Finite Element Techniques for the Simulation of Two-phase Incompressible Flows

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Free ....

Outline

Introduction:

- Standard model for two-phase flow.

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Nitsche's method for a mass transport problem:

- Explanation of the method.
- Results of numerical experiments.

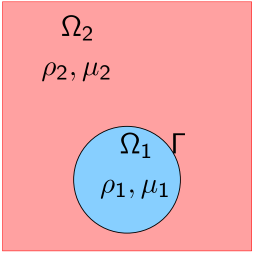
Sharp Interface Model for two-phase flows with interfacial phenomena

Fluid dynamics in the two phases

Incompressible Navier-Stokes in the subdomains:

Domains: $\Omega_1 = \Omega_1(t)$, $\Omega_2 = \Omega_2(t)$

Interface: $\Gamma = \Gamma(t)$



ρ_i: density in Ω_i
μ_i: viscosity in Ω_i

$\mathbf{D}(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T$, $\boldsymbol{\sigma} = -p\,\mathbf{I} + \mu \mathbf{D}(\mathbf{u})$

$$\begin{cases} \rho_i(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) = \operatorname{div}(\boldsymbol{\sigma}) + \rho_i \mathbf{g} \\ \qquad = -\nabla p + \operatorname{div}(\mu_i \mathbf{D}(\mathbf{u})) + \rho_i \mathbf{g} & \text{in } \Omega_i \quad \text{for } i = 1,2 \\ \operatorname{div} \mathbf{u} = 0 & \text{in } \Omega_i \end{cases}$$

Interfacial effects

$$\text{Force on } \gamma = \int_{\partial\gamma} \boldsymbol{\sigma}_\Gamma n \, ds = \int_\gamma \operatorname{div}_\Gamma \boldsymbol{\sigma}_\Gamma \, ds$$

Interfacial surface force: $\operatorname{div}_\Gamma \boldsymbol{\sigma}_\Gamma$

Coupling interface-fluid

$$\begin{aligned} V_\Gamma &= \mathbf{u} \cdot \mathbf{n} \quad \text{(immiscibility)} \\ [\mathbf{u}]_\Gamma &= 0 \quad \text{(viscosity)} \\ [\boldsymbol{\sigma}\mathbf{n}]_\Gamma &= \operatorname{div}_\Gamma \boldsymbol{\sigma}_\Gamma \quad \text{(momentum conservation)} \end{aligned}$$

Classical models

Interfacial effects

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Classical models

Clean interface: only surface tension

$$\boldsymbol{\sigma}_\Gamma = \tau \mathbf{P} \quad \text{with} \quad \mathbf{P} := \mathbf{I} - \mathbf{n}\mathbf{n}^T \quad \text{(projection on } \Gamma)$$

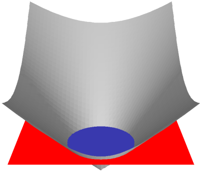
then

$$\operatorname{div}_\Gamma \boldsymbol{\sigma}_\Gamma = -\tau\kappa\mathbf{n} + \nabla_\Gamma \tau \qquad (\kappa\text{: curvature of } \Gamma)$$

"Modeling" of the interface: Level set approach

$\Gamma(t)$ = zero-level of a scalar function:

the level set function $\varphi(x,t)$



$$\varphi(x,t) = \begin{cases} < 0 & \text{for } x \text{ in phase } \Omega_1 \\ > 0 & \text{for } x \text{ in phase } \Omega_2 \\ = 0 & \text{at the interface} \end{cases}$$

should be an *"approximate signed distance function"*.

$$x(t) \in \Gamma(t) \quad \Rightarrow \quad \varphi(x(t),t) = 0.$$

Level set equation

$$\varphi_t + \mathbf{u} \cdot \nabla\varphi = 0$$

Fluid dynamics model: Navier-Stokes + LS equation

Navier-Stokes equations coupled with level set equation

$$\begin{aligned} \rho(\varphi)\Big(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\Big) - \mathrm{div}\Big(\mu(\varphi)\,\mathbf{D}(\mathbf{u})\Big) + \nabla p &= \rho(\varphi)\,g + \delta_\Gamma(\varphi)\,\mathrm{div}_\Gamma\,\boldsymbol{\sigma}_\Gamma \\ \mathrm{div}\,\mathbf{u} &= 0 \\ \varphi_t + \mathbf{u}\cdot\nabla\varphi &= 0 \end{aligned}$$

Localized force term in weak formulation

$$f_\Gamma(\mathbf{v}) = \int_\Gamma (\mathrm{div}_\Gamma\,\boldsymbol{\sigma}_\Gamma)\cdot\mathbf{v}\;ds, \qquad f_\Gamma \in H^{-1}(\Omega)$$

Accurate discretization of f_Γ is essential!.

Fluid dynamics + mass- and surfactant transport

Mass transport (or heat transport)

$$\begin{aligned} \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c &= D(\varphi)\Delta c, \\ [D(\varphi)\nabla c \cdot \mathbf{n}] &= 0 \quad \text{at the interface,} \\ c_1 &= C_H c_2 \quad \text{at the interface.} \end{aligned}$$

D: piecewise constant. Henry condition: discontinuity in c.

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Transport of surfactants: PDE on $\Gamma(t)$

$$\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S + S \mathrm{div}_\Gamma \mathbf{u} = \mathrm{div}_\Gamma (D_\Gamma \nabla_\Gamma S) \quad \text{on} \quad \Gamma$$

with D_Γ: interfacial diffusion coefficient.

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No chemical reactions considered!

Numerical issues

Numerical challenges

- Unknown interface $\Gamma(t)$.
- Highly nonlinear couplings between $\mathbf{u}$, φ, $f_{\Gamma(\varphi)}$, c, S.
- Treatment of force balance $[\boldsymbol{\sigma}\mathbf{n}]_\Gamma = \operatorname{div}_\Gamma \boldsymbol{\sigma}_\Gamma$ (driving interfacial forces)
- Discontinuities (in p, ρ, μ, c) across $\Gamma(t)$.
- PDE on the evolving interface.

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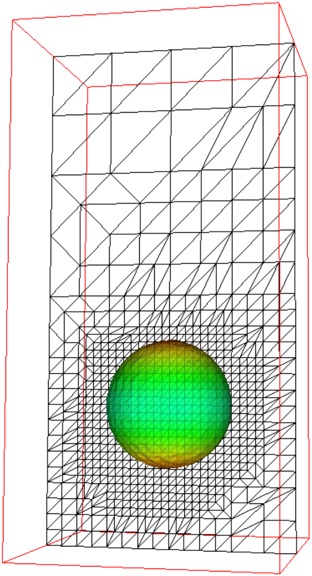
Demand for:

- Adaptive space discretization, that can handle discontinuities.
- Accurate time integration, that can handle moving discontinuities.
- Methods for PDEs on interfaces.
- Efficient and robust iterative solvers.

Examples of numerical simulations

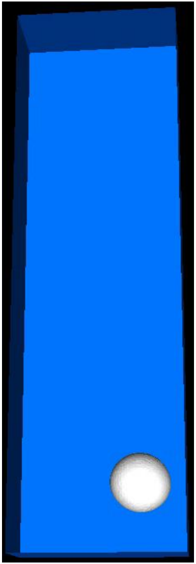
Multilevel adaptive finite elements



Rising butanol droplet: fluid dynamics

system: n-butanol/water

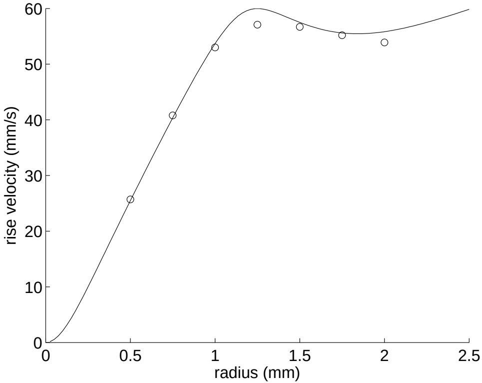
drop radius $r = 3\,mm \quad \rightsquigarrow$ wobbling

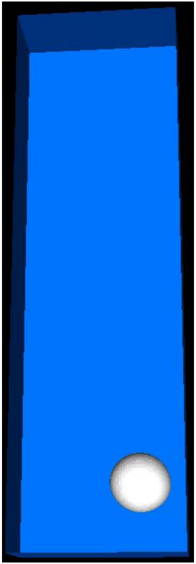


Rising butanol droplet: fluid dynamics

system: n-butanol/water

rise velocity vs. drop radius





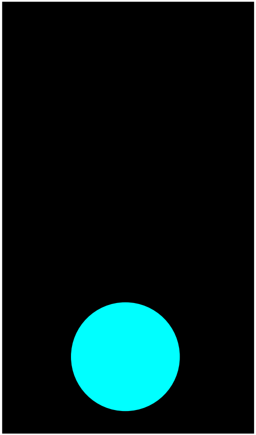
Rising droplet with surfactant transport

- gravity-driven butanol-droplet (diam. 4mm) in water, interfacial tension 1.63mN/m
- Velocity field determined from NS-equations.

$+$ surfactant eqn. $\dot{S} - D_\Gamma \Delta_\Gamma S + (\nabla_\Gamma \cdot \mathbf{v})S = 0$

- τ does **not** depend on S.

solution



Observation

- accumulation of surfactant at the bottom.

A few numerical aspects

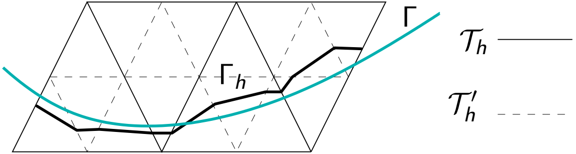
Approximation of Γ by Γ_h (hybrid level set)

Γ = zero level of φ (= level set function)

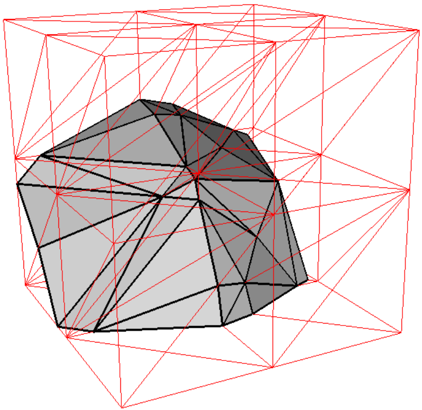
φ_h = piecewise quadratic FE approximation of φ.

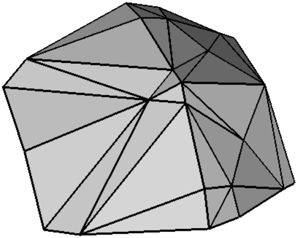
Our strategy for Γ_h:

$$\varphi_h \text{ (piecewise } P_2) \quad \rightarrow \quad I(\varphi_h) \text{ (piecewise } P_1 \text{ on refined mesh).}$$



Approximation of Γ by Γ_h: 3D illustration





Mass transport equation

Strong formulation

$$
\begin{aligned}
\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \mathrm{div}(\alpha \nabla u) &= f \quad \text{in} \ \ \Omega_i, \ \ i = 1, 2, \ \ t \in [0, T], \\
[\alpha \nabla u \cdot \mathbf{n}]_\Gamma &= 0, \\
[\beta u]_\Gamma &= 0, \\
u(\cdot, 0) &= u_0 \quad \text{in} \ \ \Omega_i, \ \ i = 1, 2, \\
u(\cdot, t) &= 0 \quad \text{on} \ \ \partial\Omega, \quad t \in [0, T].
\end{aligned}
$$

With $\alpha = \alpha_i > 0$, $\beta = \beta_i > 0$.

Space-time weak formulation

Assumptions: $u_0 = 0$, $\operatorname{div} \mathbf{w} = 0$, $V_\Gamma = \mathbf{w} \cdot \mathbf{n}$ (Γ transported by $\mathbf{w}$).
Space-time: $Q_T := \Omega \times (0, T)$,
$\Gamma_* := \{ (x, t) \mid x \in \Gamma(t),\ t \in (0, T) \}$.

$$Q_i := \{ (x, t) \mid x \in \Omega_i(t),\ t \in (0, T) \}, \quad i = 1, 2.$$

Spaces (anisotropic; $Q_T = Q_1 \cup Q_2$):

$$H^{1,0}(Q_i) = \{ u \in L^2(Q_i) \mid \frac{\partial u}{\partial x_j} \in L^2(Q_i), \ \ j = 1, 2, 3 \}$$

$$H_0^{1,0}(Q_T) = \{ u \in L^2(Q_T) \mid \frac{\partial u}{\partial x_j} \in L^2(Q_T), \ \ j = 1, 2, 3, \ \ u_{|\partial\Omega} = 0 \}$$

$$V_\beta = \{ u \in L^2(Q_T) \mid u_i \in H^{1,0}(Q_i),\ i = 1, 2,\ u_{|\partial\Omega} = 0,\ [\beta u]_{\Gamma_*} = 0 \}$$

$$W_\beta = \{ v \in V_\beta \mid \frac{\partial v}{\partial t} \in H_0^{1,0}(Q_T)' \}.$$

Well-posed weak formulation

Determine $u \in W_\beta$ with $u(\cdot,0)=0$ such that

$$\frac{\partial u}{\partial t}(v) - \int_{Q_T} u\mathbf{w}\cdot\nabla v \, dx\, dt + \sum_{i=1}^{2}\int_{Q_i}\alpha_i \nabla u_i \cdot \nabla v \, dx\, dt = \int_{Q_T} fv \, dx\, dt$$

for all $v \in H_0^{1,0}(Q_T)$

Note:

- Space-time formulation.
- Trial functions are discontinuous across Γ_*.
- Condition $[\beta u]_\Gamma = 0$ essential condition in space W_β.

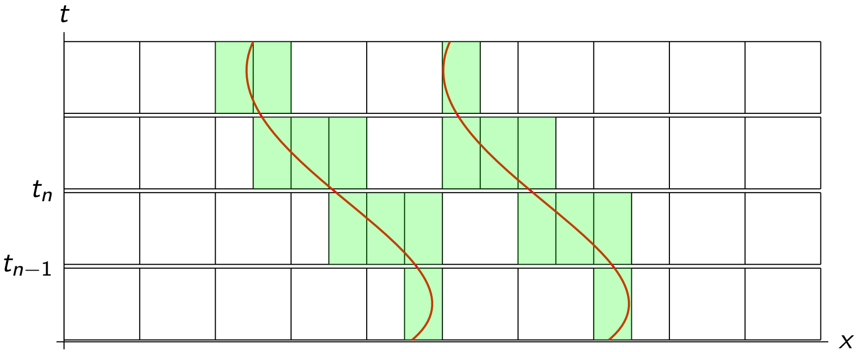
Nitsche-DG-XFEM discretization

Space-time FE.

$I_n = (t_{n-1}, t_n]$. $Q^n = \Omega \times I_n$. V_n : standard FE space on Ω.

$$W_n := \{\, v : Q^n \to \mathbb{R} \mid v(x,t) = \phi_0(x) + t\phi_1(x), \quad \phi_0, \phi_1 \in V_n \,\} \tag{1}$$

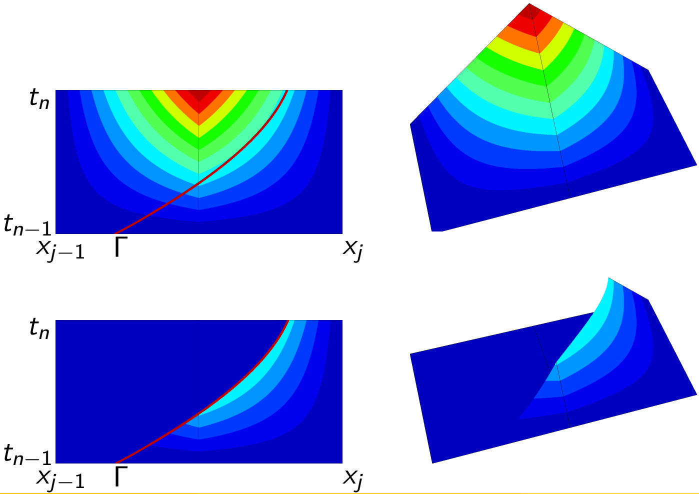
$$W := \{\, v : Q \to \mathbb{R} \mid v_{|Q^n} \in W_n \,\} \quad \text{(space-time FE).} \tag{2}$$



Space-time XFEM.

$$Q_i^n := \cup_{t \in I_n} \Omega_i(t), \quad R_i^n: \ \text{restiction to } Q_i^n$$

$$W_n^\Gamma := R_1^n W_n \oplus R_2^n W_n, \quad W^{\Gamma *} := \{\, v: \ Q \to \mathbb{R} \mid v_{|Q^n} \in W_n^\Gamma \,\}$$



Bilinear forms

$$a^n(u,v) = \sum_{i=1}^{2} \int_{Q_i^n} (\frac{\partial u_i}{\partial t} + \mathbf{w}\cdot\nabla u_i)\beta_i v_i + \alpha_i\beta_i\nabla u_i\cdot\nabla v_i \, dx\, dt$$

Discontinuous Galerkin (DG) w.r.t. time:

$$d^n(u,v) = \int_{\Omega} \beta(\cdot,t_n)[u]^{n-1} v_+^{n-1}\, dt$$

Nitsche method for Henry condition:

$$N_{\Gamma_*}^n(u,v) = -\int_{\Gamma_*^n} \{\alpha\nabla u\cdot\mathbf{n}\}_{\Gamma_*}[\beta v]_{\Gamma_*}\, ds - \int_{\Gamma_*^n} \{\alpha\nabla v\cdot\mathbf{n}\}_{\Gamma_*}[\beta u]_{\Gamma_*}\, ds$$
$$+ \lambda h_n^{-1}\int_{\Gamma_*^n} [\beta u]_{\Gamma_*}[\beta v]_{\Gamma_*}\, ds,$$

with $\{\cdot\}_{\Gamma_*}$ a suitable area weighted average. $\lambda > 0$: stablization parameter.

$$a(u,v) = \sum_{n=1}^{N} a^n(u,v), \quad \text{similarly}: \quad d(u,v),\ N_{\Gamma_*}(u,v).$$

Nitsche-DG-XFEM variational problem

Determine $U \in W^{\Gamma_*}$ such that

$$B(U,V) = f(V) \quad \text{for all} \quad V \in W^{\Gamma_*},$$
$$B(U,V) := a(U,V) + d(U,V) + N_{\Gamma_*}(U,V).$$

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Error analysis for linear FE

Theorem.

$$\|(u-U)(\cdot,t_N)\|_{L^2(\Omega)} \leq c(h^2 + \Delta t^2).$$

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Error analysis for linear FE

Theorem.

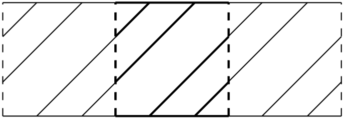
$$\|(u-U)(\cdot,t_N)\|_{L^2(\Omega)} \leq c(h^2 + \Delta t^2).$$

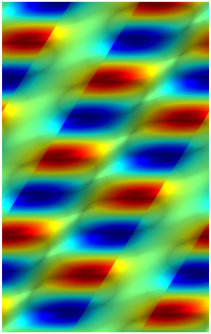
Remark: for standard space-time DG [V. Thomee] (no Nitsche, no XFEM):

$$\|(u-U)(\cdot,t_N)\|_{L^2(\Omega)} \leq c(h^2 + \Delta t^3)$$

Numerical experiment

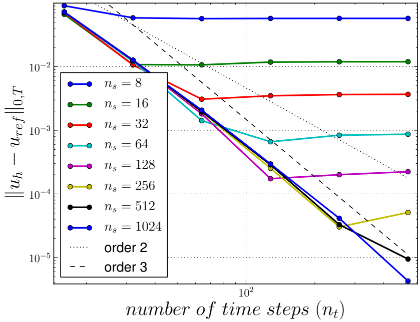
One-dimensional, linear interface velocity, periodic BC.



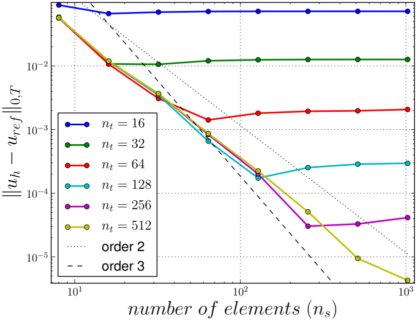


Discretization error

Error: $\|(U-u)(\cdot,t_N)\|_{L^2(\Omega)}$, $\Delta t = h$.



This indicates: $\|(U-u)(\cdot,t_N)\|_{L^2(\Omega)} \sim \Delta t^3$ if h sufficiently small.



This indicates: $\|(U-u)(\cdot,t_N)\|_{L^2(\Omega)} \sim h^2$ of Δt sufficiently small.