Development of Phase Field Methods using OpenFOAM

Part I: Method Development and Implementation

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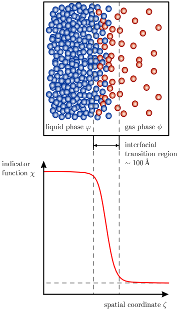
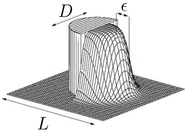
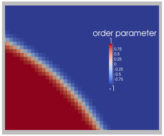
Karlsruhe Institute of Technology

July 02, 2015







10th OpenFOAM Workshop
June 29 – July 2, 2015 in Ann Arbor, Michigan, USA

Center of Smart Interfaces

Introduction & Motivation I

What is coming up?

- **Today's Objectives**

  Executive Overview of

  - **Numerical Modeling**
    (Allen-Cahn and Cahn-Hilliard in unified model framework)
    - Consistent coupling to incompressible two-phase Navier-Stokes equations
    - Enforcement of phase-volume conservation and boundedness (AC)
    - Treatment of moving contact lines
  - **Equation Discretization and Solution**
    - Enforcement of phase-volume conservation and boundedness (CH)
    - Treatment of moving contact lines
  - **Implementation into FOAM**
  - **Numerical Results**
    - Validation & Verification
    - Wetting Physics (Xuan Cai, KIT Karlsruhe)

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Sharp vs. Diffuse Interface Modeling

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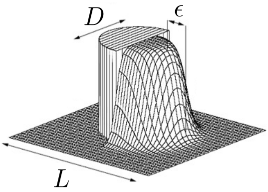
- **sharp interface models**
  - surface of zero thickness
  - discontinuity/jump of material and transport quantities
  - discontinuous phase indicator
  - methods (main representatives): Volume-Of-Fluid / Level-Set Interface-Capturing, Arbitrary Lagrangian Eulerian Interface-Tracking, Front-Tracking Methods
- **diffuse interface models**
  - surface of finite thickness
  - smooth but rapid transition of material and transport quantities
  - smooth phase indicator
  - methods (main representatives): Phase-Field Interface-Capturing Methods



Introduction & Motivation II

Sharp vs. Diffuse Interface Modeling

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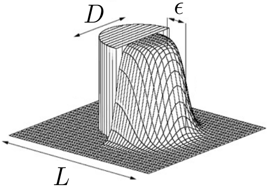

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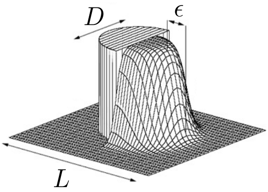

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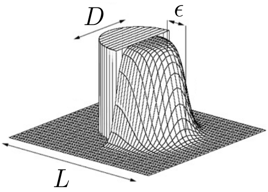

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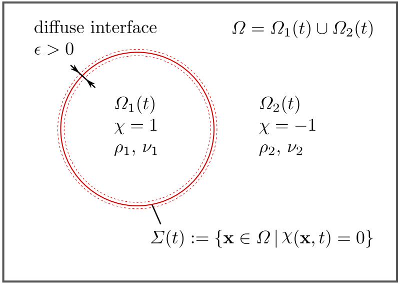

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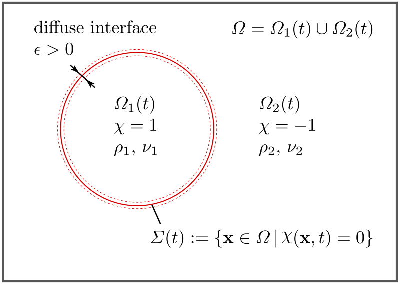
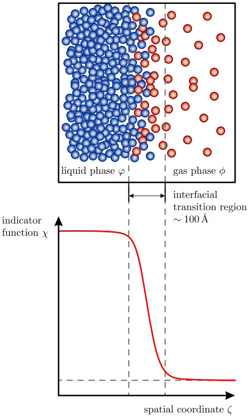


Introduction & Motivation III

Diffuse Interface Models – Characteristics

- **Phase-field methods** rely on **diffuse interface models**
  - connection to thermodynamics by a phenomenological free energy functional (model).
  - evolution of phase field governed by dissipative minimization of free energy.
- **Diffuse interface** represented as a finite thickness transition layer
  - characterized by capillary width $\epsilon > 0$ (related to interfacial thickness)
  - diffusion of phase constituents within thin transition layer
  - fluid mixing (even for immiscible fluids) and interface evolution controlled by chemical potential
  - fluid properties vary rapidly but smoothly between fluids
- **Phase-field methods for two-phase flow**
  - pioneering work: Jacqmin [1]
  - two 'flavors': Cahn-Hilliard [2] or Allen-Cahn [3]



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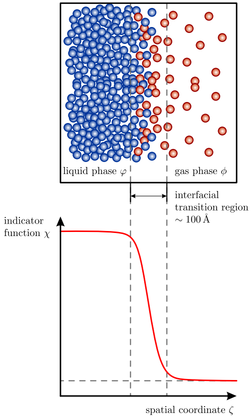

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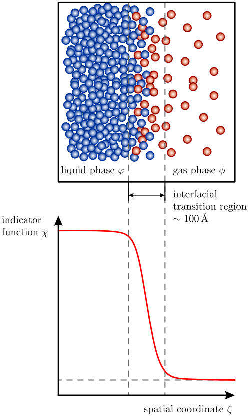

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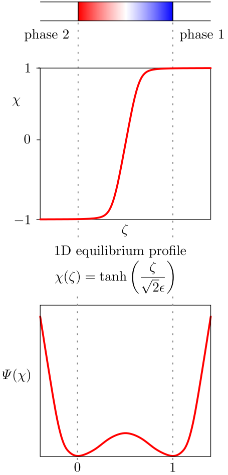
Introduction & Motivation IV

Diffuse Interface Models – Characteristics

- **Free energy**
  Free energy density model for mixing of the two-phase system

$$f(\chi) = \underbrace{\frac{\lambda}{2}|\nabla\chi|^2}_{\text{'gradient energy'}} + \underbrace{\frac{\lambda}{\epsilon^2}\Psi(\chi)}_{\text{bulk energy}}$$

  where
  - $\Psi(\chi) = (\chi^2 - 1)^2/4$: bulk energy density (Ginzburg-Landau double-well functional)
  - $\Psi'(\chi) = \chi(\chi^2 - 1)$: derivative of Ψ w.r.t. χ
  - $\Phi(\chi) = \delta F/\delta\chi$, with $F = \int_\Omega f\,d\mathbf{x}$: **chemical potential** (Cahn, 1961)
- Competition between bulk and capillary/interfacial (gradient) contribution 'controlling' surface tension and interfacial thickness.



Introduction & Motivation V

Diffuse Interface Models – Model Parameters

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- **Input model parameters** (primary parameters)
  - capillary width: ϵ
  - mobility coefficient: κ
  - viscosities and densities: $\overline{\rho}^{\varphi}$, $\overline{\nu}^{\varphi}$
  - surface tension coefficient: σ
- **Derived model parameters** (secondary parameters)
  - mixing energy parameter: $\lambda = \frac{3}{2\sqrt{2}}\sigma\epsilon.$
  - relaxation time parameter: $\gamma = \frac{\lambda\kappa}{\epsilon^2}.$

```
/*--------------------------------------------------------------------------*\
| =========                 |                                               |
| \\      /  F ield         | foam-extend: Open Source CFD                  |
|  \\    /   O peration     |                                               |
|   \\  /    A nd           | For copyright notice see file Copyright       |
|    \\/     M anipulation  |                                               |
\*--------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      phaseFieldProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

diffuseInterface
{
    //- diffusion interface model
//    type    CahnHilliard;
    type    AllenCahn;

    //- numerical method (CH only)
    method coupled;

    //- interfacial width
    epsilon                 epsilon [ 0 1 0 0 0 0 0 ] 5e-5;

    //- mobility
    kappa                   kappa [ -1 3 1 0 0 0 0 ] 10e-9;

}

// ************************************************************************* //
```

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- Starting Point: Generic structure of the phase-field equation [4,5]

$$\partial_t (\rho \chi) + \nabla\bullet (\rho \chi \mathbf{v} + \mathbf{J}_\chi) = \xi_\chi .$$

  - This can be specified into Allen-Cahn- (AC) or Cahn-Hilliard-type (CH) models via choice of either the production rate ξ_χ or flux $\mathbf{J}_\chi$ being non-zero

    $\mathbf{J}_\chi \neq 0$ and $\xi_\chi = 0$ (CH) and $\mathbf{J}_\chi = 0$ and $\xi_\chi \neq 0$ (AC)
  - Volume-Averaging yields governing equations with $C \equiv \bar{c} := \alpha_2 - \alpha_1$.

[4] W. Dreyer, J. Giesselmann and C. Kraus, *Physica D: Nonlinear Phenomena* 273 (2014).

[5] M. Heida, J. Málek and K.R. Rajagopal, *Z. Angew. Math. Phys.* 63 (2012).

Derivation of Governing Phase-Field Transport Equations

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- Allen-Cahn phase-field equation

$$\partial_t \overline{c} + \nabla\boldsymbol{\cdot} (\overline{c}\,\overline{\mathbf{u}}) = \frac{\lambda\kappa}{\epsilon^2}\nabla^2 \overline{c} - \frac{\lambda\kappa}{\epsilon^4}\Psi'(\overline{c}) \qquad \text{in } \Omega$$

$$\partial_n \overline{c} = -\frac{3}{4\lambda}\cos\theta_e(\overline{c}^{\,2} - 1) \text{ and } \partial_n \Phi = 0 \qquad \text{on } \partial\Omega$$

$$\overline{c}\,\big|_{t=0} = \overline{c}_0 \qquad \text{in } \Omega \text{ at } t = 0$$

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Numerical Modeling I

Derivation of Governing Phase-Field Transport Equations

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- Cahn-Hilliard phase-field equation

$$\partial_t \overline{c} + \nabla\cdot (\overline{c}\, \overline{\mathbf{u}}) = \kappa \nabla^2 \Phi(\overline{c}) \text{ with } \Phi(\overline{c}) = \frac{\lambda}{\epsilon^2}\Psi'(\overline{c}) - \lambda \nabla^2 \overline{c} \qquad \text{in } \Omega$$

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- Cahn-Hilliard momentum equation with (non-standard) relative density flux due to diffusion of components [6,7]

$$\partial_t(\alpha_1\,\overline{\rho}^k) + \nabla\cdot(\alpha_1\,\overline{\rho}^k\,\overline{\mathbf{u}}) = -\nabla\cdot\mathbf{J}_k \quad\Leftrightarrow\quad \partial_t\alpha_1 + \nabla\cdot(\alpha_1\,\overline{\mathbf{u}}) = -\nabla\cdot\left(\frac{\mathbf{J}_k}{\overline{\rho}^k}\right)$$

- From summation of the right equation for $k = 1, 2$, exploiting $\alpha_1 + \alpha_2 \equiv 1$

$$\frac{\mathbf{J}_1}{\overline{\rho}^1} + \frac{\mathbf{J}_2}{\overline{\rho}^2} = 0, \qquad \text{where } \mathbf{J}_k := \alpha_1\,\overline{\rho}^1(\overline{\mathbf{u}}^1 - \overline{\mathbf{u}}) + \overline{\mathbf{J}_\chi}\,,$$

i.e., insisting on volume conservation in the volume-averaged model, the volumetric diffusion fluxes are required to match – in the spirit of Cahn and Hilliard.

- Then, however, from summation of the left equation for $k = 1, 2$, the continuity equation becomes

$$\partial_t\,\overline{\rho} + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}) =: D_t\,\overline{\rho} = -\nabla\cdot(\mathbf{J}_1 + \mathbf{J}_2) \neq 0 \qquad \text{in cases where } \overline{\rho}^1 \neq \overline{\rho}^2$$

[6] H. Abels, H. Garcke and G. Grün, *Math. Models Methods Appl. Sci.* 22/3 (2012).

[7] H. Ding, P.D.M. Spelt and C. Shu, *J. Comput. Phys.* 226 (2007).

Numerical Modeling II

Coupling to Navier-Stokes Equation

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- Cahn-Hilliard momentum equation with (non-standard) relative density flux due to diffusion of components [6,7]

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Numerical Modeling III

Coupling to Navier-Stokes Equation (cont'd)

- Cahn-Hilliard momentum equation with (non-standard) relative density flux due to diffusion of components

- Linear momentum equation (l.h.s.), using $\nabla\cdot\,\overline{\mathbf{u}} = 0$,

$$\partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = \overline{\rho}\,(\partial_t\overline{\mathbf{u}} + \overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}}) - \nabla\cdot\,[\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2)] + (\mathbf{J}_1 + \mathbf{J}_2)\cdot\nabla\,\overline{\mathbf{u}},$$

which allows for an objective [8] momentum flux tensor on r.h.s.

$$\boldsymbol{\sigma} := \tilde{\boldsymbol{\sigma}} + \overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2) = -p\mathbf{I} + \boldsymbol{\tau}$$

- Then,

$$\partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) - \overline{\mathbf{u}}\,[D_t\,\overline{\rho}] = -\nabla p + \nabla\cdot\boldsymbol{\tau} - (\mathbf{J}_1 + \mathbf{J}_2)\cdot\nabla\,\overline{\mathbf{u}}$$

$$\Leftrightarrow\ \partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = -\nabla p + \nabla\cdot\boldsymbol{\tau} - \nabla\cdot\,(\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2))$$

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- Cahn-Hilliard momentum equation with (non-standard) relative density flux due to diffusion of components

- Linear momentum equation (l.h.s.), using $\nabla\cdot\, \overline{\mathbf{u}} = 0$,

$$\partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = \overline{\rho}\,(\partial_t\overline{\mathbf{u}} + \overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}}) - \nabla\cdot\,[\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2)] + (\mathbf{J}_1 + \mathbf{J}_2)\cdot\nabla\overline{\mathbf{u}},$$

which allows for an objective [8] momentum flux tensor on r.h.s.

$$\boldsymbol{\sigma} := \tilde{\boldsymbol{\sigma}} + \overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2) = -p\mathbf{I} + \tau$$

- Then,

$$\partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) - \overline{\mathbf{u}}\,[D_t\,\overline{\rho}] = -\nabla p + \nabla\cdot\tau - (\mathbf{J}_1 + \mathbf{J}_2)\cdot\nabla\overline{\mathbf{u}}$$

$$\Leftrightarrow\ \partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = -\nabla p + \nabla\cdot\tau - \nabla\cdot\,(\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2))$$

[8] H. Abels, H. Garcke and G. Grün, *Math. Models Methods Appl. Sci.* 22/3 (2012).

TECHNISCHE UNIVERSITÄT DARMSTADT

- Cahn-Hilliard momentum equation with (non-standard) relative density flux due to diffusion of components

  - Linear momentum equation (l.h.s.), using $\nabla\cdot\,\overline{\mathbf{u}} = 0$,

$$\partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = \overline{\rho}\,(\partial_t\overline{\mathbf{u}} + \overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}}) - \nabla\cdot\left[\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2)\right] + (\mathbf{J}_1 + \mathbf{J}_2)\cdot\nabla\,\overline{\mathbf{u}},$$

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$$\Leftrightarrow\ \partial_t(\overline{\rho}\,\overline{\mathbf{u}}) + \nabla\cdot(\overline{\rho}\,\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = -\nabla p + \nabla\cdot\tau - \nabla\cdot\left(\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2)\right)$$

[8] H. Abels, H. Garcke and G. Grün, *Math. Models Methods Appl. Sci.* 22/3 (2012).

Enforcement of phase-volume conservation and boundedness (AC)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Allen-Cahn phase-field equation with space-time dependent Lagrange multiplier concept [9] to enforce volume conserving property

$$\partial_t \overline{c} + \nabla\cdot(\overline{c}\,\overline{u}) = \gamma\Delta\overline{c} - \frac{\gamma}{\epsilon^2}\Psi'(\overline{c}) + \lambda(t)\Psi(\overline{c})$$

- Choose λ s.t. phase volumes are conserved, i.e.

$$\begin{aligned}\frac{d}{dt}\int_\Omega \overline{c}\,d\mathbf{x} &= \int_\Omega \partial_t\overline{c}\,d\mathbf{x} = 0\\ &= \int_\Omega \left[-\nabla\cdot(\overline{c}\,\overline{u}) + \gamma\Delta\overline{c} - \frac{\gamma}{\epsilon^2}\Psi'(\overline{c}) + \lambda(t)\Psi(\overline{c})\right] d\mathbf{x}\\ &= -\int_{\partial\Omega}\overline{c}\,\overline{\mathbf{u}}\cdot\mathbf{n}\,ds + \gamma\int_{\partial\Omega}\mathbf{n}\cdot\nabla\overline{c}\,ds - \frac{\gamma}{\epsilon^2}\int_\Omega\Psi'(\overline{c})\,d\mathbf{x} + \lambda(t)\int_\Omega\Psi(\overline{c})\,d\mathbf{x}\end{aligned}$$

$$\Rightarrow \lambda(t) = \frac{\int_{\partial\Omega}[\mathbf{n}\cdot(\overline{\mathbf{u}}\,\overline{c}) - \mathbf{n}\cdot\nabla\overline{c}]\,ds}{\int_\Omega\Psi(\overline{c})\,dx} + \frac{\gamma/\epsilon^2\int_\Omega\Psi'(\overline{c})\,dx}{\int_\Omega\Psi(\overline{c})\,dx}$$

[9] J. Kim, S. Lee and Y. Choi, *Int. J. Eng. Sci.* 84 (2014).

Enforcement of phase-volume conservation and boundedness (AC)

- Allen-Cahn phase-field equation with space-time dependent Lagrange multiplier concept [9] to enforce volume conserving property

$$\partial_t \overline{c} + \nabla\cdot(\overline{c}\,\overline{u}) = \gamma\Delta\overline{c} - \frac{\gamma}{\epsilon^2}\Psi'(\overline{c}) + \lambda(t)\Psi(\overline{c})$$

- Choose λ s.t. phase volumes are conserved, i.e.

$$\frac{d}{dt}\int_\Omega \overline{c}\,d\mathbf{x} = \int_\Omega \partial_t \overline{c}\,d\mathbf{x} = 0$$

$$= \int_\Omega \left[-\nabla\cdot(\overline{c}\,\overline{u}) + \gamma\Delta\overline{c} - \frac{\gamma}{\epsilon^2}\Psi'(\overline{c}) + \lambda(t)\Psi(\overline{c})\right] d\mathbf{x}$$

$$= -\int_{\partial\Omega} \overline{c}\,\overline{\mathbf{u}}\cdot\mathbf{n}\,ds + \gamma\int_{\partial\Omega}\mathbf{n}\cdot\nabla\overline{c}\,ds - \frac{\gamma}{\epsilon^2}\int_\Omega \Psi'(\overline{c})\,d\mathbf{x} + \lambda(t)\int_\Omega \Psi(\overline{c})\,d\mathbf{x}$$

$$\Rightarrow \lambda(t) = \frac{\int_{\partial\Omega}[\mathbf{n}\cdot(\overline{\mathbf{u}}\,\overline{c}) - \mathbf{n}\cdot\nabla\overline{c}]\,ds}{\int_\Omega \Psi(\overline{c})\,d\mathbf{x}} + \frac{\gamma/\epsilon^2\int_\Omega \Psi'(\overline{c})\,d\mathbf{x}}{\int_\Omega \Psi(\overline{c})\,d\mathbf{x}}$$

[9] J. Kim, S. Lee and Y. Choi, *Int. J. Eng. Sci.* 84 (2014).

Numerical Modeling IV

Enforcement of phase-volume conservation and boundedness (AC)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Allen-Cahn phase-field equation with space-time dependent Lagrange multiplier concept [9] to enforce volume conserving property

$$\partial_t \bar{c} + \nabla\bullet(\bar{c}\,\bar{u}) = \gamma\Delta\bar{c} - \frac{\gamma}{\epsilon^2}\Psi'(\bar{c}) + \lambda(t)\Psi(\bar{c})$$

- Choose λ s.t. phase volumes are conserved, i.e.

$$\begin{aligned}\frac{d}{dt}\int_\Omega \bar{c}\,d\mathbf{x} &= \int_\Omega \partial_t\bar{c}\,d\mathbf{x} = 0\\ &= \int_\Omega\left[-\nabla\bullet(\bar{c}\,\bar{u}) + \gamma\Delta\bar{c} - \frac{\gamma}{\epsilon^2}\Psi'(\bar{c}) + \lambda(t)\Psi(\bar{c})\right]d\mathbf{x}\\ &= -\int_{\partial\Omega}\bar{c}\,\bar{\mathbf{u}}\bullet\mathbf{n}\,ds + \gamma\int_{\partial\Omega}\mathbf{n}\bullet\nabla\bar{c}\,ds - \frac{\gamma}{\epsilon^2}\int_\Omega\Psi'(\bar{c})\,d\mathbf{x} + \lambda(t)\int_\Omega\Psi(\bar{c})\,d\mathbf{x}\end{aligned}$$

$$\Rightarrow \lambda(t) = \frac{\int_{\partial\Omega}[\mathbf{n}\bullet(\bar{\mathbf{u}}\,\bar{c}) - \mathbf{n}\bullet\nabla\bar{c}]\,ds}{\int_\Omega\Psi(\bar{c})\,d\mathbf{x}} + \frac{\gamma/\epsilon^2\int_\Omega\Psi'(\bar{c})\,d\mathbf{x}}{\int_\Omega\Psi(\bar{c})\,d\mathbf{x}}$$

[9] J. Kim, S. Lee and Y. Choi, *Int. J. Eng. Sci.* 84 (2014).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- approach: decompose 4th order Cahn-Hilliard phase-field transport equation into 2nd order Helmholtz-type equations and solve simultaneously.
- steps:
  - use FOAM's block-coupled matrix support
  - treat all coupling and transport terms fully implicit
  - reconstruct volumetric fluxes from solution of the block-coupled system
- starting point: semi-(time-)discretized form of Cahn-Hilliard transport equation [10,11]

$$\frac{\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}}{\Delta t} + \nabla\cdot(\overline{c}\,\overline{u})^{o}$$
$$= \kappa\nabla^2\left[-\lambda\nabla^2\,\overline{c}^{\,n} + \frac{\lambda}{\epsilon^2}\left((\overline{c}^{\,o})^2 - 1\right)\,\overline{c}^{\,o} + \gamma_i\frac{\lambda}{\epsilon^2}\left(\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}\right)\right],$$

with the time-discretization dependent parameters $\gamma_n = (1,\ 3/2)$, $\gamma_o = (1,\ 2)$ and $\gamma_{oo} = (0,\ 1/2)$ for Euler implicit and Gear's backward schemes, respectively.

[10] P. Yue et al., *J. Fluid Mech.* 515 (2004).

[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- approach: decompose 4th order Cahn-Hilliard phase-field transport equation into 2nd order Helmholtz-type equations and solve simultaneously.
- steps:
  - use FOAM's block-coupled matrix support
  - treat all coupling and transport terms fully implicit
  - reconstruct volumetric fluxes from solution of the block-coupled system
- starting point: semi-(time-)discretized form of Cahn-Hilliard transport equation [10,11]

$$\frac{\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}}{\Delta t} + \nabla\cdot\left(\overline{c}\,\overline{u}\right)^o$$

$$= \kappa\nabla^2\left[-\lambda\nabla^2\,\overline{c}^{\,n} + \frac{\lambda}{\epsilon^2}\left(\left(\overline{c}^{\,o}\right)^2 - 1\right)\,\overline{c}^{\,o} + \gamma_i\frac{\lambda}{\epsilon^2}\left(\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}\right)\right],$$

with the time-discretization dependent parameters $\gamma_n = (1,\ 3/2)$, $\gamma_o = (1,\ 2)$ and $\gamma_{oo} = (0,\ 1/2)$ for Euler implicit and Gear's backward schemes, respectively.

[10] P. Yue et al., *J. Fluid Mech.* 515 (2004).

[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- approach: decompose 4th order Cahn-Hilliard phase-field transport equation into 2nd order Helmholtz-type equations and solve simultaneously.
- steps:
  - use FOAM's block-coupled matrix support
  - treat all coupling and transport terms fully implicit
  - reconstruct volumetric fluxes from solution of the block-coupled system
- starting point: semi-(time-)discretized form of Cahn-Hilliard transport equation [10,11]

$$\frac{\gamma_n\,\bar{c}^{\,n} - \gamma_o\,\bar{c}^{\,o} + \gamma_{oo}\,\bar{c}^{\,oo}}{\Delta t} + \nabla\bullet\left(\bar{c}\,\bar{u}\right)^o$$

$$= \kappa\nabla^2\left[-\lambda\nabla^2\,\bar{c}^{\,n} + \frac{\lambda}{\epsilon^2}\left((\bar{c}^{\,o})^2 - 1\right)\,\bar{c}^{\,o} + \gamma_i\frac{\lambda}{\epsilon^2}\left(\gamma_n\,\bar{c}^{\,n} - \gamma_o\,\bar{c}^{\,o} + \gamma_{oo}\,\bar{c}^{\,oo}\right)\right],$$

with the time-discretization dependent parameters $\gamma_n = (1,\,3/2)$, $\gamma_o = (1,\,2)$ and $\gamma_{oo} = (0,\,1/2)$ for Euler implicit and Gear's backward schemes, respectively.

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[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- approach: decompose 4th order Cahn-Hilliard phase-field transport equation into 2nd order Helmholtz-type equations and solve simultaneously.
- steps:
  - use FOAM's block-coupled matrix support
  - treat all coupling and transport terms fully implicit
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- starting point: semi-(time-)discretized form of Cahn-Hilliard transport equation [10,11]

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[10] P. Yue et al., *J. Fluid Mech.* 515 (2004).

[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

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  - treat all coupling and transport terms fully implicit
  - reconstruct volumetric fluxes from solution of the block-coupled system
- starting point: semi-(time-)discretized form of Cahn-Hilliard transport equation [10,11]

$$\frac{\gamma_n \, \bar{c}^{\,n} - \gamma_o \, \bar{c}^{\,o} + \gamma_{oo} \, \bar{c}^{\,oo}}{\Delta t} + \nabla \bullet (\bar{c}\, \bar{u})^{o}$$

$$= \kappa \nabla^2 \left[-\lambda \nabla^2 \, \bar{c}^{\,n} + \frac{\lambda}{\epsilon^2} \left((\bar{c}^{\,o})^2 - 1 \right) \bar{c}^{\,o} + \gamma_i \frac{\lambda}{\epsilon^2} \left(\gamma_n \, \bar{c}^{\,n} - \gamma_o \, \bar{c}^{\,o} + \gamma_{oo} \, \bar{c}^{\,oo} \right) \right],$$

with the time-discretization dependent parameters $\gamma_n = (1,\, 3/2)$, $\gamma_o = (1,\, 2)$ and $\gamma_{oo} = (0,\, 1/2)$ for Euler implicit and Gear's backward schemes, respectively.

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[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution I

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

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$$\frac{\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}}{\Delta t} + \nabla\bullet\left(\overline{c}\,\overline{u}\right)^o$$

$$= \kappa\nabla^2\left[-\lambda\nabla^2\,\overline{c}^{\,n} + \frac{\lambda}{\epsilon^2}\left(\left(\overline{c}^{\,o}\right)^2 - 1\right)\,\overline{c}^{\,o} + \gamma_i\frac{\lambda}{\epsilon^2}\left(\gamma_n\,\overline{c}^{\,n} - \gamma_o\,\overline{c}^{\,o} + \gamma_{oo}\,\overline{c}^{\,oo}\right)\right],$$

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[10] P. Yue et al., *J. Fluid Mech.* 515 (2004).

[11] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

Equation Discretization and Solution II

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Sorting: explicit (r.h.s.) and implicit (l.h.s.) terms

$$-\nabla^2\left(\lambda\nabla^2\,\overline{c}^{\,n} - \gamma_i\gamma_n\frac{\lambda}{\epsilon^2}\,\overline{c}^{\,n}\right) - \frac{\gamma_n}{\kappa\Delta t}\,\overline{c}^{\,n} = S_\Psi(\,\overline{c}^{\,o},\,\overline{c}^{\,oo}),$$

where

$$S_\Psi(\,\overline{c}^{\,o},\,\overline{c}^{\,oo}) := \frac{1}{\kappa}\Bigg[-\frac{\gamma_o}{\Delta t}\,\overline{c}^{\,o} + \frac{\gamma_{oo}}{\Delta t}\,\overline{c}^{\,oo} + \nabla\cdot(\,\overline{c}\,\overline{u}\,)^{o} - \frac{\lambda\kappa}{\epsilon^2}\nabla^2\left(((\,\overline{c}^{\,o})^2 - 1 - \gamma_o\gamma_i)\,\overline{c}^{\,o} + \gamma_{oo}\gamma_i\,\overline{c}^{\,oo}\right)\Bigg]$$

- Defining auxiliary variable for separation into two Helmhotz-type equations as

$$\Psi^n := \lambda\nabla^2\,\overline{c}^{\,n} - \gamma_i\gamma_o\frac{\lambda}{\epsilon^2}\,\overline{c}^{\,n},$$

we arrive at

$$\begin{aligned} &\texttt{PsiEqn}: && \nabla^2\,\Psi^{\,n} + \frac{\gamma_o}{\kappa\Delta t}\,\overline{c}^{\,n} = -S_\Psi(\,\overline{c}^{\,o},\,\overline{c}^{\,oo}) \\ &\texttt{CEqn}: && \nabla^2\,\overline{c} - \frac{\Psi^{\,n}}{\lambda} = \frac{\gamma_i\gamma_o}{\epsilon^2}\,\overline{c}^{\,n} \end{aligned}$$

Equation Discretization and Solution II

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Sorting: explicit (r.h.s.) and implicit (l.h.s.) terms

$$-\nabla^2 \left(\lambda \nabla^2 \, \overline{c}^{\,n} - \gamma_i \gamma_n \frac{\lambda}{\epsilon^2} \, \overline{c}^{\,n} \right) - \frac{\gamma_n}{\kappa \Delta t} \, \overline{c}^{\,n} = S_\Psi (\, \overline{c}^{\,o}, \, \overline{c}^{\,oo}),$$

where

$$S_\Psi (\, \overline{c}^{\,o}, \, \overline{c}^{\,oo}) := \frac{1}{\kappa} \Bigg[- \frac{\gamma_o}{\Delta t} \, \overline{c}^{\,o} + \frac{\gamma_{oo}}{\Delta t} \, \overline{c}^{\,oo} + \nabla \cdot (\, \overline{c} \, \overline{u} \,)^{o} - \frac{\lambda \kappa}{\epsilon^2} \nabla^2 \left(((\, \overline{c}^{\,o})^2 - 1 - \gamma_o \gamma_i) \, \overline{c}^{\,o} + \gamma_{oo} \gamma_i \, \overline{c}^{\,oo} \right) \Bigg]$$

- Defining auxiliary variable for separation into two Helmhotz-type equations as

$$\Psi^n := \lambda \nabla^2 \, \overline{c}^{\,n} - \gamma_i \gamma_o \frac{\lambda}{\epsilon^2} \, \overline{c}^{\,n},$$

we arrive at

`PsiEqn` :	$\nabla^2 \, \Psi^{\,n} +$	$\frac{\gamma_o}{\kappa \Delta t} \, \overline{c}^{\,n}$	$= -S_\Psi (\, \overline{c}^{\,o}, \, \overline{c}^{\,oo})$
`CEqn` :	$\nabla^2 \, \overline{c} -$	$\frac{\Psi^{\,n}}{\lambda}$	$= \frac{\gamma_i \gamma_o}{\epsilon^2} \, \overline{c}^{\,n}$

Equation Discretization and Solution III

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Assembling the coupled system
  - improved implicitness compared to Dong [12] and Yue et al. [13] achieved by

$$S'_{\Psi}(\,\bar{c}^{\,o}, \bar{c}^{\,oo}) := \frac{1}{\kappa}\left[-\frac{\gamma_o}{\Delta t}\,\bar{c}^{\,o} + (\gamma_i - 1/\Delta t)\gamma_{oo}\,\bar{c}^{\,oo}\right]$$

  - finite volume notation of final coupled system

$$\left\{\begin{array}{ll} [\![\nabla\cdot(\nabla[\Psi])]\!] & +[\![\frac{\gamma_n}{\kappa\Delta t}\{\bar{c}\}]\!] \\ & +[\![\nabla\cdot\left(\phi\{\bar{c}\}_{f(\phi,\Gamma,\gamma=0.75)}\right)]\!] \\ & +[\![\nabla\cdot\left(\gamma(3\,\bar{c}^{\,2} - 1 - \gamma_i\gamma_o)\nabla\{\bar{c}\}\right)]\!] = -S'_{\Psi} \\ [\![\nabla\cdot(\nabla\{\bar{c}\})]\!] & -[\![\frac{1}{\lambda}[\Psi]]\!] = [\![\frac{\gamma_i\gamma_n}{\epsilon^2}\{\bar{c}\}]\!] \end{array}\right\}$$

[12] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

[13] P. Yue et al., *J. Fluid Mech.* 515 (2004).

Equation Discretization and Solution III

Enforcement of phase-volume conservation and boundedness (CH)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Assembling the coupled system
  - improved implicitness compared to Dong [12] and Yue et al. [13] achieved by

$$S'_\Psi(\bar{c}^{\,o}, \bar{c}^{\,oo}) := \frac{1}{\kappa}\left[-\frac{\gamma_o}{\Delta t}\,\bar{c}^{\,o} + (\gamma_i - 1/\Delta t)\gamma_{oo}\,\bar{c}^{\,oo}\right]$$

  - finite volume notation of final coupled system

$$\left\{\begin{array}{ll} [\![\nabla\cdot(\nabla[\Psi])]\!] & +[\![\frac{\gamma_n}{\kappa\Delta t}\{\bar{c}\}]\!] \\ & +[\![\nabla\cdot\left(\phi\{\bar{c}\}_{f(\phi,\Gamma,\gamma=0.75)}\right)]\!] \\ & +[\![\nabla\cdot\left(\gamma(3\bar{c}^{\,2} - 1 - \gamma_i\gamma_o)\nabla\{\bar{c}\}\right)]\!] = -S'_\Psi \\ [\![\nabla\cdot(\nabla\{\bar{c}\})]\!] & -[\![\frac{1}{\lambda}[\Psi]]\!] = [\![\frac{\gamma_i\gamma_n}{\epsilon^2}\{\bar{c}\}]\!] \end{array}\right\}$$

[12] S. Dong, *Comput. Methods App. Mech. Engrg.* 247–248 (2012).

[13] P. Yue et al., *J. Fluid Mech.* 515 (2004).

Implementation into FOAM I

Class overview and collaboration

- three main (base) classes
  - ▷ `diffuseInterfaceModels` holding `phaseFieldEquations`
  - ▷ `phaseContactAngle` holding `constantPhaseContactAngle` and `dynamicPhaseContactAngle`
  - ▷ `diffuseInterfaceProperties` providing mixture density and viscosity fields as well as derived (secondary) model parameters, i.e. mixing energy and relaxation time parameters
- Client point of view:
  - ▷ Top-Level Solver `phaseFieldFoam`
  - ▷ Dictionary `phaseFieldProperties`

```
-------------------------------------------------------------------------
=========                 |
\\      /  F ield         | foam-extend: Open Source CFD
 \\    /   O peration     |
  \\  /    A nd           | For copyright notice see file Copyright
   \\/     M anipulation  |
-------------------------------------------------------------------------
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      phaseFieldProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

diffuseInterface
{
    //- diffusion interface model
//    type    CahnHilliard;
    type    AllenCahn;

    //- numerical method (CH only)
    method coupled;

    //- interfacial width
    epsilon             epsilon [ 0 1 0 0 0 0 0 ] 5e-5;

    //- mobility
    kappa               kappa [ -1 3 1 0 0 0 0 ] 10e-9;

}

// ************************************************************************
```

Implementation into FOAM II

Top-level: Client/user interface

Temporal Sub-cycling

- needed in segregated mode for solution of Cahn-Hilliard equation (chemical potential as auxiliary quantity):

$$\partial_t \overline{c} + \nabla\cdot(\overline{c}\,\overline{\mathbf{u}}) = \kappa\nabla^2\Phi(\overline{c})$$

with $\Phi(\overline{c}) = \frac{\lambda}{\epsilon^2}\Psi'(\overline{c}) - \lambda\nabla^2\overline{c}$

- mass-flux accumulation yields updated

$$\begin{aligned} F_m &\equiv \alpha_{1,f}\,\overline{\rho}^1 F_1 + \alpha_{2,f}\,\overline{\rho}^2 F_2 \\ &= \left(\frac{1-\overline{c}}{2}\right)_f \overline{\rho}^1 F_1 + \left(\frac{1+\overline{c}}{2}\right)_f \overline{\rho}^2 F_2 \\ &= \frac{\overline{\rho}^2 - \overline{\rho}^1}{2}(\overline{c})_f F_1 + \frac{\overline{\rho}^2 + \overline{\rho}^1}{2} F \end{aligned}$$

for discretized momentum equation (`rhoPhi`). Note: $\alpha_{1,f} F_1 \approx \alpha_{1,f} F$.

implemented as

$$F_{m,\text{sum}} = \sum_{n_\text{asc}} \frac{\Delta t_\text{asc}}{\Delta t_\text{total}} F_{m,\text{asc}},$$

with $\Delta t_\text{asc} \equiv \frac{\Delta t_\text{total}}{n_\text{asc}}$

Implementation into FOAM II

Top-level: Client/user interface

TECHNISCHE UNIVERSITÄT DARMSTADT

Temporal Sub-cycling

- needed in segregated mode for solution of Cahn-Hilliard equation (chemical potential as auxiliary quantity):

  $$\partial_t \overline{c} + \nabla\cdot(\overline{c}\,\overline{\mathbf{u}}) = \kappa\nabla^2\Phi(\overline{c})$$

  with $\Phi(\overline{c}) = \frac{\lambda}{\epsilon^2}\Psi'(\overline{c}) - \lambda\nabla^2\overline{c}$

- mass-flux accumulation yields updated

  $$\begin{aligned} F_m &\equiv \alpha_{1,f}\,\overline{\rho}^1 F_1 + \alpha_{2,f}\,\overline{\rho}^2 F_2 \\ &= \left(\frac{1-\overline{c}}{2}\right)_f \overline{\rho}^1 F_1 + \left(\frac{1+\overline{c}}{2}\right)_f \overline{\rho}^2 F_2 \\ &= \frac{\overline{\rho}^2 - \overline{\rho}^1}{2}(\overline{c})_f F_1 + \frac{\overline{\rho}^2 + \overline{\rho}^1}{2} F \end{aligned}$$

  for discretized momentum equation (`rhoPhi`). Note: $\alpha_{1,f} F_1 \approx \alpha_{1,f} F$.

implemented as

$$F_{m,\text{sum}} = \sum_{n_\text{asc}} \frac{\Delta t_\text{asc}}{\Delta t_\text{total}} F_{m,\text{asc}},$$

with $\Delta t_\text{asc} \equiv \frac{\Delta t_\text{total}}{n_\text{asc}}$

Implementation into FOAM II

Top-level: Client/user interface

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Temporal Sub-cycling

- needed in segregated mode for solution of Cahn-Hilliard equation (chemical potential as auxiliary quantity):

$$\partial_t \overline{c} + \nabla \cdot (\overline{c}\,\overline{\mathbf{u}}) = \kappa \nabla^2 \Phi(\overline{c})$$

with $\Phi(\overline{c}) = \frac{\lambda}{\epsilon^2} \Psi'(\overline{c}) - \lambda \nabla^2 \overline{c}$

- mass-flux accumulation yields updated

$$\begin{aligned} F_m &\equiv \alpha_{1,f}\,\overline{\rho}^1 F_1 + \alpha_{2,f}\,\overline{\rho}^2 F_2 \\ &= \left(\frac{1-\overline{c}}{2}\right)_f \overline{\rho}^1 F_1 + \left(\frac{1+\overline{c}}{2}\right)_f \overline{\rho}^2 F_2 \\ &= \frac{\overline{\rho}^2 - \overline{\rho}^1}{2} (\overline{c})_f F_1 + \frac{\overline{\rho}^2 + \overline{\rho}^1}{2} F \end{aligned}$$

for discretized momentum equation (`rhoPhi`). Note: $\alpha_{1,f} F_1 \approx \alpha_{1,f} F$.

implemented as

$$F_{m,\text{sum}} = \sum_{n_\text{asc}} \frac{\Delta t_\text{asc}}{\Delta t_\text{total}} F_{m,\text{asc}},$$

with $\Delta t_\text{asc} \equiv \frac{\Delta t_\text{total}}{n_\text{asc}}$

`phaseFieldEqn.H`

```
{
    label nSubCycles
    (
        readLabel(piso.lookup("nSubCycles"))
    );

    if (nSubCycles > 1)
    {
        dimensionedScalar totalDeltaT = runTime.deltaT();
        surfaceScalarField rhoPhiSum = 0.0*rhoPhi;

        for
        (
            subCycle<volScalarField> CSubCycle(C, nSubCycles);
            !(++CSubCycle).end();
        )
        {
            // Solve the phase field equation
            // Update and return mass flux field
            rhoPhi = phaseField.solve(C, Phi);
            rhoPhiSum += (runTime.deltaT()/totalDeltaT)*rhoPhi;
        }
        rhoPhi = rhoPhiSum;
    }
    else
    {
        rhoPhi = phaseField.solve(C, Phi);
    }
}

diffuseInterface.updateProperties(rho, mu);
```

Implementation into FOAM III

Top-level: Client/user interface

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- Relative density flux due to diffusion of components (with matching volumetric diffusion fluxes – in the spirit of Cahn and Hilliard) as consequence of solenoidal condition ($\nabla \cdot \mathbf{u} = 0$):

$$\partial_t (\overline{\rho}\ \overline{\mathbf{u}}) + \nabla \cdot (\overline{\rho}\ \overline{\mathbf{u}}\ \overline{\mathbf{u}}) = - \nabla p + \nabla \cdot \tau - \nabla \cdot (\overline{\mathbf{u}} (\mathbf{J}_1 + \mathbf{J}_2))$$

- Consistency of the Allen-Cahn diffuse interface model requires a source term in the pressure equation.

part of UEqn.H

```
surfaceScalarField muf = diffuseInterface.muf();

fvVectorMatrix UEqn
(
    fvm::ddt(rho, U)
  + fvm::div(rhoPhi, U)
  − fvm::laplacian(mu, U)
  − (fvc::grad(U) & fvc::grad(mu))

  //—HM Relative density flux
  //— due to diffusion of components
  //— Abels et al. (arXiv:1011.0528, 2010)
  //— Ding et al. (JCOMP, 226, 2007)
  − phaseField.diffRhoPhi(U)

  //—HM Rhie—Chow interpolation practice
  //— buoyancy and surface tension term
  //— tansferred to pressure equation
);
```

part of pEqn.H

```
for(int nonOrth=0; nonOrth<=nNonOrthCorr; nonOrth++)
{
    fvScalarMatrix pdEqn
    (
        fvm::laplacian(rUAf, pd)
     == fvc::div(phi) + phaseField.massSource(C)
    );

    //[...]
}
```

Implementation into FOAM III

Top-level: Client/user interface

TECHNISCHE UNIVERSITÄT DARMSTADT

- Relative density flux due to diffusion of components (with matching volumetric diffusion fluxes – in the spirit of Cahn and Hilliard) as consequence of solenoidal condition ($\nabla\cdot\mathbf{u} = 0$):

$$\partial_t(\,\overline{\rho}\;\overline{\mathbf{u}}\,) + \nabla\cdot(\,\overline{\rho}\;\overline{\mathbf{u}}\;\overline{\mathbf{u}}\,)$$
$$= -\nabla p + \nabla\cdot\tau - \nabla\cdot\,(\,\overline{\mathbf{u}}\,(\mathbf{J}_1 + \mathbf{J}_2))$$

- Consistency of the Allen-Cahn diffuse interface model requires a source term in the pressure equation.

part of `UEqn.H`

```
surfaceScalarField muf = diffuseInterface.muf();

fvVectorMatrix UEqn
(
    fvm::ddt(rho, U)
  + fvm::div(rhoPhi, U)
  - fvm::laplacian(mu, U)
  - (fvc::grad(U) & fvc::grad(mu))

  //-HM Relative density flux
  //- due to diffusion of components
  //- Abels et al. (arXiv:1011.0528, 2010)
  //- Ding et al. (JCOMP, 226, 2007)
  - phaseField.diffRhoPhi(U)

  //-HM Rhie-Chow interpolation practice
  //- buoyancy and surface tension term
  //- tansferred to pressure equation
);
```

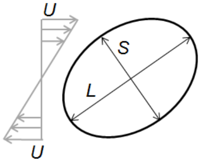
part of `pEqn.H`

```
for(int nonOrth=0; nonOrth<=nNonOrthCorr; nonOrth++)
{
    fvScalarMatrix pdEqn
    (
        fvm::laplacian(rUAf, pd)
     == fvc::div(phi) + phaseField.massSource(C)
    );

    //[...]
}
```

Results: Validation & Verification I

Test case I – Drop deformation in shear flow



$$D = \frac{L - S}{L + S}$$

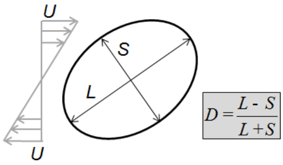
Drop deformation in shear flow

- Analytical solution [14] relates deformation parameter D to Capillary number Ca. (Assumptions: matching ν, ρ and creeping unbounded flow)
- Validation test for implementation of interfacial energy density (surface tension)
- Verification test for phase-volume conservation and boundedness

[14] G.I. Taylor, *Proc. R. Soc. London, Ser. A* 146 (1934).

Results: Validation & Verification I

Test case I – Drop deformation in shear flow



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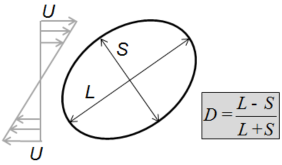

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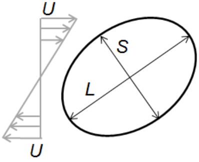
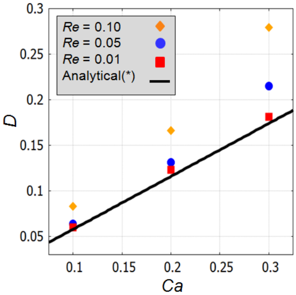
Test case I – Drop deformation in shear flow



$$D = \frac{L - S}{L + S}$$

Drop deformation in shear flow



- Analytical solution [14] relates deformation parameter D to Capillary number Ca. (Assumptions: matching ν, ρ and creeping unbounded flow)
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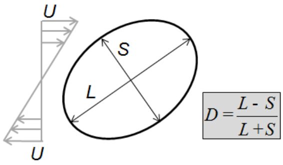
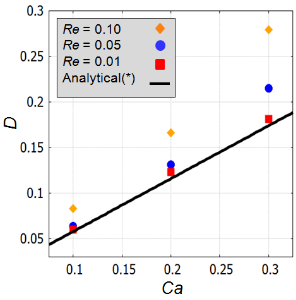
Results: Validation & Verification I

Test case I – Drop deformation in shear flow



Drop deformation in shear flow



- Analytical solution [14] relates deformation parameter D to Capillary number Ca. (Assumptions: matching ν, ρ and creeping unbounded flow)
- Validation test for implementation of interfacial energy density (surface tension)
- **Verification test for phase-volume conservation and boundedness**

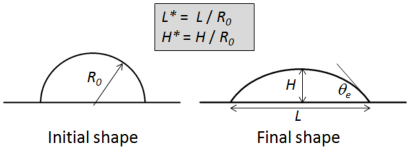
model / method	Δe_b	Δe_v /%
Allen-Cahn	$0.000E-12$	$3.054E-09$
Cahn-Hilliard / segregated	$3.900E-03$	$1.211E-06$
Cahn-Hilliard / coupled	$3.149E-04$	$4.036E-06$

Tab.: Phase-volume conservation and bounded properties.

[14] G.I. Taylor, *Proc. R. Soc. London, Ser. A* 146 (1934).

Results: Validation & Verification II

Test case II – Capillarity-driven Droplet Spreading / Dewetting



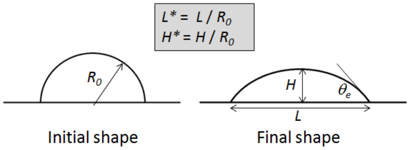
- Analytical solution [15,16] for $\mathrm{Eo} \ll 1$ (droplet shape is controlled by the capillary force) and $\mathrm{Eo} \gg 1$ (droplet shape is controlled by the gravity force)
- Validation test for implementation of (static) contact angle boundary condition
- Verification test for phase-volume conservation and boundedness

[15] Y. Chen, R. Mertz and R. Kulenovic, *Int. J. Multiphase Flow* 35/1 (2009).

[16] J.-B. Dupont and D. Legendre, *J. Comput. Phys.* 229 (2010).

Results: Validation & Verification II

Test case II – Capillarity-driven Droplet Spreading / Dewetting



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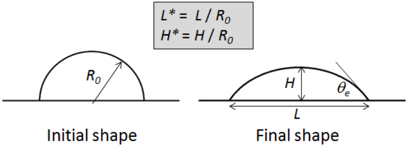

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Test case II – Capillarity-driven Droplet Spreading / Dewetting

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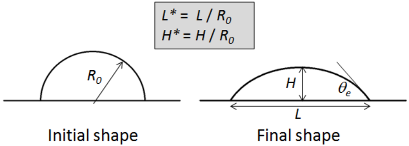

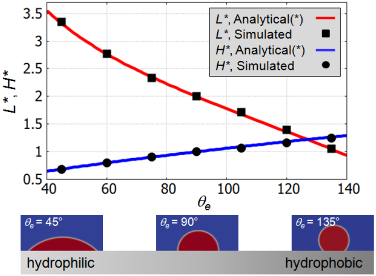

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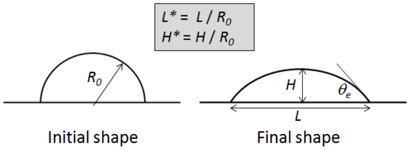

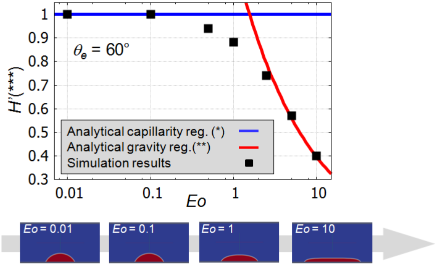

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Results: Validation & Verification II

Test case II – Capillarity-driven Droplet Spreading / Dewetting

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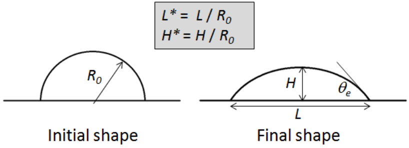

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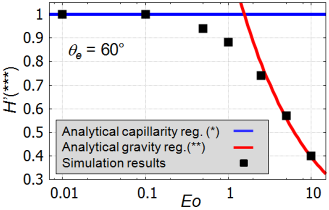

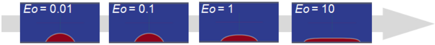

model / method	Δe_b	Δe_v /%
Allen-Cahn	$1.000E-11$	$1.076E-06$
Cahn-Hilliard / segregated	$2.577E-03$	$1.018E-09$
Cahn-Hilliard / coupled	$1.253E-03$	$8.230E-07$

Tab.: Phase-volume conservation and bounded properties.

[15] Y. Chen, R. Mertz and R. Kulenovic, *Int. J. Multiphase Flow* 35/1 (2009).

[16] J.-B. Dupont and D. Legendre, *J. Comput. Phys.* 229 (2010).

Closing I

Summary & Outlook

Summary

- Consistent coupling to incompressible two-phase Navier-Stokes equations.
- Enforcement of phase-volume conservation and boundedness.
- Quantitative validation of phase-field methods based on Allen-Cahn and Cahn-Hilliard diffuse interface models.
- Quantitative verification on phase-volume conservation and boundedness properties (ongoing work).

Outlook

- Release of the source to `foam-extend`.

Closing II

Acknowledgements...

Acknowledgements

- **Prof. Dr. Hrvoje Jasak** and **Vuko Vukčević** (Faculty of Mechanical Engineering, University of Zagreb; Wikki Limited)
- **Klas Jareteg** (Department of Applied Physics, Chalmers University of Technology)
- **Ivor Clifford** (The Idaho National Laboratory, The Pennsylvania State University)
- **Helmut Abels** (Faculty of Mathematics, University of Regensburg)

Closing II

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Thank You for Your Attention!

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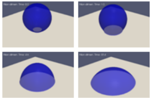
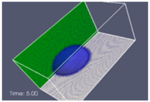

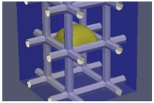
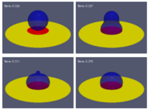
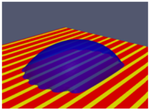
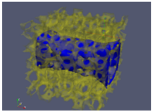

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Karlsruhe Institute of Technology

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