Diffuse interface models and their application in float forming

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Joint work with
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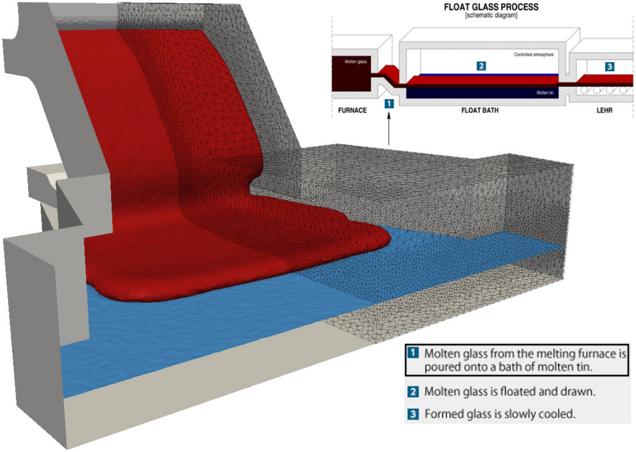
Outline

Target application

Float glass process (Pilkington process)

- standard industrial scale process for making flat glass



Multiphase flows: General concepts

Description

Simultaneous flow of materials with different

- states or phases (gas, liquid or solid)
- **chemical properties but in the same state or phase** (oil and water)

Source: photographyblogger.net/18-interesting-pictures-of-oil-in-water/

Occurrence

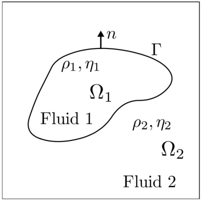
Industrial applications including

- **production of glass**, oil or gas
- food processing
- disposal of nuclear waste

Multiphase flows: Specific setting

Target

Several **immiscible (incompressible) fluids** in a **fixed domain**



Source: Junseok Kim. Phase-field models for multi-component fluid flows. *Commun. Comput. Phys.*, 12(3):613–661, 2012

Modelling approaches

1. Sharp interface (SI) approach:
   intuitive derivation vs. explicit interface tracking
2. Diffuse interface (DI) approach:
   implicit interface tracking vs. computational demands (HPC)

Theoretical issues accompanying DI approach

Variants of DI models

- matching material densities $\left\{ Model - H \right.$ ✓
- different material densities $\left\{ \begin{array}{l} Model - J \\ Model - U \\ Model - N \\ Model - G \\ Model - L \\ Model - E \end{array} \right.$

P. C. Hohenberg and B. I. Halperin. Theory of dynamic critical phenomena. *Rev. Mod. Phys.*, 49:435–479, Jul 1977

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Practical issues accompanying DI approach

1. Simulations with real parameter values
2. Development of efficient numerical algorithms

   David Kay and Richard Welford. Efficient numerical solution of Cahn-Hilliard-Navier-Stokes fluids in 2D.
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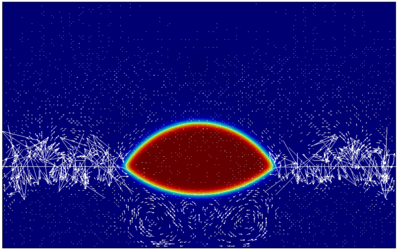
3. Development of multiphase *do-nothing* boundary condition, etc.



$\varrho_g \sim 10^3$ $\quad$ $\varrho_t \sim 10^3$ $\quad$ $\varrho_a \sim 10^0$

$\nu_g \sim 10^2$ $\quad$ $\nu_t \sim 10^{-4}$ $\quad$ $\nu_a \sim 10^{-5}$

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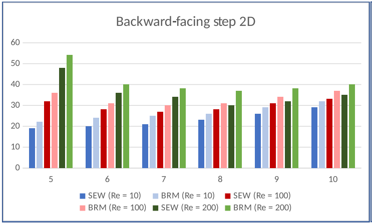

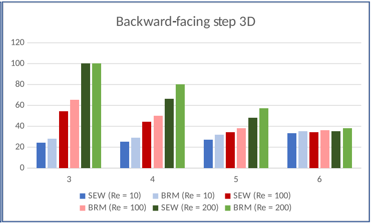

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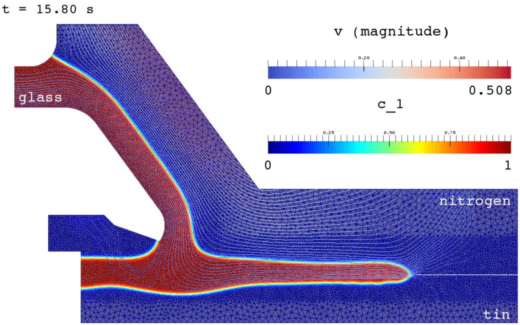

Outline

Description of the physical system

Candidates for phase field variables

- Mass fractions $c_i \approx \frac{M_i}{M} \in [0, 1]$ assuming that $M = M_1 + \ldots + M_N$
- **Volume fractions** $\phi_i \approx \frac{V_i}{V} \in [0, 1]$ assuming that $V = V_1 + \ldots + V_N$
- Partial densities $\varrho_i = \varrho c_i = \hat{\varrho}_i \phi_i$, where $\hat{\varrho}_i$ are **constants**

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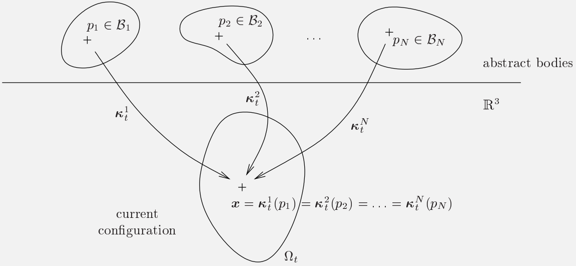
Assumption of co-occupancy



Balance equations: Individual mass balance

- Balance of mass for the i-th constituent reads

$$\frac{\partial \varrho_i}{\partial t} + \operatorname{div}(\varrho_i \boldsymbol{v}_i) = 0 \tag{1}$$

- Let $\boldsymbol{v}$ is an averaged velocity for the mixture as a whole, then

$$\frac{\partial \varrho_i}{\partial t} + \operatorname{div}(\varrho_i \boldsymbol{v}) = -\operatorname{div} \boldsymbol{\jmath}_i, \tag{2}$$

where $\boldsymbol{\jmath}_i = \varrho_i(\boldsymbol{v}_i - \boldsymbol{v})$ denotes the **diffusive mass flux**.

- The same equation in terms of mass/volume fractions read

$$\varrho \frac{\mathrm{d} c_i}{\mathrm{d} t} + c_i \left(\frac{\mathrm{d} \varrho}{\mathrm{d} t} + \varrho \operatorname{div} \boldsymbol{v} \right) = -\operatorname{div} \boldsymbol{\jmath}_i, \tag{3}$$

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$$\operatorname{div} \boldsymbol{v} = -\operatorname{div} \widetilde{\boldsymbol{J}}, \qquad \widetilde{\boldsymbol{J}} = \sum_{i=1}^{N} \widetilde{\boldsymbol{\jmath}}_i \tag{6}$$

- **Mass averaged** velocity

$$\boldsymbol{v}^{\mathrm{m}} \stackrel{\mathrm{def}}{=} \frac{1}{\varrho} \sum_{i=1}^{N} \varrho_i \boldsymbol{v}_i$$

leads to $\boldsymbol{J} = \boldsymbol{0}$, but generally $\widetilde{\boldsymbol{J}} \neq \boldsymbol{0}$.

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Balance equations

Other balance equations [$v = v^{\mathrm{m}}$]

Linear momentum	$\varrho \frac{\mathrm{d}^{\mathrm{m}} \boldsymbol{v}^{\mathrm{m}}}{\mathrm{d}t} = \operatorname{div} \mathbb{T}^{\mathrm{m}} + \varrho \boldsymbol{b}$
Angular momentum	$\mathbb{T}^{\mathrm{m}} = \left(\mathbb{T}^{\mathrm{m}}\right)^{\top}$
Total energy	$\varrho \frac{\mathrm{d}^{\mathrm{m}} E^{\mathrm{m}}}{\mathrm{d}t} = \operatorname{div} \left(\left(\mathbb{T}^{\mathrm{m}}\right)^{\top} \boldsymbol{v}^{\mathrm{m}} - \boldsymbol{q}^{\mathrm{m}} \right) + \varrho \boldsymbol{v}^{\mathrm{m}} \cdot \boldsymbol{b} + \sum_{i=1}^{N} \boldsymbol{\jmath}_i^{\mathrm{m}} \cdot \boldsymbol{b}_i + \varrho q$
Internal energy	$\varrho \frac{\mathrm{d}^{\mathrm{m}} e^{\mathrm{m}}}{\mathrm{d}t} = \mathbb{T}^{\mathrm{m}} : \mathbb{D}^{\mathrm{m}} - \operatorname{div} \boldsymbol{q}_e^{\mathrm{m}} + \sum_{i=1}^{N} \boldsymbol{\jmath}_i^{\mathrm{m}} \cdot (\boldsymbol{b}_i - \boldsymbol{b}) + \varrho q$
Entropy	$\varrho \frac{\mathrm{d}^{\mathrm{m}} \eta}{\mathrm{d}t} = -\operatorname{div} \boldsymbol{q}_\eta^{\mathrm{m}} + \varrho s + \xi$

Linear momentum

$$\varrho \frac{\mathrm{d}^{\mathrm{V}} \boldsymbol{v}^{\mathrm{V}}}{\mathrm{d}t} = \operatorname{div} \mathbb{T}^{\mathrm{V}} + \varrho \boldsymbol{b} - \left[\left(\operatorname{div} \boldsymbol{v}^{\mathrm{V}}\right) \mathbb{I} + \nabla \boldsymbol{v}^{\mathrm{V}}\right] \boldsymbol{J}^{\mathrm{V}} - \frac{\mathrm{d}^{\mathrm{V}} \boldsymbol{J}^{\mathrm{V}}}{\mathrm{d}t}$$

Angular momentum

$$\mathbb{T}^{\mathrm{V}} = \left(\mathbb{T}^{\mathrm{V}}\right)^{\top}$$

Total energy

$$\varrho \frac{\mathrm{d}^{\mathrm{V}} E^{\mathrm{V}}}{\mathrm{d}t} = \operatorname{div} \left(\left(\mathbb{T}^{\mathrm{V}}\right)^{\top} \boldsymbol{v}^{\mathrm{V}} - \frac{1}{2} \left|\boldsymbol{v}^{\mathrm{V}}\right|^2 \boldsymbol{J}^{\mathrm{V}} - \boldsymbol{q}^{\mathrm{V}} \right) + E^{\mathrm{V}} \operatorname{div} \boldsymbol{J}^{\mathrm{V}} + \sum_{i=1}^{N} \boldsymbol{\jmath}_i^{\mathrm{V}} \cdot \boldsymbol{b}_i + \varrho q + \boldsymbol{v}^{\mathrm{V}} \cdot \left(\varrho \boldsymbol{b} - \left(\operatorname{div} \boldsymbol{v}^{\mathrm{V}}\right) \boldsymbol{J}^{\mathrm{V}} \right) - \frac{\mathrm{d}(\boldsymbol{v}^{\mathrm{V}} \cdot \boldsymbol{J}^{\mathrm{V}})}{\mathrm{d}t}$$

Internal energy

$$\varrho \frac{\mathrm{d}^{\mathrm{V}} e^{\mathrm{V}}}{\mathrm{d}t} = \mathbb{T}^{\mathrm{V}} : \left(\mathbb{D}^{\mathrm{V}} + \nabla_{\mathrm{sym}} \left(\varrho^{-1} \boldsymbol{J}^{\mathrm{V}} \right) \right) + e^{\mathrm{V}} \operatorname{div} \boldsymbol{J}^{\mathrm{V}} - \operatorname{div} \boldsymbol{q}_e^{\mathrm{V}} + \varrho q + \sum_{i=1}^{N} \boldsymbol{\jmath}_i^{\mathrm{V}} \cdot (\boldsymbol{b}_i - \boldsymbol{b}) + \varrho^{-1} \boldsymbol{J}^{\mathrm{V}} \cdot \left(\left[\left(\operatorname{div} \boldsymbol{v}^{\mathrm{V}}\right) \mathbb{I} + \nabla \boldsymbol{v}^{\mathrm{V}}\right] \boldsymbol{J}^{\mathrm{V}} + \frac{\mathrm{d}^{\mathrm{V}} \boldsymbol{J}^{\mathrm{V}}}{\mathrm{d}t} \right)$$

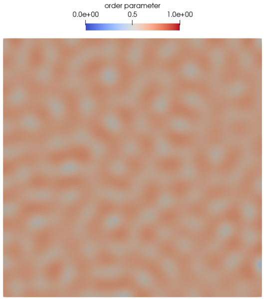
Entropy

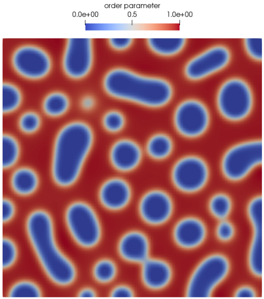
$$\varrho \frac{\mathrm{d}^{\mathrm{V}} \eta}{\mathrm{d}t} = \eta \operatorname{div} \boldsymbol{J}^{\mathrm{V}} - \operatorname{div} \boldsymbol{q}_\eta^{\mathrm{V}} + \varrho s + \xi$$

Thermodynamic considerations

How to ensure separation of phases?

With suitable choice of constitutive assumption for the **free energy**





J. W. Cahn and J. E. Hilliard. Free Energy of a Nonuniform System. I. Interfacial Free Energy. *J. Chem. Phys.*, 28(2):258–267, 1958

Thermodynamic considerations

Naive scenario

Assumption of co-occupancy

+ balance equations (mass, momenta, energy) for all individual phases
+ interaction terms (tricky modeling business)
+ free energy constitutive assumption

→ "complete description"

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Q: "Do we need a sledgehammer to crack a nut?"

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Q: "Do we need a sledgehammer to crack a nut?"

Model reduction

- Neglect *"less important"* interactions (may be difficult to decide)
- Reduce the number of governing equations
  - balance of mass for individual components
  - other balance equations for the mixture as a whole

Thermodynamic considerations

Martin Heida, Josef Málek, and K. R. Rajagopal. On the development and generalizations of Cahn-Hilliard equations within a thermodynamic framework.
Z. Angew. Math. Phys., 63(1):145–169, 2012

Two options:

1. I will bother you with the identification of the entropy production . . .
2.

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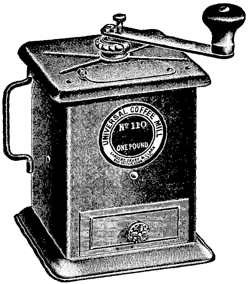

or we will quickly rotate the handle (several turns) ...

Governing equations

...and voilà → system of PDEs for unknowns ϕ, $\boldsymbol{v}$ and p
(as we have used the grinder in the **isothermal setting**)

Incompressible CHNS model

$$\frac{\partial \phi_i}{\partial t} + \mathrm{div}\,(\phi_i \boldsymbol{v}) = \mathrm{div}\,(M_{\mathbf{0}}\,\nabla \chi_i), \quad i = 1, \ldots, N-1,$$

$$\chi_i = \frac{b}{\varepsilon} \sum_{j=1}^{N-1} \ell_{ij} \frac{\partial F}{\partial \phi_j} - \frac{a\varepsilon}{2} \Delta \phi_i, \quad i = 1, \ldots, N-1,$$

$$\mathrm{div}\,\boldsymbol{v} = 0,$$

$$\varrho(\boldsymbol{\phi}) \frac{\partial \boldsymbol{v}}{\partial t} + (\nabla \boldsymbol{v})\,(\varrho(\boldsymbol{\phi})\boldsymbol{v} + \boldsymbol{J}(\nabla \boldsymbol{\chi})) = -\nabla p + \mathrm{div}\,(2\nu(\boldsymbol{\phi})\mathbb{D}) - \frac{a\varepsilon}{2} \sum_{i,j=1}^{N-1} \lambda_{ij}\,\mathrm{div}\,(\nabla \phi_j \otimes \nabla \phi_i) + \varrho(\boldsymbol{\phi})\boldsymbol{b},$$

Helmut Abels, Harald Garcke, and Günther Grün. Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Math. Models Methods Appl. Sci.*, 22(3):1150013, 40, 2012

Franck Boyer and Céline Lapuerta. Study of a three component Cahn-Hilliard flow model. *ESAIM: Mathematical Modelling and Numerical Analysis*, 40:653–687, 7 2006

Governing equations

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Quasi-incompressible CHNS model

$$\frac{\partial \phi_i}{\partial t} + \operatorname{div}(\phi_i \boldsymbol{v}) = \operatorname{div}(M_{\mathbf{0}} \nabla \chi_i), \quad i = 1, \ldots, N-1,$$

$$\chi_i = \frac{b}{\varepsilon} \sum_{j=1}^{N-1} \ell_{ij} \frac{\partial F}{\partial \phi_j} - \frac{a\varepsilon}{2} \Delta \phi_i + \Upsilon(p), \quad i = 1, \ldots, N-1,$$

$$\operatorname{div} \boldsymbol{v} \neq 0,$$

$$\varrho(\boldsymbol{\phi}) \frac{\partial \boldsymbol{v}}{\partial t} + (\nabla \boldsymbol{v})\left(\varrho(\boldsymbol{\phi})\boldsymbol{v} + \boldsymbol{J}(\nabla \boldsymbol{\chi})\right) = -\nabla p + \operatorname{div}(2\nu(\boldsymbol{\phi})\mathbb{D}) - \frac{a\varepsilon}{2} \sum_{i,j=1}^{N-1} \lambda_{ij} \operatorname{div}\left(\nabla \phi_j \otimes \nabla \phi_i\right) + \varrho(\boldsymbol{\phi})\boldsymbol{b},$$

J. Lowengrub and L. Truskinovsky. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. *R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci.*, 454(1978):2617–2654, 1998

Martin Heida, Josef Málek, and K. R. Rajagopal. On the development and generalizations of Cahn-Hilliard equations within a thermodynamic framework. *Z. Angew. Math. Phys.*, 63(1):145–169, 2012

Extension of existing models

How about using the grinder in **non-isothermal setting**?

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$\rightarrow$ appropriate **modification** of the free energy brings us to the following

Temperature equation

$$\varrho(\phi)c_V(\phi)\left(\frac{\partial\vartheta}{\partial t} + \boldsymbol{v}\cdot\nabla\vartheta\right) = 2\nu(\phi)\mathbb{D}:\mathbb{D} + \operatorname{div}\left(\kappa(\phi)\,\nabla\vartheta\right) + \ [\ldots]$$

Martin Řehoř. *Diffuse interface models in theory of interacting continua.*
PhD thesis, Mathematical Institute of Charles University, Czech Republic, in prep. 2017

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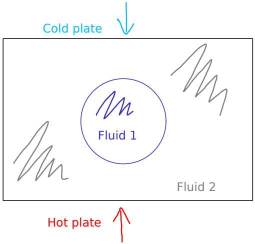

Outline

1. Motivation
2. Diffuse interface models in a unified framework
3. **Computer simulations**

Discretization schemes

Space discretization using FEM

- $\mathbb{P}_{k+1}/\mathbb{P}_k$ to aproximate $\boldsymbol{v}$ and p
- equal order elements to approximate $\boldsymbol{\phi}$ and $\boldsymbol{\chi}$, typically $\mathbb{P}_m$ with $m = k$

Monolithic scheme

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \operatorname{div}\left(\phi_i^{n+\theta}\boldsymbol{v}^{n+\theta}\right) = \operatorname{div}\left(M_0\,\nabla\chi_i^{n+1}\right), \quad i = 1, \ldots, N-1,$$

$$\chi_i^{n+1} = \frac{b}{\varepsilon}\sum_{j=1}^{N-1}\ell_{ij}\boldsymbol{d}_j^F(\boldsymbol{\phi}^{n+1}, \boldsymbol{\phi}^n) - \frac{a\varepsilon}{2}\Delta\phi_i^{n+\theta}, \quad i = 1, \ldots, N-1,$$

$$\operatorname{div}\boldsymbol{v}^{n+\theta} = 0,$$

$$\frac{\varrho^{n+1}\boldsymbol{v}^{n+1} - \varrho^n\boldsymbol{v}^n}{\Delta t} + \operatorname{div}\left(\boldsymbol{v}^{n+\theta}\otimes\left(\varrho^{n+\theta}\boldsymbol{v}^{n+\theta} + \boldsymbol{J}^{n+\theta}\right)\right) = -\nabla p^{n+\theta} + \operatorname{div}\left(2\nu^{n+\theta}\mathbb{D}^{n+\theta}\right) + \boldsymbol{f}_{ca}^{n+\theta} + \varrho^{n+\theta}\boldsymbol{b}^{n+\theta}.$$

$$g^{n+\theta} = g(t^{n+\theta})\theta g(t^n) + (1-\theta)g(t^{n+1})$$

Different levels of decoupling

Semi-decoupled scheme

CH part

$$\frac{\partial \phi_i}{\partial t} + \operatorname{div}(\phi_i \boldsymbol{v}) = \operatorname{div}(M_0 \nabla \chi_i), \quad i = 1, \dots, N-1,$$

$$\chi_i = \frac{b}{\varepsilon} \sum_{j=1}^{N-1} \ell_{ij} \frac{\partial F}{\partial \phi_j} - \frac{a\varepsilon}{2} \Delta \phi_i, \quad i = 1, \dots, N-1,$$

NS part

$$\operatorname{div} \boldsymbol{v} = 0,$$

$$\varrho(\boldsymbol{\phi}) \frac{\partial \boldsymbol{v}}{\partial t} + (\nabla \boldsymbol{v})(\varrho(\boldsymbol{\phi})\boldsymbol{v} + \boldsymbol{J}) = -\nabla p + \operatorname{div}(2\nu(\boldsymbol{\phi})\mathbb{D}) - \frac{a\varepsilon}{2} \sum_{i,j=1}^{N-1} \lambda_{ij} \operatorname{div}(\nabla \phi_j \otimes \nabla \phi_i) + \varrho(\boldsymbol{\phi})\boldsymbol{b},$$

Sebastian Minjeaud. An unconditionally stable uncoupled scheme for a triphasic Cahn-Hilliard/Navier-Stokes model.
Numerical Methods for Partial Differential Equations, 29(2):584–618, 2013

Discretization schemes

Different levels of decoupling

Semi-decoupled scheme vs. Fully-decoupled scheme

CH part

$$\frac{\partial \phi_i}{\partial t} + \operatorname{div}(\phi_i \boldsymbol{v}) = \operatorname{div}(M_0 \nabla \chi_i), \quad i = 1, \dots, N-1,$$

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S. Dong. Wall-bounded multiphase flows of n immiscible incompressible fluids: Consistency and contact-angle boundary condition.
Journal of Computational Physics, 338:21 – 67, 2017

Software tools

- Extensive testing of various models and discretization schemes is required
- Appropriate tool is needed
- **FEniCS** project `<fenicsproject.org>`
  - FEM based solution environment for solving PDEs
  - offers automated code generation → fast prototyping
- **MUFLON**: MUltiphase FLow simulatioN
  - software package build on top of FEniCS
  - developed as part of the thesis

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Convergence tests

Exact (manufactured) solution for $N = 4$ in 2D:

$$
\begin{aligned}
v_1 &= A_0 \sin(ax) \cos(\pi y) \sin(\omega_0 t), \\
v_2 &= -\frac{A_0 a}{\pi} \cos(ax) \sin(\pi y) \sin(\omega_0 t), \\
p &= A_0 \sin(ax) \sin(\pi y) \cos(\omega_0 t), \\
\phi_1 &= \frac{1}{6} \left[1 + A_1 \cos(a_1 x) \cos(b_1 y) \sin(\omega_1 t)\right], \\
\phi_2 &= \frac{1}{6} \left[1 + A_2 \cos(a_2 x) \cos(b_2 y) \sin(\omega_2 t)\right], \\
\phi_3 &= \frac{1}{6} \left[1 + A_3 \cos(a_3 x) \cos(b_3 y) \sin(\omega_3 t)\right].
\end{aligned}
$$

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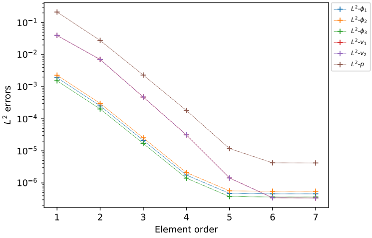
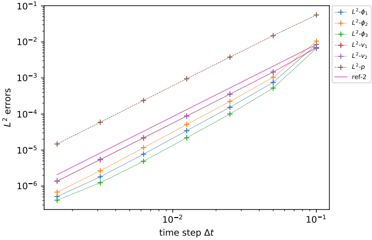
Convergence tests

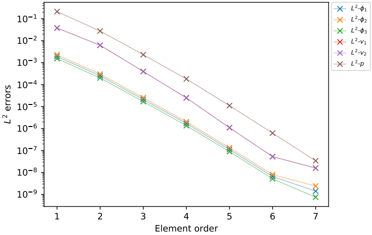
Results for fully-decoupled scheme

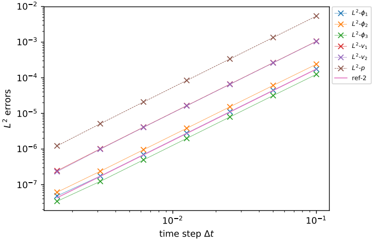




Convergence tests

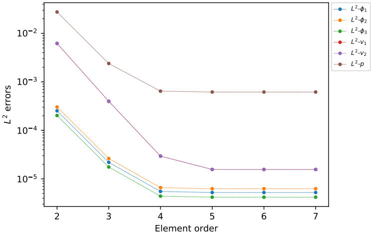
Results for monolithic scheme (with $\theta = \frac{1}{2}$)

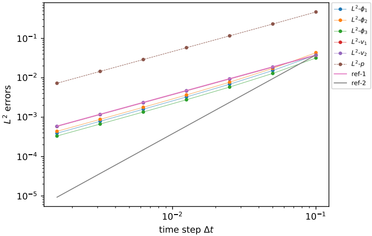




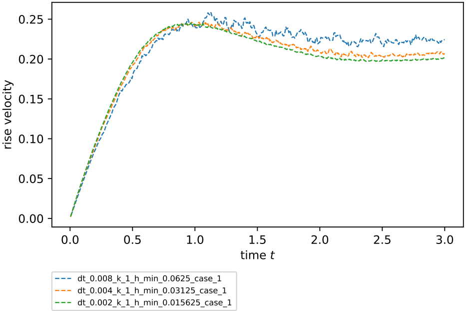
Convergence tests

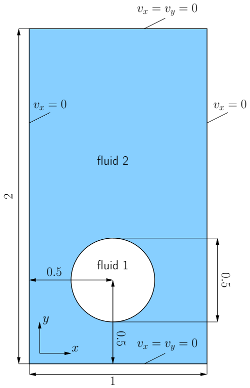
Results for semi-decoupled scheme

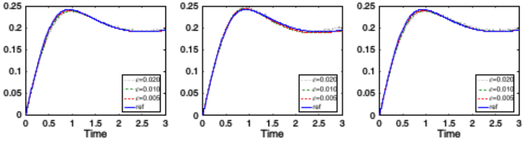




Rising bubble benchmark







S. Aland and A. Voigt. Benchmark computations of diffuse interface models for two-dimensional bubble dynamics.
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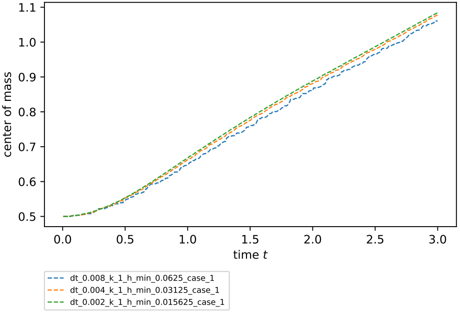
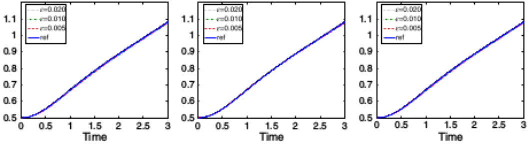
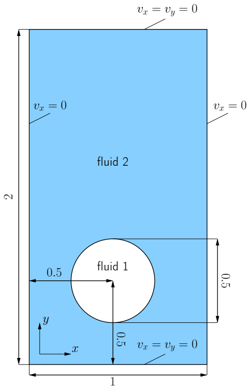
Rising bubble benchmark







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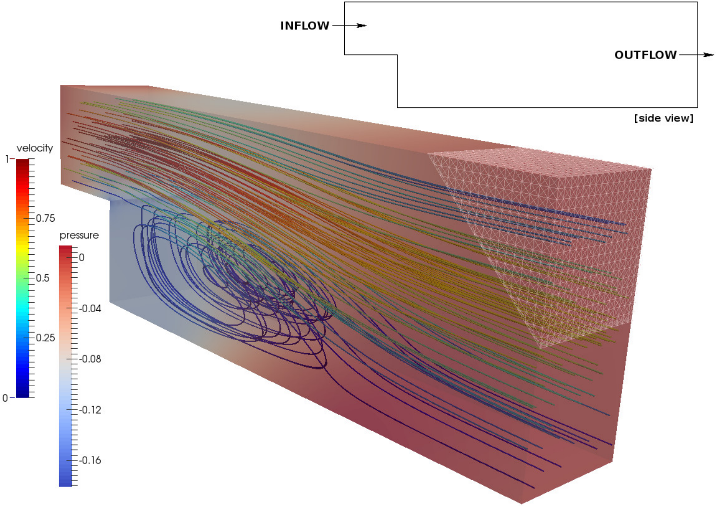
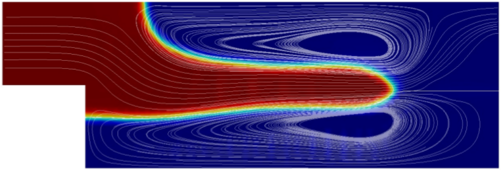
PCD preconditioning

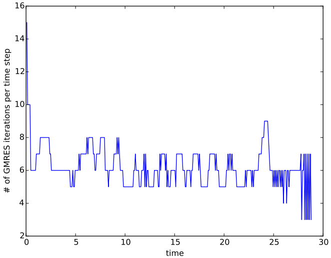


FENaPack: FEniCS Navier-Stokes preconditioning package

MUFLON + FENaPack

- Coefficients ρ and ν are both spatially and time dependent.
- At each time step:
  - Cahn–Hilliard is resolved using MUMPS
  - Oseen type problem is resolved using GMRES with PCD preconditioning



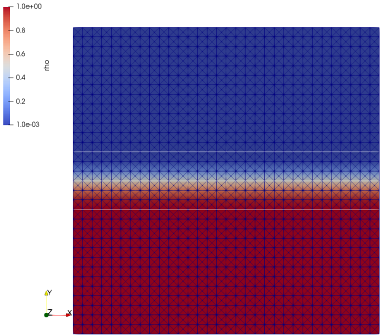


- **Modelling challenges:**
  - Outflow boundary condition for variable density flow.

Spurious velocities

Stationary Stokes equations with variable coefficients

$$-\operatorname{div}(2\nu(\phi)\mathbb{D}) = -\nabla p + \varrho(\phi)\boldsymbol{b},$$
$$\operatorname{div}\boldsymbol{v} = 0.$$



Spurious velocities

Stationary Stokes equations with variable coefficients

$$-\operatorname{div}\left(2\nu(\phi)\mathbb{D}\right) = -\nabla p + \varrho(\phi)\boldsymbol{b},$$
$$\operatorname{div}\boldsymbol{v} = 0.$$

- ϕ is a given function of $r = y - \frac{1}{2}$, namely

$$\phi(r) = \begin{cases} 0, & r \in \left(\frac{\varepsilon}{2}, \frac{1}{2}\right], \\ \frac{1}{2} - \frac{r}{\varepsilon} - \frac{1}{2\pi}\sin\left(\frac{2\pi r}{\varepsilon}\right), & r \in \left[-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right], \\ 1, & r \in \left[-\frac{1}{2}, -\frac{\varepsilon}{2}\right). \end{cases}$$

- $\varrho(\phi) = (\varrho_1 - \varrho_2)\phi + \varrho_2$ with $\varrho_1 \approx 10^3$, $\varrho_2 \approx 1$
- $\nu(\phi) = (\nu_1 - \nu_2)\phi + \nu_2$ with $\nu_1 \approx 10^{-3}$, $\varrho_2 \approx 10^{-5}$
- $\boldsymbol{b} = [0, -g_a]^\top$ is gravitational acceleration with $g_a \approx 10$
- analytic solution: $\boldsymbol{v} = \boldsymbol{0}$, $p = -g_a \int_0^y \varrho(\phi(y' - \frac{1}{2}))\mathrm{d}y'$

Spurious velocities

Stationary Stokes equations with variable coefficients

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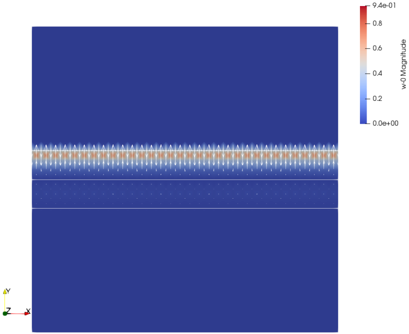

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MOdelling REvisited + MOdel REduction
ERC-CZ project LL1202 - MORE

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