Phase-field modeling and computation of mixture flows

Marco ten Eikelder

TU Darmstadt

DFG: Walter Benjamin project EI 1210/1-1.0

(version without videos)

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Motivation

Situation

Modeling assumptions:

- Multiple fluids
- Incompressible fluids
- Viscous fluids
- Isothermal fluids

Prototypical phase-field model: Navier-Stokes Cahn-Hilliard model

Navier-Stokes Cahn-Hilliard models

Navier-Stokes model

$$\partial_t(\rho \mathsf{v}) + \operatorname{div}(\rho \mathsf{v} \otimes \mathsf{v}) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} = 0,$$
$$\operatorname{div}\mathsf{v} = 0.$$

Cahn-Hilliard model

$$\partial_t c - \operatorname{div}(\mathsf{M}\nabla\mu) = 0,$$
$$\mu - \frac{\sigma}{\epsilon}F'(c) + \sigma\epsilon\Delta c = 0.$$

Navier-Stokes Cahn-Hilliard models

Navier-Stokes model

$$\partial_t(\rho \mathrm{v}) + \mathrm{div}\,(\rho \mathrm{v} \otimes \mathrm{v}) - \mathrm{div}\mathrm{T} - \rho \mathrm{b} = 0,$$
$$\mathrm{div}\mathrm{v} = 0.$$

Notation Navier-Stokes model:

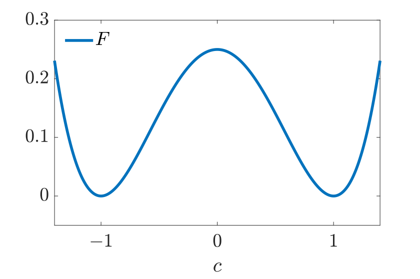
- ρ density
- v velocity
- T stress
- b body force

Notation Cahn-Hilliard model:

- σ surface energy parameter
- ϵ interface width parameter
- M mobility, c concentration

Cahn-Hilliard model

$$\partial_t c - \mathrm{div}\,(\mathrm{M}\nabla\mu) = 0,$$
$$\mu - \frac{\sigma}{\epsilon}F'(c) + \sigma\epsilon\Delta c = 0.$$



Navier-Stokes Cahn-Hilliard models

Navier-Stokes model

$$\begin{aligned} \partial_t(\rho \mathsf{v}) + \mathrm{div}\,(\rho \mathsf{v} \otimes \mathsf{v}) - \mathrm{div}\mathsf{T} - \rho \mathsf{b} &= 0, \\ \mathrm{div}\mathsf{v} &= 0. \end{aligned}$$

Cahn-Hilliard model

$$\begin{aligned} \partial_t c - \mathrm{div}\,(\mathsf{M}\nabla\mu) &= 0, \\ \mu - \frac{\sigma}{\epsilon}F'(c) + \sigma\epsilon\Delta c &= 0. \end{aligned}$$

Navier-Stokes model + Cahn-Hilliard model?

$$\begin{aligned} \partial_t(\rho \mathsf{v}) + \mathrm{div}\,(\rho \mathsf{v} \otimes \mathsf{v}) - \mathrm{div}\mathsf{T} - \rho \mathsf{b} &= 0, \\ \mathrm{div}\mathsf{v} &= 0, \\ \partial_t c - \mathrm{div}\,(\mathsf{M}\nabla\mu) &= 0, \\ \mu - \frac{\sigma}{\epsilon}F'(c) + \sigma\epsilon\Delta c &= 0. \end{aligned}$$

Constant density $\rightarrow$ [Hohenberg and Halperin, Rev. Mod. Phys., 1977]

Non-matching densities - Navier-Stokes Cahn-Hilliard model

Mass-averaged velocity model - Lowengrub and Truskinovsky:

$$\begin{aligned} \rho\partial_t \mathrm{v} + \rho\mathrm{v}\cdot\nabla\mathrm{v} + \nabla\check{p} - \mathrm{div}\check{\tau} \; + \sigma\epsilon\mathrm{div}(\rho\nabla c\otimes\nabla c) &= 0, \\ \partial_t\rho + \mathrm{div}(\rho\mathrm{v}) &= 0, \\ \rho(\partial_t c \; + \mathrm{v}\cdot\nabla c) - \mathrm{div}\left(\check{m}\nabla\check{\mu}\right) &= 0, \\ \check{\mu} + \rho^{-2}\frac{\partial\rho}{\partial c}p - \frac{\sigma}{\epsilon}f'(c) + \sigma\epsilon\rho^{-1}\mathrm{div}(\rho\nabla c) &= 0. \end{aligned}$$

Notation:

- order parameter: concentration difference $c = c_1 - c_2$
- density ρ $\rho^{-1}(c) = \rho_1^{-1}c_1 + \rho_2^{-1}c_2$
- velocity v: mass-averaged $\rho\mathrm{v} = \tilde{\rho}_1\mathrm{v}_1 + \tilde{\rho}_2\mathrm{v}_2$, with $\tilde{\rho}_\alpha = \rho c_\alpha$
- mobility $\check{m} = \mathrm{const} \geq 0$

[Lowengrub and Truskinovsky, Proc. R. Soc. A, 1998]

Non-matching densities - Navier-Stokes Cahn-Hilliard model

Volume-averaged velocity model - Abels, Garcke, Grün:

$$
\begin{aligned}
\partial_t(\rho \mathrm{u}) + \mathrm{div}(\rho \mathrm{u} \otimes \mathrm{u}) + \mathrm{div}\,(\mathrm{u} \otimes \mathrm{J}) + \nabla \hat{p} - \mathrm{div}\hat{\boldsymbol{\tau}} + \sigma\epsilon \mathrm{div}(\nabla\phi \otimes \nabla\phi) &= 0, \\
\mathrm{div}\mathrm{u} &= 0, \\
\partial_t \phi + \mathrm{u} \cdot \nabla\phi - \mathrm{div}\,(\hat{m}\nabla\hat{\mu}) &= 0, \\
\hat{\mu} - \frac{\sigma}{\epsilon} F'(\phi) + \sigma\epsilon\Delta\phi &= 0.
\end{aligned}
$$

Notation:

- order parameter: volume fraction difference $\phi = \phi_1 - \phi_2$
- density ρ $\rho(\phi) = \rho_1\phi_1 + \rho_2\phi_2$
- velocity u: volume-averaged $\mathrm{u} = \phi_1 \mathrm{u}_1 + \phi_2 \mathrm{v}_2$, with $\tilde{\rho}_\alpha = \rho_\alpha \phi_\alpha$
- mobility $\hat{m} = \hat{m}(\phi) \geq 0$
- diffusive flux $\mathrm{J} = \frac{\rho_1 - \rho_2}{2} \hat{m} \nabla \hat{\mu}$

[Abels, Garcke, Grün, M3AS, 2013]

Overview Navier-Stokes Cahn-Hilliard models

Model	Velocity	Order param.	Free energy	Mobility	Energy law
Abels et al., Math. Mod. Meth. Appl. Sci. 2012	u	ϕ	Ψ	non-deg./deg.	✓
Aki et al., Math. Mod. Meth. Appl. Sci. 2014	v	ϕ	Ψ	non-deg.	✓
Boyer, Comput. Fluids 2002	u	ϕ	Ψ	deg.	✗
Ding et al., J. Comput. Phys. 2007	u	ϕ	Ψ	deg.	✗
Lowengrub and Truskinovsky, Proc. R. Soc. A, 1998	v	c	ψ	non-deg.	✓
Shen et al. Commun. Comput. Phys. 2013	v	ϕ	Ψ	non-deg.	✓
S. Roudbari et al., Math. Mod. Meth. Appl. Sci. 2018	v	ϕ	Ψ	non-deg.	✓

Objective

Modeling assumptions:

- Multiple fluids
- Incompressible fluids
- Viscous fluids
- Isothermal fluids

Observation:

- Same physics, yet different **Navier-Stokes** **Cahn-Hilliard (Allen-Cahn)** models
  $\rightarrow$ similar situation for N-phase flow

Objective:

- A **unified framework** for **Navier-Stokes** **Cahn-Hilliard (Allen-Cahn)** models
- **A mixture-theory compatible phase-field framework**

Phase-field mixture models

Preliminaries

Definitions:

Partial constituent density: $\tilde{\rho}_\alpha(\mathrm{x}, t) := \lim_{|V|\to 0} \frac{M_\alpha(V)}{|V|}$

Specific constituent density: $\rho_\alpha(\mathrm{x}, t) := \lim_{|V|\to 0} \frac{M_\alpha(V)}{|V_\alpha|}$

Constituent volume fraction: $\phi_\alpha(\mathrm{x}, t) := \lim_{|V|\to 0} \frac{|V_\alpha|}{|V|}$

Constituent concentration: $c_\alpha(\mathrm{x}, t) := \lim_{|V|\to 0} \frac{M_\alpha(V)}{M(V)}$

Mixture density: $\rho(\mathrm{x}, t) := \lim_{|V|\to 0} \frac{M(V)}{|V|}$

Relations:

$$\rho = \sum_\alpha \tilde{\rho}_\alpha \qquad 1 = \sum_\alpha \phi_\alpha \qquad 1 = \sum_\alpha c_\alpha \qquad \tilde{\rho}_\alpha = \rho_\alpha \phi_\alpha \qquad \tilde{\rho}_\alpha = c_\alpha \rho$$

Two sets of equations

Balance laws constituents:

$$
\begin{aligned}
\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) &= \gamma_\alpha, \\
\partial_t \mathsf{m}_\alpha + \operatorname{div}\left(\mathsf{m}_\alpha \otimes \mathsf{v}_\alpha\right) - \operatorname{div}\mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha &= \boldsymbol{\pi}_\alpha, \\
\mathsf{T}_\alpha - \mathsf{T}_\alpha^T &= \mathsf{N}_\alpha, \\
\partial_t \left(\tilde{\rho}_\alpha \left(\epsilon_\alpha + \|\mathsf{v}_\alpha\|^2/2\right)\right) + \operatorname{div}\left(\tilde{\rho}_\alpha \left(\epsilon_\alpha + \|\mathsf{v}_\alpha\|^2/2\right) \mathsf{v}_\alpha\right) & \\
-\operatorname{div}\left(\mathsf{T}_\alpha \mathsf{v}_\alpha\right) - \tilde{\rho}_\alpha \mathsf{b}_\alpha \cdot \mathsf{v}_\alpha + \operatorname{div}\mathsf{q}_\alpha - \tilde{\rho}_\alpha r_\alpha &= e_\alpha.
\end{aligned}
$$

Balance laws mixture (consequence):

$$
\begin{aligned}
\partial_t \rho + \operatorname{div}(\rho \mathsf{v}) &= 0, & \textstyle\sum_\alpha \gamma_\alpha &= 0 \\
\partial_t (\rho \mathsf{v}) + \operatorname{div}\left(\rho \mathsf{v} \otimes \mathsf{v}\right) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} &= 0, & \textstyle\sum_\alpha \boldsymbol{\pi}_\alpha &= 0 \\
\mathsf{T} - \mathsf{T}^T &= 0, & \textstyle\sum_\alpha N_\alpha &= 0 \\
\partial_t \left(\rho \left(\epsilon + \|\mathsf{v}\|^2/2\right)\right) + \operatorname{div}\left(\rho \left(\epsilon + \|\mathsf{v}\|^2/2\right) \mathsf{v}\right) & \\
-\operatorname{div}\left(\mathsf{T} \mathsf{v}\right) - \rho \mathsf{b} \cdot \mathsf{v} + \operatorname{div}\mathsf{q} - \rho r &= 0, & \textstyle\sum_\alpha e_\alpha &= 0.
\end{aligned}
$$

[Truesdell, Toupin, 1960]

Two sets of equations

Balance laws constituents:

$$
\begin{aligned}
\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) &= \gamma_\alpha, \\
\partial_t \mathsf{m}_\alpha + \operatorname{div}\left(\mathsf{m}_\alpha \otimes \mathsf{v}_\alpha\right) - \operatorname{div} \mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha &= \boldsymbol{\pi}_\alpha, \\
\mathsf{T}_\alpha - \mathsf{T}_\alpha^T &= \mathsf{N}_\alpha, \\
\partial_t \left(\tilde{\rho}_\alpha \left(\epsilon_\alpha + \|\mathsf{v}_\alpha\|^2/2\right)\right) + \operatorname{div}\left(\tilde{\rho}_\alpha \left(\epsilon_\alpha + \|\mathsf{v}_\alpha\|^2/2\right) \mathsf{v}_\alpha\right) & \\
-\operatorname{div}\left(\mathsf{T}_\alpha \mathsf{v}_\alpha\right) - \tilde{\rho}_\alpha \mathsf{b}_\alpha \cdot \mathsf{v}_\alpha + \operatorname{div} \mathsf{q}_\alpha - \tilde{\rho}_\alpha r_\alpha &= e_\alpha.
\end{aligned}
$$

Balance laws mixture (consequence):

$$
\begin{aligned}
\partial_t \rho + \operatorname{div}(\rho \mathsf{v}) &= 0, \\
\partial_t (\rho \mathsf{v}) + \operatorname{div}\left(\rho \mathsf{v} \otimes \mathsf{v}\right) - \operatorname{div} \mathsf{T} - \rho \mathsf{b} &= 0, \\
\mathsf{T} - \mathsf{T}^T &= 0, \\
\partial_t \left(\rho \left(\epsilon + \|\mathsf{v}\|^2/2\right)\right) + \operatorname{div}\left(\rho \left(\epsilon + \|\mathsf{v}\|^2/2\right) \mathsf{v}\right) & \\
-\operatorname{div}\left(\mathsf{T} \mathsf{v}\right) - \rho \mathsf{b} \cdot \mathsf{v} + \operatorname{div} \mathsf{q} - \rho r &= 0.
\end{aligned}
$$

[Truesdell, Toupin, 1960]

Two sets of equations

Balance laws constituents:

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$

$$\partial_t \mathsf{m}_\alpha + \operatorname{div}(\mathsf{m}_\alpha \otimes \mathsf{v}_\alpha) - \operatorname{div}\mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha = \boldsymbol{\pi}_\alpha.$$

Balance laws mixture (consequence):

$$\partial_t \rho + \operatorname{div}(\rho \mathsf{v}) = 0,$$

$$\partial_t(\rho \mathsf{v}) + \operatorname{div}(\rho \mathsf{v} \otimes \mathsf{v}) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} = 0.$$

[Truesdell, Toupin, 1960]

Two sets of equations

Balance laws constituents:

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$
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Balance laws mixture (consequence):

$$\partial_t \rho + \operatorname{div}(\rho \mathsf{v}) = 0,$$
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Objective 1: Phase-field modeling framework - Navier-Stokes Cahn-Hilliard

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$
$$\partial_t(\rho \mathsf{v}) + \operatorname{div}(\rho \mathsf{v} \otimes \mathsf{v}) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} = 0.$$

Two sets of equations

Balance laws constituents:

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$
$$\partial_t \mathsf{m}_\alpha + \operatorname{div}(\mathsf{m}_\alpha \otimes \mathsf{v}_\alpha) - \operatorname{div}\mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha = \boldsymbol{\pi}_\alpha.$$

Balance laws mixture (consequence):

$$\partial_t \rho + \operatorname{div}(\rho \mathsf{v}) = 0,$$
$$\partial_t (\rho \mathsf{v}) + \operatorname{div}(\rho \mathsf{v} \otimes \mathsf{v}) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} = 0.$$

Objective 1: Phase-field modeling framework - Navier-Stokes Cahn-Hilliard

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$
$$\partial_t (\rho \mathsf{v}) + \operatorname{div}(\rho \mathsf{v} \otimes \mathsf{v}) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} = 0.$$

Objective 2: Phase-field modeling framework - Full mixture

$$\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) = \gamma_\alpha,$$
$$\partial_t \mathsf{m}_\alpha + \operatorname{div}(\mathsf{m}_\alpha \otimes \mathsf{v}_\alpha) - \operatorname{div}\mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha = \boldsymbol{\pi}_\alpha.$$

Navier-Stokes Cahn-Hilliard model - two components

Balance laws mixture - mass-averaged formulation:

$$\begin{aligned} \partial_t \rho + \mathrm{div}(\rho \mathsf{v}) &= 0, \\ \partial_t(\rho \mathsf{v}) + \mathrm{div}\left(\rho \mathsf{v} \otimes \mathsf{v}\right) - \mathrm{div}\mathsf{T} - \rho \mathsf{b} &= 0, \\ \partial_t \phi + \mathrm{div}\left(\phi \mathsf{v}\right) + \mathrm{div}\mathsf{h} &= 0, \end{aligned}$$

- **Constitutive models** for T and $\mathsf{h} = \phi_1(\mathsf{v}_1 - \mathsf{v}) - \phi_2(\mathsf{v}_2 - \mathsf{v})$

[ten Eikelder et al., M3AS, 2023]

Navier-Stokes Cahn-Hilliard model - two components

Balance laws mixture - mass-averaged formulation:

$$
\begin{aligned}
\partial_t \rho + \mathrm{div}(\rho \mathsf{v}) =&\ 0, \\
\partial_t(\rho \mathsf{v}) + \mathrm{div}\left(\rho \mathsf{v} \otimes \mathsf{v}\right) - \mathrm{div}\,\mathsf{T} - \rho \mathsf{b} =&\ 0, \\
\partial_t \phi + \mathrm{div}\left(\phi \mathsf{v}\right) + \mathrm{div}\mathsf{h} =&\ 0,
\end{aligned}
$$

- **Constitutive models** for T and $\mathsf{h} = \phi_1(\mathsf{v}_1 - \mathsf{v}) - \phi_2(\mathsf{v}_2 - \mathsf{v}) \longrightarrow$ **Energy-dissipation law**:

NSCH model - mass-averaged formulation:

$$
\begin{aligned}
\partial_t \rho + \mathrm{div}(\rho \mathsf{v}) =&\ 0, \\
\partial_t(\rho \mathsf{v}) + \mathrm{div}\left(\rho \mathsf{v} \otimes \mathsf{v}\right) + \nabla p - \mathrm{div}\boldsymbol{\tau} + \phi \nabla \mu - \rho \mathsf{b} =&\ 0, \\
\partial_t \phi + \mathrm{div}(\phi \mathsf{v}) - \mathrm{div}\left(\mathsf{M} \nabla (\mu + \alpha p)\right) =&\ 0.
\end{aligned}
$$

[ten Eikelder et al., M3AS, 2023]

Navier-Stokes Cahn-Hilliard model - two components

Balance laws mixture - volume-averaged formulation:

$$
\begin{aligned}
\operatorname{div} \mathsf{u} &= 0, \\
\partial_t(\rho \mathsf{u} + \mathsf{J}) + \operatorname{div}\left(\rho \mathsf{u} \otimes \mathsf{u} + \mathsf{J} \otimes \mathsf{u} + \mathsf{u} \otimes \mathsf{J} + \frac{1}{\rho}\mathsf{J} \otimes \mathsf{J}\right) - \operatorname{div}\mathsf{T} - \rho \mathsf{b} &= 0, \\
\partial_t \phi + \operatorname{div}(\phi \mathsf{v}) + \operatorname{div}\mathsf{h} &= 0,
\end{aligned}
$$

- **Constitutive models** for T and $\mathsf{h} = \phi_1(\mathsf{v}_1 - \mathsf{v}) - \phi_2(\mathsf{v}_2 - \mathsf{v})$ $\longrightarrow$ **Energy-dissipation law**:

NSCH model - volume-averaged formulation:

$$
\begin{aligned}
\operatorname{div} \mathsf{u} &= 0, \\
\partial_t(\rho \mathsf{u} + \hat{\mathsf{J}}) + \operatorname{div}\left(\rho \mathsf{u} \otimes \mathsf{u} + \hat{\mathsf{J}} \otimes \mathsf{u} + \mathsf{u} \otimes \hat{\mathsf{J}} + \frac{1}{\rho}\hat{\mathsf{J}} \otimes \hat{\mathsf{J}}\right) + \nabla p - \operatorname{div}\boldsymbol{\tau} + \phi \nabla \mu - \rho \mathsf{b} &= 0, \\
\partial_t \phi + \operatorname{div}(\phi \mathsf{v}) - \operatorname{div}\left(\mathsf{M} \nabla(\mu + \alpha p)\right) &= 0.
\end{aligned}
$$

[ten Eikelder et al., M3AS, 2023]

NSCH model - mass-averaged formulation:

$$
\begin{aligned}
\partial_t \rho + \mathrm{div}(\rho \mathbf{v}) =&\ 0,\\
\partial_t(\rho \mathbf{v}) + \mathrm{div}\left(\rho \mathbf{v} \otimes \mathbf{v}\right) + \nabla p - \mathrm{div}\boldsymbol{\tau} + \phi \nabla \mu - \rho \mathbf{b} =&\ 0,\\
\partial_t \phi + \mathrm{div}(\phi \mathbf{v}) - \mathrm{div}\left(\mathbf{M}\nabla(\mu + \alpha p)\right) =&\ 0.
\end{aligned}
$$

- **Variable transformations** $\rho \mathbf{v} = \rho \mathbf{u} + \hat{\mathbf{J}}$:

NSCH model - volume-averaged formulation:

$$
\begin{aligned}
\mathrm{div}\mathbf{u} =&\ 0,\\
\partial_t(\rho \mathbf{u} + \hat{\mathbf{J}}) + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \hat{\mathbf{J}} \otimes \mathbf{u} + \mathbf{u} \otimes \hat{\mathbf{J}} + \frac{1}{\rho}\hat{\mathbf{J}} \otimes \hat{\mathbf{J}}\right) + \nabla p - \mathrm{div}\boldsymbol{\tau} + \phi \nabla \mu - \rho \mathbf{b} =&\ 0,\\
\partial_t \phi + \mathbf{u} \cdot \nabla \phi - \mathrm{div}\left(\hat{\mathbf{M}}\nabla(\mu + \alpha p)\right) =&\ 0.
\end{aligned}
$$

[ten Eikelder et al., M3AS, 2023]

Navier-Stokes Cahn-Hilliard model - N-components

NSCH model - mass-averaged formulation:

$$\begin{aligned}
\partial_t \tilde{\rho}_\alpha + \mathrm{div}(\tilde{\rho}_\alpha \mathbf{v}) + \mathrm{div}\hat{\mathbf{J}}_\alpha &= 0,\\
\partial_t(\rho \mathbf{v}) + \mathrm{div}\left(\rho \mathbf{v} \otimes \mathbf{v}\right) + \sum_\beta \phi_\beta \nabla(\mu_\alpha + p) - \mathrm{div}\boldsymbol{\tau} - \rho \mathbf{b} &= 0,\\
\hat{\mathbf{J}}_\alpha + \sum_\beta m_{\alpha\beta} \nabla g_\beta &= 0, \qquad g_\alpha = \rho_\alpha^{-1}(\mu_\alpha + p)
\end{aligned}$$

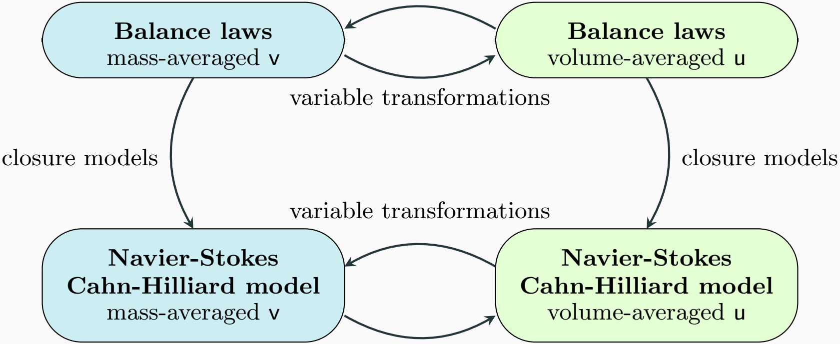
- **Variable transformations** $\rho \mathbf{v} = \rho \mathbf{u} + \sum_\alpha \hat{\mathbf{J}}_\alpha^u$ and $\hat{\mathbf{J}}_\alpha^u = \hat{\mathbf{J}}_\alpha - \tilde{\rho}_\alpha \sum_\beta \rho_\beta^{-1} \hat{\mathbf{J}}_\beta$:

NSCH model - volume-averaged formulation:

$$\begin{aligned}
\partial_t \tilde{\rho}_\alpha + \mathrm{div}(\tilde{\rho}_\alpha \mathbf{u}) + \mathrm{div}\hat{\mathbf{J}}_\alpha^u &= 0,\\
\partial_t(\rho \mathbf{v}) + \mathrm{div}\left(\rho \mathbf{v} \otimes \mathbf{v}\right) + \sum_\beta \phi_\beta \nabla(\mu_\alpha + p) - \mathrm{div}\boldsymbol{\tau} - \rho \mathbf{b} &= 0,
\end{aligned}$$

[ten Eikelder, arxiv.org, 2024]

Invariance of set of fundamental variables

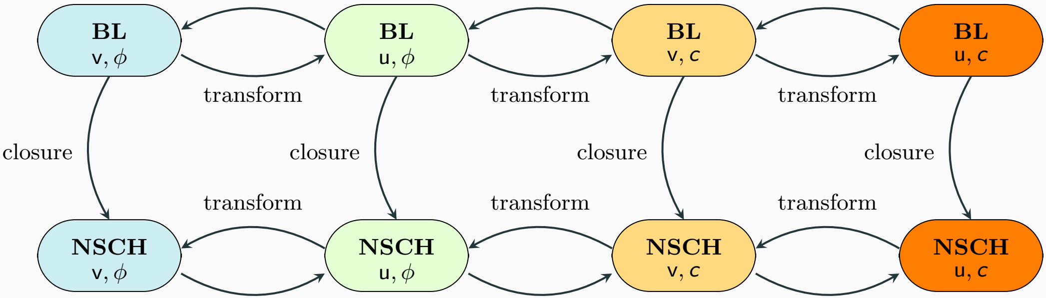


Observation:

- NSCH mixture theory framework invariant to set of variables

[ten Eikelder et al., M3AS, 2023; ten Eikelder, arxiv.org, 2024]

Invariance of set of fundamental variables



Observation:

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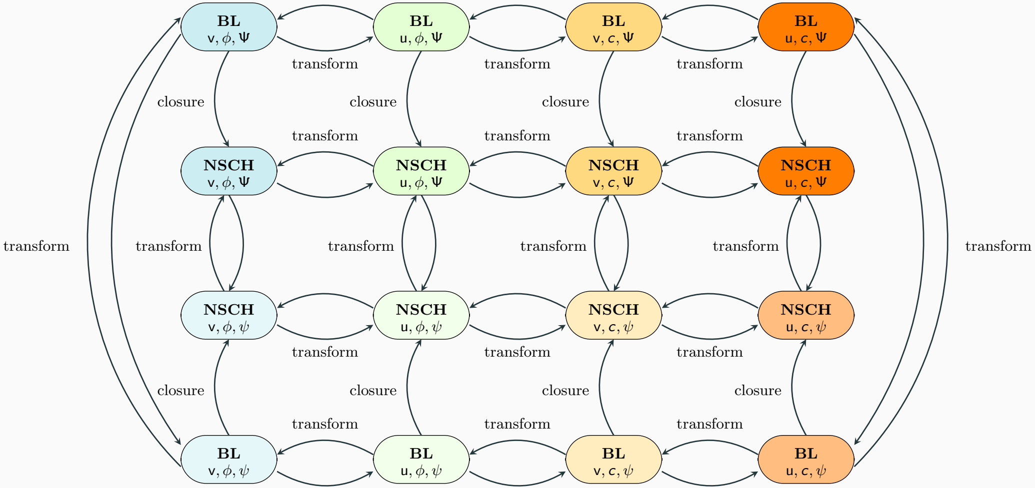
Invariance of set of fundamental variables



[ten Eikelder et al., M3AS, 2023; ten Eikelder, arxiv.org, 2024]

Phase-field full mixture model

Balance laws constituents:

$$\begin{aligned} \partial_t \tilde{\rho}_\alpha + \mathrm{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) &= 0 \\ \partial_t(\tilde{\rho}_\alpha \mathsf{v}_\alpha) + \mathrm{div}\left(\tilde{\rho}_\alpha \mathsf{v}_\alpha \otimes \mathsf{v}_\alpha\right) - \mathrm{div}\mathsf{T}_\alpha - \tilde{\rho}_\alpha \mathsf{b}_\alpha &= \boldsymbol{\pi}_\alpha \end{aligned}$$

Constitutive models for T_α and $\boldsymbol{\pi}_\alpha$ $\longrightarrow$ **Second law of thermodynamics for mixtures**:

$$\begin{aligned} \partial_t \tilde{\rho}_\alpha + \mathrm{div}(\tilde{\rho}_\alpha \mathsf{v}_\alpha) &= 0, \\ \partial_t(\tilde{\rho}_\alpha \mathsf{v}_\alpha) + \mathrm{div}\left(\tilde{\rho}_\alpha \mathsf{v}_\alpha \otimes \mathsf{v}_\alpha\right) + \phi_\alpha \nabla \left(p + \hat{\mu}_\alpha\right) & \\ -\mathrm{div}(\nu_\alpha(2D_\alpha + \lambda_\alpha(\mathrm{div}\mathsf{v}_\alpha)\mathsf{I}) - \tilde{\rho}_\alpha \mathsf{b} &= \sum_\beta R_{\alpha\beta}(\mathsf{v}_\beta - \mathsf{v}_\alpha). \end{aligned}$$

[ten Eikelder et al., JFM, 2024]

Phase-field full mixture model

Mixture model:

$$
\begin{aligned}
\partial_t \tilde{\rho}_\alpha + \operatorname{div}(\tilde{\rho}_\alpha \mathrm{v}_\alpha) =&\ 0,\\
\partial_t(\tilde{\rho}_\alpha \mathrm{v}_\alpha) + \operatorname{div}\left(\tilde{\rho}_\alpha \mathrm{v}_\alpha \otimes \mathrm{v}_\alpha\right) + \phi_\alpha \nabla\left(p + \hat{\mu}_\alpha\right) &\\
-\operatorname{div}(\nu_\alpha(2D_\alpha + \lambda_\alpha(\operatorname{div}\mathrm{v}_\alpha)\mathrm{I}) - \tilde{\rho}_\alpha \mathrm{b} =&\ \sum_\beta R_{\alpha\beta}(\mathrm{v}_\beta - \mathrm{v}_\alpha),\\
\hat{\mu}_\alpha - \frac{\partial \Psi_\alpha}{\partial \phi_\alpha} + \operatorname{div}\frac{\partial \Psi_\alpha}{\partial \nabla \phi_\alpha} =&\ 0
\end{aligned}
$$

Phase-field characteristics:

- ✓ Phase-field/order parameters ϕ_α / c_α
- ✓ Diffuse-interface (thickness ϵ_α)
- ✓ Chemical potentials $\hat{\mu}_\alpha$
- ✓ Energy-dissipation/thermodynamics
- ✗ Mobility m
- ✓ Gradient theory ($\nabla \phi_\alpha$)
- ✗ Chemical potential in phase-field equation
- ✓ Energy depends on interface thickness
- ✓ Tanh-interface profile possible
- ✓ Order parameter $0 \leq \phi_\alpha, c_\alpha \leq 1$

[ten Eikelder et al., JFM, 2024]

Comparison

	Mixture model	**NSCHAC model**
Mixture theory	✓	✗
Modeling restriction	Second law	Approximation second law
# mass balance laws	N	N
# momentum balance laws	N	1
Diffusive flux	Evolution equation	Constitutive model

[ten Eikelder et al., JFM, 2024, ten Eikelder, arxiv.org, 2024]

Computation

Objective

Objective:

- **Benchmark Navier-Stokes Cahn-Hilliard unified framework**
- **Structure-preserving discretization Navier-Stokes Cahn-Hilliard model**

Benchmarking NSCH unified framework

NSCH model - volume-averaged formulation:

$$
\begin{aligned}
\mathrm{div}\,\mathrm{u} &= 0,\\
\partial_t(\rho \mathrm{u} + \hat{\mathrm{J}}) + \mathrm{div}\left(\rho \mathrm{u}\otimes\mathrm{u} + \hat{\mathrm{J}}\otimes\mathrm{u} + \mathrm{u}\otimes\hat{\mathrm{J}} + \frac{1}{\rho}\hat{\mathrm{J}}\otimes\hat{\mathrm{J}}\right) + \nabla p - \mathrm{div}\boldsymbol{\tau} + \phi\nabla\mu - \rho\mathrm{b} &= 0,\\
\partial_t\phi + \mathrm{u}\cdot\nabla\phi - \mathrm{div}\left(\hat{\mathrm{M}}\nabla(\mu + \alpha p)\right) &= 0.
\end{aligned}
$$

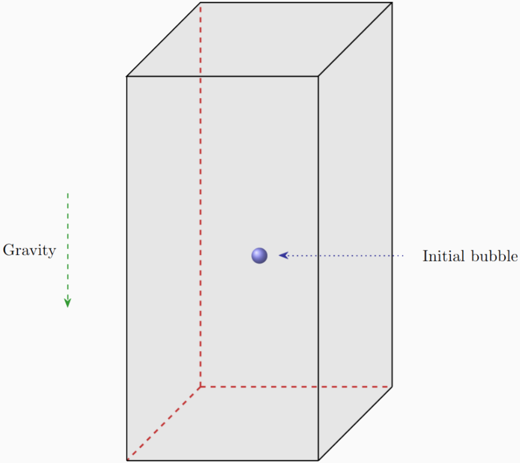
[ten Eikelder and Schillinger, JCP, 2024]

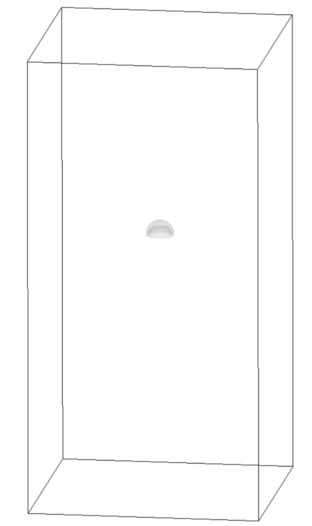
Rising bubble

- isogeometric discretization
- divergence conforming spaces [J.A. Evans and T.J.R. Hughes, J. Comput. Phys., 2013]
- no stabilization required
- midpoint time stepping

[ten Eikelder and Schillinger, JCP, 2024]

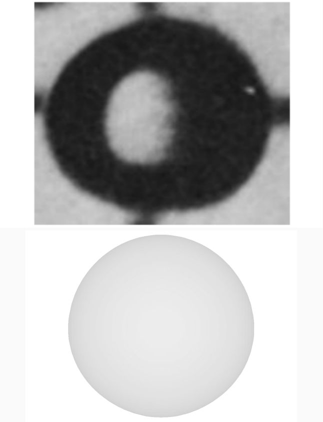
Rising bubble



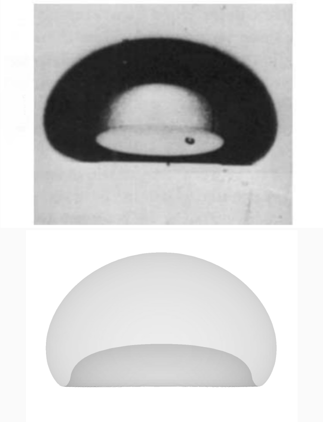


[ten Eikelder and Schillinger, JCP, 2024]

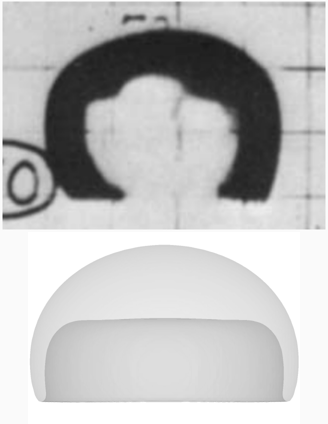
Rising bubble



(a) Case 1



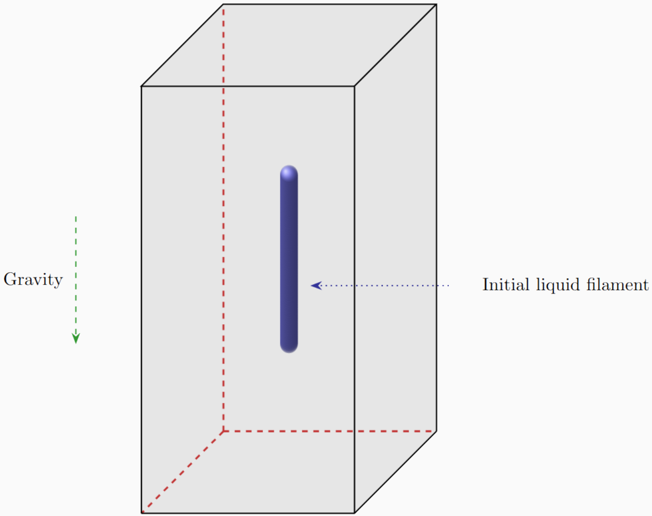
(b) Case 2



(c) Case 3

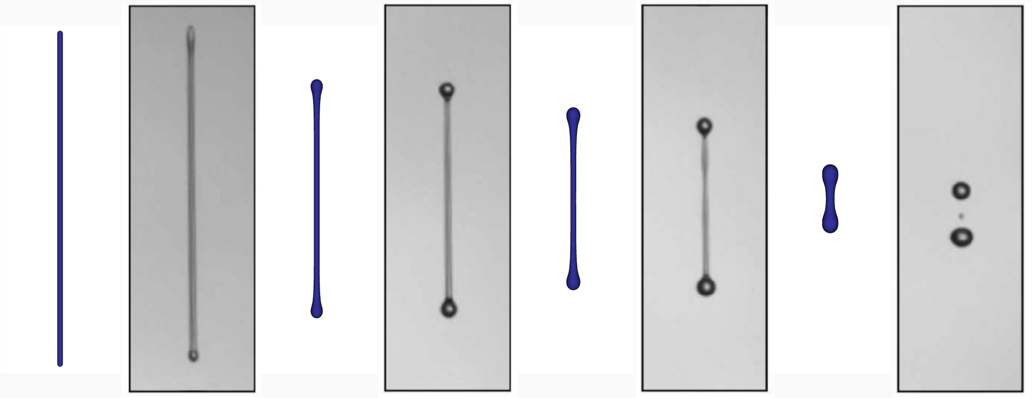
Rising bubble problem. Final bubble shape. Top: [Bhaga and Weber, JFM 1981], Bottom: [ten Eikelder and Schillinger, JCP, 2024].

Liquid filament contraction



[ten Eikelder and Schillinger, JCP, 2024]

Liquid filament contraction



time(ms):

$t = 0.0$ $t = 4.0$ $t = 6.3$ $t = 10.7$

[ten Eikelder and Schillinger, JCP, 2024]

NSCH model - alternative mass-averaged formulation:

$$\begin{aligned} \mathrm{div}\, v - \alpha \mathrm{div}\left(\mathrm{M}\nabla(\mu + \alpha p)\right) =&\ 0, \\ \frac{\mathrm{v}}{2}\partial_t \rho + \rho \partial_t \mathrm{v} + \frac{1}{2}\mathrm{v}\,\mathrm{div}(\rho \mathrm{v}) + \rho \mathrm{v} \cdot \nabla \mathrm{v} + \nabla p - \mathrm{div} \boldsymbol{\tau} + \phi \nabla \mu - \rho \mathrm{b} =&\ 0, \\ \partial_t \phi + \mathrm{div}(\phi \mathrm{v}) - \mathrm{div}\left(\mathrm{M}\nabla(\mu + \alpha p)\right) =&\ 0. \end{aligned}$$

Structure-preserving scheme satisfies the conservation of phase, mass, and the energy dissipation law:

$$\langle \phi_h^{n+1}, 1\rangle = \langle \phi_{0,h}, 1\rangle, \qquad \langle \rho(\phi_h^{n+1}), 1\rangle = \langle \rho(\phi_{0,h}), 1\rangle,$$

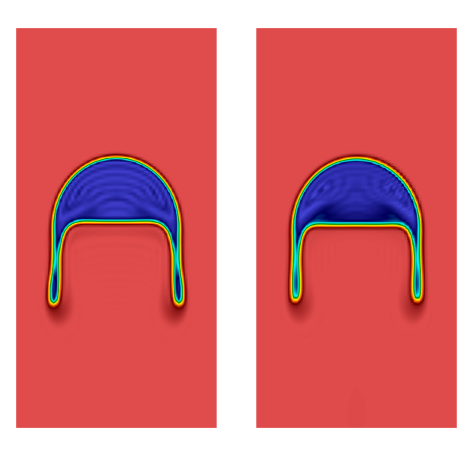
$$E(\phi_h^{n+1}, \mathrm{v}_h^{n+1}) + \Delta t \mathcal{D}^{n+1} \leq E(\phi_h^n, \mathrm{v}_h^n)$$

[Brunk, ten Eikelder, 2025]

Structure preserving scheme - preliminary results

[Brunk, ten Eikelder, 2025]

Structure preserving scheme - preliminary results



Volume-averaged Mass-averaged

[Brunk, ten Eikelder, 2025]

Structure preserving scheme - N-phase - preliminary results

[ten Eikelder, Brunk, 2025] Smaller gravity Larger gravity

Conclusions

Modeling:

1. NSCH mixture theory framework invariant to set of variables
2. Mixture model is a phase-field model but not Cahn-Hilliard (Allen-Cahn) type

Computation:

3. NSCH mixture model benchmark
4. Structure-preserving schemes NSCH mixture model

Outlook

- Bound-preservation
- Temperature
- N-component flows
- Sharp-interface limits
- Model comparison
- more ...

Flory-Huggins

Ginzburg-Landau

[ten Eikelder, Khanwale, Stanford CTR Proc., 2024]

Thank you for your attention!

Marco ten Eikelder - marco.eikelder@tu-darmstadt.de

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