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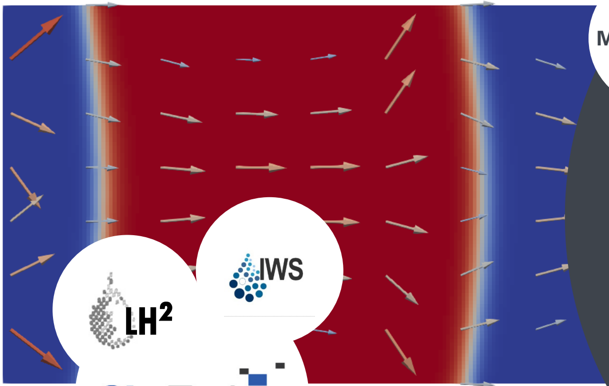


Mathis Kelm

Upscaling of phase-field models for two-phase flow based on fluid morphology

Structure

Introduction

1

Motivation

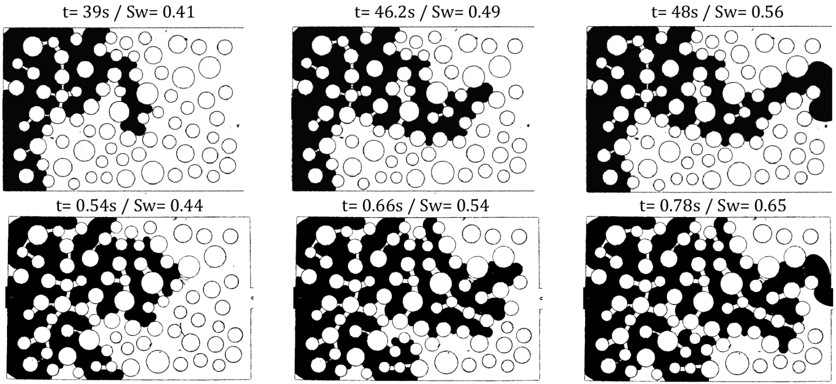
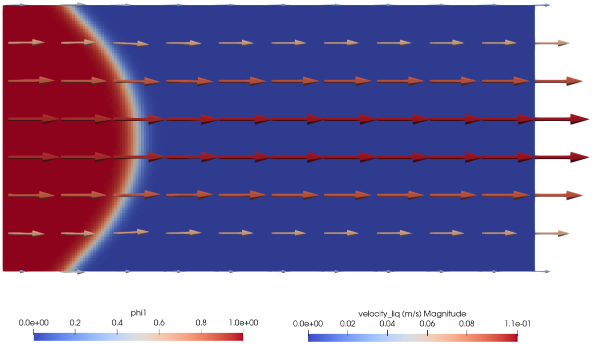


Figure: Fluid distribution in microfluidic experiments under different flow rates*.

*Yiotis, A., Karadimitriou, N. K., Zarikos, I., and Steeb, H. (Feb, 2021) Pore-scale effects during the transition from capillary- to viscosity-dominated flow dynamics within microfluidic porous-like domains. Scientific Reports, 11(1), 3891.

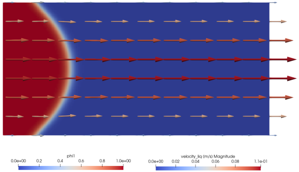
Model scope

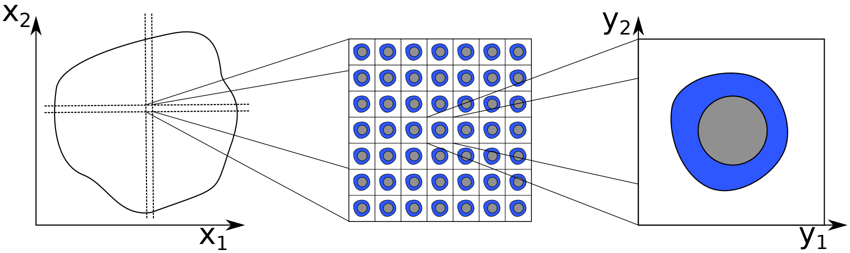
- Formulate diffuse-interface models at pore-scale capturing fluid distribution and interfacial effects



Model scope

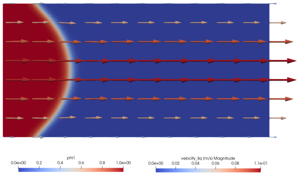
- Formulate diffuse-interface models at pore-scale capturing fluid distribution and interfacial effects
- Derive two-scale model through periodic homogenization

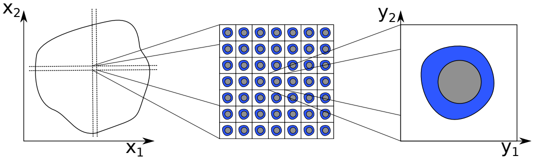


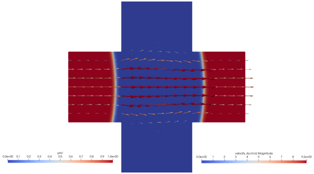


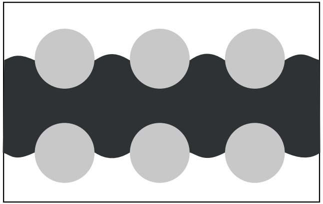
Model scope

- Formulate diffuse-interface models at pore-scale capturing fluid distribution and interfacial effects
- Derive two-scale model through periodic homogenization
- Implement pore-scale solver and couple to macro-scale model
- Relate effective parameters to the local phase distribution and idealised fluid morphologies







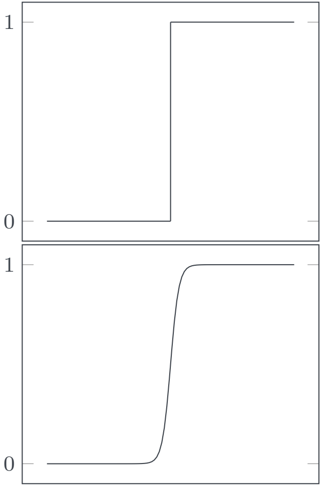


Modeling concepts

2

Diffuse interface approach

- Approximates characteristic functions with smooth phase-field functions
- Allows for a diffuse transition zone between phases
- Defines a unified model for the combined domain
- Interface conditions are captured by additional volume terms
- Implicitly captures topology changes
- Eases upscaling process



Allen-Cahn Navier-Stokes model

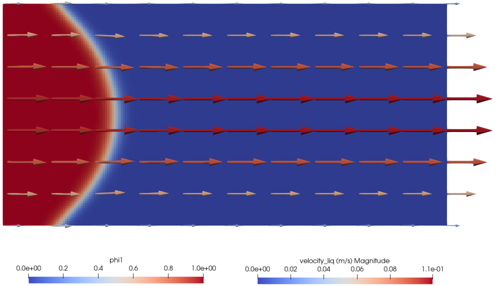
$$\partial_t \phi + \nabla \cdot (\vec{v}\phi) = m(\nabla^2\phi - \xi^{-2}P'(\phi)) \qquad \text{in } \Omega\,, \qquad (1a)$$

$$P(\phi) = 8\phi^2(1-\phi)^2\,, \qquad (1b)$$

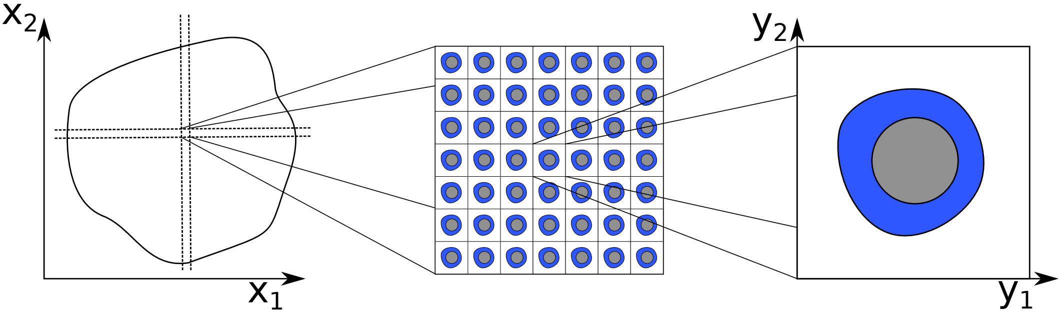
$$\partial_t(\rho(\phi)\vec{v}) + \nabla \cdot (\rho(\phi)\vec{v} \otimes \vec{v}) = -\nabla p - \nabla \cdot \tau(\phi, \vec{v}) - \frac{3}{2}\xi\gamma\nabla \cdot (\nabla\phi \otimes \nabla\phi) \qquad \text{in } \Omega\,, \qquad (1c)$$

$$\partial_t \rho(\phi) + \nabla \cdot (\rho(\phi)\vec{v}) = 0 \qquad \text{in } \Omega\,. \qquad (1d)$$

- Width of diffuse transition zone controlled by $\xi > 0$
- Evolution governed by phase-field mobility $m > 0$
- Second order nonlinear phase-field equation
- Compressible (Navier-)Stokes equation
- Tightly coupled through advection, density, viscosity and surface tension flux



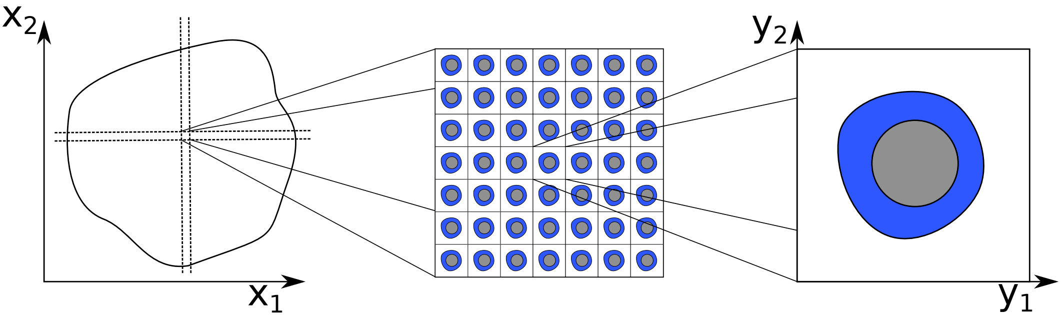
Periodic homogenization



- Two characteristic length scales $l < L$
- Scale separation $\epsilon = l/L \ll 1$
- Coordinates for slow (x) and fast (y) spatial variability
- Represent porous medium with periodic arrangement of decoupled micro-scale cells ϵY
- Assume asymptotic expansion in ϵ with periodicity in y

$$\phi(x) = \phi_0(x, y) + \epsilon\phi_1(x, y) + \epsilon^2\phi_2(x, y) + \dots \tag{2}$$

Periodic homogenization



- Non-dimensionalized model
- Flow regime affects scaling of dimensionless numbers
- Match leading order terms
- Cell-problems account for local phase-distribution and yield effective parameters
- Macro-scale equations using parameters informed by pore-scale behaviour
- Nonlinear phase-field cell-problems

Upscaling Results

3

Pore-scale model

- Constant fluid properties ρ_1, μ_1 and ρ_2, μ_2
- Mixture properties $\rho(\phi) = \rho_2 + \phi(\rho_1 - \rho_2)$, $\mu(\phi) = \mu_2 + \phi(\mu_1 - \mu_2)$

Phase-field model with slip length $\lambda > 0$ and contact angle θ

$$\partial_t \phi + \nabla \cdot (\vec{v}\phi) = m(\nabla^2 \phi - \xi^{-2} P'(\phi)) \quad \text{in } \Omega\,, \tag{3a}$$

$$\partial_t(\rho(\phi)\vec{v}) + \nabla \cdot (\rho(\phi)\vec{v} \otimes \vec{v}) = -\nabla p - \nabla \cdot \tau(\phi, \vec{v}) - \frac{3}{2}\xi\gamma\nabla \cdot (\nabla\phi \otimes \nabla\phi) \quad \text{in } \Omega\,, \tag{3b}$$

$$\partial_t \rho(\phi) + \nabla \cdot (\rho(\phi)\vec{v}) = 0 \quad \text{in } \Omega\,, \tag{3c}$$

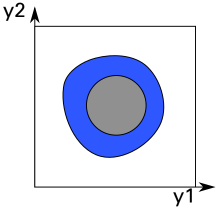
$$\nabla\phi \cdot \vec{n} = -\frac{4}{\xi}\phi(1-\phi)\cos(\theta) \quad \text{on } \partial\Omega\,, \tag{3d}$$

$$\vec{v} \cdot \vec{n} = 0 \quad \text{on } \partial\Omega\,, \tag{3e}$$

$$\nabla v_t \cdot \vec{n} = -\frac{1}{\lambda} v_t \quad \text{on } \partial\Omega\,, \tag{3f}$$

$$p = p_D \quad \text{on } \partial\Omega\,. \tag{3g}$$

Two-scale model: Cell-problems



Using $\mathrm{Eu} = \epsilon^{-2}\overline{\mathrm{Eu}} \in \mathcal{O}(\epsilon^{-2})$, $\mathrm{Pe} \in \mathcal{O}(\epsilon^{0})$ and $m = \epsilon^{-1}\bar{m} \in \mathcal{O}(\epsilon^{-1})$
Cell-Problems for reference cells $Y = [0,1]^2 = \mathcal{P} \cup \mathcal{G} \cup \partial\mathcal{G}$

$$\begin{cases} \nabla_y \cdot (\vec{v}_0\phi_0) = \bar{m}\nabla_y^2\phi_0 - \bar{m}\xi^{-2}P'(\phi_0) & \text{in } \mathcal{P}\,, \\ \nabla_y\phi_0 \cdot \vec{n} = 0 & \text{on } \partial\mathcal{G}\,, \\ \phi_0 \text{ is } Y\text{-periodic and } \int_{\mathcal{P}} \phi_0 = \Phi S^{(1)}\,, \end{cases} \tag{4}$$

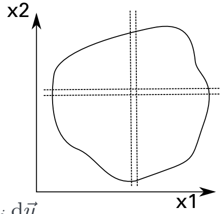
as well as

$$\begin{cases} \overline{\mathrm{Eu}}(e_j + \nabla_y\Pi_j) = \frac{1}{\mathrm{Re}}\nabla_y \cdot \tau(\phi_0, \vec{w}_j), & \text{in } \mathcal{P}\,, \\ \nabla_y \cdot (\phi_0\vec{w}_j) = 0, & \text{in } \mathcal{P}\,, \\ \vec{w}_j = -\lambda(\partial v_t/\partial n)\vec{t}, & \text{on } \partial\mathcal{G}\,, \\ \Pi_j, \vec{w}_j \text{ are } Y\text{-periodic and } \int_{\mathcal{P}} \Pi_j \,\mathrm{d}\vec{y} = 0, \end{cases} \tag{5}$$

for $j \in \{1, \ldots, d\}$ and

$$\begin{cases} \nabla_y\Pi_0 = \nabla_y \cdot \tau(\phi_0, \vec{w}_0) - \frac{1}{\mathrm{ReCa}}\frac{3\xi}{2}\nabla_y \cdot (\nabla_y\phi_0 \otimes \nabla_y\phi_0), & \text{in } \mathcal{P}\,, \\ \nabla_y \cdot (\phi_0\vec{w}_0) = 0, & \text{in } \mathcal{P}\,, \\ \vec{w}_0 = -\lambda(\partial v_t/\partial n)\vec{t}, & \text{on } \partial\mathcal{G}\,, \\ \Pi_0, \vec{w}_0 \text{ are } Y\text{-periodic and } \int_{\mathcal{P}} \Pi_0 \,\mathrm{d}\vec{y} = 0\,. \end{cases} \tag{6}$$

Two-scale model: Macro-scale flow



Effective parameters

$$\mathbf{K}_{ij}^{(1)} = \int_{\mathcal{P}} \phi_0 (\vec{w}_j)_i \, \mathrm{d}\vec{y} \,, \qquad \mathbf{M}_i^{(1)} = \int_{\mathcal{P}} \phi_0 (\vec{w}_0)_i \, \mathrm{d}\vec{y} \,,$$
$$\mathbf{K}_{ij}^{(2)} = \int_{\mathcal{P}} (1-\phi_0) (\vec{w}_j)_i \, \mathrm{d}\vec{y} \,, \quad \mathbf{M}_i^{(2)} = \int_{\mathcal{P}} (1-\phi_0) (\vec{w}_0)_i \, \mathrm{d}\vec{y} \tag{7}$$

Macro-scale equations ($i = 1, 2$)

$$\bar{v}^{(i)} = \mathbf{K}^{(i)} \nabla_x p_0 + \mathbf{M}^{(i)} \,, \tag{8a}$$
$$0 = \Phi \partial_t S^{(i)} + \nabla_x \cdot \bar{v}^{(i)} \tag{8b}$$

Reconstructed pore-scale velocity

$$\vec{v}_0 = \sum_{j=1}^{d} \vec{w}_j \partial_{x_j} p_0 + \vec{w}_0 \tag{9}$$

Numerical Simulations

4

Numerical implementation

- Implemented in DuMu^{X}*
- Discretized using implicit Euler and finite volume method
- Momentum equations discretized using a staggered grid
- Shifted control volumes for each velocity component
- Degrees of freedom placed at faces of original finite volume faces
- Discretization of surface tension flux requires enlarged stencil

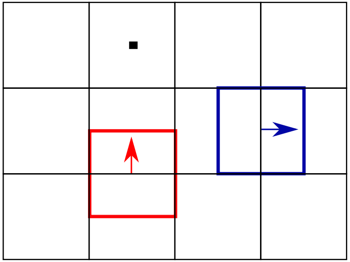


Figure: Sketch of staggered discretization scheme.

*T. Koch, D. Gläser, K. Weishaupt, et al., Dumux 3 - an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling, *Computers & Mathematics with Applications*, vol. 81, pp. 423-443, 2021.

Two-phase flow

Distribution of two fluid phases, surface tension of advected interface alters flow-field

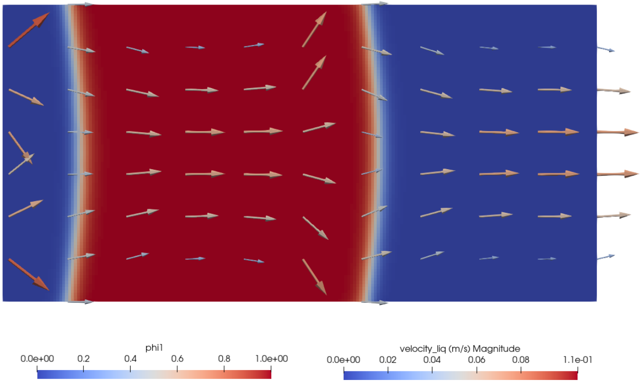


Figure: Simulation of two-phase flow in a capillary.

Pore throat and bodies

Two-phase flow through a throat connecting two pore bodies

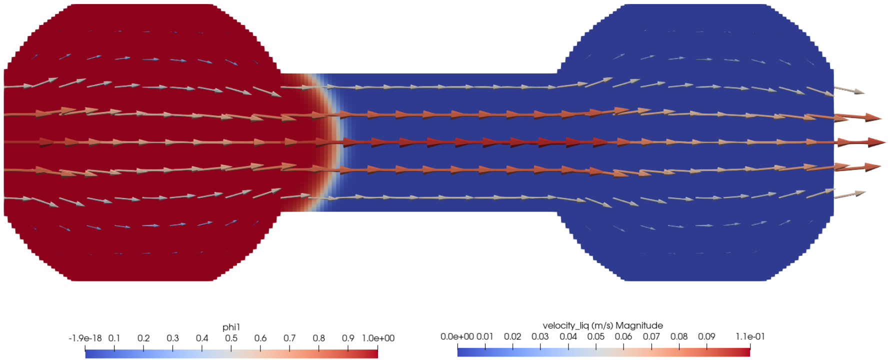


Figure: Simulation of flow through a pore throat.

Cell problems

Preliminary results for cell-problem simulations with periodic boundary conditions

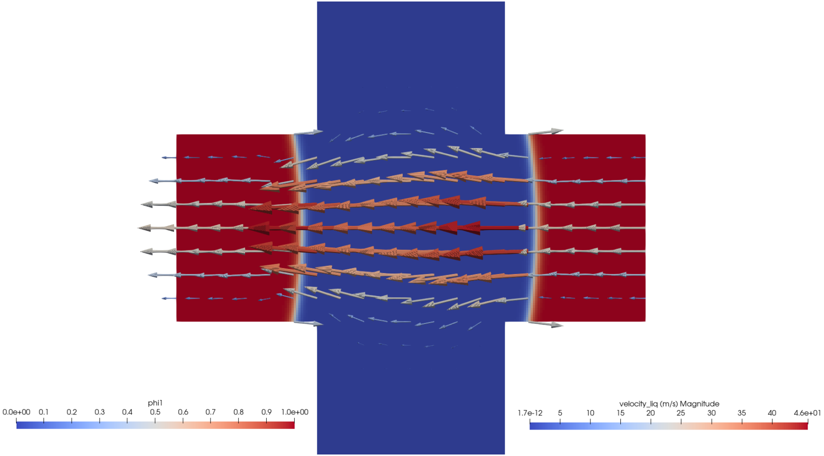


Figure: Interface-driven velocity w_0.

Cell problems

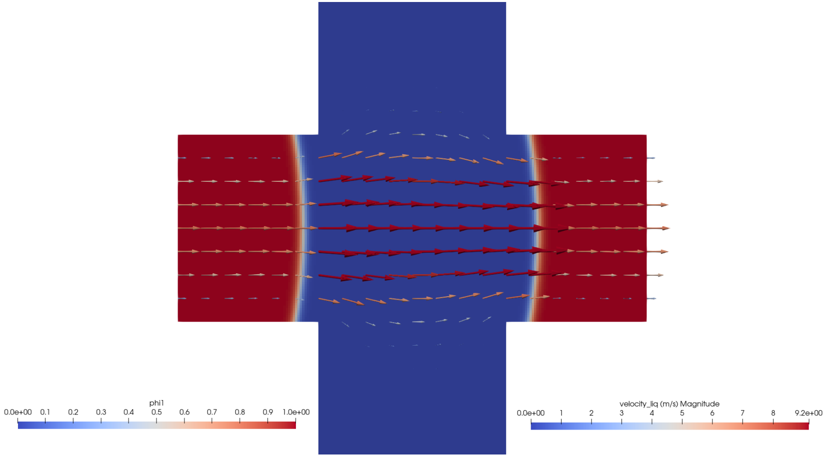


Figure: Pressure-driven velocity w_1.

Cell problems

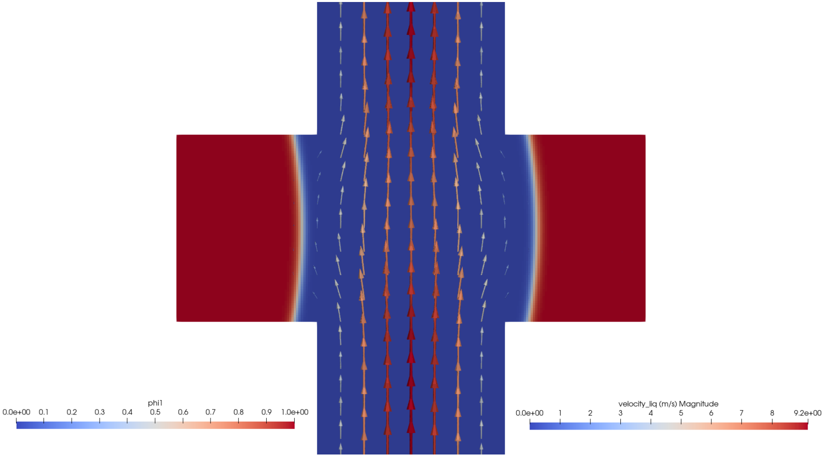


Figure: Pressure-driven velocity w_2.

Summary and Outlook

5

Summary and outlook

- Pore-scale Allen-Cahn Navier-Stokes model captures interfacial interactions
- Periodic homogenization incorporates micro-scale fluid morphology and interface effects through decoupled cell-problems
- Implementation of fully coupled pore-scale model and cell-problems in DuMu^X

- Investigate relation between effective parameters and phase distribution/saturation
- Prescribe meaningful solutions to phase-field cell-problems
- Adapt upscaling to fluid morphology
- Solve two-scale problem using coupling library preCICE

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Thank You!

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