technische universität dortmund

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Isogeometric Analysis of Cahn–Hilliard phase field-based Binary-Fluid–Structure Interaction based on an ALE variational formulation

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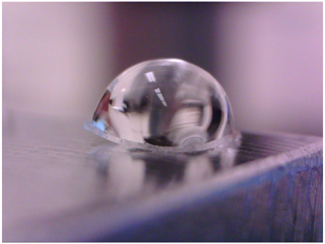
Motivation



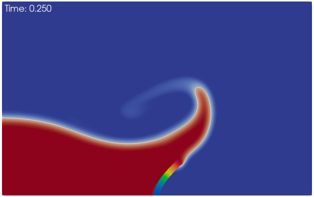
Definition

Elasto-capillarity: Ability of capillary forces or surface tensions to deform elastic solids through a complex interplay between the energy of the surfaces and the elastic strain energy in the solid.

Objective: Develop a robust **computational multiphysics model** capable of capturing the complex physics behind the intriguing phenomena of **Binary-Fluid–Structure Interaction (BFSI aka Elasto-capillarity)**.

Idea:

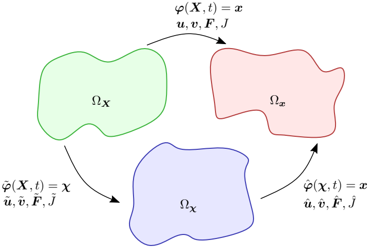
Combine a sharp interface monolithic ALE-FSI method with a diffuse interface two-phase flow method and use IGA



Two-phase flow, Navier–Stokes–Cahn–Hilliard system

$$
\begin{aligned}
\rho(\varphi)\left(\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right) - \nabla\cdot\left(\mu(\varphi)\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T\right)\right) &= -\nabla p + \rho(\varphi)\boldsymbol{b} \\
&\quad - \hat{\sigma}\varepsilon\,\nabla\cdot(\nabla\varphi\otimes\nabla\varphi) && \text{in } \Omega_T, \\
\nabla\cdot\boldsymbol{v} &= 0 && \text{in } \Omega_T, \\
\frac{\partial\varphi}{\partial t} + \boldsymbol{v}\cdot\nabla\varphi - \nabla\cdot(m(\varphi)\nabla\eta) &= 0 && \text{in } \Omega_T, \\
\eta - \hat{\sigma}\varepsilon^{-1}\,\frac{d\psi(\varphi)}{d\varphi} + \hat{\sigma}\varepsilon\,\nabla^2\varphi &= 0 && \text{in } \Omega_T, \\
\varphi(\boldsymbol{x},0) = \varphi_0(\boldsymbol{x}), \quad \boldsymbol{v}(\boldsymbol{x},0) &= \boldsymbol{v}_0(\boldsymbol{x}) && \text{in } \Omega, \\
\boldsymbol{v} &= \boldsymbol{v}_D && \text{on } (\partial\Omega_T)_D, \\
\nabla\varphi\cdot\boldsymbol{n} = \frac{1}{\varepsilon\sqrt{2}}\,\cos(\theta)(1-\varphi^2), \quad \nabla\eta\cdot\boldsymbol{n} &= 0 && \text{on } (\partial\Omega_T)_N, \\
\left(-p\boldsymbol{I} + \mu(\varphi)\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T\right)\right)\cdot\boldsymbol{n} &= \boldsymbol{t} && \text{on } (\partial\Omega_T)_N
\end{aligned}
$$

Fluid–Structure Interaction, Compressible solid



$$\begin{aligned}\boldsymbol{\varphi}\colon \overline{\Omega}_{\boldsymbol{X}} \times [0,T] &\longrightarrow \overline{\Omega}_{\boldsymbol{x}} \times [0,T]\\ (\boldsymbol{X},t) &\longmapsto \boldsymbol{\varphi}(\boldsymbol{X},t)=(\boldsymbol{x},t)\end{aligned}$$

$$\boldsymbol{\varphi}(\boldsymbol{X},t)=\boldsymbol{X}+\boldsymbol{u}(\boldsymbol{X},t)$$

$$\boldsymbol{v}(\boldsymbol{X},t)=\left.\frac{\partial \boldsymbol{u}}{\partial t}\right|_{\boldsymbol{X}}$$

$$\boldsymbol{F} := \boldsymbol{F}(\boldsymbol{X},\boldsymbol{u}) := \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{X}} = \nabla_{\boldsymbol{X}}\boldsymbol{\varphi}(\boldsymbol{X}) = \boldsymbol{I}+\nabla_{\boldsymbol{X}}\,\boldsymbol{u}$$

$$J := \det(\boldsymbol{F})$$

Elastodynamics (Lagrangian perspective):

$$\begin{aligned} J\rho\frac{\partial \boldsymbol{v}}{\partial t} - \nabla_{\boldsymbol{X}}\cdot\boldsymbol{P} &= J\rho\boldsymbol{b} && \text{in } \Omega_{\boldsymbol{X}}\times I,\\ \frac{\partial \boldsymbol{u}}{\partial t} - \boldsymbol{v} &= 0 && \text{in } \Omega_{\boldsymbol{X}}\times I,\\ \boldsymbol{u}(\cdot,0)=\mathring{\boldsymbol{u}}, \boldsymbol{v}(\cdot,0) &= \mathring{\boldsymbol{v}} && \text{in } \Omega_{\boldsymbol{X}},\\ \boldsymbol{u} &= \boldsymbol{u}_D && \text{on } \Gamma_{D,\boldsymbol{X}}\times I,\\ \boldsymbol{P}\,\boldsymbol{n}_0 &= \boldsymbol{g}_0 && \text{on } \Gamma_{N,\boldsymbol{X}}\times I. \end{aligned}$$

- St. Venant–Kirchhoff material

$$\boldsymbol{P} := \lambda\,\mathrm{tr}\,(\boldsymbol{E})\,\boldsymbol{F} + 2\mu\boldsymbol{F}\boldsymbol{E}$$

- Neo–Hookean material

$$\boldsymbol{P} := \mu(\boldsymbol{F}-\boldsymbol{F}^{-T}) + \lambda\log(\det\boldsymbol{F})\boldsymbol{F}^{-T}$$

Hyperelastic material: $\hat{\boldsymbol{P}}(\boldsymbol{X},\boldsymbol{F}) = \frac{\partial \hat{W}}{\partial \boldsymbol{F}}(\boldsymbol{X},\boldsymbol{F})$
Green–St. Venant strain tensor:

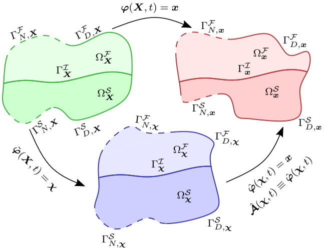
$$\boldsymbol{E} := 1/2\left(\nabla_{\boldsymbol{X}}\boldsymbol{u} + (\nabla_{\boldsymbol{X}}\boldsymbol{u})^T + (\nabla_{\boldsymbol{X}}\boldsymbol{u})^T\,\nabla_{\boldsymbol{X}}\boldsymbol{u}\right)$$

Fluid–Structure Interaction, Incompressible fluid

Incompressible Newtonian flow (Eulerian perspective):

$$
\begin{aligned}
\rho\left(\frac{\partial \boldsymbol{v}}{\partial t}\bigg|_{\boldsymbol{x}} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right) &= \nabla\cdot\boldsymbol{\sigma} + \rho\boldsymbol{b} && \text{in } \Omega^{\mathcal{F}}_{\boldsymbol{x}}(t), t\in I,\\
\nabla\cdot\boldsymbol{v} &= 0 && \text{in } \Omega^{\mathcal{F}}_{\boldsymbol{x}}(t), t\in I,\\
p(\cdot,0) = \mathring{p}, \boldsymbol{v}(\cdot,0) &= \mathring{\boldsymbol{v}} && \text{in } \Omega^{\mathcal{F}}_{\boldsymbol{x}}(0),\\
\boldsymbol{v} &= \boldsymbol{v}_D && \text{on } \Gamma^{\mathcal{F}}_{D,\boldsymbol{x}}(t), t\in I,\\
\boldsymbol{\sigma}\cdot\boldsymbol{n} &= \boldsymbol{g} && \text{on } \Gamma^{\mathcal{F}}_{N,\boldsymbol{x}}(t), t\in I.
\end{aligned}
$$

$$\boldsymbol{\sigma} := -p\boldsymbol{I} + \mu(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)$$



FSI coupling conditions:

- Geometric coupling: Fluid- and solid-domains never detach or overlap
- Continuity of velocity: $\boldsymbol{v}^{\mathcal{F}} = \boldsymbol{v}^{\mathcal{S}}$ on $\Gamma^{\mathcal{I}}_{\boldsymbol{x}}(t)$
- Continuity of normal stresses: $\boldsymbol{\sigma}^{\mathcal{F}}\cdot\boldsymbol{n}^{\mathcal{F}}_{\boldsymbol{x}} = -\boldsymbol{\sigma}^{\mathcal{S}}\cdot\boldsymbol{n}^{\mathcal{S}}_{\boldsymbol{x}}$ on $\Gamma^{\mathcal{I}}_{\boldsymbol{x}}(t)$

Strategy for combination into one conservation equation: **Rewrite fluid equations in a “structure-appropriate” framework (ALE)**

Binary-Fluid–Structure Interaction, Governing equations

$$\hat{J}\left(\frac{\partial\varphi}{\partial t}\Big|_{\boldsymbol{\chi}} + \nabla_{\boldsymbol{\chi}}\varphi\left(\hat{\boldsymbol{F}}^{-1}(\boldsymbol{v}^{\mathcal{F}} - \partial_t\hat{\boldsymbol{\mathcal{A}}})\right) - \nabla_{\boldsymbol{\chi}}\cdot\left(\hat{J}\hat{\boldsymbol{F}}^{-1}m(\varphi)\nabla_{\boldsymbol{\chi}}\eta\right)\right) = 0 \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{F}}\times I,$$

$$\hat{J}\left(\eta - \hat{\sigma}\varepsilon^{-1}\frac{d\psi(\varphi)}{d\varphi} + \hat{\sigma}\varepsilon\,\nabla_{\boldsymbol{\chi}}\cdot\left(\hat{J}\hat{\boldsymbol{F}}^{-1}\nabla_{\boldsymbol{\chi}}\varphi\right)\right) = 0 \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{F}}\times I,$$

$$\begin{aligned}&\hat{J}\rho^{\mathcal{F}}(\varphi)\left(\frac{\partial\boldsymbol{v}^{\mathcal{F}}}{\partial t}\Big|_{\boldsymbol{\chi}} + \nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}}\left(\hat{\boldsymbol{F}}^{-1}(\boldsymbol{v}^{\mathcal{F}} - \partial_t\hat{\boldsymbol{\mathcal{A}}})\right)\right)\\ &-\nabla_{\boldsymbol{\chi}}\cdot\left(-\hat{\sigma}\varepsilon\,\hat{\boldsymbol{F}}^{-T}\nabla_{\boldsymbol{\chi}}\varphi\otimes\hat{\boldsymbol{F}}^{-T}\nabla_{\boldsymbol{\chi}}\varphi\right)\\ -\nabla_{\boldsymbol{\chi}}\cdot\left(\hat{J}\left(-p^{\mathcal{F}}\boldsymbol{I} + \mu^{\mathcal{F}}(\varphi)\left(\nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}}\hat{\boldsymbol{F}}^{-1} + \hat{\boldsymbol{F}}^{-T}(\nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}})^T\right)\right)\hat{\boldsymbol{F}}^{-T}\right) &= \hat{J}\rho^{\mathcal{F}}(\varphi)\boldsymbol{b}^{\mathcal{F}} \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{F}}\times I,\end{aligned}$$

$$\nabla_{\boldsymbol{\chi}}\cdot\left(\hat{J}\hat{\boldsymbol{F}}^{-1}\boldsymbol{v}^{\mathcal{F}}\right) = 0 \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{F}}\times I,$$

$$\hat{J}\rho^{\mathcal{S}}\frac{\partial\boldsymbol{v}^{\mathcal{S}}}{\partial t}\Big|_{\boldsymbol{\chi}} - \nabla_{\boldsymbol{\chi}}\cdot\hat{\boldsymbol{P}}^{\mathcal{S}} = \hat{J}\rho^{\mathcal{S}}\boldsymbol{b}^{\mathcal{S}} \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{S}}\times I,$$

$$\frac{\partial\boldsymbol{u}^{\mathcal{S}}}{\partial t} - \boldsymbol{v}^{\mathcal{S}} = 0 \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{S}}\times I,$$

$$\nabla_{\boldsymbol{\chi}}\cdot\left(\alpha_u\hat{J}^{-1}\nabla_{\boldsymbol{\chi}}\boldsymbol{u}^{\mathcal{F}}\right) = 0 \qquad \text{in } \Omega_{\boldsymbol{\chi}}^{\mathcal{F}}\times I,$$

$+$ initial and boundary conditions (e.g. nonlinear contact angle b.c. etc.).

BFSI, Function spaces

$$\boldsymbol{\mathcal{T}} := \{\boldsymbol{\mathcal{T}}^{\boldsymbol{v},\mathcal{F}} \times \boldsymbol{\mathcal{T}}^{\boldsymbol{v},\mathcal{S}} \times \boldsymbol{\mathcal{T}}^{\boldsymbol{u},\mathcal{F}} \times \boldsymbol{\mathcal{T}}^{\boldsymbol{u},\mathcal{S}} \times \mathcal{L}^{\mathcal{F}} \times \mathcal{L}^{\mathcal{S}}\}$$
$$\boldsymbol{\mathcal{W}} := \{\boldsymbol{\mathcal{W}}^{\boldsymbol{v},\mathcal{F}} \times \boldsymbol{\mathcal{W}}^{\boldsymbol{v},\mathcal{S}} \times \boldsymbol{\mathcal{W}}^{\boldsymbol{u},\mathcal{F}} \times \boldsymbol{\mathcal{W}}^{\boldsymbol{u},\mathcal{S}} \times \mathcal{L}^{\mathcal{F}} \times \mathcal{L}^{\mathcal{S}}\}$$

- Displacement trial and test spaces in the fluid domain:

$$\boldsymbol{\mathcal{T}}^{\boldsymbol{u},\mathcal{F}} := \{\boldsymbol{u}^{\mathcal{F}} \in \boldsymbol{\mathcal{H}}^1(\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}) \,|\, \boldsymbol{u}^{\mathcal{F}} = \boldsymbol{u}^{\mathcal{S}} \text{ on } \Gamma^{\mathcal{I}}_{\chi}, \boldsymbol{u}^{\mathcal{F}} = \boldsymbol{u}^{\mathcal{F}}_D \text{ on } \Gamma^{\mathcal{F}}_{D,\boldsymbol{\chi}}\}$$
$$\boldsymbol{\mathcal{W}}^{\boldsymbol{u},\mathcal{F}} := \{\boldsymbol{\phi}^{\boldsymbol{u},\mathcal{F}} \in \boldsymbol{\mathcal{H}}^1_0(\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}; \Gamma^{\mathcal{F}}_{D,\boldsymbol{\chi}}) \,|\, \boldsymbol{\phi}^{\boldsymbol{u},\mathcal{F}} = \boldsymbol{\phi}^{\boldsymbol{u},\mathcal{S}} \text{ on } \Gamma^{\mathcal{I}}_{\chi}\}$$

- Velocity trial and test spaces in the fluid domain:

$$\boldsymbol{\mathcal{T}}^{\boldsymbol{v},\mathcal{F}} := \{\boldsymbol{v}^{\mathcal{F}} \in \boldsymbol{\mathcal{H}}^1(\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}) \,|\, \boldsymbol{v}^{\mathcal{F}} = \boldsymbol{v}^{\mathcal{S}} \text{ on } \Gamma^{\mathcal{I}}_{\chi}, \boldsymbol{v}^{\mathcal{F}} = \boldsymbol{v}^{\mathcal{F}}_D \text{ on } \Gamma^{\mathcal{F}}_{D,\boldsymbol{\chi}}\}$$
$$\boldsymbol{\mathcal{W}}^{\boldsymbol{v},\mathcal{F}} := \{\boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}} \in \boldsymbol{\mathcal{H}}^1_0(\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}; \Gamma^{\mathcal{F}}_{D,\boldsymbol{\chi}}) \,|\, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}} = \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{S}} \text{ on } \Gamma^{\mathcal{I}}_{\chi}\}$$

- Phase field functions search space in the fluid domain: $\mathcal{H}^1(\Omega^{\mathcal{F}}_{\boldsymbol{\chi}})$
- Displacement trial and test space in the solid domain:

$$\boldsymbol{\mathcal{T}}^{\boldsymbol{u},\mathcal{S}} := \{\boldsymbol{u}^{\mathcal{S}} \in \boldsymbol{\mathcal{H}}^1(\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}) \,|\, \boldsymbol{u}^{\mathcal{S}} = \boldsymbol{u}^{\mathcal{S}}_D \text{ on } \Gamma^{\mathcal{S}}_{D,\boldsymbol{\chi}}\}, \qquad \boldsymbol{\mathcal{W}}^{\boldsymbol{u},\mathcal{S}} := \boldsymbol{\mathcal{H}}^1_0(\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}; \Gamma^{\mathcal{S}}_{D,\boldsymbol{\chi}})$$

- Velocity trial and test space in the solid domain:

$$\boldsymbol{\mathcal{T}}^{\boldsymbol{v},\mathcal{S}} := \{\boldsymbol{v}^{\mathcal{S}} \in \boldsymbol{\mathcal{H}}^1(\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}) \,|\, \boldsymbol{v}^{\mathcal{S}} = \boldsymbol{v}^{\mathcal{S}}_D \text{ on } \Gamma^{\mathcal{S}}_{D,\boldsymbol{\chi}}\}, \qquad \boldsymbol{\mathcal{W}}^{\boldsymbol{v},\mathcal{S}} := \boldsymbol{\mathcal{H}}^1_0(\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}; \Gamma^{\mathcal{S}}_{D,\boldsymbol{\chi}})$$

- Pressure function search spaces: $\mathcal{L}^m := \mathcal{L}^2(\Omega^m_{\boldsymbol{\chi}})/\mathbb{R}, \qquad m \in \{\mathcal{F}, \mathcal{S}\}$

BFSI, Operator splitting solution algorithm

while $t \leq T$ **do**

1. **Solve the nonlinear Cahn–Hilliard phase field problem**:
   Find $\varphi(\boldsymbol{x},t)$, $\eta(\boldsymbol{x},t) \in \mathcal{S} \times (0,T)$, s.t. $\forall\, \phi^{\varphi}, \phi^{\eta} \in \mathcal{V}$ it holds:

   $$\mathcal{F}_{\mathsf{CH}}((\varphi,\eta);(\phi^{\varphi},\phi^{\eta})) = 0 \qquad \text{Semilinear form}$$

   In each Newton iteration k,

   Find $\delta\varphi, \delta\eta \in \mathcal{S} \times (0,T)$, s.t.

   $$\mathcal{F}'_{\mathsf{CH}}((\varphi^k,\eta^k);(\delta\varphi,\delta\eta),(\phi^{\varphi},\phi^{\eta})) = -\mathcal{F}_{\mathsf{CH}}((\varphi^k,\eta^k);(\phi^{\varphi},\phi^{\eta})) \qquad \forall\, \phi^{\varphi}, \phi^{\eta} \in \mathcal{V}$$

   $$(\varphi^{k+1},\eta^{k+1}) = (\varphi^k,\eta^k) + \omega\,(\delta\varphi,\delta\eta)$$

2. **Solve the nonlinear monolithic (two-phase) FSI problem**:
   Find $\boldsymbol{U}(\boldsymbol{x},t) \in \boldsymbol{\mathcal{T}} \times (0,T)$, s.t. $\forall\, \boldsymbol{\Phi} \in \boldsymbol{\mathcal{W}}$ it holds

   $$\mathcal{F}_{\mathsf{FSI}}(\boldsymbol{U};\boldsymbol{\Phi}) = \sum_i \mathcal{F}_{\mathsf{FSI},i}(\boldsymbol{U};\boldsymbol{\Phi}) = 0 \qquad \text{Semilinear form}$$

   In each Newton iteration k,

   Find $\delta\boldsymbol{U}(\boldsymbol{x},t) \in \boldsymbol{\mathcal{T}} \times (0,T)$, s.t.

   $$\mathcal{F}'_{\mathsf{FSI}}(\boldsymbol{U}^k;\delta\boldsymbol{U},\boldsymbol{\Phi}) = -\mathcal{F}_{\mathsf{FSI}}(\boldsymbol{U}^k;\boldsymbol{\Phi}), \qquad \forall \boldsymbol{\Phi} \in \boldsymbol{\mathcal{W}}$$

   $$\boldsymbol{U}^{k+1} = \boldsymbol{U}^k + \omega\,\delta\boldsymbol{U},$$

end

BFSI, Variational formulation

$$
{}^{1}\mathcal{F}_{\mathsf{CH}}((\varphi,\eta);(\phi^{\varphi},\phi^{\eta})) :=
$$

$$
\left(\hat{J}\left(\frac{\partial\varphi}{\partial t}\Big|_{\boldsymbol{\chi}} + \nabla_{\boldsymbol{\chi}}\varphi\left(\hat{\boldsymbol{F}}^{-1}(\boldsymbol{v}^{\mathcal{F}} - \partial_t\hat{\boldsymbol{\mathcal{A}}})\right)\right), \phi^{\varphi}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}} + \hat{J}\left(\hat{J}\hat{\boldsymbol{F}}^{-1} m(\varphi)\nabla_{\boldsymbol{\chi}}\eta, \nabla_{\boldsymbol{\chi}}\phi^{\varphi}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}
$$

$$
+ \left(\hat{J}\left(\eta - \hat{\sigma}\varepsilon^{-1}\frac{d\psi(\varphi)}{d\varphi}\right), \phi^{\eta}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}} - \left(\hat{J}\hat{\sigma}\varepsilon\left(\hat{J}\hat{\boldsymbol{F}}^{-1}\nabla_{\boldsymbol{\chi}}\varphi\right), \nabla_{\boldsymbol{\chi}}\phi^{\eta}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}
$$

$+$ "contact angle b.c.".

$$
\mathcal{F}_{\mathsf{FSI}}(\boldsymbol{U};\boldsymbol{\Phi}) = \sum_i \mathcal{F}_{\mathsf{FSI},i}(\boldsymbol{U};\boldsymbol{\Phi})
$$

$$
\boldsymbol{U} := \{\boldsymbol{v}^{\mathcal{F}}, \boldsymbol{v}^{\mathcal{S}}, \boldsymbol{u}^{\mathcal{F}}, \boldsymbol{u}^{\mathcal{S}}, p^{\mathcal{F}}, p^{\mathcal{S}}\},
$$

$$
\boldsymbol{\Phi} := \{\boldsymbol{\phi}^{v,\mathcal{F}}, \boldsymbol{\phi}^{v,\mathcal{S}}, \boldsymbol{\phi}^{u,\mathcal{F}}, \boldsymbol{\phi}^{u,\mathcal{S}}, \phi^{p,\mathcal{F}}, \phi^{p,\mathcal{S}}\}.
$$

[1] $(\cdot,\cdot)_X := (\cdot,\cdot)_{\mathcal{L}^2(X)}$, and $\|\cdot\|_X := \|\cdot\|_{\mathcal{L}^2(X)}$

BFSI, Variational formulation

$$\mathcal{F}_{\mathsf{FSI},1}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(\hat{J}\rho^{\mathcal{F}}(\varphi)\left(\frac{\partial \boldsymbol{v}^{\mathcal{F}}}{\partial t}\bigg|_{\boldsymbol{\chi}} + \nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}}\left(\hat{\boldsymbol{F}}^{-1}(\boldsymbol{v}^{\mathcal{F}} - \partial_t\hat{\boldsymbol{\mathcal{A}}})\right)\right), \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}$$

$$+\left(\hat{J}\left(-p^{\mathcal{F}}\boldsymbol{I} + \mu^{\mathcal{F}}(\varphi)\left(\nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}}\hat{\boldsymbol{F}}^{-1} + \hat{\boldsymbol{F}}^{-T}(\nabla_{\boldsymbol{\chi}}\boldsymbol{v}^{\mathcal{F}})^T\right)\right)\hat{\boldsymbol{F}}^{-T}, \nabla_{\boldsymbol{\chi}}\boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}$$

$$+\left(\hat{\sigma}\varepsilon\,\hat{\boldsymbol{F}}^{-T}\nabla_{\boldsymbol{\chi}}\varphi \otimes \hat{\boldsymbol{F}}^{-T}\nabla_{\boldsymbol{\chi}}\varphi, \nabla_{\boldsymbol{\chi}}\boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}} - \left(\hat{J}\rho^{\mathcal{F}}(\varphi)\boldsymbol{f}^{\mathcal{F}}, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}} - \left(\boldsymbol{g}_0^{\mathcal{F}}, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{F}}\right)_{\Gamma^{\mathcal{F}}_{N,\boldsymbol{\chi}}}.$$

$$\mathcal{F}_{\mathsf{FSI},2}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(\nabla_{\boldsymbol{\chi}}\cdot\left(\hat{J}\hat{\boldsymbol{F}}^{-1}\boldsymbol{v}^{\mathcal{F}}\right), \phi^{p,\mathcal{F}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}.$$

$$\mathcal{F}_{\mathsf{FSI},3}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(\hat{J}\rho^{\mathcal{S}}\frac{\partial \boldsymbol{v}^{\mathcal{S}}}{\partial t}\bigg|_{\boldsymbol{\chi}}, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{S}}\right)_{\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}} + \left(\hat{\boldsymbol{P}}^{\mathcal{S}}, \nabla_{\boldsymbol{\chi}}\boldsymbol{\phi}^{\boldsymbol{v},\mathcal{S}}\right)_{\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}}$$

$$-\left(\hat{J}\rho^{\mathcal{S}}\boldsymbol{b}^{\mathcal{S}}, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{S}}\right)_{\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}} - \left(\boldsymbol{g}_0^{\mathcal{S}}, \boldsymbol{\phi}^{\boldsymbol{v},\mathcal{S}}\right)_{\Gamma^{\mathcal{S}}_{N,\boldsymbol{\chi}}}.$$

$$\mathcal{F}_{\mathsf{FSI},4}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(\frac{\partial \boldsymbol{u}^{\mathcal{S}}}{\partial t}\bigg|_{\boldsymbol{\chi}} - \boldsymbol{v}^{\mathcal{S}}, \boldsymbol{\phi}^{\boldsymbol{u},\mathcal{S}}\right)_{\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}}.$$

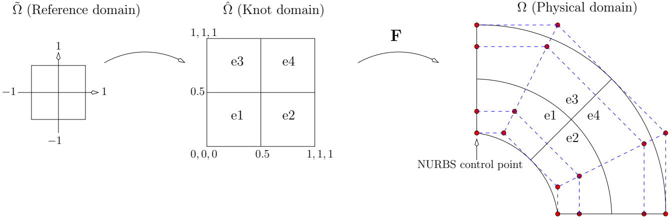
$$\mathcal{F}_{\mathsf{FSI},5}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(p^{\mathcal{S}}, \phi^{p,\mathcal{S}}\right)_{\Omega^{\mathcal{S}}_{\boldsymbol{\chi}}}.$$

$$\mathcal{F}_{\mathsf{FSI},6}(\boldsymbol{U};\boldsymbol{\Phi}) := \left(\alpha_u\hat{J}^{-1}\nabla_{\boldsymbol{\chi}}\boldsymbol{u}^{\mathcal{F}}, \nabla_{\boldsymbol{\chi}}\boldsymbol{\phi}^{\boldsymbol{u}}\right)_{\Omega^{\mathcal{F}}_{\boldsymbol{\chi}}}.$$

BFSI, Discrete Isogeometric approximation spaces

Approximation of velocity and pressure functions with LBB-stable Taylor-Hood like non-uniform rational B-spline space pairs $\hat{\mathbf{V}}_h^{TH}/\hat{Q}_h^{TH}$

$$\hat{\mathbf{V}}_h^{TH} \equiv \hat{\mathbf{V}}_h^{TH}(\mathbf{p},\boldsymbol{\alpha}) = \boldsymbol{\mathcal{N}}_{\alpha,\alpha}^{p+1,p+1} = \mathcal{N}_{\alpha,\alpha}^{p+1,p+1} \times \mathcal{N}_{\alpha,\alpha}^{p+1,p+1}$$
$$\hat{Q}_h^{TH} \equiv \hat{Q}_h^{TH}(\mathbf{p},\boldsymbol{\alpha}) = \mathcal{N}_{\alpha,\alpha}^{p,p}$$



Corresponding spaces $\mathbf{V}_h^{TH}$ and Q_h^{TH} in the physical domain Ω obtained via component-wise mapping using parametrization $\mathbf{F} : \hat{\Omega} \to \Omega$

$$\mathbf{V}_h^{TH} = \{\mathbf{v}_h = \hat{\mathbf{v}}_h \circ \mathbf{F}^{-1}, \hat{\mathbf{v}}_h \in \hat{\mathbf{V}}_h^{TH}\}, Q_h^{TH} = \{q_h = \hat{q}_h \circ \mathbf{F}^{-1}, \hat{q}_h \in \hat{Q}_h^{TH}\}$$

BFSI, Discrete problems

- Variational formulation of CH problem

$$\begin{cases} \mathcal{S}_h := \mathcal{H}^1(\Omega) \cap V_h^{TH} \\ \mathcal{V}_h := \mathcal{H}^1_0(\Omega) \cap V_h^{TH} \\ \text{Find } \varphi_h, \eta_h \in \mathcal{S}_h \times (0,T), \text{ s.t.} \\ \mathcal{F}_{\mathsf{CH}}((\varphi_h, \eta_h); (\phi_h^{\varphi}, \phi_h^{\eta})) = 0 \qquad \forall\, \phi_h^{\varphi}, \phi_h^{\eta} \in \mathcal{V}_h \end{cases}$$

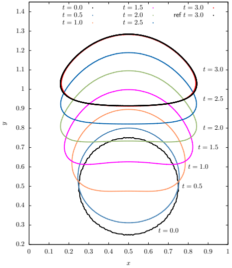
- Variational formulation of monolithic FSI problem

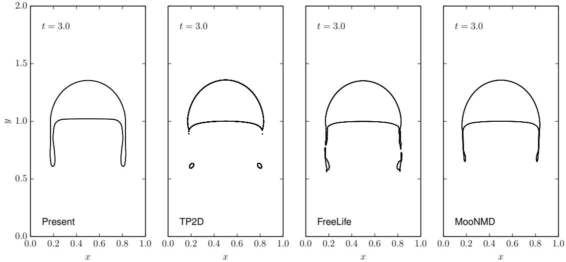
$$\begin{cases} \text{Let } f \in \{\boldsymbol{v}, \boldsymbol{u}\}, m \in \{\mathcal{F}, \mathcal{S}\} \\ \boldsymbol{\mathcal{T}}_h := \{\left(\boldsymbol{\mathcal{T}}^{f,m} \cap \mathbf{V}_h^{TH}\right) \times \left(\mathcal{L}^m \cap Q_h^{TH}\right)\} \\ \boldsymbol{\mathcal{W}}_h := \{\left(\boldsymbol{\mathcal{W}}^{f,m} \cap \mathbf{V}_h^{TH}\right) \times \left(\mathcal{L}^m \cap Q_h^{TH}\right)\} \\ \text{Find } \boldsymbol{U}_h = \{\boldsymbol{v}_h^{\mathcal{F}}, \boldsymbol{v}_h^{\mathcal{S}}, \boldsymbol{u}_h^{\mathcal{F}}, \boldsymbol{u}_h^{\mathcal{S}}, p_h^{\mathcal{F}}, p_h^{\mathcal{S}}\} \in \boldsymbol{\mathcal{T}}_h \times (0,T), \text{ s.t.} \\ \forall\, \boldsymbol{\Phi}_h = \{\boldsymbol{\phi}_h^{v,\mathcal{F}}, \boldsymbol{\phi}_h^{v,\mathcal{S}}, \boldsymbol{\phi}_h^{u,\mathcal{F}}, \boldsymbol{\phi}_h^{u,\mathcal{S}}, \phi_h^{p,\mathcal{F}}, \phi_h^{p,\mathcal{S}}\} \in \boldsymbol{\mathcal{W}}_h \\ \mathcal{F}_{\mathsf{FSI}}(\boldsymbol{U}_h; \boldsymbol{\Phi}_h) = 0 \end{cases}$$

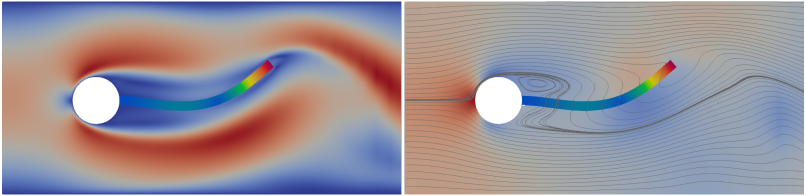
- Time discretization: Shifted Crank-Nicolson ($\theta = \frac{1}{2} + O(\delta t)$)

Model validation/Numerical experiments and results

- FeatFlow's Two-phase flow & FSI (Turek+Hron) benchmarks







- **Converged Two-phase flow & FSI results of high accuracy!**

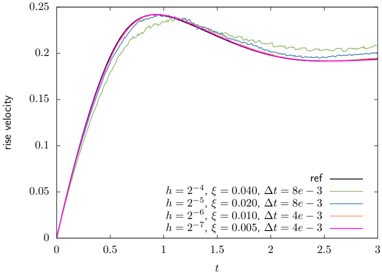
Model validation, RB, case 1, quantities over time

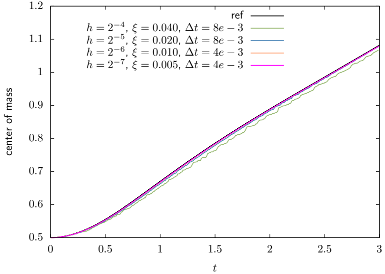
$$A_b = \int_{\Omega_2} 1 \, \mathrm{d}\boldsymbol{x},$$

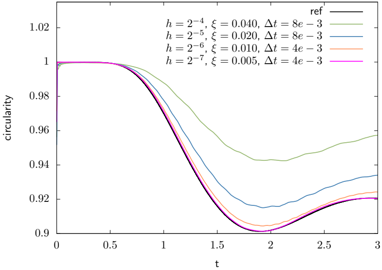
$$V_b = \int_{\Omega_2} \boldsymbol{v}.y \, \mathrm{d}\boldsymbol{x} / A_b \text{ (rise velocity)},$$

$$Y_b = \int_{\Omega_2} \boldsymbol{x}.y \, \mathrm{d}\boldsymbol{x} / A_b \text{ (center of mass)},$$

$$\not{c} = \frac{P_a}{P_b} = \frac{2\pi\sqrt{A_b/\pi}}{P_b} \text{ (circularity)}$$







Model validation, RB, case 1, convergence orders

$$\|e\|_1 = \frac{\sum_{t=1}^{N} |q_{t,\mathsf{ref}} - q_t|}{\sum_{t=1}^{N} |q_{t,\mathsf{ref}}|}, \; \|e\|_2 = \left(\frac{\sum_{t=1}^{N} |q_{t,\mathsf{ref}} - q_t|^2}{\sum_{t=1}^{N} |q_{t,\mathsf{ref}}|^2} \right)^{1/2}, \; \|e\|_\infty = \frac{\max_t |q_{t,\mathsf{ref}} - q_t|}{\max_t |q_{t,\mathsf{ref}}|},$$

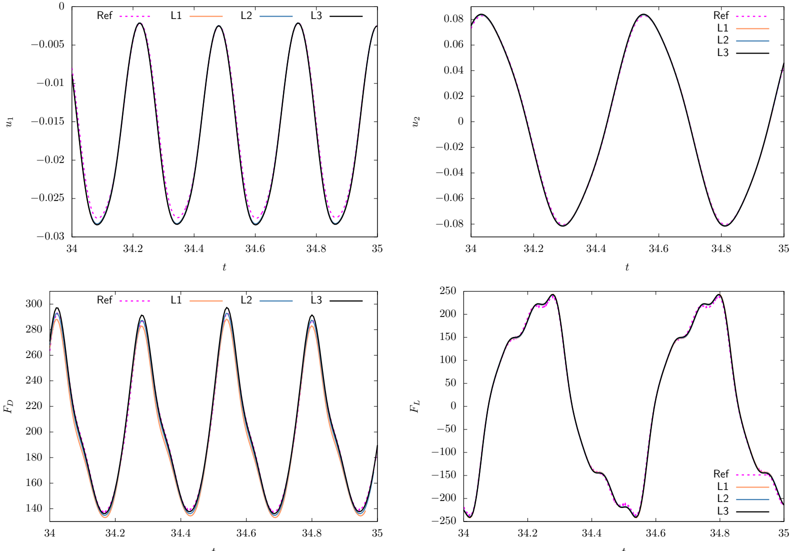
$$\mathsf{EOC}_{(\cdot)} = \frac{\log(\|e_{i-1}\|_{(\cdot)}/\|e_i\|_{(\cdot)})}{\log(h_{i-1}/h_i)}$$

q	h	EOC_1	$\mathsf{EOC}_1^{\mathsf{self,L7}}$	EOC_2	$\mathsf{EOC}_2^{\mathsf{self,L7}}$	EOC_∞	$\mathsf{EOC}_\infty^{\mathsf{self,L7}}$
Y_b	2^{-5}	1.7049	2.0024	1.6818	1.9263	1.4755	1.6026
	2^{-6}	1.4633	2.5718	1.5127	2.5136	1.5947	2.2132
	2^{-7}	0.5312		0.5706		0.8730	
V_b	2^{-5}	1.3263	1.3883	1.3518	1.3969	1.2714	1.2100
	2^{-6}	2.0064	2.3780	1.8934	2.3116	1.4112	2.0974
	2^{-7}	1.1755		1.0575		0.9790	
¢	2^{-5}	1.4927	1.5363	1.5095	1.5463	1.5051	1.1128
	2^{-6}	2.0446	2.3055	2.0443	2.2597	1.9111	1.6609
	2^{-7}	2.1778		2.0334		1.6871	

Order of convergence between 1 and ~ 2 in all norms

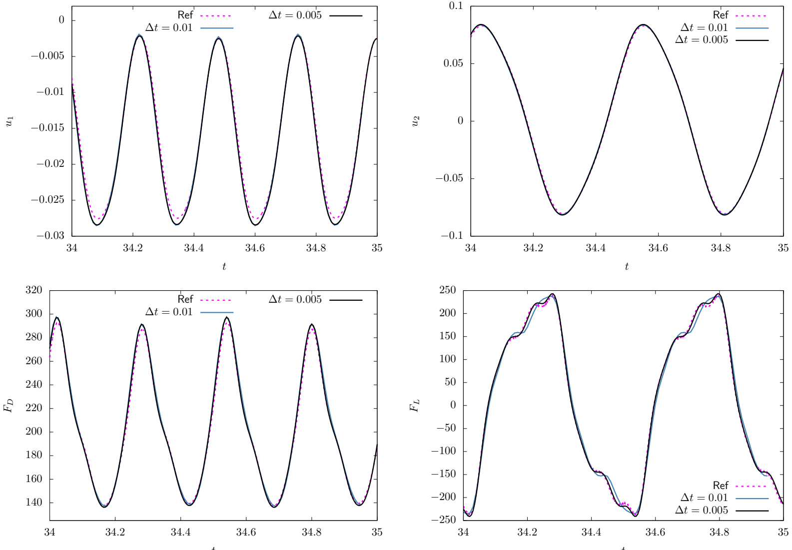
Model validation, FSI, case 2

Converged displacement ($\boldsymbol{u}$), Drag (F_D), Lift (F_L) profiles for $h \to 0$:



Model validation, FSI, case 2

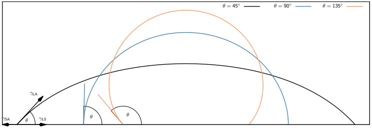
Converged displacement ($\boldsymbol{u}$), Drag (F_D), Lift (F_L) profiles for $\Delta t \to 0$:



Model validation, BFSI, Wetting

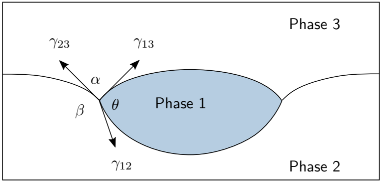
Young-Dupré equation (Static wetting law of a flat rigid solid):

$$\gamma_{SA} = \gamma_{LS} + \cos\theta_E\,\gamma_{LA}$$

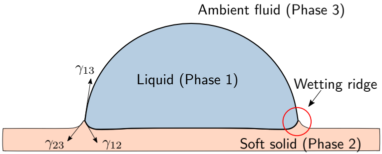


Neumann's law (3 immiscible fluids):

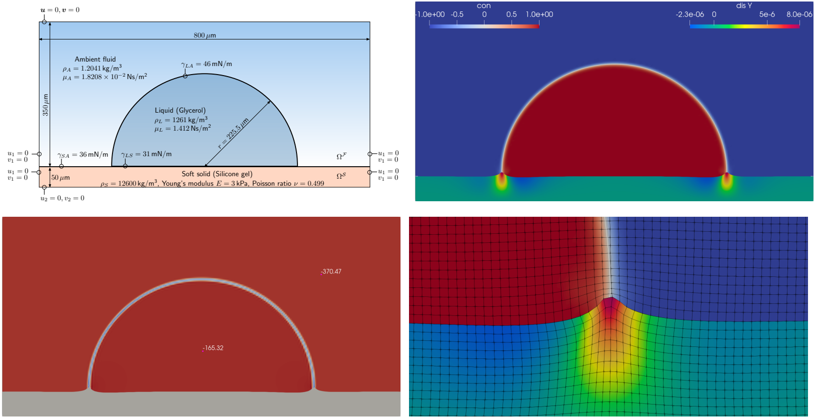
$$\gamma_{12}\,\boldsymbol{t}_{12} + \gamma_{13}\,\boldsymbol{t}_{13} + \gamma_{23}\,\boldsymbol{t}_{23} = \boldsymbol{0}$$



Wetting behavior of soft solids: Deformation of elastic solid as the result of the competition between surface forces and bulk elastic stresses.

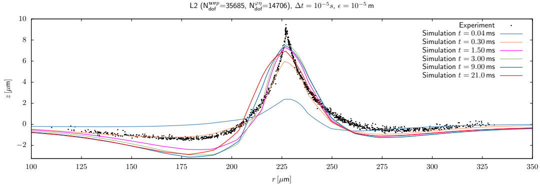


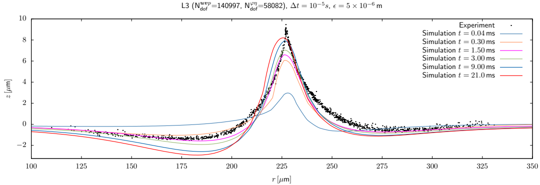
Model validation, BFSI, Wetting of soft solids

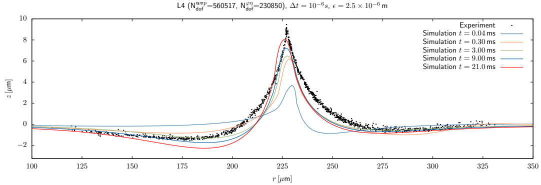


Laplace-Young law: $\delta p = \gamma_{LA}/r, \quad \rightsquigarrow |\delta p - \delta p_{\text{approx}}|/|\delta p| \approx 0.35\%$

Model validation, BFSI, Wetting of soft solids

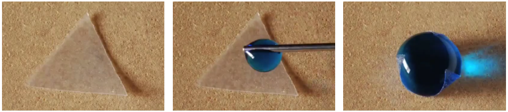






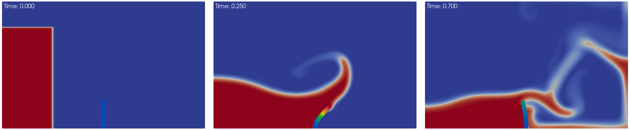
Summary

- Robust computational physics model for BFSI



- Idea: Sharp interface monolithic ALE-FSI method $\oplus$ Diffuse interface two-phase flow method

- "Quasi"-monolithic computational model + Isogeometric Analysis (Geometry, Analysis) $\rightarrow$ Robust BFSI system with
  - highly accurate numerical results for two-phase flow and single-phase FSI
  - "acceptable" numerical results for BFSI (work in progress..)



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