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One-component Single-phase Flow Simulator and Two-component Binary Flow Simulator with Applications in Porous Media

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Cahn–Hilliard–Navier–Stokes System

Mathematical Model

- The unknown variables are **order parameter** c, **chemical potential** μ, **velocity** $\boldsymbol{v}$, and **pressure** p.

$$\begin{aligned} \partial_t c - \nabla \cdot (M(c)\, \nabla \mu) + \nabla \cdot (c\boldsymbol{v}) &= 0 \quad \text{in } (0,T) \times \Omega\,, \\ \mu &= \beta\, \Phi'(c) - \alpha\, \Delta c \quad \text{in } (0,T) \times \Omega\,, \\ \rho_0(\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}) - \mu_s \Delta \boldsymbol{v} &= -\nabla p + \mu \nabla c \quad \text{in } (0,T) \times \Omega\,, \\ \nabla \cdot \boldsymbol{v} &= 0 \quad \text{in } (0,T) \times \Omega\,. \end{aligned}$$

- For flow through porous media scenarios, the model is supplemented with physically and mathematically **consistent boundary conditions** at the inlet and outlet.
- Total energy F equals kinetic energy plus Helmholtz free energy:

$$F(c, \boldsymbol{v}) = \int_\Omega \frac{\rho_0}{2} |\boldsymbol{v}|^2 + \int_\Omega \left(\beta\, \Phi(c) + \frac{\alpha}{2} |\nabla c|^2 \right)\,,$$

where $\Phi(c)$ denotes the **chemical energy density**.
- Popular expressions of Φ include **Ginzburg–Landau potential** and **Flory–Huggins potential**.
- A closed Cahn–Hilliard–Navier–Stokes system enjoys the properties of **mass conservation** and **energy dissipation**.

Numerical Method

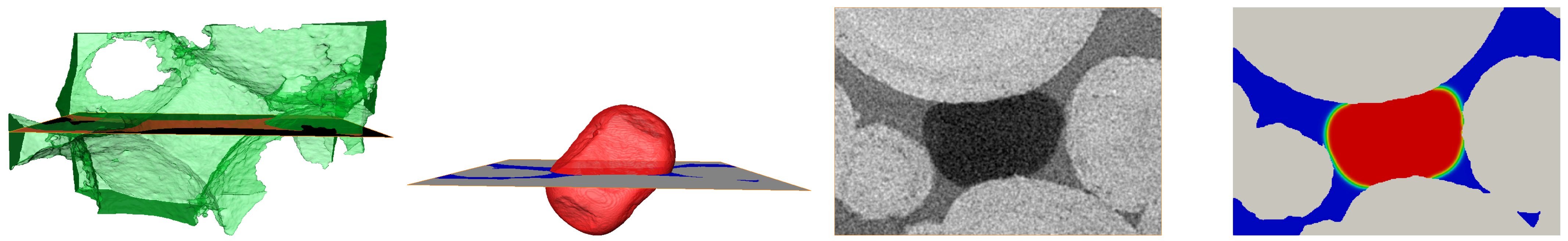
- **Hierarchical bases** with orthogonal basis functions enable arbitrary order of approximation.
- **Interior penalty DG** methods for space discretization.
- **Implicit-explicit** scheme for time discretization.
- **Pressure-correction projection** in conjunction with **div-div correction technique** ensures a pointwise solenoidal velocity field.
- Momentum balance equation: linearized by **Picard splitting**. Nonlinear solution is obtained by fixed-point iteration.
- Mass balance equation: linearized by **Newton's method**. **Dissipates discrete free energy** by utilizing a **convex–concave decomposition**. Scheme reduces to **cell-centered finite volumes** with the use of element-wise constants basis [1].

[1] F. Frank, C. Liu, F. O. Alpak, S. Berg, and B. Rivière. "Direct numerical simulation of flow on pore-scale images using the phase-field method". In: *SPE Journal* (2018). SPE-182607-PA. Accepted.

[2] F. Frank, C. Liu, A. Scanziani, F. O. Alpak, and B. Rivière. "An energy-based contact angle boundary condition on jagged surfaces for the Cahn–Hilliard equation". In: *Journal of Colloid and Interface Science* (2018). Accepted.

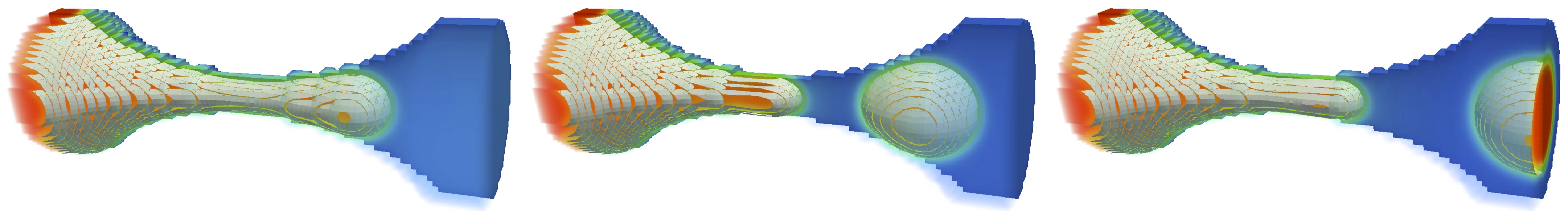
Pore-scale Numerical Simulations

Ketton–brine–decane System



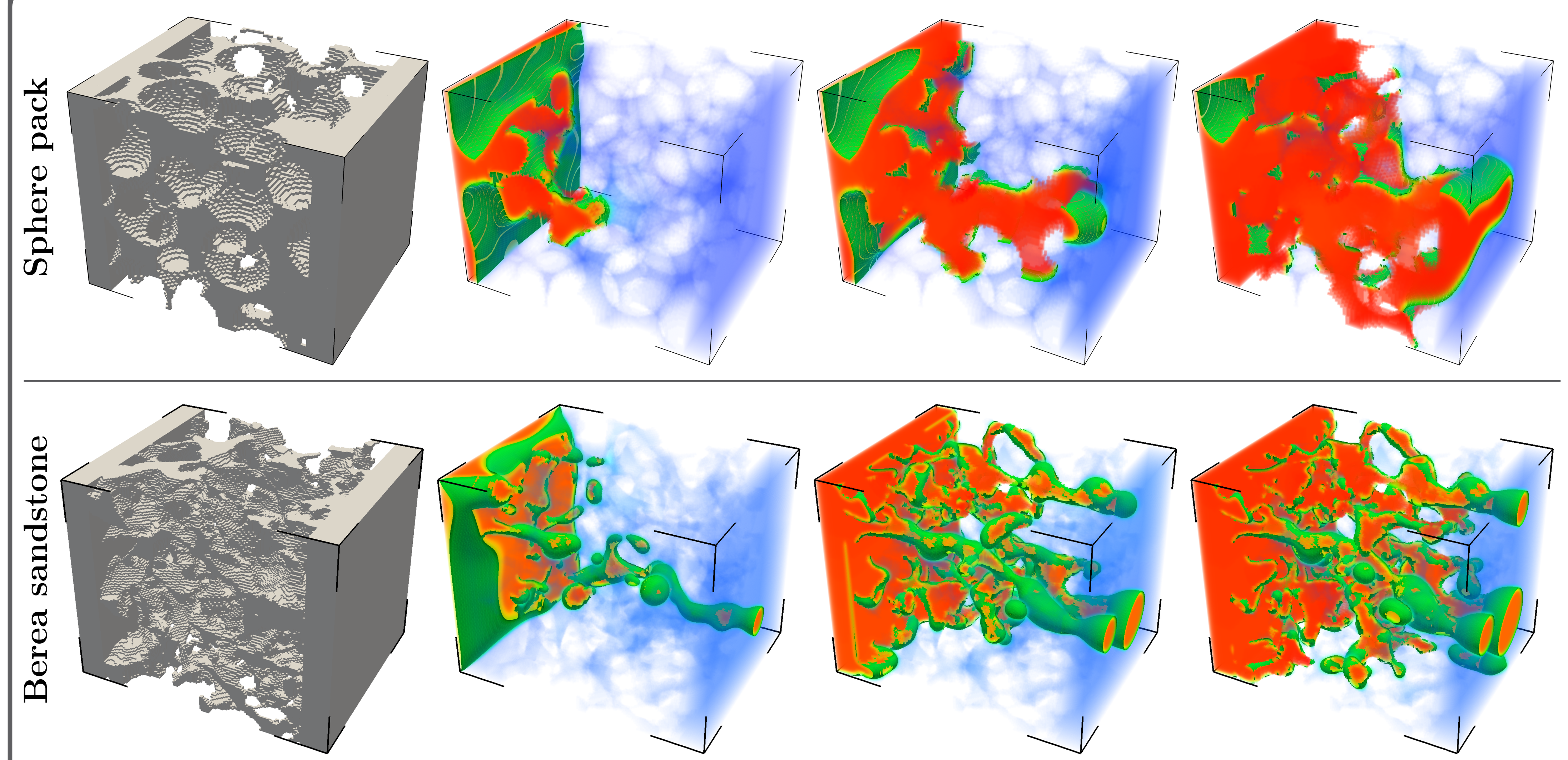
The simulation of equilibrium state **wetting phenomena** is validated by comparing numerical results against segmented micro-CT data from an experimental setup: The pore space (left) contains 62.6% brine and 37.4% decane, the latter of which forms a ganglion (2nd from left) with a contact angle of 37.5° at steady state. The simulation data (right) matches the segmented image data from the physical experiment (2nd from right) [2].

Snap-off Phenomenon



Three dimensional views of the evolution of the **order parameter** c (interface center is shown in gray and phase B is blue). Capillary forces cause droplets to snap off through the geometric constriction of the pore space.

Two-phase Flow through Porous Domains



Micro-CT scan creates **porous images** at micrometer scale in which **voxel sets** represent the structure of porous media. The figure shows the **computational domain** including **buffers** and the order parameter field (red for phase A, green for the interface center, and blue / transparent for phase B).

Upscaling: Permeability Estimation

- The classical incompressible Navier–Stokes model is employed in the one-component single-phase flow simulation module.
- Basis principle for **estimating permeability** is Darcy's law.

Permeability of Pipes – Physical Validation

Permeability estimations of cylindrical pipes

radius [m]	theoretical [mD]	estimated [mD]	error
2.25 E−4	1.020 E+0	9.853 E−1	3.40%
4.00 E−4	1.019 E+1	1.014 E+1	0.49%
7.00 E−4	9.554 E+1	9.670 E+1	1.21%
1.25 E−3	9.714 E+2	9.535 E+2	1.84%
2.25 E−3	1.020 E+4	9.822 E+3	3.71%
4.00 E−3	1.019 E+5	1.014 E+5	0.49%

Permeability estimations of squared pipes

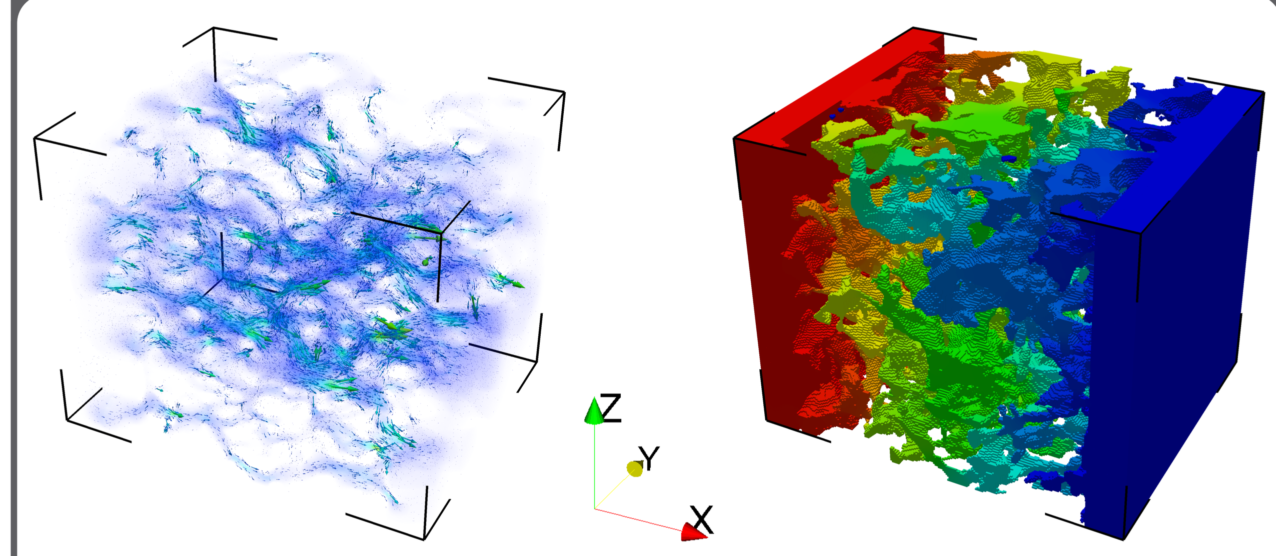
edge length [m]	theoretical [mD]	estimated [mD]	error
4.09 E−4	9.965 E−1	1.036 E+0	3.96%
7.28 E−4	1.000 E+1	9.499 E+0	5.01%
1.30 E−3	1.017 E+2	9.967 E+1	2.00%
2.30 E−3	9.965 E+2	9.814 E+2	1.52%
4.09 E−3	9.965 E+3	1.034 E+4	3.76%
7.28 E−3	1.000 E+5	9.475 E+4	5.25%

Permeability estimations of equilateral-triangular pipes

side length [m]	theoretical [mD]	estimated [mD]	error
6.53 E−4	9.972 E−1	9.954 E−1	0.18%
1.17 E−3	1.028 E+1	1.067 E+1	3.79%
2.07 E−3	1.007 E+2	1.015 E+2	0.79%
3.67 E−3	9.949 E+2	1.004 E+3	0.91%
6.53 E−3	9.972 E+3	9.928 E+3	0.44%
1.17 E−2	1.028 E+5	1.066 E+5	3.70%

- Theoretical permeability of a particular pipe is obtained from Darcy's law based analytical formula as standard reference.

Berea Sandstone



- Velocity field (left) and pressure field (right) at the steady state.
- Mesh resolution: 1/235. Number of elements: 2 931 419. Number of unknowns per time step: 35 177 028.
- Estimated permeability of this sample in X-direction: 761.8 mD.