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A curvature-free level set FEM approach for multiphase flow problems

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Modeling of two phase flows

- The incompressible Navier-Stokes equations

$$\rho(\Gamma)\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) - \nabla\cdot\boldsymbol{\tau} + \nabla p = 0,$$

$$\nabla\cdot\boldsymbol{u} = 0$$

- Viscous stress

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s = 2\mu(\Gamma)\mathbf{D}(\boldsymbol{u})$$

- Interfacial boundary conditions

$$[\boldsymbol{u}]\,|_\Gamma = 0$$

$$-\left[-p\mathbf{I} + \tau\right]_{|\Gamma}\cdot\boldsymbol{n} = \sigma\kappa\boldsymbol{n}$$

Direct interface conditions implementation is impractical due to the

unknown interface location Γ

Interface Tension Force

- Implicit interface condition by restriction of volume force

$$\boldsymbol{f}_{\mathrm{st}|_\Gamma} = \sigma\kappa\boldsymbol{n}, \quad \kappa = -\nabla\cdot\boldsymbol{n} \quad on \quad \Gamma$$

- Non-homogeneous incompressible Navier-Stokes equations

$$\rho(\Gamma)\left(\frac{\partial\boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) - \nabla\cdot(2\mu(\Gamma)\mathbf{D}(\boldsymbol{u})) + \nabla p = \boldsymbol{f}_{st},$$

$$\nabla\cdot\boldsymbol{u} = 0$$

Challenges

Surface tension forces pose some challenging problems

- As a source term, it is not appropriately treated w.r.t. to mixed FE approximation of Navier-Stokes problem
- If treated explicitly leads to the capillary time step restriction

$$\triangle t^{(ca)} < \sqrt{\frac{\langle \rho \rangle h^3}{2\pi\sigma}}$$

Aim

Remove the surface tension as force term

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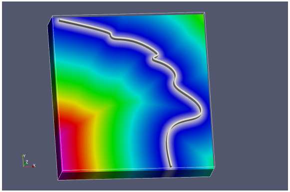
Methodology

- Embedding the interface in a higher dimentional function



The level Zero represents the interface.

- Governing equation for level set function

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi = 0$$

This transport equation can be efficiently solved due to the choice of a smooth level set function

Advantages

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- Exact representation of the interface e. g.

$$\Gamma = \{\boldsymbol{x} \in \Omega, \varphi = 0\},$$

- Provides the geometric quantities $\boldsymbol{n}$ and κ

$$\boldsymbol{n} = \frac{\nabla \varphi}{\|\nabla \varphi\|}, \quad \kappa = -\nabla \cdot \boldsymbol{n}$$

- Flexible w.r.t. topological changes

The signed distance function is the natural choice for the level set !

Volume integrals of surface force

Finite element methods allow for surface internal as a volume integral

- Introducing the δ_Γ function

$$\int_\Gamma \boldsymbol{f}_{st} \boldsymbol{v} dx = \int_\Gamma \kappa\sigma \boldsymbol{n}_{|_\Gamma} \boldsymbol{v} dx = \int_\Omega \kappa\sigma \boldsymbol{n} \delta_\Gamma \boldsymbol{v} dx$$

$$\boldsymbol{f}_{\mathrm{CSF},1} = \kappa\sigma \boldsymbol{n} \delta_\Gamma$$

- Regularization of δ_Γ with the help of level set function

$$\delta_\Gamma^\epsilon(x) = \begin{cases} \frac{1}{\epsilon}\varphi(x/\epsilon) & \text{if } |x| \leq \epsilon = mh \\ 0 & \text{if } |x| > \epsilon = mh \end{cases}$$

$$\boldsymbol{f}_{\mathrm{st}} = \kappa\sigma \boldsymbol{n}_{|_\Gamma} \longrightarrow \boldsymbol{f}_{\mathrm{CSF},1} = \kappa\sigma \boldsymbol{n} \delta_\Gamma \simeq \kappa\sigma \boldsymbol{n} \delta_\Gamma^\epsilon$$

Problems and Challenges

Explicit treatment

- Surface tension forces
  - Capillary time step restriction
  - Not appropriately treated w.r.t. to mixed regularity of physical quantities, velocity and pressure.
- Reinitialization: Brute force, PDE, Algebraic Newton, $\cdots$
  - Requires perfect description of the interface w.r.t. FE
    $\longrightarrow$ in a conflictual with the Eulerian approach of level set $\longleftarrow$

Towards a fully implicit treatment

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Volume integrals of surface force

Finite element methods allow for surface internal as a volume integral

- Introducing finite element cutoff function ψ

$$\psi(\varphi) = \begin{cases} +1 & \text{if } \varphi \geq 0 \\ 0 & \text{if } \varphi < 0 \end{cases} \longrightarrow \quad \begin{aligned} \int_\Gamma \boldsymbol{f}_{st} \boldsymbol{v} dx &= \int_\Gamma \kappa\sigma \boldsymbol{n}_{|\Gamma} \boldsymbol{v} dx \\ &= \int_\Omega \kappa\sigma\nabla\psi \boldsymbol{v} dx \end{aligned}$$

$$\boldsymbol{f}_{\mathrm{CSF},2} = \sigma\kappa\nabla\psi$$

- Advantages
  - Enhances the accuracy
  - ψ is material characteristic and can be used for conservative level set
- Disadvantages
  - Explicit treatment of curvature requires high regularity of ψ

$$\kappa = -\nabla \cdot \boldsymbol{n}, \quad \boldsymbol{n} = \frac{\nabla\psi}{\|\nabla\psi\|}.$$

Implicit treatment of curvature

$$\kappa = -\nabla \cdot \boldsymbol{n}, \quad \boldsymbol{n} = \frac{\nabla\psi}{\|\nabla\psi\|}.$$

Then,

$$\begin{aligned}
\boldsymbol{f}_{\mathrm{CSF},2} &= -\sigma\nabla\cdot\left(\frac{\nabla\psi}{\|\nabla\psi\|}\right)\nabla\psi \\
&= -\sigma\left(\frac{\nabla\cdot\nabla\psi}{\|\nabla\psi\|} - \frac{\nabla\|\nabla\psi\|\,\nabla\psi}{\|\nabla\psi\|^2}\right)\nabla\psi \\
&= -\sigma\left(\frac{1}{\|\nabla\psi\|}\triangle\psi\nabla\psi - \nabla\|\nabla\psi\|\right).
\end{aligned}$$

Moreover, we have

$$\triangle\psi\nabla\psi = \nabla\cdot(\nabla\psi\otimes\nabla\psi) - \frac{1}{2}\nabla\|\nabla\psi\|^2.$$

Implicit treatment of curvature

$$\frac{1}{\|\nabla\psi\|}\triangle\psi\nabla\psi = \frac{\nabla\cdot(\nabla\psi\otimes\nabla\psi)}{\|\nabla\psi\|} - \frac{1}{2}\frac{\nabla\|\nabla\psi\|^2}{\|\nabla\psi\|}$$
$$= \nabla\cdot\left(\frac{\nabla\psi\otimes\nabla\psi}{\|\nabla\psi\|}\right) + \frac{(\nabla\psi\otimes\nabla\psi)\nabla\|\nabla\psi\|}{\|\nabla\psi\|^2} - \nabla\|\nabla\psi\|$$
$$= \nabla\cdot\left(\frac{\nabla\psi\otimes\nabla\psi}{\|\nabla\psi\|}\right) - \left(\mathbf{I} - \frac{\nabla\psi}{\|\nabla\psi\|}\otimes\frac{\nabla\psi}{\|\nabla\psi\|}\right)\nabla\|\nabla\psi\|$$
$$= \nabla\cdot\left(\frac{\nabla\psi\otimes\nabla\psi}{\|\nabla\psi\|}\right) - \nabla_s\|\nabla\psi\|$$

where $\nabla_s = (\mathbf{I} - \boldsymbol{n}\otimes\boldsymbol{n})\nabla$

$$\boldsymbol{f}_{\mathrm{CSF},2} = -\sigma\left\{\nabla\cdot\left(\frac{\nabla\psi\otimes\nabla\psi}{\|\nabla\psi\|}\right) - \nabla\|\nabla\psi\|\right\}.$$

Curvature-free CSF

$$\boldsymbol{f}_{\text{CSF},3} = -\sigma\nabla \cdot \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|} \right)$$

where the pressure

$$\nabla p_{\text{CSF},3} = \nabla p_{\text{CSF},1/2} - \sigma\nabla \|\nabla\psi\|$$

$$\begin{aligned}\int_\Omega \boldsymbol{f}_{\text{CSF},3} \boldsymbol{v} \, d\Omega &= \int_\Omega -\sigma\nabla \cdot \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|} \right) \boldsymbol{v} dx \\ &= \int_\Omega \sigma \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|} \right) : \mathbf{D}(\boldsymbol{v}) \, dx\end{aligned}$$

Less regularity requirement for ψ

Curvature-free multiphase flows

New multiphase stress $\boldsymbol{\tau}_m$

$$\boldsymbol{\tau}_m = -\sigma \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|} \right)$$

New set of equations for multiphase flows

$$\begin{cases} \rho(\psi) \left(\dfrac{\partial \boldsymbol{u}}{\partial t} + u \cdot \nabla \boldsymbol{u} \right) - \operatorname{div} \boldsymbol{\tau} + \nabla p = 0 \\ \nabla \cdot \boldsymbol{u} = 0 \\ \boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_m \end{cases}$$

where the stresses

$$\boldsymbol{\tau}_m = -\sigma \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|} \right), \quad \tau_s = 2\mu(\psi)\mathbf{D}(\boldsymbol{u})$$

The momentum equation gets rid of the CSF force terms

Preserving signed distance function

The distance based level set equations have the constraint

$$\|\nabla\varphi\| = 1 \quad \Longleftrightarrow \quad \boldsymbol{n}\cdot\nabla\varphi = 1,\ \boldsymbol{n} = \frac{\nabla\varphi}{\|\nabla\varphi\|}$$

Impose the constraint on the variational formulation

- Variational formulation

$$\int_\Omega \left(\frac{\partial\varphi}{\partial t} + \boldsymbol{u}\cdot\nabla\varphi\right)\phi\,dx + \gamma_{nd}\int_\Omega (\boldsymbol{n}\cdot\nabla\varphi)\ (\boldsymbol{n}\cdot\nabla\phi)\ dx = \gamma_{nd}\int_\Omega \boldsymbol{n}\cdot\nabla\phi\,dx \qquad \forall\phi\in H^1(\Omega)$$

- Continuous problem

$$\frac{\partial\varphi}{\partial t} + \boldsymbol{u}\cdot\nabla\varphi - \gamma_{nd}\nabla\cdot\left(\left(\frac{\nabla\varphi}{\|\nabla\varphi\|}\cdot\nabla\varphi - 1\right)\frac{\nabla\varphi}{\|\nabla\varphi\|}\right) = 0$$

where γ_{nd} is a relaxation parameter.

Characteristic material PDE

- The material cutoff function ψ can be derived directly from the signed distance function

$$\psi^{\epsilon}(\varphi) = \frac{-1}{1+\exp(\varphi/\epsilon)} + 0.5$$

- PDE for ψ

$$\frac{\partial \psi}{\partial \tau} + \underbrace{\nabla \cdot (\gamma_{nc}\psi(1-\psi)\nabla\varphi)}_{\textbf{Conv. normal}} - \underbrace{\nabla \cdot (\gamma_{nd}(\nabla\psi \cdot \nabla\varphi)\ \nabla\varphi)}_{\textbf{Diff. normal}} = 0$$

Conv. normal: nonlinear convection tends to build the Heaviside step function

Diff. normal: normal diffusion control the sharpness of the interface

Curvature-free level set PDE

$$\begin{cases} \rho(\psi)\left(\frac{\partial \boldsymbol{u}}{\partial t} + u \cdot \nabla \boldsymbol{u}\right) - \operatorname{div} \boldsymbol{\tau} + \nabla p = 0 \\ \nabla \cdot \boldsymbol{u} = 0 \\ \boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_m \end{cases}$$

- viscous stress

$$\tau_s = 2\mu(\psi)\mathbf{D}(\boldsymbol{u})$$

- multiphase stress

$$\boldsymbol{\tau}_m = -\sigma \left(\frac{\nabla\psi \otimes \nabla\psi}{\|\nabla\psi\|}\right)$$

- new level set PDE

$$\begin{cases} \frac{\partial \varphi}{\partial t} + \boldsymbol{u} \cdot \nabla\varphi - \gamma_{nd} \nabla \cdot \left(\left(\frac{\nabla\varphi}{\|\nabla\varphi\|} \cdot \nabla\varphi - 1\right)\frac{\nabla\varphi}{\|\nabla\varphi\|}\right) = 0 \\ \frac{\partial \psi}{\partial \tau} + \nabla \cdot (\gamma_{nc}\psi(1-\psi)\nabla\varphi) - \nabla \cdot (\gamma_{nd}(\nabla\psi \cdot \nabla\varphi)\ \nabla\varphi) = 0 \end{cases}$$

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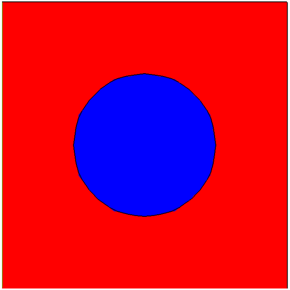
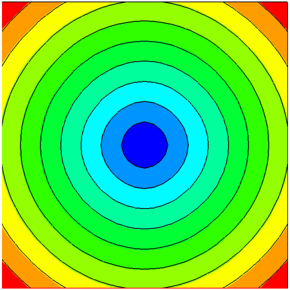
Distance based level set function

Distance based level set function φ out of Heaviside step function ψ via PDE

$$\frac{\partial\varphi}{\partial\tau} - \gamma_{nd}\nabla\cdot\left(\left(\frac{\nabla\varphi}{\|\nabla\varphi\|}\cdot\nabla\varphi - 1\right)\frac{\nabla\varphi}{\|\nabla\varphi\|}\right) = 0$$

Initial Heaviside step function ψ (Left), the final distance based level set function φ (Right) with the penalty parameter $\gamma_{nd} = 10^2$



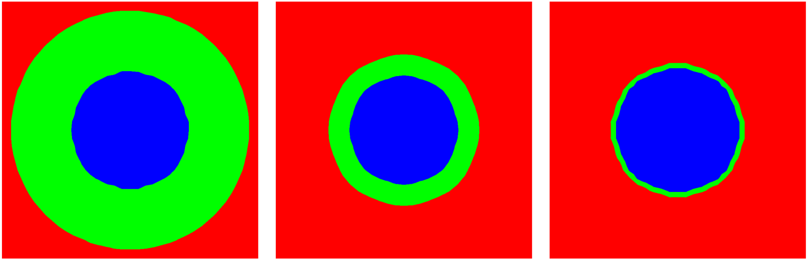


Characteristic material function

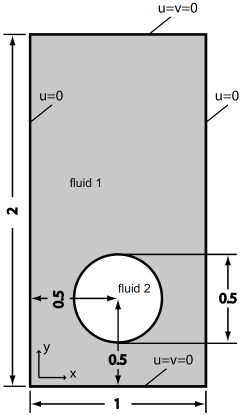
Heaviside step function ψ out of level set function φ via PDE

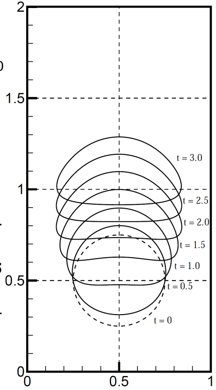
$$\frac{\partial\psi}{\partial\tau} + \underbrace{\nabla\cdot(\gamma_{nc}\psi(1-\psi)\nabla\varphi)}_{\textbf{Conv. normal}} - \underbrace{\nabla\cdot(\gamma_{nd}(\nabla\psi\cdot\nabla\varphi)\ \nabla\varphi)}_{\textbf{Diff. normal}} = 0$$

Heaviside step function ψ for different normal diffusion parameters $\gamma_{nd} = 1.0, 0.1, 0.01$ (Left-Right), the nonlinear convective parameter $\gamma_{nc} = 0.01$, and the initial level set function $\varphi = \sqrt{x^2+y^2} - 0.5$



Rising bubble benchmark





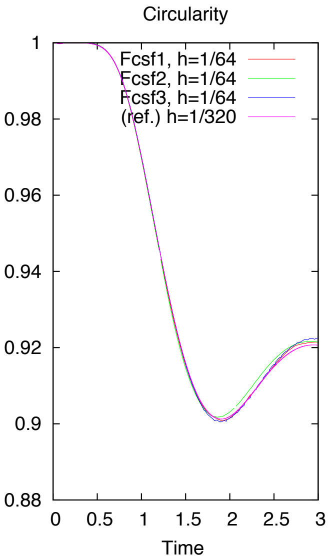
Center point $\mathbf{X}_c = \dfrac{\int_{\Omega_2} \mathbf{x}\, d\Omega}{\int_{\Omega_2} \mathbf{1}\, d\Omega}$

Circularity $c = \dfrac{\pi P_a}{P_d}$

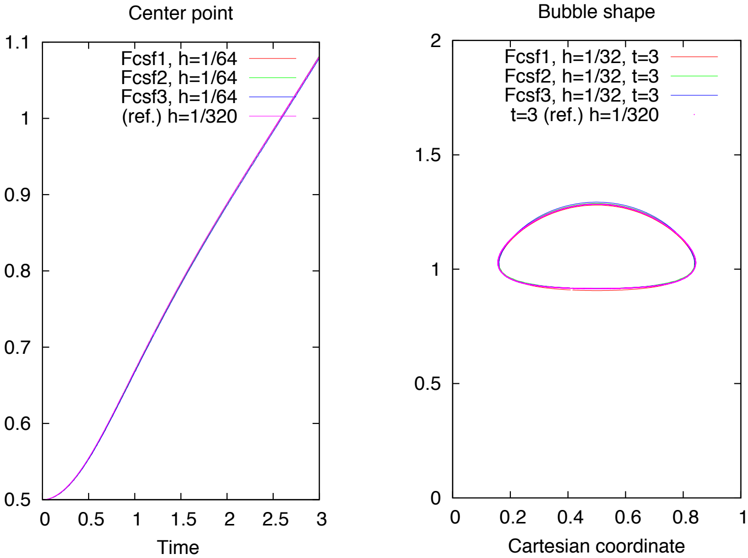
Rising velocity $\mathbf{U}_c = \dfrac{\int_{\Omega_2} \boldsymbol{u}\, d\Omega}{\int_{\Omega_2} 1\, d\Omega}$

ρ_1	ρ_1	μ_1	μ_2	g	σ	Re	Eo	ρ_1/ρ_1	μ_1/μ_2
1000	100	10	1	0.98	24.5	35	10	10	10

Rising bubble benchmark



Rising bubble benchmark



Summary and outlook

New curvature-free level set FEM method is introduced and numerically validated for multiphase phase flow problems where

- no explicit calculation of curvature and normals
- a monolithic treatment of multiphase flow problems is possible
- no capillary time step restriction remains
- a conservative level set can be used
- multiphase flow problems can be simulated with a standard Navier-Stokes solver with homogenous force
- special FEM for the multiphase stress can be used