

# The numerical solution of the micro-scale phase-field equation and its role in a two-scale two-phase flow model

**Manuela Bastidas<sup>1,2</sup>**  
Sohely Sharmin<sup>2</sup>, Carina Bringedal<sup>3</sup> and Sorin Pop<sup>2</sup>

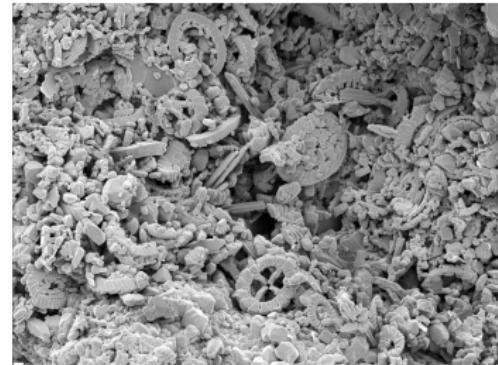
<sup>1</sup> Inria, Paris  
<sup>2</sup>Hasselt University  
<sup>3</sup>Stuttgart University

**Interpore 2022**  
14th Annual Meeting  
Abu Dhabi, United Arab Emirates.

# Motivation

## Pore/Micro Scale

- ★ Size of nm-mm.
- ★ Detailed mathematical models.
- ★ Simulations are complicated/impossible?



## Darcy/Macro Scale

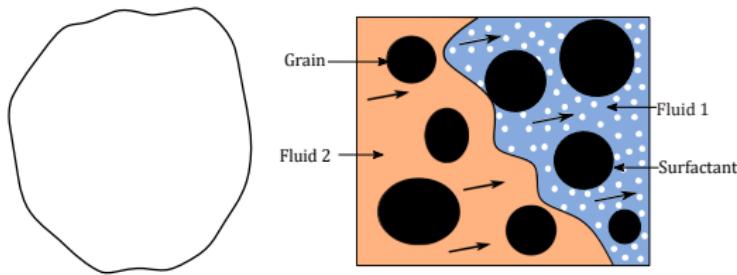
- ★ Size of cm-km.
- ★ Detail mathematical models are complicated.
- ★ Simulations are possible.



# 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.

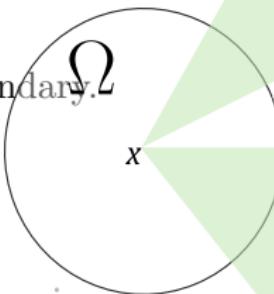


- ✓ **Main interest:** Averaged behaviour of the system at the Darcy scale.
- ✓ **Goal:** Numerical strategies for the Darcy-scale models incorporating pore-scale information.

# Upscaling: simple to complex media

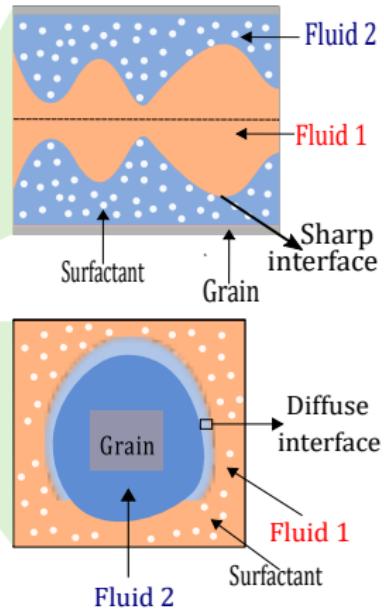
## Thin strip:

- ★ Simple geometry.
- ★ Fluid-fluid interface: Free boundary.
- ★ Darcy scale: 1D, simple model.



## Periodic porous medium:

- ★ Complex domain.
- ★ Fluid-fluid interface: Phase field.
- ★ Darcy scale: 2D or 3D, more general model.



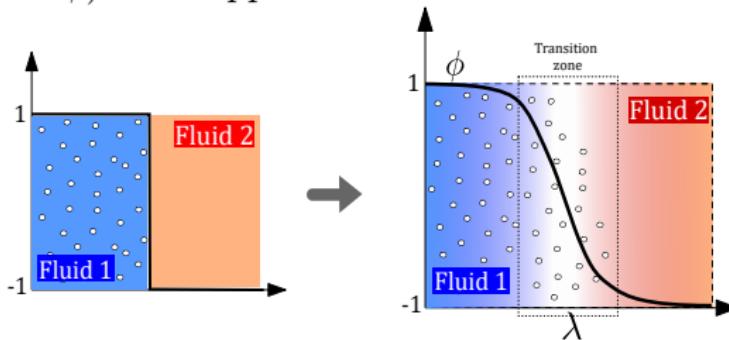
- S. SHARMIN, C. BRINGEDAL, I.S. POP, ON UPSCALING PORE-SCALE MODELS FOR TWO-PHASE FLOW WITH EVOLVING INTERFACES, ADV. WATER RESOUR., 2021.

- S. SHARMIN, M. BASTIDAS, C. BRINGEDAL, I.S. POP, UPSCALING A NAVIER-STOKES-CAHN-HILLIARD MODEL FOR TWO-PHASE POROUS-MEDIUM FLOW WITH SOLUTE-DEPENDENT SURFACE TENSION EFFECTS, APPL. ANAL., 2022.

# The pore-scale model (periodic porous medium)

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

- $\Omega_T := \Omega \times (0, T]$  → fixed domain.
- $\phi : \Omega_T \rightarrow \mathbb{R}$  → phase indicator  $\approx 1$  for fluid1 and  $\approx -1$  for fluid2.
- $\gamma(c)$  → concentration-dependent surface tension.
- $I(\phi) = \frac{1}{2}(1 + \phi)$  → Approximate the characteristic function.



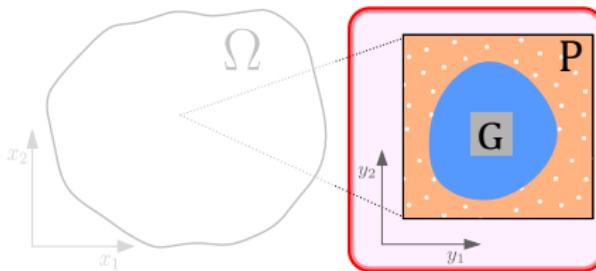
$$\partial_t \phi + \nabla \cdot (\mathbf{v} \phi) = m \lambda \Delta \psi \quad \text{in } \Omega_T,$$

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

# The pore-scale model

## 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).

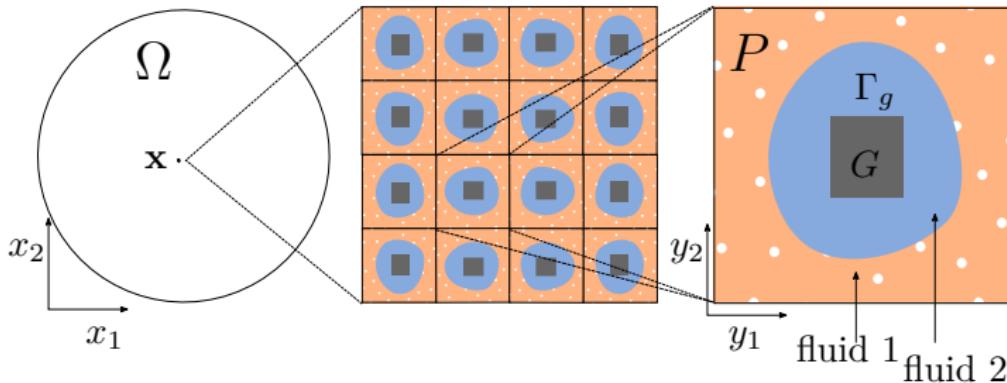


$$\begin{aligned}\partial_t(I(\phi)c) + \nabla \cdot (I(\phi)\mathbf{v}c) &= \nabla \cdot (D I(\phi)\nabla c) && \text{in } \Omega_T, \\ \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega_T,\end{aligned}$$

$$\begin{aligned}\partial_t (\rho(\phi)\mathbf{v}) + \nabla \cdot (\rho(\phi)\mathbf{v} \otimes \mathbf{v}) - \nabla \cdot (-p\mathbf{I} + 2\mu(\phi)\mathcal{E}(\mathbf{v}) + \mathbf{v} \otimes \rho'(\phi)\lambda m \nabla \psi) \\ = \left( \frac{\mathcal{C}}{\lambda} \gamma(c) P'(\phi) - \nabla \cdot (\mathcal{C} \lambda \gamma(c) \nabla \phi) \right) \nabla \phi + \left( \frac{\mathcal{C} \lambda}{2} |\nabla \phi|^2 + \frac{\mathcal{C}}{\lambda} P(\phi) \right) \nabla \gamma(c) &\text{ in } \Omega_T.\end{aligned}$$

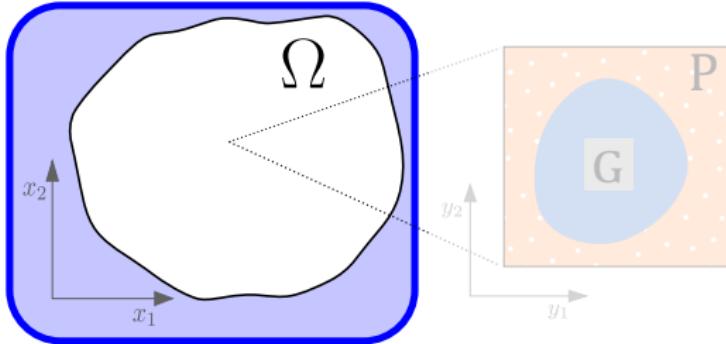
# The upscaling

- ★  $\Omega \rightarrow$  porous media (Darcy scale).
- ★  $Y = (P \cup G \cup \Gamma_g) \rightarrow$  Pore scale.



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

# The Darcy scale



$$\bar{\mathbf{v}} = -\mathcal{K} \nabla p - \mathbf{M} \gamma(c), \quad \text{in } \Omega_T,$$

$$\nabla \cdot \bar{\mathbf{v}} = 0, \quad \text{in } \Omega_T,$$

$$\Phi \partial_t S + \frac{1}{2} \nabla \cdot \bar{\mathbf{v}}_\phi = 0, \quad \text{in } \Omega_T,$$

$$\bar{\mathbf{v}}_\phi = -\mathcal{K}_\phi \nabla p - \mathbf{M}_\phi \gamma(c), \quad \text{in } \Omega_T,$$

$$\Phi \partial_t (Sc) + \frac{1}{2} \nabla \cdot (c(\bar{\mathbf{v}} + \bar{\mathbf{v}}_\phi)) = \frac{1}{\text{Pe}_c} \nabla \cdot (\mathcal{B} \nabla c + \mathbf{H} c), \quad \text{in } \Omega_T.$$

# The pore scale

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

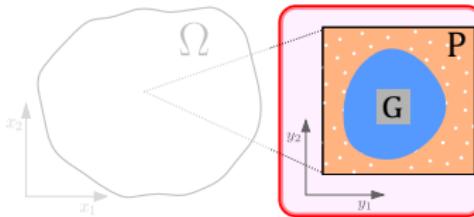
$$\nabla_{\mathbf{y}} \cdot (\mathbf{v}\phi) = \overline{\mathbf{A}_\phi} \lambda \Delta_{\mathbf{y}} \psi, \quad \text{in } P,$$

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

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

Pore scale velocity

$$\mathbf{v}_0 = \mathbf{v}(t, \mathbf{x}, \mathbf{y}) = - \sum_{j=1}^d \mathbf{w}_j(t, \mathbf{x}, \mathbf{y}) \partial_{x_j} p_0(t, \mathbf{x}) - \mathbf{w}_0(t, \mathbf{x}, \mathbf{y}) \gamma(c_0(t, \mathbf{x})).$$



# The effective parameters

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

$$\mathcal{K}_{i,j} := \int_P \mathbf{w}_{i,j} \, d\mathbf{y}$$

$$\mathcal{K}_\phi{}_{i,j} := \int_P \mathbf{w}_{i,j} \phi \, d\mathbf{y}$$

$$\mathcal{B}_{i,j} := \int_P I(\phi) (\delta_{ij} + \partial_{y_i} \chi_j) \, d\mathbf{y}$$

$$\mathbf{M}_i := \int_P \mathbf{w}_{0,i} \, d\mathbf{y}$$

$$\mathbf{M}_\phi{}_i := \int_P \mathbf{w}_{0,i} \phi \, d\mathbf{y}$$

$$\mathbf{H}_i := \int_P I(\phi) \partial_{y_i} \chi_0 \, d\mathbf{y}$$

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

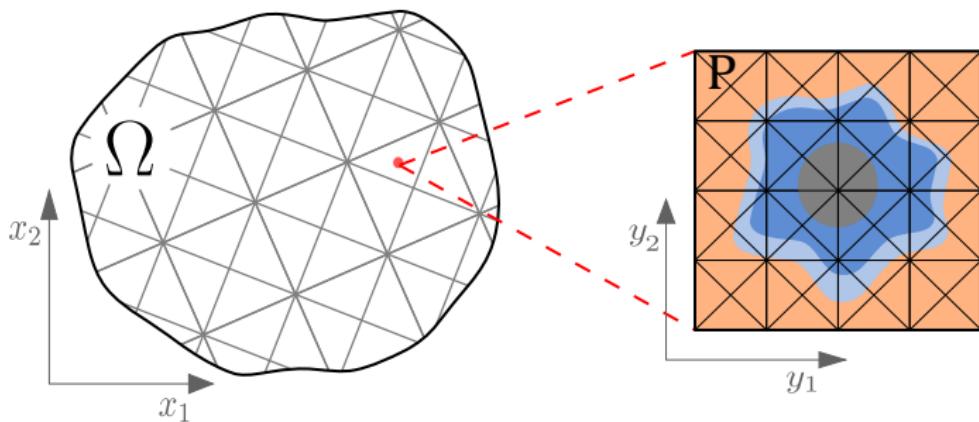
$$\overline{\text{Eu}} \nabla_{\mathbf{y}} \Pi_0 = -\frac{1}{\overline{\text{Re}}} \nabla_{\mathbf{y}} \cdot (2\mu(\phi) \mathcal{E}_y(\mathbf{w}_0)) + \frac{1}{\overline{\text{Re}} \overline{\text{Ca}}} \left( \frac{\mathcal{C}}{\lambda} P'(\phi) - \mathcal{C} \lambda \Delta_{\mathbf{y}} \phi \right)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

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

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

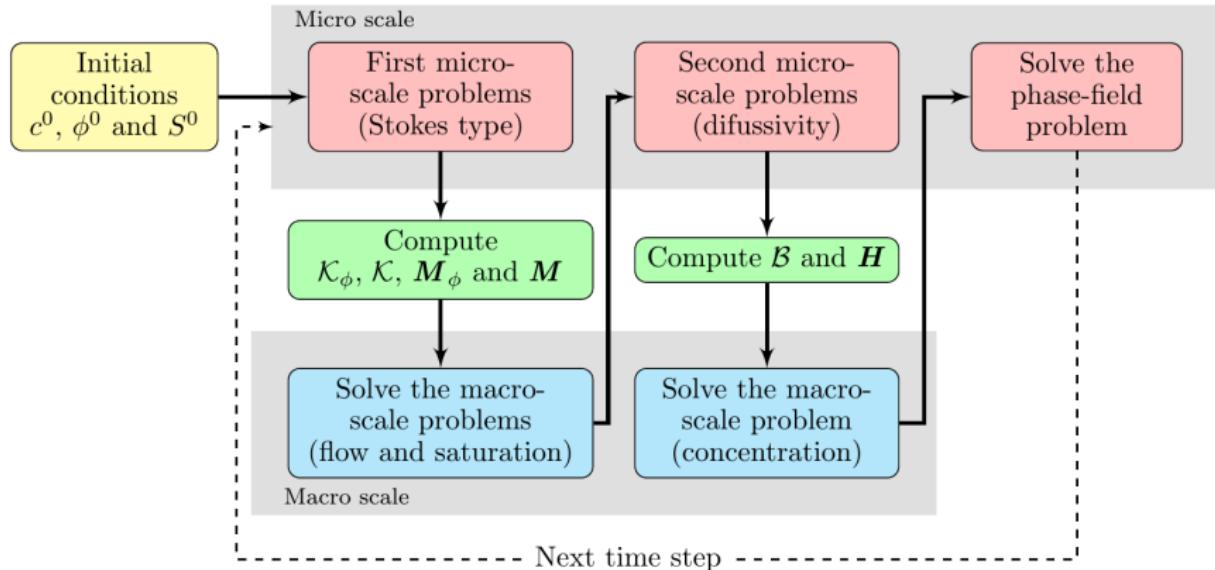
$\Pi_0, \mathbf{w}_0$  are  $Y$ -periodic and  $\int_P \Pi_0 \, d\mathbf{y} = 0$ .

# The two-scale discretization

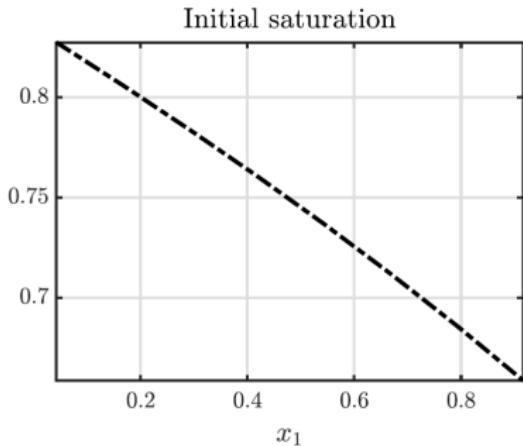
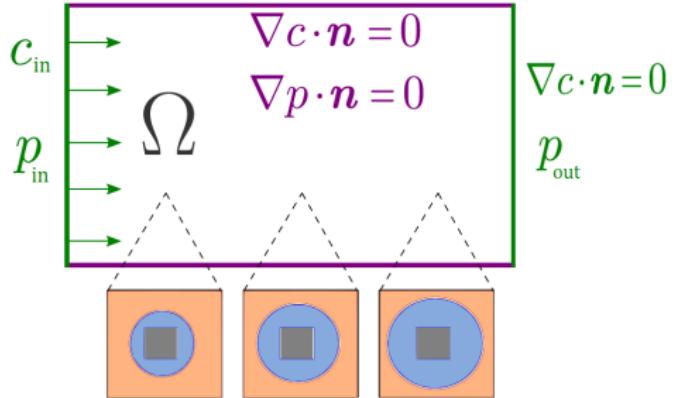


Mixed finite element method (MFEM) at both scales and Euler explicit in time.

# The explicit two-scale scheme

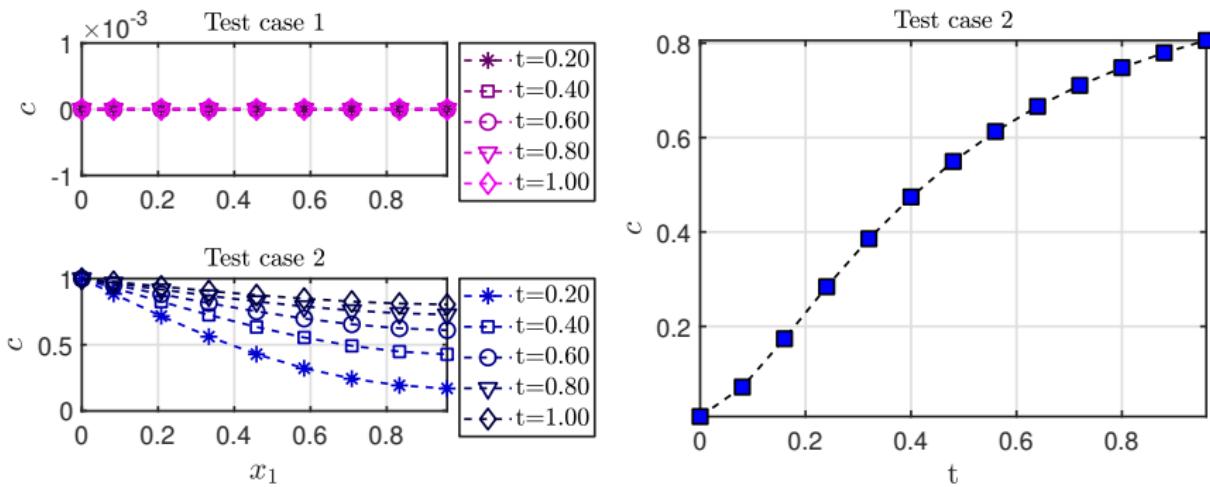


# A numerical example



- ★ Surface tension:  $\gamma(c) = -(100c + 1)$ .
- ★ **Test case 1:** Constant surface tension  $c_{in} = 0$ .
- ★ **Test case 2:** Variable surface tension  $c_{in} = 1$ .
- ★ Pressure  $p_{in} = 2$  and  $p_{out} = 0$ .

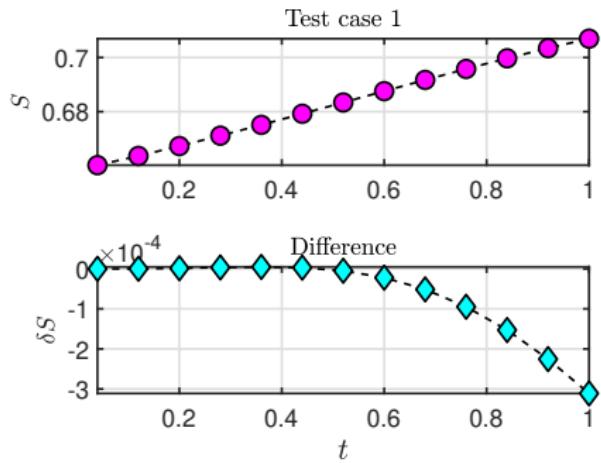
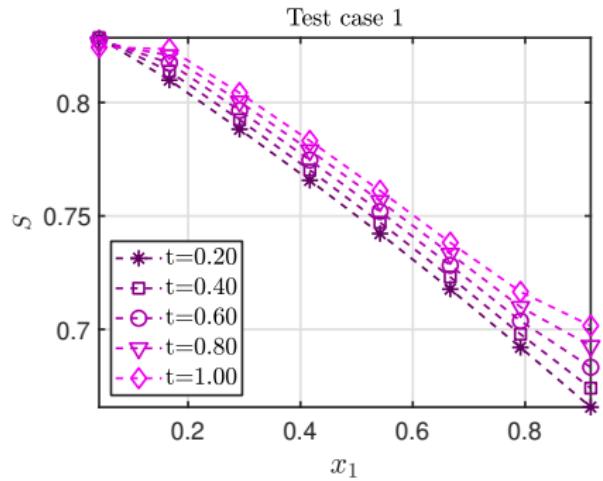
# Changes in concentration



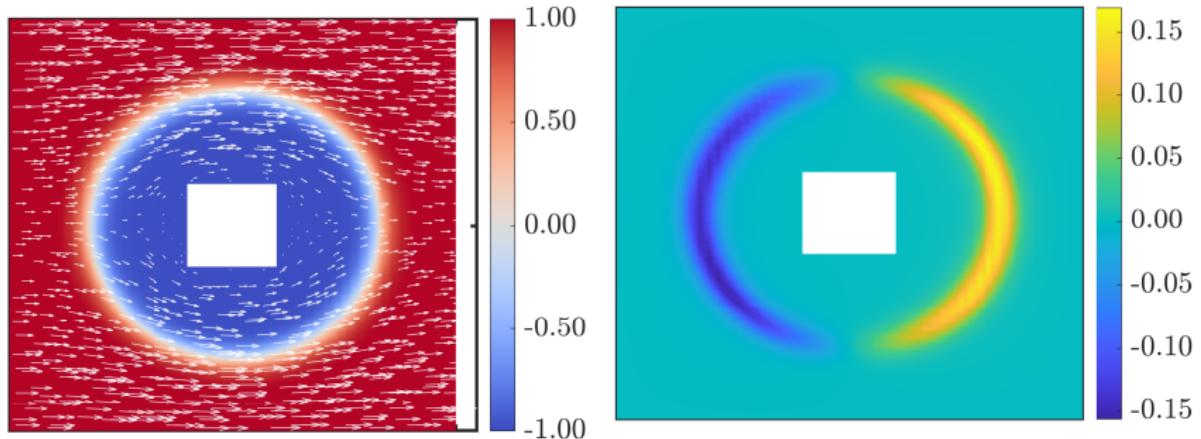
The changes in the concentration in space and the evolution of the concentration at one macro-scale point (test 2).

# Changes in Saturation

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



## The micro-scale phase field



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

## Conclusions and future work

- ✓ Periodic homogenization for a two-phase flow model with evolving interfaces.
- ✓ Rational derivation of the upscaled model from a pore-scale model.
- ✓ Darcy type laws involving effective parameters.
- ✓ Two-scale numerical solution for two-phase flow.

## Conclusions and future work

- ✓ Periodic homogenization for a two-phase flow model with evolving interfaces.
  - ✓ Rational derivation of the upscaled model from a pore-scale model.
  - ✓ 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!

