t,n}) = -G(\mathbf{X}^{t,n})$$

Numerical Experiments

- **1D Advection-Dominated (Constant Temperature):**
  - Pure water, single-phase and supercritical fluid flow
  - Pure water, two-phase flow



- **2D Convection-Dominated (Constant Heat Flux) without gravity:**



Implementation in PorePy [1]:

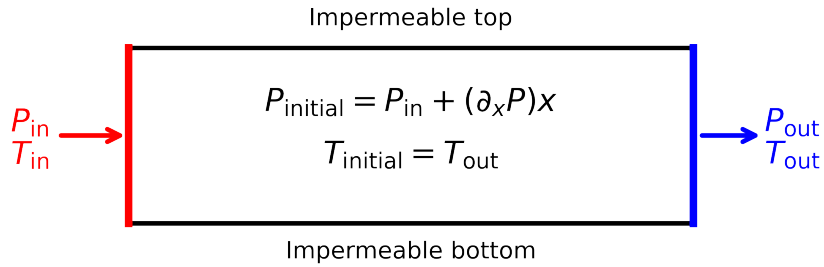
Benchmark with CSMP++ (developed by Stephan Matthai and colleagues at ETH Zurich) [2].

[1] Keilegavlen, E., Berge, R., Fumagalli, A., Starnoni, M., Stefansson, I., Varela, J., & Berre, I. (2021). Porepy: An open-source software for simulation of multiphysics processes in fractured porous media. Computational Geosciences, 25, 243-265.
[2] Weis, P., Driesner, T., Coumou, D., & Geiger, S. (2014). Hydrothermal, multiphase convection of H2O-NaCl fluids from ambient to magmatic temperatures: A new numerical scheme and benchmarks for code comparison. Geofluids, 14(3), 347-371.

1D Advection-Dominated

Common model parameters:

- Domain: 2000×10m
- Abs perm: 10^{-15}m^2 (isotropic)
- Component: H_20
- Relperm: linear
- Pressure and energy equations are active
- $\mathbf{x} = (p, h)$
- Grid cell size: 10m



- At BCs and ICs: $h := \tilde{h}(p, T)$
- $\delta t \in [100, 365]$ days
- Convergence tol: 10^{-3}

1D Advection Dominated (Single-Phase)

Three Cases: Single-Phase/Fluid Flow

Case 1: Liquid Phase

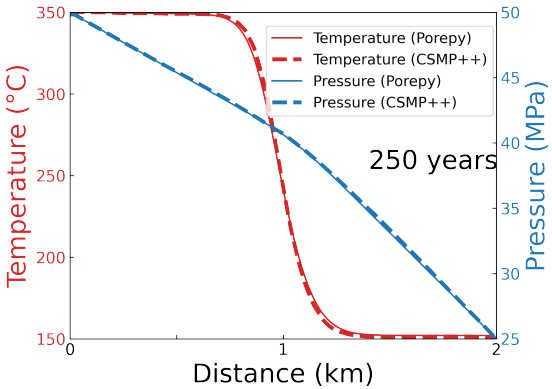
- $p_{\text{in}} = 50\,\text{MPa}$, $p_{\text{out}} = 25\,\text{MPa}$
- $T_{\text{in}} = 350°\text{C}$, $T_{\text{out}} = 150°\text{C}$

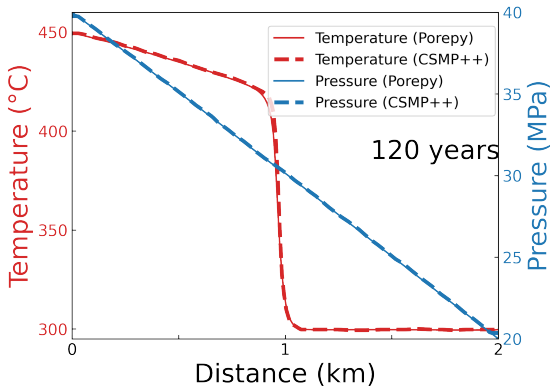
Case 2: Supercritical Fluid

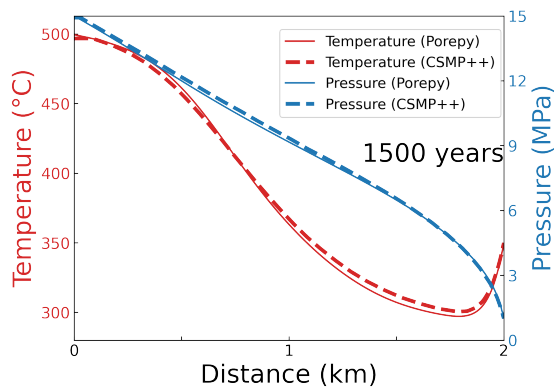
- $p_{\text{in}} = 40\,\text{MPa}$, $p_{\text{out}} = 20\,\text{MPa}$
- $T_{\text{in}} = 450°\text{C}$, $T_{\text{out}} = 300°\text{C}$

Case 3: Vapor Phase

- $p_{\text{in}} = 15.0\,\text{MPa}$, $p_{\text{out}} = 1.0\,\text{MPa}$
- $T_{\text{in}} = 500°\text{C}$, $T_{\text{out}} = 300°\text{C}$







1D Advection Dominated (Two-Phase)

Case 1: Pure Water Two-Phase (High Pressure Gradient)

- BCs:
  - $p_{\text{in}} = 20.0\text{MPa},\ p_{\text{out}} = 1.0\,\text{MPa}$
  - $T_{\text{in}} = 400^{\circ}\text{C},\ T_{\text{out}} = 150^{\circ}\text{C}$
- Residual liquid saturation (R_l): 0.3
- Residual vapour saturation (R_v): 0.0
- Relperm of liquid:

$$k_{rl}(s_l) = \begin{cases} 0 & \text{if } s_l \leq R_l \\ \frac{s_l - R_l}{1-(R_l+R_v)} & \text{if } s_l > R_l \end{cases}$$

- Relperm of vapor:

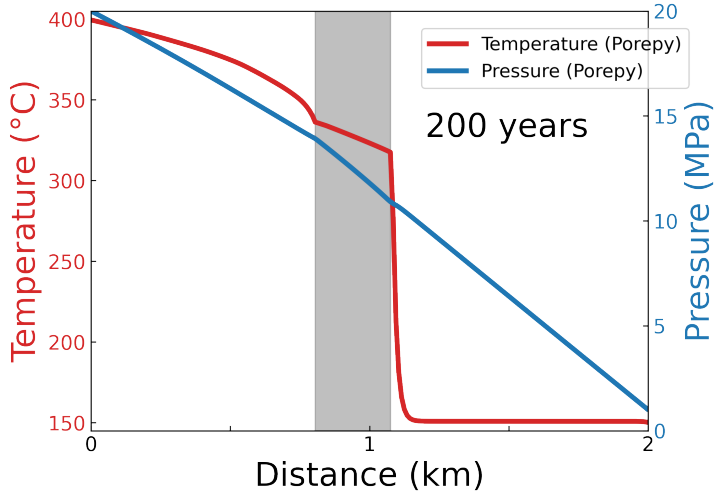
$$k_{rv}(s_v) = \frac{s_v - R_v}{1-(R_l+R_v)}$$

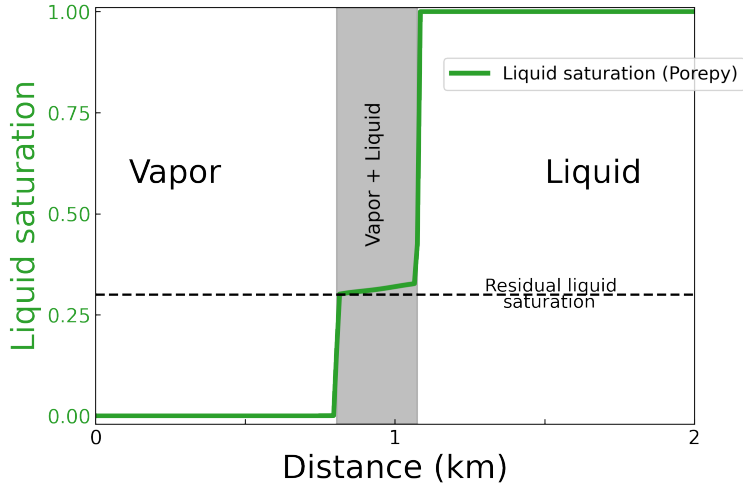
1D Advection Dominated (Two-Phase)

Case 1: Pressure -Temperature and Saturation Progressions

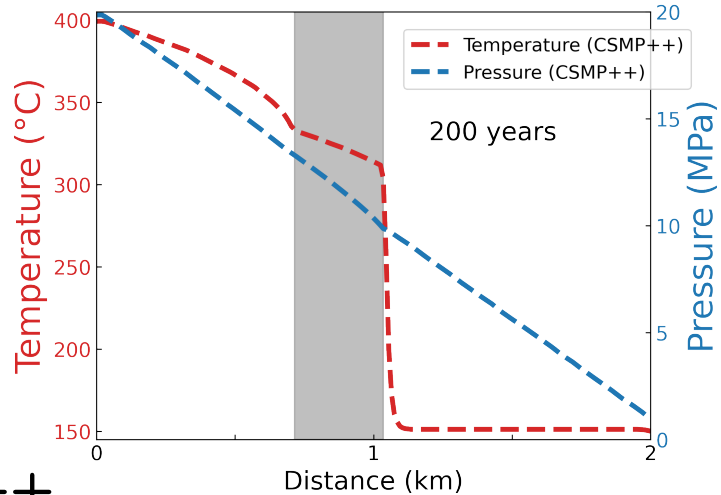
(High Pressure Gradient)

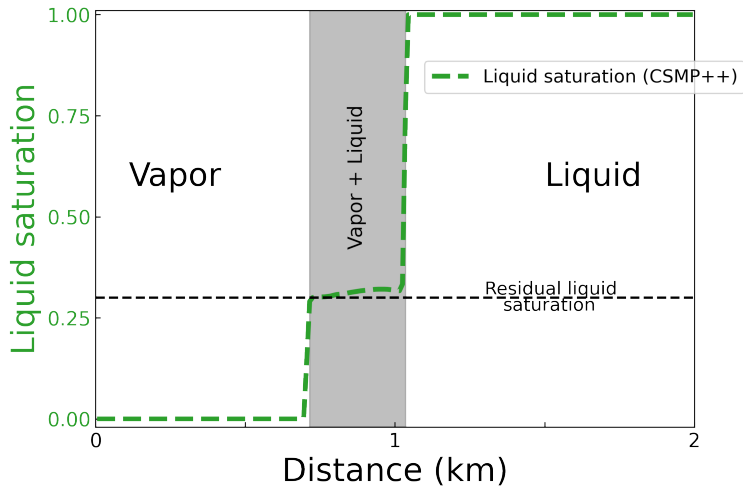
Porepy





CSMP++





1D Advection Dominated (Two-Phase)

Case 2: Pure Water Two-phase Flow (Low Pressure Gradient)

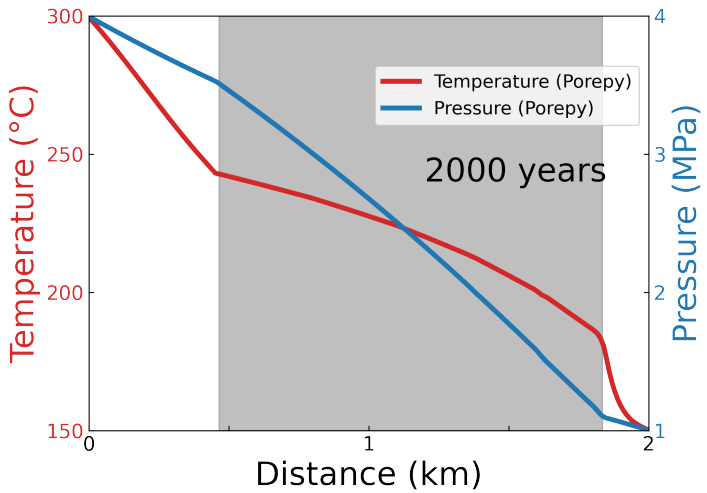
- BCs:
  - $p_{\text{in}} = 4.0\text{MPa},\ p_{\text{out}} = 1.0\,\text{MPa}$
  - $T_{\text{in}} = 300^{\circ}\text{C},\ T_{\text{out}} = 150^{\circ}\text{C}$
- Residual liquid saturation (R_l): 0.3
- Residual vapour saturation (R_v): 0.0
- Relperm of liquid and vapour: same with high pressure gradient case

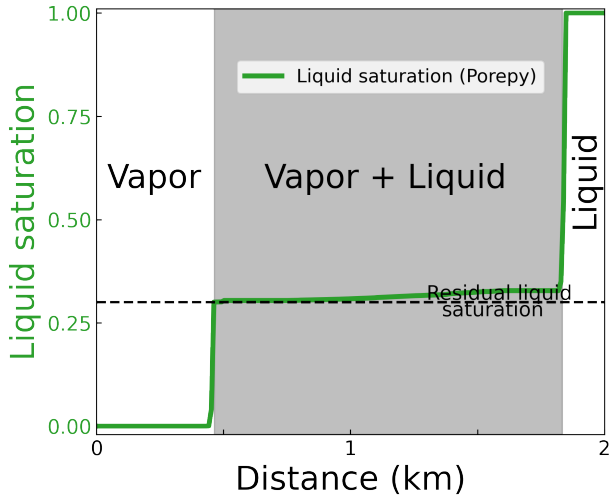
1D Advection Dominated (Two-Phase)

Case 1: Pressure-Temperature and Saturation Progressions

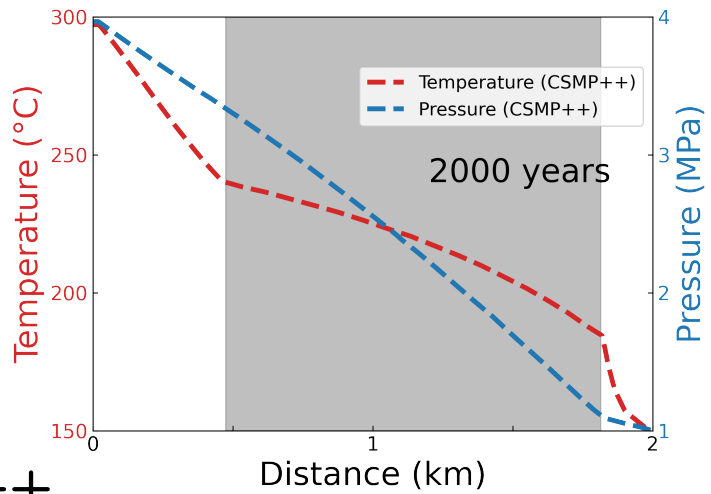
(Low Pressure Gradient)

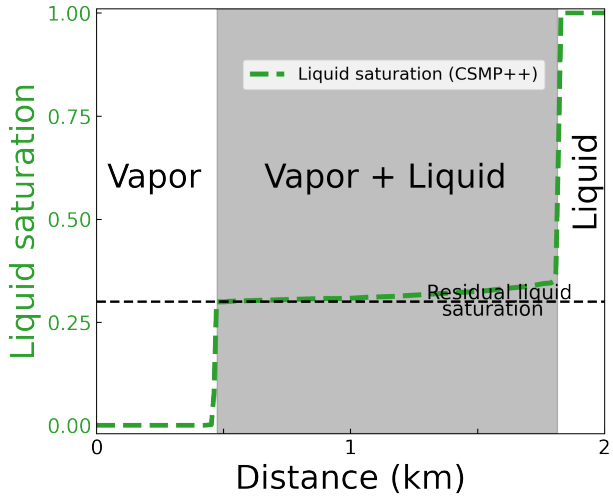
Porepy





CSMP++

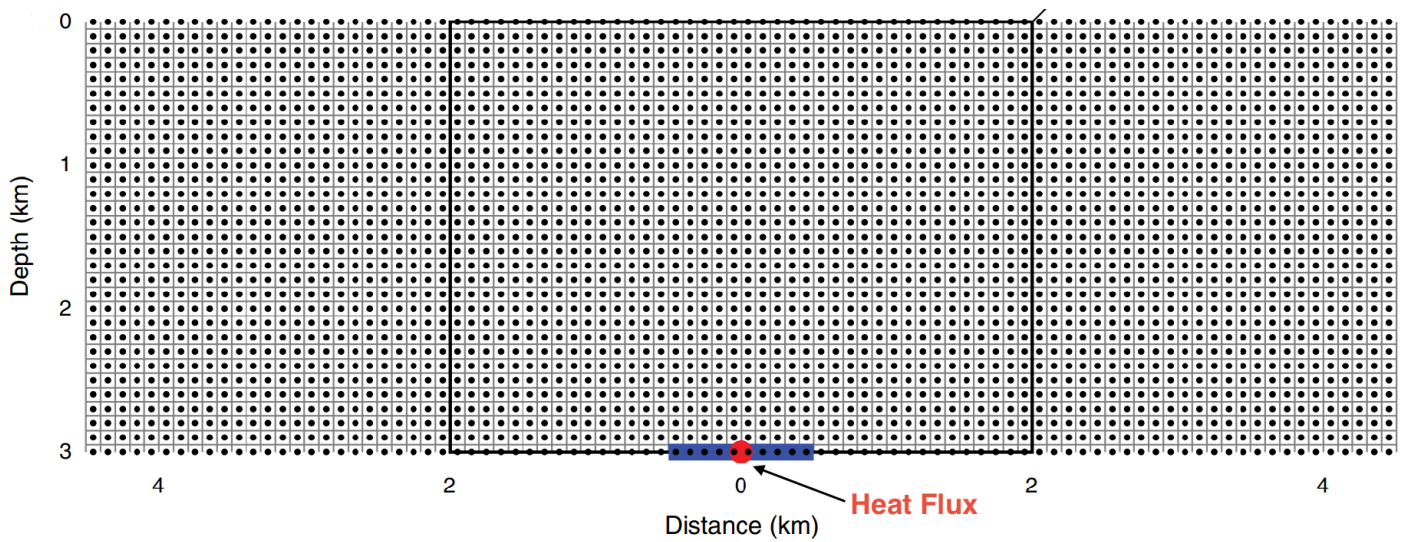




2D Convection-Dominated with Constant Heat Flux

Pure Water Liquid Phase

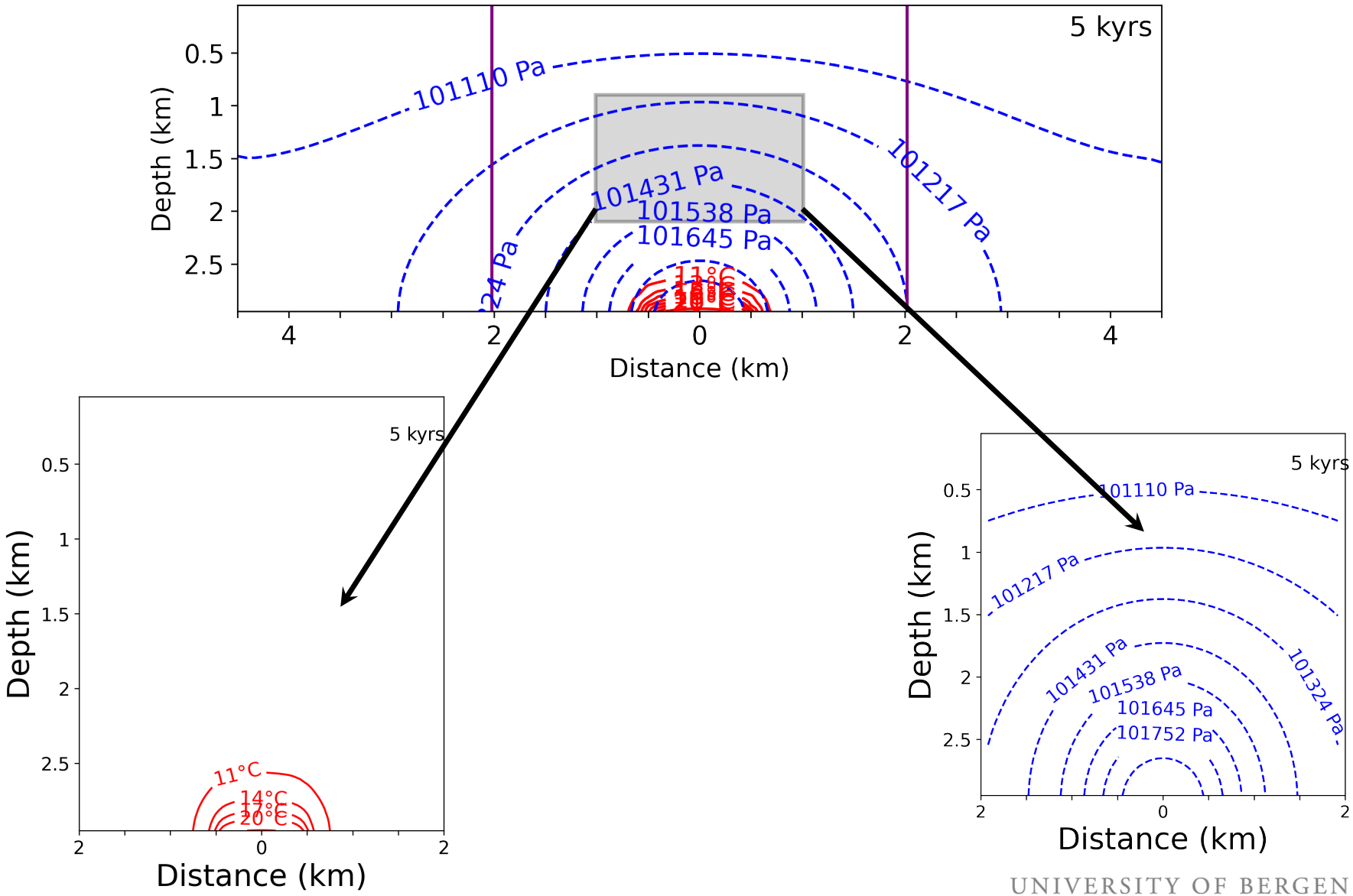
- Domain: 9×3 km
- BCs:
  - $p_{\text{top}} = 0.1\text{MPa}$, $T_{\text{top}} = 10^{\circ}\text{C}$
  - Imperbeable sides and bottom
- ICs: $p_{\text{initial}} =$ hydrostatic pressure, $T_{\text{initial}} = 10^{\circ}\text{C}$
- Constant heat flux (q_e) over 1km at bottom center: 5W/m^3
- No gravity



[1] Weis, P., Driesner, T., Coumou, D., & Geiger, S. (2014). Hydrothermal, multiphase convection of H2O-NaCl fluids from ambient to magmatic temperatures: A new numerical scheme and benchmarks for code comparison. Geofluids, 14(3), 347-371.

2D Convection-Dominated with Constant Heat Flux

Temperature-Pressure Evolution after 5 kyrs



Conclusion

- Developed a unified compositional model combined with pre-computed flash calculation for multiphase geothermal reservoir simulation
- Implemented in PorePy for high-enthalpy and single component two-phase flow
- Achieved good agreement with existing benchmark models
- Applications in geothermal energy extraction, predicting temperature-pressure dynamics and phase transitions

Local Equilibrium Model

Motivation:

- Avoid interpolation and additional error.
- Advanced strategies for equilibrium calculations without relying on an a-priori discretized thermodynamic space.
- Step towards generality in terms of thermodynamic modeling (EoS) and parameter space (p, T, h, u, v).

Outline of unified flash

The persistent variable approach requires a *uniform formulation* of the phase equilibrium conditions [1].

- Static phase context $\gamma = 1, 2, \ldots, N_p$.
- Phase appearance & disappearance is handled with inequality constraints $0 \leq y_\gamma \leq 1$.
- Introduction of extended partial fractions $\tilde{\chi}_{\xi\gamma}$ for each phase γ

$$\chi_{\xi\gamma} = \begin{cases} \tilde{\chi}_{\xi\gamma} & y_\gamma > 0 \\ \frac{\tilde{\chi}_{\xi\gamma}}{\sum_\zeta \tilde{\chi}_{\zeta\gamma}} & y_\gamma = 0 \end{cases}, \quad 0 \leq 1 - \sum_{\zeta=1}^{N_p} \tilde{\chi}_{\zeta\gamma} \ ,$$

as mathematical extensions for the case $y_\gamma = 0$.

[1] Ben Gharbia et al. An analysis of the unified formulation for the equilibrium problem of compositional multiphase mixtures. ESAIM (55) 6, 2981-3016 (2021)

Unified equilibrium conditions: Optimization approach

Locally, we consider the thermodynamic state of the fluid defined in terms of z_ξ and two additional state functions σ

$$\sigma \in \{\{p, T\}, \{p, h\}, \{v, T\}, \{v, u\}, \{v, h\}\}.$$

Secondary Variables ($N_p N_c + 2(N_p - 1)$ fractions):

$$\tilde{\mathbf{y}}_\sigma = \{p \text{ and/or } T\} \cup \{s_\gamma : \gamma = 1, \ldots, N_p - 1\} \cup \{y_\gamma : \gamma = 1, \ldots, N_p - 1\}$$
$$\cup \{\tilde{\chi}_{\xi\gamma} : \xi = 1, \ldots, N_c,\ \gamma = 1, \ldots, N_p\}.$$

Reference phase parameters (Closure relation 3):

$$s_{N_p} := 1 - \sum_{\gamma=1}^{N_p-1} s_\gamma, \quad y_{N_p} := 1 - \sum_{\gamma=1}^{N_p-1} y_\gamma$$

$\rightarrow$ primary variables can be seen as *transport of thermodynamic target state*,
$\rightarrow$ secondary variables as local, non-linear alteration of transport.

Find $\mathbf{y}_\sigma^\star$ such that

$$\mathbf{y}_\sigma^\star = \arg\min_{\mathbf{y}} \; f_\sigma(\mathbf{y})$$

$$\text{with:} \quad z_\xi - \sum_{\gamma=1}^{N_p} \tilde{\chi}_{\xi\gamma} y_\gamma = 0, \; \forall \xi,$$

$$y_\gamma \geq 0, \; \forall \gamma.$$

$f_\sigma(\mathbf{y})$ is a function to be minimized depending target state σ . In fact, we again obtain a map

$$\tau_\sigma^\star : \; \mathbf{x} \longmapsto \tau_\sigma^\star(\mathbf{x}) = \mathbf{y}^\star \; ,$$

with $\tau_\sigma^\star$ not being an interpolation, but the solution to the σ-flash problem.
Exemplarily,

$$f_{p,T} = g \;\; \text{(Gibbs energy minimization)},$$
$$f_{p,h} = -S = \frac{1}{T}(g - h) \;\; \text{(entropy maximization)}.$$

By virtue of thermodynamic relations, the target function can always be chosen to be of the following form [1]:

$$f_\sigma(\mathbf{y}) = f_\sigma(\mathbf{y}, g(\mathbf{y}))$$

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[1] Lipovac et al. Unified Flash Calculations with Isenthalpic and Isochoric Constraints. FPE 578, 113991 (2023)

With $f_\sigma(\mathbf{y}) = f_\sigma(\mathbf{y}, g(\mathbf{y}))$ and standard optimization techniques, the semi-smooth first-order conditions are of form

$$F_\sigma(\mathbf{x}, \mathbf{y}) = \nabla_{\mathbf{y}} f_\sigma = \begin{bmatrix} \Lambda(\mathbf{y}) \\ \Upsilon_\sigma(\mathbf{y}) \\ \min\{\Gamma(\mathbf{y}), \lambda(\mathbf{y})\} \end{bmatrix} = 0 \ ,$$

with

$$\Lambda(\mathbf{y}) = \begin{bmatrix} \left(\tilde{\chi}_{\xi\gamma} - \tilde{\chi}_{\xi N_p} \frac{\varphi_{\xi N_p}}{\varphi_{\xi\gamma}} \right)_{\substack{\xi=1\ldots N_c \\ \gamma=1\ldots N_p-1}} \\ \left(z_\xi - \sum_{\gamma=1}^{N_p} \tilde{\chi}_{\xi\gamma} y_\gamma \right)_{\xi=1\ldots N_c} \end{bmatrix}, \ \Gamma(\mathbf{y}) = \left[(y_\gamma)_{\gamma=1\ldots N_p} \right], \ \lambda(\mathbf{y}) = \left[\left(1 - \sum_{\xi=1}^{N_c} \tilde{\chi}_{\xi,\gamma} \right)_{\gamma=1\ldots N_p} \right].$$

Using the unified formulation and an optimization approach, we arrived at a general mathematical structure of the flash problem, where only Υ_σ varies:

$$\Upsilon_{pT} = [-], \quad \Upsilon_{ph} = \left[h - \sum_{\gamma=1}^{N_p} y_\gamma h_\gamma(\mathbf{y}) \right].$$

Coupling with flow & transport

With $G(\mathbf{x}^t, \mathbf{y}^t)$ denoting the discretized balance equations and $\mathbf{x} = [p, h, z_1, \ldots, z_{N_c-1}]$, the unified compositional formulation using the isenthalpic flash can be written as

$$\begin{bmatrix} G(\mathbf{x}^t, \mathbf{y}^t) \\ F_{ph}(\mathbf{x}^t, \mathbf{y}^t) \end{bmatrix} = 0.$$

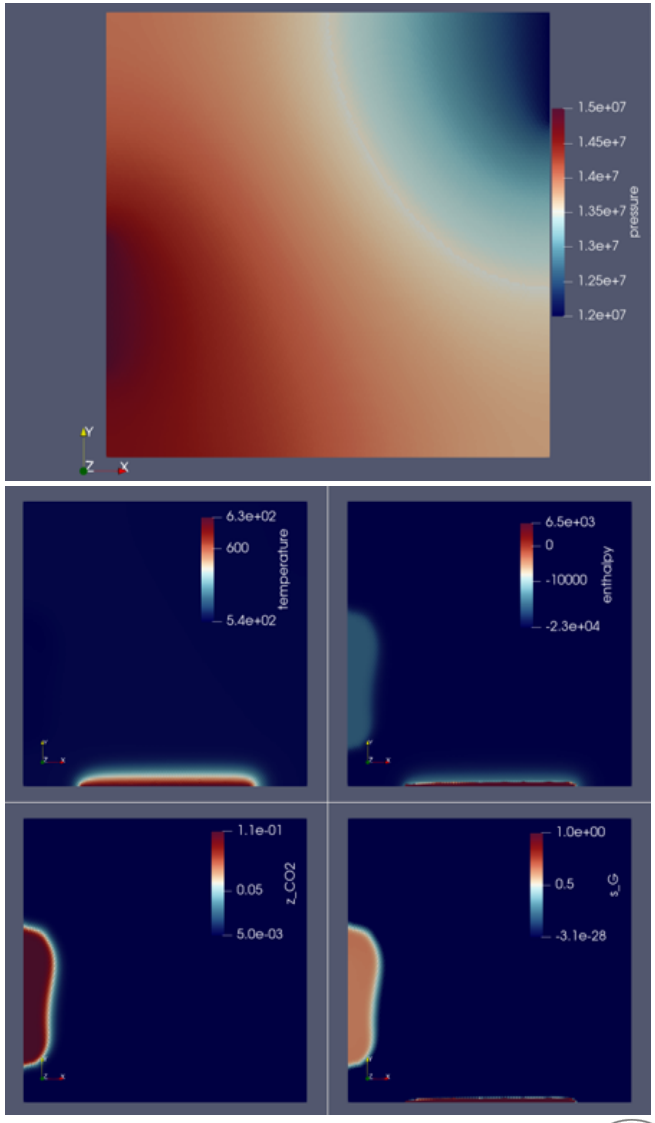
Numerical Solution strategies

While flow & transport progress in some non-zero characteristic time, the local phase equilibrium is instantaneous.

The stiffness of the system in the general case (EoS) makes it difficult to solve above system without a splitting-type approach.

2D Flash calculations as resolutions of instant-time scale for multiple flow regimes

- A Semi-smooth Newton solver with a Schur complement technique is applied on the global system.
- In between iterations, the flash problem is solved in every cell in parallel.
- The numerical method to obtain $\tau^\star(\mathbf{x}_i^t)$ can be any suitable optimization algorithm [1].
- The pT-flash as a subset of the ph-flash can be used in areas with a less volatile flow regime.
- Ongoing work explores above mentioned options.



[1] Vu et al.A new approach for solving nonlinear algebraic systems with complementarity conditions. Application to compositional multiphase equilibrium problems, IMACS (190), 1243-1274 (2021)

Conclusion

- A persistent variable formulation for both flow & transport problem, and thermodynamic equilibrium problem leads to a global and closed mathematical model.
- Flash calculations can be used to resolve the instantaneous timescale.
- Computational cost, as a price for flexibility, can be significantly compensated for using the unified formulation and an efficient parallelization.