Monolithic Newton-Multigrid Solver for Multiphase Flow Problems with Surface Tension

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1 Motivation

- Q Governing Equations
- Oiscretization/Solver
- 4 Test Case 1: Static Bubble
 - Numerical Results
- 5 Test Case 2: Oscillating Bubble
 - Numerical Results
- 6 Benchmark: Rising Bubble
 - Numerical Results

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Multiphase flows in Nature and Industry

Gas-Liquid

- Condensation
- Boiling
- Spray cooling
- Biological flows

Solid-Liquid

- Emulsification
- Slurries
- food processing

Gas-Solid

- Fluidization
- Coal burners

Liquid-Liquid

- Petroleum extraction
- Oil exploration:

4-phases



Interface tracking: Immersed boundary,¹ Front tracking²

Interface capturing: Volume of fluid,³ Phase field,^{4,5} Level set^{6,7}



Continuum surface force (CSF): Interface as a smooth transition^{8,9}

Continuum surface stress (CSS): Surface force term as the divergence of the stress $tensor^{8, 10}$

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CSF Formulation

The incompressible Navier Stokes equations

$$\begin{cases} \rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) - \nabla \cdot 2\mu \mathbf{D}(\boldsymbol{u}) + \nabla \boldsymbol{p} = \boldsymbol{f}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega. \end{cases}$$
(1)

• $\rho = \text{density}$ • $\mathbf{D}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ • p = pressure• f = external force

$$f = \kappa \sigma \mathbf{n} \delta_{\Gamma} \tag{2}$$

- $\kappa = \text{curvature}$ n = normal to the interface
- $\sigma =$ surface tension constant $\delta_{\Gamma} =$ delta function

$$\begin{cases} \rho(\Gamma) \Big(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \Big) - \nabla \cdot 2\mu(\Gamma) \mathbf{D}(\boldsymbol{u}) + \nabla \boldsymbol{p} = \kappa \sigma \boldsymbol{n} \delta_{\Gamma}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega. \end{cases}$$
(3)

• Interface capturing by level set method

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0 \tag{4}$$

• $\phi = \text{level set function}$

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

• Exact representation of the interface

$$\Gamma = \{ x \in \Omega, \phi = 0 \}$$
(5)

• Provides derived geometrical quantities (n, κ)

$$\boldsymbol{n} = \frac{\nabla \phi}{\|\nabla \phi\|}, \quad \kappa = -\nabla \cdot \boldsymbol{n}$$
(6)

• The surface tension force in terms of the level set function

$$f = \kappa \sigma \mathbf{n} \delta_{\Gamma}(\phi) \tag{7}$$

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

Problems and Challenges

• Spurious velocity Unphysical flows near the interface

- Unphysical interface movement
- Misinterpret the flow physics

Large surface tension

- Spurious velocity may grow
- Destroy the interface
- **Observed** \longrightarrow explicit/implicit interface representation
- Explicit treatment of surface tension Capillary time restriction
- Explicit reinitialization Requires perfect interface description

Towards a fully implicit treatment

Material cut-off function

$$\psi(x,t) = \begin{cases} +\frac{1}{2} & \text{if } \phi(x,t) \ge 0\\ -\frac{1}{2} & \text{if } \phi(x,t) < 0 \end{cases}$$
(8)

Features

- Enhances the accuracy
- ψ is material characteristic \longrightarrow conservative level set
- Regularization of material cut-off function

$$\psi = \frac{-1}{1 + \exp(\frac{\phi}{\epsilon_{\psi}})} + 0.5 \tag{9}$$

New set of equations for multiphase flow

$$\begin{cases} \rho(\psi) \Big(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \Big) - di \boldsymbol{v} \boldsymbol{\tau} + \nabla \boldsymbol{p} = \boldsymbol{0}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = \boldsymbol{0}, & \text{in } \Omega, \\ \frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \boldsymbol{0}, & \text{in } \Omega, \\ \psi - \Big(\frac{-1}{1 + \exp(\frac{\phi}{\epsilon_{\psi}})} + \boldsymbol{0}.5 \Big) = \boldsymbol{0}, & \text{in } \Omega. \end{cases}$$
(10)

- $\bullet \ \phi = {\rm level \ set \ function}$
- $\epsilon_{\psi} = \text{interface thickness}$

• $au = (au_s + au_m)$ full stress tensor

•
$$\psi = \text{cut-off function}$$

Viscous stress

$$\boldsymbol{\tau}_{s}=2\mu(\psi)\mathbf{D}(\boldsymbol{u})$$

Multiphase stress

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

Signed distance function needs to satisfy the constraint

$$\|\nabla \phi\| = 1 \quad \Longleftrightarrow \quad \mathbf{n} \cdot \nabla \phi = 1$$

• For implicit approach, constraint is imposed

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi - \underbrace{\nabla \cdot (\gamma_{nd} (\boldsymbol{n} \cdot \nabla \phi - 1) \boldsymbol{n})}_{reinitialization} = 0$$

• γ_{nd} = penalty parameter

Curvature-Free Level Set¹¹

$$\begin{cases} \rho(\psi) \Big(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \Big) - \nabla \cdot \Big(2\mu(\psi) \mathbf{D}(\boldsymbol{u}) + \sigma \Big(\frac{\nabla \psi \otimes \nabla \psi}{\|\nabla \psi\|} \Big) \Big) + \nabla \boldsymbol{p} = 0, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \\ \frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi - \nabla \cdot \Big(\gamma_{nd} \Big(\frac{\nabla \phi}{\|\nabla \phi\|} \cdot \nabla \phi - 1 \Big) \frac{\nabla \phi}{\|\nabla \phi\|} \Big) = 0, & \text{in } \Omega, \end{cases}$$
(11)
$$\psi - \Big(\frac{-1}{1 + \exp(\frac{\phi}{\epsilon_{\psi}})} + 0.5 \Big) = 0, & \text{in } \Omega. \end{cases}$$

Advantages

- Fully implicit and requires less regularity
- Neither \boldsymbol{n} nor κ are explicitly calculated
- No capillary time restriction
- Reinitialization is integrated within the formulation
- Navier-Stokes with homogeneous force terms

The momentum equation gets rid of the CSF force terms

PDE for the material cut-off function with fictitious time¹²

$$\frac{\partial \psi}{\partial \tau} + \underbrace{\nabla \cdot \left(\gamma_{nc}\psi(1-\psi)\boldsymbol{n}\right)}_{\text{Conv. normal}} - \underbrace{\nabla \cdot \left(\gamma_{nd}(\nabla\psi\cdot\boldsymbol{n})\boldsymbol{n}\right)}_{\text{Diff. normal}} = 0$$
(12)

- **Conv. normal**: nonlinear convection tends to build the Heaviside step function
- Diff. normal: normal diffusion control the sharpness of the interface

Curvature-Free Cut-off Function¹¹

$$\begin{cases} \rho(\psi) \Big(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \Big) - \nabla \cdot \Big(2\mu(\psi) \mathbf{D}(\boldsymbol{u}) + \sigma \Big(\frac{\nabla \psi \otimes \nabla \psi}{\|\nabla \psi\|} \Big) \Big) + \nabla \boldsymbol{p} = 0, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \\ \frac{\partial \psi}{\partial t} + \boldsymbol{u} \cdot \nabla \psi + \nabla \cdot \Big(\gamma_{nc} (0.5 + \psi) (0.5 - \psi) \frac{\nabla \psi}{\|\nabla \psi\|} \Big) - \nabla \cdot \Big(\gamma_{nd} \Big(\nabla \psi \cdot \frac{\nabla \psi}{\|\nabla \psi\|} \Big) \frac{\nabla \psi}{\|\nabla \psi\|} \Big) = 0, & \text{in } \Omega. \end{cases}$$
(13)

• $\gamma_{nc} = \text{nonlinear convection}$

• $\gamma_{nd} = \text{normal diffusion}$

Advantages

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The momentum equation gets rid of the CSF force terms

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Oiscretization/Solver

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Discretization/Solver

- Time discretization: Crank-Nicolson
- Space discretization: FEM Q_2 , P_1^{disc} for \boldsymbol{u} , p and Q_2 for ϕ, ψ



Newton-multigrid solver

- Nonlinearity: Treated by Newton solver
- Linear problem: Solved by multigrid

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Test Case 1: Static Bubble

•
$$\Omega = [0, 1]^2$$
 with bubble centred at origin $[0.5, 0.5]$

•
$$\sigma = \mu = \rho = 1$$
, $g = 0$, $r = 0.25$, $t_f = 10$

Pressure field should satisfy Laplace Young law

$$p_i = p_o + \frac{\sigma}{r} \tag{14}$$



• $p_i/p_o =$ pressure inside/outside the bubble

		CSF formu	lation (3)		S. Turek et al. ¹³				
L	$\frac{\ \mathbf{p_i} - \mathbf{p_o}\ }{(\sigma/r)}$	$\left\ u-u_{h}\right\ _{0}$	$\ \boldsymbol{u}-\boldsymbol{u}_h\ _{1,h}$	NL/LL	$rac{\ \mathbf{p_i}-\mathbf{p_o}\ }{(\sigma/r)}$	$\left\ u-u_{h}\right\ _{0}$	$\ \boldsymbol{u}-\boldsymbol{u}_h\ _{1,h}$	NL/LL	
4	1.040583	1.22×10^{-3}	5.63×10^{-2}	4/1	0.954349	2.61×10^{-3}	2.08×10^{-1}	5/1	
5	0.999839	9.58×10^{-5}	1.28×10^{-2}	5/1	0.979682	9.71×10^{-4}	1.54×10^{-1}	5/1	
6	1.000969	4.98×10^{-5}	5.26×10^{-3}	5/1	0.992961	3.62×10^{-4}	1.13×10^{-1}	4/1	
7	1.000204	2.10×10^{-6}	1.03×10^{-3}	6/1	0.997166	1.38×10^{-4}	8.21×10^{-2}	4/1	

Numerical Results:¹⁴ Static Bubble

Curvature-Free Level Set

Curvature-Free Cut-off Material



Mass is conserved!

Curvature-Free Level Set: Static Bubble



Curvature-Free Cut-off Function: Static Bubble



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Test Case 2:14 Oscillating Bubble

• $\Omega = [0, 1]^2$, bubble centred at origin [0.5, 0.5]

•
$$\sigma = \mu = \rho = 1$$
, $g = 0$, $r_x = 0.25$, $r_y = 0.125$

•
$$t_f = 100, \ \Delta t = 10^{-2}$$

Evaluate

- Mass conservation? \longrightarrow Surface area¹⁴
- Bubble shape \longrightarrow Interface position¹⁴

Expected behaviour¹⁵







Curvature-Free Level Set: Oscillating Bubble



Curvature-Free Cut-off Function: Oscillating Bubble





Less oscillations, mass is conserved!

Curvature-Free Cut-off Function

$$\rho(\psi) \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \left(2\mu(\psi) \mathsf{D}(u) + \sigma \left(\frac{\nabla \psi \otimes \nabla \psi}{\|\nabla \psi\|} \right) \right) + \nabla \rho = 0, \quad \text{in } \Omega,$$

$$\nabla \cdot u = 0, \quad \text{in } \Omega,$$

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Advantages

- No need for the level set function
- Fully implicit and requires less regularity
- Neither \boldsymbol{n} nor κ are explicitly calculated
- No capillary time restriction

Investigate the effects of γ_{nc} and γ_{nd}

Effects of γ_{nc} and γ_{nd} : Static Bubble



Big $\gamma_{nc} \rightarrow$ disturbs ψ range



 ψ range recovers \rightarrow suitable value of γ_{nd}

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Benchmark: Rising Bubble¹⁶

• $\Omega = \Omega_1 \cup \Omega_2$, bubble of radius r = 0.25

• centred at origin [0.5, 0.5]

Parameters¹⁶

ρ_1	ρ_2	μ_1	μ_2	g	σ	Re	Eo	$ ho_1/ ho_2$	μ_1/μ_2
1000	100	10	1	0.98	24.5	35	10	10	10

Evaluate

• rise velocity
$$U_c = \int_{\Omega_2} u dx / \int_{\Omega_2} 1 dx$$

• center of mass $X_c = \int_{\Omega_2} u dx / \int_{\Omega_2} 1 dx$

• circularity
$$c = P_a/P_b = \pi d_a/P_b$$

bubble shape



Curvature-Free Cut-off Function: Rising Bubble



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A monolithic Newton-multigrid solver for multiphase flow problems is developed

- Solves velocity, pressure and interface position simultaneously
- Nonlinearity: Treated with a Newton solver
- Linearized system: Solved by geometrical multigrid
- Requires less regularity
- No explicit calculation of ${\it n}$ and κ
- No capillary time restriction
- Reinitialization issue is integrated within the formulations

Sr. No.	Problem Formulations	Static Bubble	Oscillating Bubble	Rising Bubble
		(Test Case 1)	(Test Case 2)	(Benchmark)
1	Level Set Approach	√	\checkmark	
2	Level Set with Material Cut-off Function	~	\checkmark	
3	Curvature-Free Level Set	√	\checkmark	
4	Curvature-Free Cut-off Material Function	√	\checkmark	√

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Thank you for your Attention!

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