Upscaling of two-phase porous-media flows with solute-dependent surface tension effects.

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KNOWLEDGE IN ACTION

CMAT

Motivation

Pore/Micro Scale

- ⋆ Size of nm-mm.
- ⋆ Modelling is possible.
- ⋆ Simulations are complicated/impossible?

Darcy/Macro Scale

- ⋆ Size of cm-km.
- ⋆ Modelling is complicated.
- ⋆ Simulations are possible.

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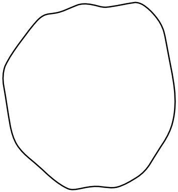
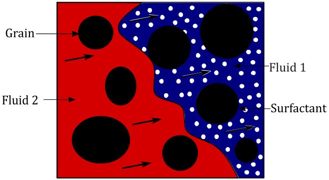
Motivation

Pore-scale models:

- ⋆ Flow of two immiscible and incompressible fluids.
- ⋆ Interface separating two fluids: free boundary problem.
- ⋆ Soluble surfactant present in one fluid phase.
- ⋆ Concentration-dependent surface tension.





- ✓ Main interest: Averaged behaviour of the system at the Darcy scale.
- ✓ Goal: Derive Darcy-scale models incorporating pore-scale information.

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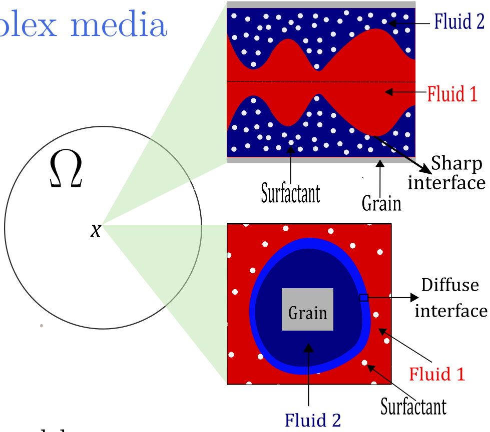
Upscaling: simple to complex media



Thin strip:

- ⋆ Simple geometry.
- ⋆ Free boundary.
- ⋆ Darcy scale:1D, simple model.

Periodic porous medium:

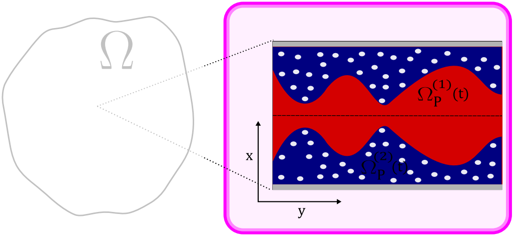
- ⋆ Complex domain.
- ⋆ Phase field.
- ⋆ Darcy scale:2D, more general model.

- S. Sharmin, C. Bringedal, I.S. Pop, On upscaling pore-scale models for two-phase flow with evolving interfaces, Adv. Water Resour., 2021.
- S. Sharmin, M. Bastidas, C. Bringedal, I.S. Pop, Upscaling a Navier-Stokes-Cahn-Hilliard model for two-phase porous-media flow with solute-dependent surface tension effects, Appl. Anal., 2022.

The pore-scale model (thin strip)

Two-phase flow and transport:

- ⋆ $\mathtt{i} = 1, 2$-fluid phases.
- ⋆ $\mathbf{v}^{(\mathtt{i})}$-fluid $\mathtt{i}$ velocity.
- ⋆ $p^{(\mathtt{i})}$-pressure inside fluid $\mathtt{i}$.
- ⋆ c-surfactant concentration.



- $\Omega_P^{(\mathtt{i})}(t)$-pore space occupied by fluid $\mathtt{i}$ (time dependent).
- If constant viscosity and density, momentum and mass conservation:

$$\rho^{(\mathtt{i})}\partial_t \mathbf{v}^{(\mathtt{i})} + \rho^{(\mathtt{i})}\left(\mathbf{v}^{(\mathtt{i})}\cdot\nabla\right)\mathbf{v}^{(\mathtt{i})} = -p^{(\mathtt{i})}\mathbf{I} + \mu^{(\mathtt{i})}\nabla^2\mathbf{v}^{(\mathtt{i})}, \quad \text{in } \Omega_P^{(\mathtt{i})}(t),$$

$$\nabla\cdot\mathbf{v}^{(\mathtt{i})} = 0, \quad \text{in } \Omega_P^{(\mathtt{i})}(t),$$

$$\partial_t c + \nabla\cdot\left(\mathbf{v}^{(2)}c\right) = D\nabla\cdot(\nabla c), \quad \text{in } \Omega_P^{(2)}(t).$$

The pore-scale model (thin strip)

Evolving fluid-fluid interfaces (sharp-interface formulation):

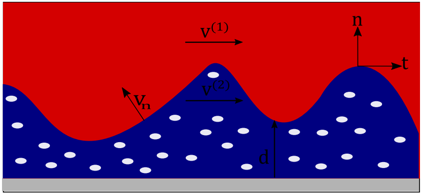
- $d(x,t)$-thickness of the fluid 2 layer.
- $\sigma^{(\mathtt{i})} := -p^{(\mathtt{i})}\mathbf{I} + \mu^{(\mathtt{i})}\left(\left(\nabla \mathbf{v}^{(\mathtt{i})}\right) + \left(\nabla \mathbf{v}^{(\mathtt{i})}\right)^T\right)$-stress tensor.
- $\Gamma_f(t)$:=$\{(x,y) \in \mathbb{R}^2 | 0 < x < L, y = -l + d(x,t)\}$-fluid-fluid interface (model unknown).

- $\Gamma_f(t)$ evolves due to flow and surface tension:

$$\mathbf{v}^{(\mathtt{i})} \cdot \mathbf{n} = v_n,$$

$$\left[\sigma^{(\mathtt{i})} \cdot \mathbf{n}\right] \cdot \mathbf{n} = \gamma(c)(\nabla \cdot \mathbf{n}),$$

$$\left[\sigma^{(\mathtt{i})} \cdot \mathbf{n}\right] \cdot \mathbf{t} = -\mathbf{t} \cdot \nabla \gamma(c).$$



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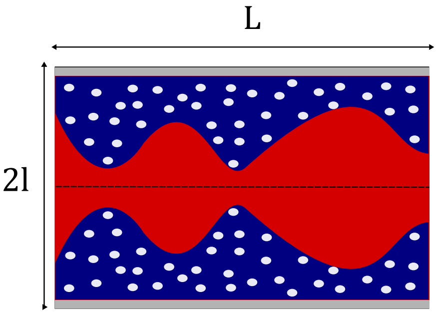
The upscaling (thin strip)

The dimensionless analysis:

- ⋆ $\epsilon = \frac{l}{L} > 0$-scale separation parameter.
- ⋆ $\nabla = (\partial_x, \frac{1}{\epsilon}\partial_y)$-scaling of local variable.
- ⋆ M$= \frac{\mu^{(2)}}{\mu^{(1)}}$-viscosity ratio.
- ⋆ Ca$= \frac{\mu^{(2)}\mathbf{v}_{\text{ref}}}{\gamma_{\text{ref}}}$-Capillary number.



$$\epsilon^2\left(\partial_t \mathbf{v}_\epsilon^{(1)} + \left(\mathbf{v}_\epsilon^{(1)}\cdot\nabla\right)\mathbf{v}_\epsilon^{(1)}\right) + \nabla p_\epsilon^{(1)} - \frac{\epsilon^2}{\text{M}}\nabla^2\mathbf{v}_\epsilon^{(1)} = 0, \text{ in } \Omega_{\epsilon,P}^{(1)}(t),$$

$$\left[\sigma_\epsilon^{(\text{i})}\cdot\mathbf{n}_\epsilon\right]\cdot\mathbf{n}_\epsilon = \frac{\epsilon^2}{\text{Ca}}\gamma(c_\epsilon)\nabla\cdot\mathbf{n}_\epsilon, \text{ on } \Gamma_{\epsilon,f}(t),$$

$$\left[\sigma_\epsilon^{(\text{i})}\cdot\mathbf{n}_\epsilon\right]\cdot\mathbf{t}_\epsilon = -\frac{\epsilon^2}{\text{Ca}}\left(\mathbf{t}_\epsilon\cdot\nabla\gamma(c_\epsilon)\right), \text{ on } \Gamma_{\epsilon,f}(t).$$

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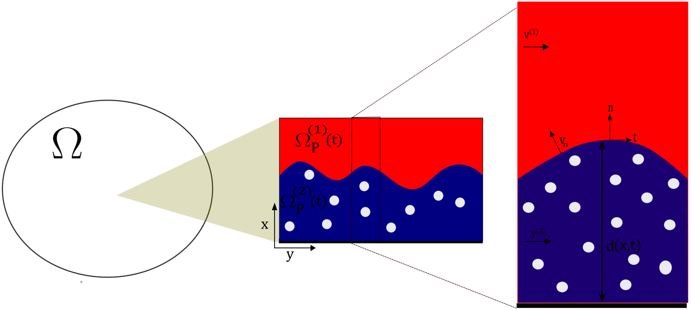
The upscaling (thin strip)

Asymptotic expansion method:

- ⋆ Assume homogenization ansatz:
  $v_\epsilon^{(\mathtt{i,k})}(x,y,t) = v_0^{(\mathtt{i,k})}(x,y,t) + \epsilon v_1^{(\mathtt{i,k})}(x,y,t) + \mathcal{O}(\epsilon^2)$.



- ⋆ Insert expansions, equate terms of same order in ϵ and use transversal integration $\bar{v}_0^{(1,1)}(x,t) := \int_{-1+d_0}^{0} v_0^{(1,1)}(x,y,t)\,dy$.
- ⋆ Derive Darcy-scale 1D model for different regimes
  $\mathrm{Ca} = \epsilon^\beta\,\overline{\mathrm{Ca}}, \beta = 0, 1, 2, 3.$

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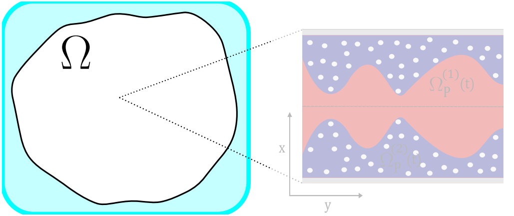
The Darcy-scale model (thin strip)

Two-phase flow with solute-dependent surface tension:

- ⋆ $\mathrm{Ca} = \epsilon\,\overline{\mathrm{Ca}}$-flow regime.
- ⋆ $d_0(x,t)$-saturation.

For every $0 < x < 1$ and $t > 0$:



$$\partial_t d_0 = -\partial_x \bar{v}_0^{(2,1)},$$

$$\partial_t d_0 = \partial_x \bar{v}_0^{(1,1)},$$

$$\bar{v}_0^{(2,1)} = -\frac{{d_0}^2\,(3-d_0)}{6}\,\partial_x p_0 + \frac{{d_0}^2}{2\,\overline{\mathrm{Ca}}}\,\partial_x \gamma(c_0),$$

$$\bar{v}_0^{(1,1)} = -\left(\frac{\mathrm{M}(1-d_0)^3}{3} + \frac{d_0\,(1-d_0)\,(2-d_0)}{2}\right)\partial_x p_0 + \frac{(1-d_0)\,d_0}{\overline{\mathrm{Ca}}}\,\partial_x \gamma(c_0),$$

$$\partial_t\,(c_0\,d_0) = -\partial_x\left(c_0\,\bar{v}_0^{(2,1)}\right) + \partial_x(D\,d_0\,\partial_x c_0).$$

- Capillary pressure is zero ($p_0 = p_0^{(1)} = p_0^{(2)}$).
- Marangoni effect is visible.

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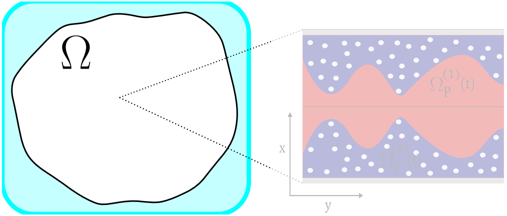
The Darcy-scale model (thin strip)

Two-phase flow with constant surface tension:

- ⋆ $\mathrm{Ca} = \epsilon^3\, \overline{\mathrm{Ca}}$-flow regime.
- ⋆ d-saturation.

For every $0 < x < 1$ and $t > 0$:



$$\partial_t d_0 = -\partial_x \bar{v}_0^{(2,1)},$$

$$\partial_t d_0 = \partial_x \bar{v}_0^{(1,1)},$$

$$\bar{v}_0^{(2,1)} = -\frac{{d_0}^3}{3}\,\partial_x p_0^{(2)} - \frac{(1-d_0)\,{d_0}^2}{2}\,\partial_x p_0^{(1)},$$

$$\bar{v}_0^{(1,1)} = -\left[\frac{\mathrm{M}\,(1-d_0)^3}{3} + d_0\,(1-d_0)^2\right]\partial_x p_0^{(1)} - \frac{(1-d_0)\,{d_0}^2}{2}\,\partial_x p_0^{(2)},$$

$$p_0^{(1)} - p_0^{(2)} = \frac{\partial_{xx} d_0}{\overline{\mathrm{Ca}}}.$$

- Capillary pressure depends on second-order derivative (curvature) of the saturation d_0.

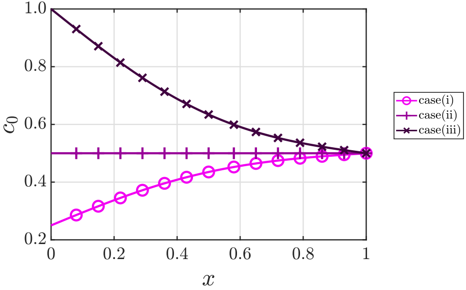
The numerical validation (thin strip)

Test cases:

case(i): corresponds to negative gradient of c_0.

case(ii): constant concentration.

case(iii): positive gradient of c_0.



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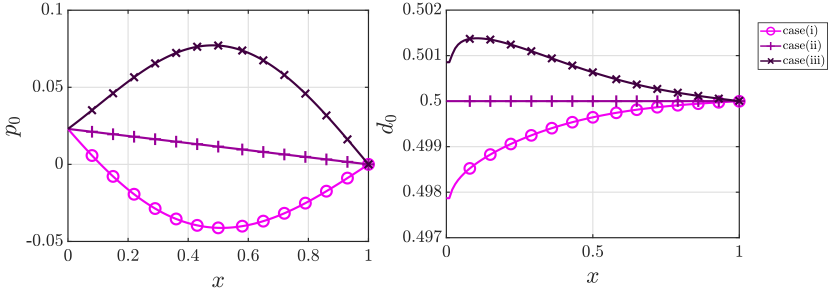
The numerical validation (thin strip)

Comparison of the pressure (left) and the saturation (right) of the upscaled mode for the Marangoni flow.



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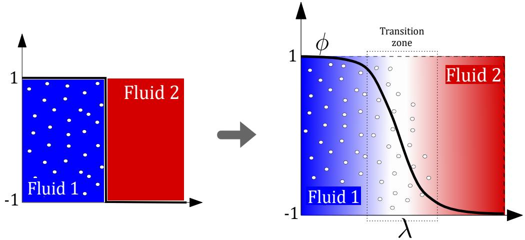
The pore-scale model (periodic porous medium)

Evolving fluid-fluid interfaces (diffuse-interface formulation):

- $Q = (0, \infty) \times \Omega_P$-fixed domain.
- $\phi : Q \to \mathbb{R}$-phase indicator.
- $\gamma(c)$-concentration-dependent surface tension.
- $I(\phi) = \frac{1}{2}(1 + \phi)$-characteristic function.



$$\partial_t \phi + \nabla \cdot (\mathbf{v}\phi) = m\,\lambda\,\Delta\psi, \qquad \text{in } Q,$$

$$\psi = -\nabla \cdot (\mathcal{C}\lambda\gamma(c)\nabla\phi) + \gamma(c)\left(\frac{\mathcal{C}P'(\phi)}{\lambda} + \frac{I'(\phi)}{\beta}\right), \qquad \text{in } Q.$$

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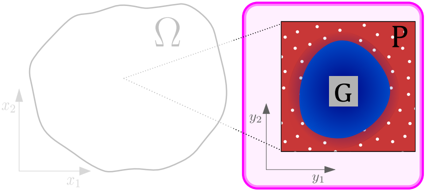
The pore-scale model (periodic porous medium)

Modified flow and transport equations:

- ⋆ $\rho(\phi) = \frac{\rho^{(1)} \cdot (1+\phi)}{2} + \frac{\rho^{(2)} \cdot (1-\phi)}{2}$-density of the mixture.
- ⋆ $\mathbf{v}$-velocity of the mixture (volume averaged).



$$\partial_t (I(\phi)c) + \nabla \cdot (I(\phi)\mathbf{v}c) = \nabla \cdot (D\, I(\phi)\nabla c)\,, \text{in } Q,$$

$$\nabla \cdot \mathbf{v} = 0, \text{in } Q,$$

$$\partial_t\,(\rho(\phi)\mathbf{v}) + \nabla \cdot (\rho(\phi)\mathbf{v} \otimes \mathbf{v}) - \nabla \cdot (-p\mathbf{I} + 2\mu(\phi)\mathcal{E}(\mathbf{v}) + \mathbf{v} \otimes \rho'(\phi)\lambda\, m\, \nabla\psi)$$

$$= \left(\frac{\mathcal{C}}{\lambda}\gamma(c)P'(\phi) - \nabla \cdot (\mathcal{C}\lambda\gamma(c)\nabla\phi)\right)\nabla\phi + \left(\frac{\mathcal{C}\lambda}{2}|\nabla\phi|^2 + \frac{\mathcal{C}}{\lambda}P(\phi)\right)\nabla\gamma(c), \text{in } Q.$$

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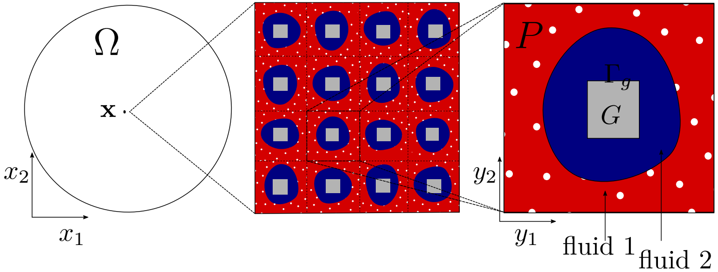
The upscaling (periodic porous medium)

- ⋆ Ω-porous media (Darcy scale).
- ⋆ $Y = (P \cup G \cup \Gamma_g)$-Pore scale.



- Rapidly changing characteristics (at the pore scale).
- Two-scale model: separation between Darcy-scale variable $\mathbf{x}$ and Pore-scale varibale $\mathbf{y} = \frac{\mathbf{x}}{\epsilon}$.

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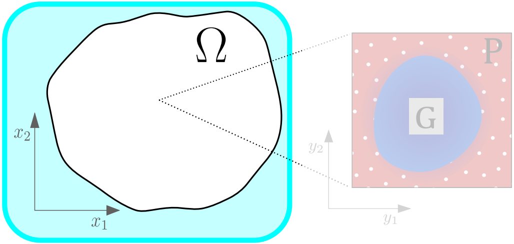
The Darcy scale (periodic porous medium)



$$
\begin{aligned}
\bar{\mathbf{v}} &= -\mathcal{K}\,\nabla p - \mathcal{M}\,\gamma(c), && \text{in } \Omega_{\mathrm{T}} := \Omega \times (0,\mathrm{T}],\\
\nabla \cdot \bar{\mathbf{v}} &= 0, && \text{in } \Omega_{\mathrm{T}},\\
\Phi \partial_t S + \frac{1}{2}\nabla \cdot \bar{\mathbf{v}}_\phi &= 0, && \text{in } \Omega_{\mathrm{T}},\\
\bar{\mathbf{v}}_\phi &= -\mathcal{K}_\phi\,\nabla p - M_\phi\,\gamma(c), && \text{in } \Omega_{\mathrm{T}},\\
\Phi \partial_t (Sc) + \frac{1}{2}\nabla \cdot (c\,(\bar{\mathbf{v}} + \bar{\mathbf{v}}_\phi)) &= \frac{1}{\mathrm{Pe}_c}\nabla \cdot (\mathcal{B}\,\nabla c + H\,c), && \text{in } \Omega_{\mathrm{T}}.
\end{aligned}
$$

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The pore scale (periodic porous medium)

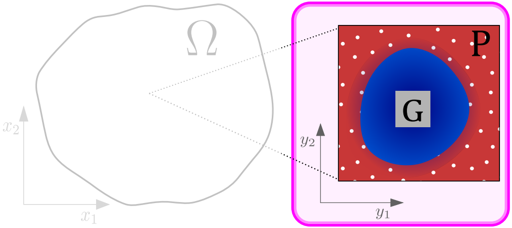
For every $\mathbf{x} \in \Omega$ and $t > 0$:

$$\nabla_{\mathbf{y}} \cdot (\mathbf{v}\phi) = \overline{\mathrm{A}_{\phi}} \lambda \Delta_{\mathbf{y}} \psi, \qquad \text{in } P,$$

$$\psi = \overline{\mathrm{A}_{\psi}} \gamma(c) \left(\frac{\mathcal{C} P'(\phi)}{\lambda} + \frac{I'(\phi)}{\beta} - \mathcal{C} \lambda \Delta_{\mathbf{y}} \phi \right), \qquad \text{in } P,$$

ϕ and ψ are Y-periodic, no flux on Γ_g, $\frac{1}{\Phi} \int_P \phi \, d\mathbf{y} = 2S - 1$.

Here pore scale velocity
$\mathbf{v}_0 = \mathbf{v}(t, \mathbf{x}, \mathbf{y}) = -\sum_{\mathrm{j}=1}^{d} \mathbf{w}_{\mathrm{j}}(t, \mathbf{x}, \mathbf{y}) \, \partial_{x_{\mathrm{j}}} p_0(t, \mathbf{x}) - \mathbf{w}_0(t, \mathbf{x}, \mathbf{y}) \, \gamma(c_0(t, \mathbf{x}))$.



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The effective parameters (periodic porous medium)

$(\mathtt{i},\mathtt{j} \in \{1,2\})$

$\mathcal{K}_{\mathtt{i},\mathtt{j}} := \int_P \mathbf{w}_{\mathtt{i},\mathtt{j}} \, d\mathbf{y}$	$\mathcal{M}_{\mathtt{i}} := \int_P \mathbf{w}_{\mathtt{i},0} \, d\mathbf{y}$
$\mathcal{K}^{\phi}_{\mathtt{i},\mathtt{j}} := \int_P \mathbf{w}_{\mathtt{i},\mathtt{j}}\phi \, d\mathbf{y}$	$\mathcal{M}^{\phi}_{\mathtt{i}} := \int_P \mathbf{w}_{\mathtt{i},0}\phi \, d\mathbf{y}$
$\mathcal{B}_{\mathtt{i},\mathtt{j}} := \int_P I(\phi)\left(\delta_{\mathtt{ij}} + \partial_{y_{\mathtt{i}}}\chi_{\mathtt{j}}\right) \, d\mathbf{y}$	$\mathcal{H}_{\mathtt{i}} := \int_P I(\phi)\partial_{y_{\mathtt{i}}}\chi_0 \, d\mathbf{y}$

Cell problems: For every $\mathbf{x} \in \Omega$ and $t > 0$

$$\overline{\mathrm{Eu}}\nabla_{\mathbf{y}}\Pi_0 = -\frac{1}{\overline{\mathrm{Re}}}\nabla_{\mathbf{y}} \cdot (2\mu(\phi)\mathcal{E}_y(\mathbf{w}_0)) + \frac{1}{\overline{\mathrm{Re}}\,\overline{\mathrm{Ca}}}\left(\frac{\mathcal{C}}{\lambda}P'(\phi) - \mathcal{C}\lambda\Delta_{\mathbf{y}}\phi\right)\nabla_{\mathbf{y}}\phi, \quad \text{in } P,$$

$$\nabla_{\mathbf{y}} \cdot \mathbf{w}_0 = 0, \quad \text{in } P,$$

$$\mathbf{w}_0 = \mathbf{0}, \quad \text{on } \Gamma_g,$$

$\Pi_0, \mathbf{w}_0$ are Y-periodic and $\displaystyle\int_P \Pi_0 \, d\mathbf{y} = 0.$

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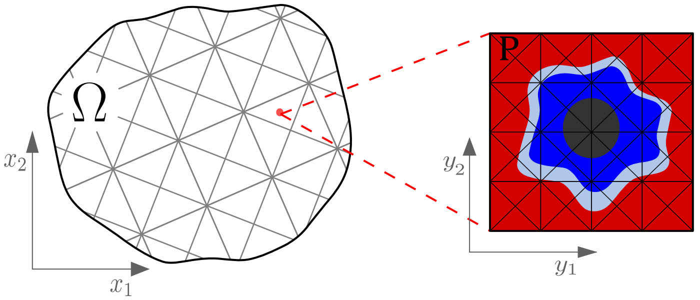
The two-scale discretization



Mixed finite element method (MFEM) at both scales and Euler explicit in time.

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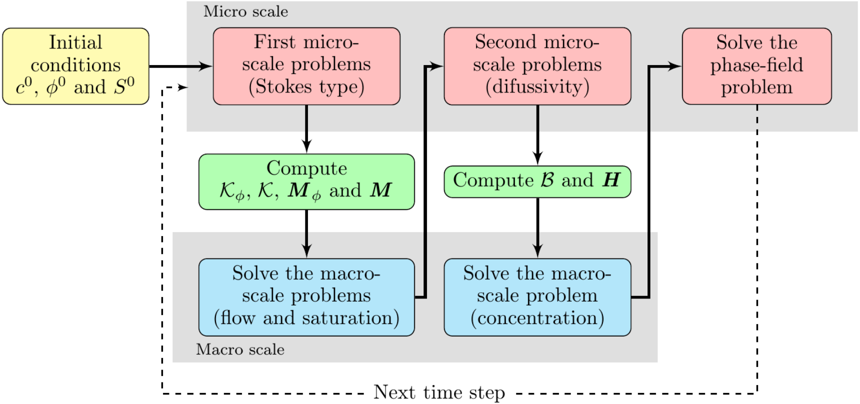
The explicit two-scale scheme



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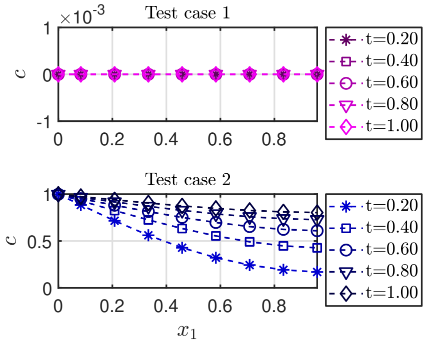
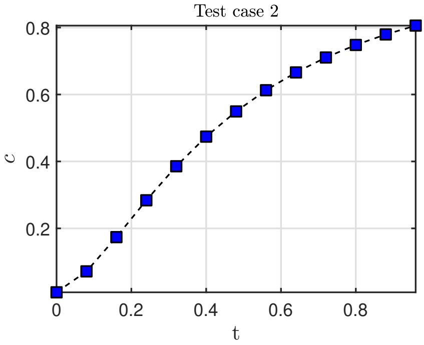
The numerical solution (periodic porous medium)

Test case 1 and 2 correspond to constant and variable surface tension, respectively.





Goal: Variable surface tension effect.

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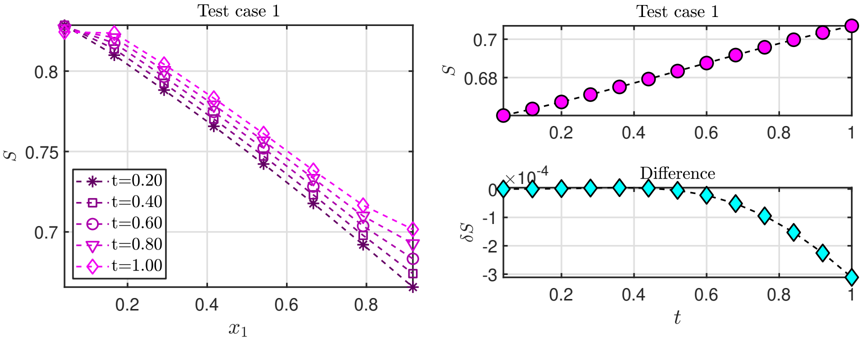
The numerical solution (periodic porous medium)

Decrease in saturation due to effective parameters which depends on the phase field.



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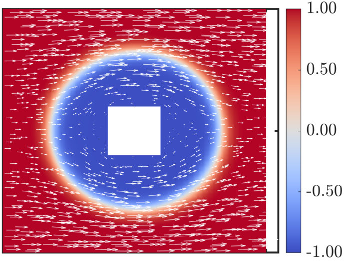
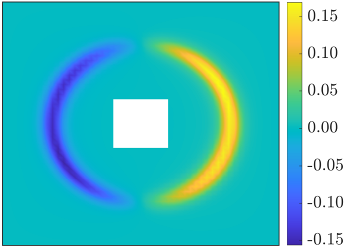
The numerical solution (periodic porous medium)

The evolution of the pore-scale phase field in the test case 1 (left) and the difference of the phase field $\delta\phi$ between the two test cases (right).





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Conclusions and future work

- ✓ Thin strip and periodic homogenization for two-phase flow model with evolving interfaces.
- ✓ Rational derivation of the upscaled model from pore-scale model.
- ✓ For thin-strip model:

  Darcy type laws with Marangoni effect.
  Capillary pressure involving second order derivative of the saturation.
- ✓ For periodic porous media:

  Darcy type laws involving effective parameters.
  Two-scale numerical solution for two-phase flow.

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Conclusions and future work

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  Darcy type laws with Marangoni effect.
  Capillary pressure involving second order derivative of the saturation.
- ✓ For periodic porous media:

  Darcy type laws involving effective parameters.
  Two-scale numerical solution for two-phase flow.
- ⋆ Different flow regimes.
- ⋆ More robust numerical solutions (iterations and adaptive computations).

  BASTIDAS OLIVARES, M. ET AL. APPL. MATH. COMPUT (2021).

Thank you for your attention!

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