A Unified Eulerian Variational Framework for Multiphase Fluid-Structure Interaction

by

Xiaoyu Mao

M.Sc., National University of Singapore, 2017

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

Doctor of Philosophy

in

THE FACULTY OF GRADUATE AND POSTDOCTORAL STUDIES
(Mechanical Engineering)

The University of British Columbia
(Vancouver)

August 2023

© Xiaoyu Mao, 2023
The following individuals certify that they have read, and recommend to the Faculty of Graduate and Postdoctoral Studies for acceptance, the thesis entitled:

**A Unified Eulerian Variational Framework for Multiphase Fluid-Structure Interaction**

submitted by Xiaoyu Mao in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mechanical Engineering.

**Examining Committee:**

Rajeev Jaiman, Associate Professor, Mechanical Engineering, UBC  
*Supervisor*

Jasmin Jelovica, Assistant Professor, Mechanical Engineering, UBC  
*Supervisory Committee Member*

Anthony Wachs, Professor, Mathematics, UBC  
*University Examiner*

Dana Grecov, Professor, Mechanical Engineering, UBC  
*University Examiner*

Hector Gomez, Professor, Mechanical Engineering, Purdue University  
*External Examiner*

**Additional Supervisory Committee Members:**

Carl Ollivier-Gooch, Professor, Mechanical Engineering, UBC  
*Supervisory Committee Member*

James Feng, Professor, Chemical and Biological Engineering, UBC  
*Supervisory Committee Member*
Abstract

Multiphase fluid-structure interaction (FSI) involving multiphase flow and contact between immersed solids is omnipresent in numerous processes in nature, biology, and engineering applications. Examples include bio-inspired avian-aquatic vehicles, aneurysm and cardiovascular diseases in biomedical engineering, and marine vessels in ocean engineering. Of particular interest to the present study is the ice-going ships in the Arctic environment. Numerical simulation of this complex system involves modeling dynamics of disparate materials, evolving multiphase interfaces, and collisions between solids. The development of a novel three-dimensional multiphase and multiphysics computational framework based on unified continuum mechanics laws is the focus of the present dissertation.

In the proposed numerical framework, we employ a fully Eulerian description for the continua of different phases, which facilitates topological changes of their interfaces during the evolution and contact processes. The interfaces and phase components are captured by the phase-field-based diffuse interface description. While the diffuse interface description circumvents the complexity of explicit interface reconstruction, it poses challenges in consistent interface transition and accurate geometric representation. To address these challenges, we developed an interface and geometry preserving phase-field method, which is the key contribution of this dissertation and lays the foundation for the success of the current framework in handling multiphase interfaces. With the phase components, we unify the mass and momentum conservations by phase-dependent interpolation. The kinematics of solid phases in an Eulerian frame of reference is resolved by evolving the left Cauchy-Green tensor.

The unified Eulerian framework for two-phase and multiphase FSI is imple-
mented in a partitioned-block iterative manner within the in-house 3D parallel vari-
ational multiphysics solver. The solver is systematically explored for a variety of
cases of two-phase flow with surface tension effect, single-phase FSI, multiphase
FSI, and contact of immersed deformable solids. The study is concluded by a 3D
demonstration of ice-going ships sailing across floating ice floes. The unified Eu-
lerian variational framework with a parallel implementation based on the novel in-
terface and geometry preserving phase-field method provides a general and robust
approach for investigating a wide range of multiphase FSI problems.
Lay Summary

In recent years, the Arctic region has gained strategic importance for finding new ship routes. Motivated by the need for high-fidelity simulation of ice-going ships, we propose a novel multiphase FSI formulation and develop a first-of-its-kind parallelized 3D finite element solver for large-scale computations. In the computational framework, the physical fields of the wind flow, marine hydrodynamics, ship structure and ice sheets are unified as a consistent continuum formulation over a spatially fixed Eulerian mesh. To capture the interfaces in the fixed Eulerian mesh, we develop a novel interface and geometry preserving phase-field method. The momentum and mass conservation equations are integrated through phase-dependent interpolation. The kinematics of the solids are resolved by evolving the left Cauchy-Green strain tensor. The solver is systematically assessed with the two-phase flow with surface tension effect, single-phase FSI and contact of immersed solids. Finally, we demonstrate our framework for an ice-going ship.
Preface

This Ph.D. thesis entitled A Unified Eulerian Variational Framework for Multiphase Fluid-Structure Interaction presents the original research conducted by Xiaoyu Mao under the supervision of Dr. Rajeev Jaiman.

Chapters 2, 3, 4 and 5: Part of literature review in Chapter 2, part of review and methodology in Chapter 3, Chapter 4 and Chapter 5 have been published in the following journal articles and presented in conferences:


X. Mao and R. Jaiman. A conservative and accurate interface-preserving vari-
tional scheme for fully-Eulerian fluid-structure interaction. In 16th US National
Congress on Computational Mechanics, 2021. Contributions from the authors:

Chapter 6 is in preparation for submission as an original journal paper.
# Table of Contents

Abstract ................................................................. iii

Lay Summary ........................................................... v

Preface ................................................................. vi

Table of Contents ..................................................... viii

List of Tables ......................................................... xii

List of Figures ......................................................... xiii

Nomenclature ......................................................... xxi

Acknowledgments ................................................... xxiv

1 Introduction ......................................................... 1
  1.1 Background and motivation ................................ 1
  1.2 Objectives and methodology ............................. 5
  1.3 Contributions and impact ................................. 7
  1.4 Organization of the thesis ............................... 9

2 Literature Review .................................................. 12
  2.1 Review of multiphase FSI formulations ............. 13
    2.1.1 Kinematic descriptions for fluids and solids .. 13
    2.1.2 Interface techniques ............................ 15
4.7 Summary .................................................... 81

5 Geometry-preserving phase-field for fluid-structure interaction . . . 84
  5.1 Background ............................................. 85
  5.2 Review of interface-preserving parameters .................... 85
  5.3 Gradient-minimizing velocity field .......................... 89
  5.4 FSI dynamics and solid kinematics in Eulerian frame ......... 91
    5.4.1 Conservation laws for the fully Eulerian FSI .......... 91
    5.4.2 Evolution of the left Cauchy-Green tensor .......... 93
    5.4.3 Summary for the Eulerian FSI formulation .......... 97
  5.5 Variational implementation .............................. 98
    5.5.1 Temporal discretization ............................ 98
    5.5.2 Semi-discrete form of equations ..................... 99
    5.5.3 Linearization of the solid stress .................... 102
    5.5.4 Implementation details ............................. 104
  5.6 Test cases .............................................. 105
    5.6.1 Convection of square and circular interfaces ....... 105
    5.6.2 Deformation of a solid block under lid-driven cavity flow 109
    5.6.3 Channel flow passing a fixed deformable block .......... 113
    5.6.4 Application to the cylinder-flexible plate problem .... 118
  5.7 Summary ................................................. 125

6 Combined multiphase flow and fluid-structure interaction ........ 126
  6.1 Background .............................................. 127
  6.2 Initialization of the phase-field variable .................. 128
    6.2.1 Calculation of the distance function ................ 128
    6.2.2 Determination of the sign on a node .............. 130
  6.3 Examples of order parameter initialization ................ 132
    6.3.1 Interface meshes for sphere and cube ............. 132
    6.3.2 Calculation with multiple grid cells ................ 134
    6.3.3 Demonstration with ship hull ...................... 134
  6.4 Fully Eulerian formulation for multiphase FSI ............. 136
    6.4.1 Conservation laws for the multiphase FSI system .... 136

x
List of Tables

Table 4.1  Quantification of the errors for 2D rising bubble case: convergence with respect to $\varepsilon$ at a constant $\eta$. .................................................. 72
Table 4.2  Quantification of the errors for 2D rising bubble case: variation of $\varepsilon$ and $\eta$ ................................................................. 74
Table 4.3  Quantification of the errors for the 3D rising bubble benchmark .................................................... 79
Table 6.1  Geometry of the ice floes ................................................................. 147
List of Figures

Figure 1.1 Multiphase FSI in nature and biology: (a) droplet rolling on leaf [1], (b) pet dog drinking water [2], (c) dolphin jumping out of free surface [3], and (d) human swimming in water [4].

Figure 1.2 Multiphase FSI in engineering systems: (a) tugboat with free surface effect [5], (b) avian-aquatic vehicle [6], (c) offshore wind turbines [7], and (d) drilling vessel-riser system [8].

Figure 1.3 Illustration of ship-ice interaction: (a) Louis S. St-Laurent ice breaker of the Canadian Coast Guard, and schematic diagrams showing combined effects of hydrodynamics and ice floes interacting with a ship hull in (b) side and (c) top views.

Figure 1.4 An abstract representation of fluid-fluid and fluid-solid interfaces in multiphase FSI problems. The diffuse interface in the Eulerian mesh is shown as the shaded region.

Figure 1.5 Illustration for the organization of the thesis.

Figure 2.1 Illustration of kinematic descriptions for fluids and solids. (Portraits from Wiki)

Figure 2.2 Illustration of various interface techniques: (a) fully Lagrangian approach, (b) ALE! (ALE!) method, (c) mixed Lagrangian Eulerian approach, and (d) fully Eulerian approach.

Figure 2.3 Illustration of the marker field for the solid kinematics.

Figure 2.4 Illustration of interface capturing in 2D: the interface plotted with red line is captured in the $X-Y$ plane as the zero isoline of the phase indicator $\phi$ visualized by its contour.
Figure 3.1 Illustration of (a) diffuse interface representation of a circular interface via the order parameter field, and (b) function value of $\phi$ at the cross section $x = 0$.

Figure 3.2 Illustration of (a) the bulk energy defined as a double-well function $F(\phi)$, (b) the phase transition and (c) the resulting interfacial energy.

Figure 3.3 Equilibrium hyperbolic tangent interface profile of the phase-field diffuse interface profile.

Figure 3.4 Illustration of the convective distortion on 1D interface profile: (a) initialized hyperbolic tangent profile, (b) thinned diffuse interface region due to a compressional velocity field, and (c) thickened diffuse interface region due to an extensional velocity field.

Figure 3.5 Illustration of the interface regularization effect by free energy minimization.

Figure 3.6 Illustration of (a) curvature flow and (b) volume-conserved mean curvature flow.

Figure 4.1 Illustrations of the interface dynamics of the convective form of the conservative Allen-Cahn equation: (a) one-dimensional equilibrium interface profile $\phi_{eq}$ and the actual interface profile $\phi(x,t)$ subjected to an extensional velocity field, and (b) volume-conserved mean curvature flow velocity $\mathbf{v}_\kappa(x,t)$ and the convective velocity $\mathbf{v}(x,t)$ of the interface $\phi(x,t) = 0$. The free energy minimization described by the equation balances the convective distortion with $\phi_{eq}$ in (a), and induces $\mathbf{v}_\kappa(x,t)$ in (b).

Figure 4.2 Schematic diagram of the diffuse interface in non-dimensional moving orthogonal curvilinear coordinate system. The coordinate system ($\tilde{n}_m$, $\tilde{\xi}_1$ and $\tilde{\xi}_2$) is attached on the moving interface indicated by $\phi(x,t)$ convected in the velocity field $\mathbf{v}(x,t)$. The thickness of the diffuse interface in the coordinate system is $\sim O(1)$ due to the non-dimensionalization.
Figure 4.3 Convergence study of phase-field solver for a generic bistable convection-diffusion-reaction system: (a) the variation of the derivative of $\phi$ with respect to domain length $L$, and (b) the relative $L^2$ error ($e_2$) as a function of grid size $h$. 57

Figure 4.4 Accuracy assessment of fully-implicit finite element formulation for a generic bistable convection-diffusion-reaction system: (a) steady state plateau-like solution as a function of distance $x$, and (b) the height of the solution $f$, (c) half-width of the solution $v$, (d) inverse width of the diffuse interface $w$ as a function of Damköhler number $Da$. 58

Figure 4.5 Schematic diagram showing the computational domain for the convection of a one-dimensional planer interface in a prescribed extensional velocity field. $\Omega_1$ and $\Omega_2$ are domains of the two phases. A zero flux boundary condition for the order parameter is applied on the left and the right boundaries. 59

Figure 4.6 Convergence of a convecting planar diffuse interface with a prescribed velocity: (a) the variation of the derivative of $\phi$ with respect to domain length $L$, and (b) the relative $L^2$ error ($e_2$) as a function of mesh resolution $\varepsilon/h$. 60

Figure 4.7 Convection of a planar interface in a prescribed velocity field: the interface profiles corresponding to various distortion parameter $\xi$. 61

Figure 4.8 Schematic diagram showing the computational domain for the convection of a curved interface in a prescribed incompressible velocity field illustrated with streamlines. $\Omega_1$ and $\Omega_2$ are domains of the two phases. A zero flux Neumann boundary conditions for the order parameter is applied on all the boundaries. 63

Figure 4.9 Convection of a curved interface with $\xi = 0.1$: the contours of $\phi$ at (a) $t = 0$, (b) $t = 0.25$, (c) $t = 0.5$, (d) $t = 0.75$, and (e) the time history of the non-dimensional interface thickness $\tilde{\varepsilon}_d$ on the bottom boundary $\theta = 0$ and the left boundary $\theta = \pi/2$ with the comparison to the equilibrium interface thickness $\tilde{\varepsilon}_{eq}$. 65
Figure 4.10  Dependence of the interface errors on the convective distortion parameter $\xi$: (a) the relative interface thickness error $e_\varepsilon$, and (b) the relative surface tension error $e_\sigma$. .......................... 66

Figure 4.11  Correlations of the interface errors as a function of RMS convective distortion parameter $\eta$: (a) the relative interface thickness error $e_\varepsilon$, and (b) the relative surface tension error $e_\sigma$. . . 67

Figure 4.12  Two-dimensional rising bubble problem: (a) schematic diagram of the computational domain, and (b) contour of the order parameter at $t = 0$. .......................... 69

Figure 4.13  Volume-conserved mean curvature flow convergence study for 2D rising bubble benchmark case: (a) circularity of the bubble, (b) interface shape at $t = 3$, (c) rise velocity, and (d) center of mass. .......................... 71

Figure 4.14  The interface-preserving capability convergence study for 2D rising bubble benchmark case: (a) circularity of the bubble (b) interface shape at $t = 3$ (c) rise velocity, and (d) center of mass. 73

Figure 4.15  Comparison of the constant and the time-dependent mobility model in 2D rising bubble case: contour of the order parameter at $t = 3$ simulated with (a) constant mobility coefficient $\gamma = 1$, (b) time-dependent mobility model at $\eta = 0.1$, and the difference in (c) rise velocity, and (d) the time history of the RMS convective distortion parameter $\eta$. .......................... 75

Figure 4.16  Three-dimensional rising bubble problem: (a) schematic diagram of the computational domain, and (b) contour of the order parameter at $t = 0$. .......................... 77

Figure 4.17  Convergence study for the 3D bubble rising problem: (a) sphericity of the bubble, (b) bubble diameters in X and Y directions, (c) rise velocity, and (d) center of mass. . . . 80

Figure 4.18  Two rising bubbles merging with a free surface problem: (a) schematic diagram showing the computational domain, and (b) unstructured finite element mesh at the plane $x = 0.5$ . . . . 82
Figure 4.19 Two rising bubbles merging with a free surface: the evolution of the interface $\phi = 0$ at different time instants $t = (a) 0.1$, (b) 1.1, (c) 1.6, (d) 1.7, (e) 1.8, (f) 1.9, (g) 2.2, (h) 2.4, and (i) 2.7.

Figure 5.1 Illustration of the concept of the IGP method.

Figure 5.2 Illustration on the construction of the gradient-minimizing velocity field. Streamlines of $-\varepsilon \nabla \phi$ which passes $\mathbf{w}$ in the normal direction throughout the diffuse interface region are shown as the blue arrows in the left figure, while the magnitude of the velocity in the normal direction $-\varepsilon \nabla \phi \cdot \mathbf{n}$ is shown in the right figure.

Figure 5.3 Illustration of the material coordinates of a deformable solid in an Eulerian mesh.

Figure 5.4 The interface distortion of the circular and square interfaces in the velocity field $v_x = x$, $v_y = -y$ until $t = 0.8$. The diffuse interface region is shown as the space between $\phi = 0.9$ (solid line) and $\phi = -0.9$ (dashed line).

Figure 5.5 Diffuse interface regions at $t = 0.8$ given by purely convection, the IP method and the IGP method in the convection of circular and square interfaces, and the corresponding time histories of the mobility coefficient for quantifying the volume-conserved mean curvature flow.

Figure 5.6 Convergence study for the discretization of IGP in the interface distortion of circular and square interfaces: (a) spatial error, and (b) temporal error.

Figure 5.7 Schematic diagram of an elastic solid block under lid-driven cavity flow.

Figure 5.8 Mesh convergence study for the deformation of a solid block under lid-driven cavity flow: (a) interface position, and (b) relative $L^2$ error of the order parameter field.

Figure 5.9 Convergence of the diffuse interface model in the deformation of a solid block under lid-driven cavity flow. The subscripts denote the times of bisection ($\eta_n = (1/2)^n \eta_0, \varepsilon_n = (1/2)^n \varepsilon_0$).
Figure 5.10  Channel flow passing a fixed deformable block: (a) schematic diagram showing the computational domain, and (b) structured finite element mesh covering the block and the surrounding unstructured mesh.

Figure 5.11  Channel flow passing a fixed deformable block: (a) diffuse interface region at $t = 5$ given by the IP method and the IGP method, and (b) time histories of the mobility coefficient.

Figure 5.12  Channel flow passing a fixed deformable block: (a) spatial convergence, and (b) temporal convergence.

Figure 5.13  Convergence of the diffuse interface model in the channel flow passing a fixed deformable block. The subscripts denote the times of bisection ($\eta_n = (1/2)^n \eta_0$, $\epsilon_n = (1/2)^n \epsilon_0$): (a) interface position represented by $\phi = 0$, and (b) time histories of the X-displacement of the marker point.

Figure 5.14  Channel flow passing a fixed deformable block: Comparison of the flow field $v_x$ and the deformed solid depicted by $\phi > 0$ at $t = 5$ from (a) IGP-based fully Eulerian solver, and (b) monolithic ALE solver.

Figure 5.15  Channel flow passing a fixed block with different shear modulus: (a) interface position represented by $\phi = 0$, and (b) the X-displacement of the marker point.

Figure 5.16  Channel flow passing a fixed block with different shear modulus: flow field for (a) $\mu_s L = 2 \times 10^5$, and (b) $\mu_s L = 2 \times 10^4$.

Figure 5.17  Cylinder-flexible plate problem: (a) schematic diagram showing the computational domain, and (b) unstructured finite element mesh covering the area where the flexible plate sweeps through.

Figure 5.18  Cylinder-flexible plate problem: (a) displacement of the marker in the $Y$-direction, and (b) time histories of the mobility coefficient.

Figure 5.19  Cylinder-flexible plate problem: phase of the normalized mobility and the $Y$-displacement.
Figure 5.20 Convergence of the diffuse interface model in the cylinder-flexible plate problem. The subscripts denote the number of times of scaling down by the factor of $1/\sqrt{2}$. ($\eta_n = (1/\sqrt{2})^n \eta_0, \epsilon_n = (1/\sqrt{2})^n \epsilon_0$). The mesh resolution is kept as three elements across the diffuse interface region by taking $h = 4/3 \epsilon$.

Figure 5.21 Cylinder-flexible plate problem: demonstration of the flow field $v_x$ and the flexible plate depicted by $\phi > 0$ at (a) $t = 3.1$, and (b) $t = 3.2$.

Figure 6.1 Illustration of ray casting algorithm: conditions for ray (a) crossing and (b) missing the surface element.

Figure 6.2 Illustration of ray casting algorithm: (a) case where the relaxed condition is satisfied but the ray doesn’t cross the surface element (b) classification of cross types.

Figure 6.3 Illustration of the interface meshes for two simple geometries: (a) sphere and (b) cube.

Figure 6.4 Convergence of the signed distance function for two representative meshes: (a) sphere and (b) cube.

Figure 6.5 Contours of (a) signed distance function and (b) order parameter field calculated with multiple grid cells.

Figure 6.6 An illustration of a tugboat represented by (a) interface mesh and (b) isosurface of $\phi = 0$.

Figure 6.7 Schematic diagram of a rotating disk in lid-driven cavity flow.

Figure 6.8 Rotating disk in lid-driven cavity flow: (a) temporal and (b) interface convergence study for the center of mass of the disk.

Figure 6.9 Schematic of a rotating sphere in lid-driven cavity flow.

Figure 6.10 Rotating sphere in lid-driven cavity flow: (a) temporal and (b) interface convergence study for the center of mass of the sphere in $X-Z$ plane.

Figure 6.11 Rotating sphere in lid-driven cavity flow: the evolution of the interface $\phi = 0$ at different time instants $t = (a) 1$, (b) 3, (c) 4, (d) 6, (e) 8, (f) 10.
Figure 6.12  Schematic of the case setup for falling and bouncing back of an elastic sphere. ............................................. 143
Figure 6.13  Falling and bouncing back of an elastic sphere: (a) temporal and (b) interface convergence study for the center of mass of the sphere. ................................................................. 143
Figure 6.14  Falling and bouncing back of an elastic sphere: the evolution of the interface $\phi = 0$ at different time instants $t = (a) 0.1, (b) 2, (c) 2.9, (d) 3.8, (e) 3.9, (f) 4.7$. .............................................................. 144
Figure 6.15  Schematic diagram of collision of two elastic spheres. ......... 145
Figure 6.16  Collision of two elastic spheres: superposition of the interfaces $\phi^i = 0$ at different time instants $t = (a) 0.1, (b) 0.9, (c) 1.1, (d) 1.8, (e) 2.8, (f) 6.8$. .............................................................. 146
Figure 6.17  Schematic diagram of an ice-going ship with free surface and ice floes. .............................................................. 147
Figure 6.18  Representative results of ship-ice interaction: superposition of the interfaces $\phi^i = 0$ at different time instants $t = (a) 0.25, (b) 2.5, (c) 5, (d) 7.5, (e) 10, (f) 11.25$. .............................................................. 148
Figure A.1  Schematic diagram of the convective distortion of the thickness between the level sets of $\phi = \phi_1$ and $\phi = \phi_2$ due to different normal velocities. .............................................................. 170
# Nomenclature

## Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>Two-dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three-dimensional</td>
</tr>
<tr>
<td>ALE</td>
<td>Arbitrary Lagrangian-Eulerian</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite element method</td>
</tr>
<tr>
<td>FSI</td>
<td>Fluid-structure interaction</td>
</tr>
<tr>
<td>GMRES</td>
<td>Generalized minimal residual method</td>
</tr>
<tr>
<td>GMV</td>
<td>Gradient minimizing velocity</td>
</tr>
<tr>
<td>IGP</td>
<td>Interface and geometry preserving</td>
</tr>
<tr>
<td>IP</td>
<td>Interface preserving</td>
</tr>
<tr>
<td>PDEs</td>
<td>Partial differential equations</td>
</tr>
<tr>
<td>RMS</td>
<td>Root mean square</td>
</tr>
</tbody>
</table>

## Domains

<table>
<thead>
<tr>
<th>Domain</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_D^{(\cdot)}$</td>
<td>Dirichlet boundary</td>
</tr>
<tr>
<td>$\Gamma_H^{(\cdot)}$</td>
<td>Neumann boundary</td>
</tr>
<tr>
<td>$\mathbb{R}$</td>
<td>Real numbers</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>General domain</td>
</tr>
</tbody>
</table>
\( \Omega^f \) Fluid domain

\( \Omega^s \) Solid domain

**Mathematical spaces**

\( H^h(\cdot) \) Space of test solution

\( H^{(\cdot)} \) Sobolev space

\( L^{(\cdot)} \) Lebesgue space

\( S^h_{(\cdot)} \) Space of trial solution

**Operators**

\( ||\cdot||_2 \) \( L^2 \) norm operator

\( \lfloor \cdot \rfloor \) Floor operator

max Maximum operator

min Minimum operator

\( \nabla(\cdot) \) Gradient operator

\( \nabla \cdot (\cdot) \) Divergence operator

\( \partial_t(\cdot) \) Partial time derivative

**Physical parameters**

\( \eta \) RMS interface distortion number

\( \gamma \) Mobility coefficient

\( \mu \) Viscosity

\( \mu_L \) Shear modulus

\( \rho \) Density

\( \epsilon \) Diffuse interface thickness parameter
Variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi$</td>
<td>Finite element test function for vector or tensor</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress tensor</td>
</tr>
<tr>
<td>$B$</td>
<td>Left Cauchy-Green tensor</td>
</tr>
<tr>
<td>$I$</td>
<td>Identity matrix tensor</td>
</tr>
<tr>
<td>$n$</td>
<td>Normal vector</td>
</tr>
<tr>
<td>$u$</td>
<td>Displacement vector</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity vector</td>
</tr>
<tr>
<td>$w$</td>
<td>Gradient minimizing velocity</td>
</tr>
<tr>
<td>$x$</td>
<td>Spatial coordinates</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Free energy</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Phase indicator (or order parameter)</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Finite element test function for scalar</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>General variable</td>
</tr>
<tr>
<td>$d$</td>
<td>Signed distance function</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$q$</td>
<td>Finite element test function for pressure</td>
</tr>
<tr>
<td>$t$</td>
<td>Temporal variable</td>
</tr>
</tbody>
</table>
Acknowledgments

It was a long journey. I can still remember the young man who was completely innocent, hence courageous enough to step onto this adventure. From Singapore to Canada, from swift globalization to post pandemic recovery stage, from machine learning to high-performance scientific computing, his life and the world were changing so rapidly that it took all his focus and energy to live what he had at the moment, even to the extent that he was emotionally blunt enough to overlook the changes happening around and on himself. Until this moment, he breaks the barrier and overwhelms me with all the sceneries and all his feelings. Well, quite a journey, and what a journey!

Among the few who consistently accompanied me on the journey, my supervisor, Dr. Rajeev K. Jaiman makes all these possible. To me, scientific research resembles treasure hunting in a dark sea. Sometimes one can be too depressed to go further and unconsciously denies the glimpse of light. Sometimes the same person can be obsessed with legends to overestimate his capability. My supervisor is not a map - no one really knows what is ahead, whether it looks like a barren land or a golden city. He is a mirror, from whom I can see who and where I am objectively. The reflection helps me to throw away imaginary difficulties thus being brave enough to hold on to the position, filter out aimless passion to focus on things that are truly necessary, and cool the mind obsessed with optimism bias and vain glory. The time we spent together fundamentally shaped my way of thinking and helped me to become wise and mature enough to achieve the current piece of work. My sincere and deepest gratitude to you!

Popcorn movies usually have short flashbacks about home, which empower the heroic protagonist to beat the challenge and embrace the moment of destiny. While
the rest parts can all be imaginary, this is surprisingly true in real life: home rarely appears explicitly in the journey, but it is everywhere along with it. It is the reason for departure, the harbor for rest, and the final destination. Due to COVID-19, it has been straight five years since I met my parents. The last time I saw them, they still enjoyed traveling and heavy food. Now they are both retired at home and plan for healthy diet everyday. While we missed each other so much, the emotion was always clumsily hidden behind, and sometimes sneaked out mildly - like the rapid flow below a clam water surface. ”True love is self-restraint and consideration for others”, my mother Meiying Zhang once said, and my father Zhenye Mao practiced it with smoke and beers when we talked across the pacific ocean and 16 time zones. I won’t say I owe you so much. We are a family, we live, laugh and suffer together. But still, it is good to be the son of yours.

If my supervisor and family are the skeleton of the story, my friends are the flesh that makes it so thrilling and meaningful. Every encounter is a fascinating and unforgettable story. Special thanks to Yumeng Zou, who influenced me with her care about surrounding people, enthusiasm for life, optimism, and confidence. Thanks to Vaibhav and Amir for the visit to North Vancouver and the birthday party at Granville Island. Thanks to Rui Gao for the delicious foods we enjoyed, the fun gaming time we had, and the interesting talks about life philosophy and global politics. Thanks to Nihar, Biswajeet, and Indu, who successfully altered my flavor to Indian style - I’m going to miss that! A researcher is always immersed in an abstract rational world. Countless boring repetitions, restless explorations, and relentless failures only for ecstasy at the moment of revealing the true knowledge that stands eternally. Although it is worthwhile, a flesh body cannot sustain for long. Thank you all for dragging me back to the real life. There is sunshine, beach, food, and game to comfort ordinary people. And above all, friends.

Now I’m almost at the end of this journey. But the endpoint of one journey is always the start point of another. Dear Siyu Yan, we shared the good old days in our high school, witnessed and encouraged each other all the way towards our Ph.D. degrees. You are always optimistic, energetic, and curious about life, with strong determination deep inside. Your personality and experiences keep reminding me that there are always things to look forward to. How about the reunion around the corner? Are you looking forward to it as well?
Chapter 1

Introduction

1.1 Background and motivation

Multiphase FSI can be found easily in numerous processes in nature, biology and in engineering applications. Multiphase flow typically includes multiple immiscible fluids with free-form deformation of fluid-fluid interfaces. When the multiphase flow interacts with an elastic solid body, the solid body will be deformed and/or displaced due to fluid loading. In turn, this change in structural configuration influences the dynamics of the fluid flow through a feedback process. This process can happen to multiple solids, which may further interact with each other through contact. In this thesis, the entire complex interaction is referred to as the multiphase FSI, one of the most widespread and fundamental phenomena. Multiphase FSI can be observed in our day-to-day life, for example, a water droplet rolling on tree leaves, one’s pet dog drinking water with its tongue, a dolphin jumping out of the free surface, and human swimming near the water level, as shown in Fig. 1.1. In all these examples, there exists a strong two-way coupling between the fluid flow and the structure.

In the context of coastal and offshore engineering, multiphase FSI is found to be the core of enormous situations where the coupled nonlinear dynamics need to be analyzed for immersed or floating structures. Examples include tugboats that help to maneuver large vessels at the port, avian-aquatic vehicles, wind turbines that provide clean energy, and oil extraction by drilling vessel-riser system. These
Figure 1.1: Multiphase FSI in nature and biology: (a) droplet rolling on leaf [1], (b) pet dog drinking water [2], (c) dolphin jumping out of free surface [3], and (d) human swimming in water [4].

Example applications are illustrated in Fig. 1.2. Strong nonlinearity in coupled dynamics between multiphase fluid flow and multiple solids of distinct physical properties are the common features in these problems. The coupling occurs at multiphase interfaces, which usually experience significant topological changes such as large deformation, translational/rotational motion and interface merging and breaking-up. They are mostly transient processes and have multi-scale nature.

*Image from internet:
Droplet rolling on leaf: "Hydrophobicity: Will the drop stop or roll?" from Science Friday.
Pet dog drinking water: "How much water does a puppy need?" from PetPlace.
Dolphin jump out of free surface: "Why do dolphins jump out of the water?" from animalwised.
Human swimming in water: "Fastest swimmers make webbed hands out of water" from NBC news.
from time to time. All these characteristics make the multiphase FSI challenging to analyze and predict in theoretical and experimental approaches, giving rise to the need for computational tools.

Figure 1.2: Multiphase FSI in engineering systems: (a) tugboat with free surface effect [5], (b) avian-aquatic vehicle [6], (c) offshore wind turbines* [7], and (d) drilling vessel-riser system [8].

Of particular interest is the ship-ice interaction in the Arctic region. Located at the north pole and surrounded by lands, the Arctic region encompassing various terrains, enormous biodiversity and rich resources, is now the home to indigenous people of over 40 communities and a total population of four million [9–11]. Under the effect of global warming, the Arctic Ocean may be seasonally ice-free by 2050

*Image from internet: Offshore wind turbines : "Offshore vs. onshore wind farms" from AZOclean-tech
This creates huge opportunities for extracting natural resources and finding new routes for transcontinental transportation. With the growing strategic importance of Arctic transportation, it is required to design and manufacture marine vessels which is reliable and safe when sailing across ocean environment with ice sheets and floes. Substantial technical improvements in ship design, manufacturing, and operation are essential to overcome such a colossal challenge.

The problem of ship-ice interaction involves interactions between ice mechanics, ship structure, hydrodynamics and wind flow. The ice floating on the sea level can vary in size and geometry: from small-scale ice rubble to large-scale ice ridges and floes. During the sailing of ships, they are in contact with the ship hull, accelerated, pushed aside, or submerged, which creates loads and deformation on both sides. Then, as a source of disturbance, the moving ices can interact with surrounding static ices and cause drifting and rotating motions. The ice and ship hull interaction happens near the water-air interface under the gravitational force. As the ship moves forward, the wave runs up and entrains air bubbles inside. The bubbles then break apart and become sea foam. The sea foam propagates along with waves surrounding the ship and interacts with floating ice and ship hull, as illustrated in Fig. 1.3. They are all coupled and interacting through interfaces of different types, forming a highly complex nonlinear dynamic system of multiphase and multi-physics nature, resulting in both the global resistance and local load on the ship. They play important roles in different ways: the global resistance affects the operation of a ship, such as maneuverability and fuel consumption, while the local load is critical for the safety of ship structure.

Over the past few decades, significant research efforts have been devoted to the ship-ice interaction problem, both experimentally and numerically. While the ice resistance, as a time-averaged value, has been understood to some extent, the local load was rarely discussed. Experimentally, collecting detailed stress information on the ship hull is difficult, and results from model tests are hard to be scaled accurately to the actual scale of ship structures. In terms of the numerical efforts, most models for the ship-ice interaction were semi-empirical and highly phenomenological, which may miss details of the dynamics and underpredict the local load. Therefore, studying ship-ice interaction with first-principle-based continuum mechanics, which captures relevant physics completely and provides a
detailed understanding of the dynamics, is of particular importance. The development of such a fully coupled continuum mechanics framework is the focus of the current thesis. The framework can capture the dynamic response of a marine vessel navigating through ice-covered Arctic waters. Accurate prediction of multiphase fluid-structure-ice interaction can be further utilized in developing industry guidelines for ship design and operation as well as ship routing strategies.

1.2 Objectives and methodology

The strong interactions between multiphase fluids and elastic structures form a highly nonlinear complex dynamic system, which requires fully-coupled model-
ing. During the modeling of multiphase FSI, interfaces between different phases and physical fields pose significant challenges in mathematical modeling and numerical simulation. Fluid-fluid and fluid-solid interfaces can undergo complex geometric changes during multiphase FSI. The mutual dependence between the geometry and the underlying dynamics of interfaces is very sensitive and error-prone in numerical simulations. Handling the discontinuity of physical properties along evolving interfaces needs careful considerations from both physical modeling and computational standpoint. The different kinematic description of solids and fluids introduces intrinsic conflict and poses fundamental difficulties during the integration between the fluid and solid equations in a unified manner. Furthermore, multiphase FSI involves other well-known computational mechanics challenges with regard to satisfying conservation (e.g., mass and energy), handling high density and viscosity ratios, and turbulence effects.

Motivated by the need for modeling the ship-ice interaction, the current work aims to develop a computational framework using a continuum mechanics based approach and a consistent variational formulation to solve multiphase FSI problems. The simulation framework should be able to handle two types of interfaces: the atmospheric-ocean interface and the fluid-structure interface. This work builds upon our previous study of [8], where the moving solid surface is evolved with the ALE method and the air-water interface is captured with the phase-field diffuse interface description based on free energy minimization. However, in the current context of simulating ice-going ships, new challenges emerge such as (i) How to handle the drifting and rotational motion of ship and ice? (ii) How to model the contact between ice and ship hull? and (iii) How to accurately capture the hydrodynamic effects during strong ice-structure interaction?

Analogous to the interface-capturing approach employed for multiphase flow interfaces, we intend to resolve these difficulties by generalizing the phase-field diffuse interface description to fluid-solid interface and solid-solid contact problems. This leads to the main research question of the current thesis:

*Can we employ the free energy principle and the diffuse interface description to simulate the interactions among fluids of multiple phases and immersed elastic solid bodies?*
There are four key objectives around this broad research question:

1. Develop a consistent formulation for the continuum mechanics of fluids and solids with different physical properties;

2. Evolve the deformation and strain of solids in an Eulerian frame of reference;

3. Represent and evolve the fluid-fluid and fluid-solid interfaces accurately via the phase-field method;

4. Solve large-scale 3D problems using an unstructured finite element mesh with complex geometries.

To realize Objective 1, we use a unified momentum and mass conservation equation for the dynamics of the continua, including both fluids and solids. The differences in physical properties are integrated via phase-dependent interpolation. While Objective 2 is achieved by temporally integrating the evolution of the left Cauchy-Green tensor, we further develop the phase-field method for Objective 3 by preserving interface and geometry properties, therefore significantly improving the performance and broadening the application range of the phase-field interface capturing method. The Objective 4 is achieved by discretizing the unified continuum system via a fully implicit finite-element framework with parallel implementation.

1.3 Contributions and impact

While research efforts have been devoted to understanding the ice-ship interaction, the current state-of-the-art methods for calculating coupled hydrodynamics-structure-ice interactions are semi-empirical and highly phenomenological, which do not include detailed physical understanding and first-principle-based continuum mechanics. On the other hand, scale model tests give insight into the phenomenon of ice-structure interaction, but they cannot be scaled accurately to the real scale of ship structures. To overcome these drawbacks, the current thesis aims to develop a unified Eulerian variational framework for solving multiphase FSI. The motion of multiphase fluids and solids will be consistently solved through unified continuum mechanics formulation via the Eulerian description. The variational finite element
discretization and the phase-field diffuse interface description allow the description of large motion and deformation of fluid and solid interfaces over unstructured meshes. The contributions in this dissertation help to advance the field of computational mechanics for multiphase FSI problems. Specifically, the current work enables us to simulate free-form motions and deformations of solid objects and multiphase flow interfaces with unified and accurate dynamics.

For the first time, this thesis provides a comprehensive study of the diffuse interface methods for the application to multiphase FSI problems. The fluid-fluid interface $\Gamma^{ff}$, fluid-solid interface $\Gamma^{fs}$ and solid-solid interface $\Gamma^{ss}$ between the fluid domains $\Omega^f$ and the solid domains $\Omega^s$ are modeled as a diffuse region with continuous variation, as illustrated in Fig. 1.4. With this approach, the requirement of resolving the interface to satisfy the velocity and traction continuity conditions with standard finite element method is circumvented. The main difficulty now is

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1_4.png}
\caption{An abstract representation of fluid-fluid and fluid-solid interfaces in multiphase FSI problems. The diffuse interface in the Eulerian mesh is shown as the shaded region.}
\end{figure}

of resolving the interface to satisfy the velocity and traction continuity conditions with standard finite element method is circumvented. The main difficulty now is
the accuracy of the interfaces to couple multiphase fluids with freely moving/deforming solids in an Eulerian description. Some of the specific contributions from the current work to solve this difficulty while achieving the objectives can be summarized as:

- A time-dependent mobility model for preserving the hyperbolic tangent profile of the phase-field method and the resulting accurate surface tension force calculation.
- A gradient-minimizing velocity field for reducing the curvature flow of the phase-field method and its application in preserving geometry details of solids in Eulerian description.
- Generalization to complex interactions and contact between multiphase fluids and multiple solids.
- An integrated, stable and robust 3D unified Eulerian finite element solver with parallel implementation.

Using our multiphase FSI framework, for the first time, we will study ship-ice interaction with nonlinear hydrodynamics effects. Such advanced modeling and simulations can provide physical understanding for ice crushing, ice induced vibrations and the resulting noise, serve as tools for efficient, reliable and low-noise operations of marine vessels, and help to develop improved industry guidelines for ship design and operation. In addition to high-fidelity modeling, the framework can allow quantifying uncertainties due to incomplete knowledge of constitutive laws, basal topography and boundary conditions. These uncertainties can be estimated by assimilating observational data into the model. Together with the development of industry guidelines, these reliable and efficient multiphysics predictions can reduce the noise emitted by Arctic shipping and enable less interruptive shipping.

1.4 Organization of the thesis

The organization of the current dissertation is illustrated in Fig. 1.5. In Chapter 2, we comprehensively review existing methods for simulating the multiphase FSI problems. We begin with the frame of reference for describing the motion of
continuum, and numerical techniques for connecting different frames of reference at the interface location. Through the review, we explain why the fully Eulerian approach is adequate for the current multiphase FSI problems. In the fully Eulerian description, we further look into the description of the solid kinematics and the interface capturing methods. Through comparison, the evolution of the left Cauchy-Green tensor and the phase-field methods are used in the current work.

The phase-field diffuse interface description is discussed in detail in Chapter 3. We systematically review the dynamics of the convective phase-field method. The source and control parameters of the convective distortion, the interface regularization and the curvature flow effect are explained in detail.

The phase-field diffuse interface description is then applied to the fluid-fluid interface in Chapter 4. While the hyperbolic tangent interface profile is the key to the consistency in phase transition across the diffuse interface and interface dynamics, its importance is further elevated for the fluid-fluid interface with surface tension effect. To maintain the hyperbolic tangent profile against the distortion due to convection, we develop an interface-preserving (IP) phase-field method based on a novel time-dependent mobility model, which adaptively regularizes the interface
with free energy minimization according to the intensity of convective distortion. The model is proved to be effective in a series of benchmark comparisons of 2D and 3D rising bubble cases and demonstrated in the case of two rising bubbles merging with a free surface.

In Chapter 5, we apply the phase-field method to the fluid-structure interface, where accurate solid geometry is required. However, the artifact curvature flow from the interface regularization disturbs the evolution of the interface, which further deteriorates the interface geometry. We resolve this dilemma with a novel interface and geometry preserving (IGP) method. In the IGP method, the phase-field variable is convected by an auxiliary velocity field termed as the gradient-minimizing velocity field (GMV). The GMV attains the solid velocity inside the solid and extends the solid velocity along the normal direction across the diffuse interface region. With this construction, the normal velocity gradient in the normal direction is reduced, which decreases the convective distortion, therefore reducing the required interface regularization and further the curvature flow. The method is shown to be effective in the case of a channel flow passing a solid block and the cylinder-flexible plate problem.

Integrating the methods developed for fluid-fluid and fluid-solid interfaces, we present the 3D multiphase FSI framework in Chapter 6. We first introduce the initialization of the hyperbolic tangent profile for complex interfaces. After that, the computational framework for the dynamics of the multiphase FSI is discussed. The framework solves a single mass and momentum conservation equation for the entire computational domain based on phase-dependent interpolation. For each phase of fluids, a set of IP equations is solved, while for each phase of solids, a set of IGP equations and the evolution of the left Cauchy-Green tensor is solved. It is worth noting that the contact between multiple solids can be naturally handled in the framework. The framework is validated through the problem of a rotating disk in lid-driven cavity flow, and further demonstrated in problems of rotational sphere, falling and bouncing back of a sphere, and collision of two solid spheres. Finally, we demonstrate the framework to simulate the interaction between ice floes and a moving ship.

Lastly, we summarize the thesis as conclusions and make some recommendations in Chapter 7.
Chapter 2

Literature Review *

Multiphase FSI can involve interacting fields of a wide range of length and time scales and disparate physical properties. The different kinematic descriptions of solids and fluids introduce intrinsic conflict and pose fundamental difficulties during the integration between the fluid and solid equations in a unified manner. Furthermore, the modeling of multiphase FSI encounters other well-known computational mechanics challenges with regard to satisfying conservation (e.g., mass and energy), handling high density and viscosity ratios, and turbulence effects. By considering proper modeling assumptions and mathematical considerations, various approaches are being explored in the literature. In this chapter, we conduct a systematic review of existing approaches and justify the current methodology in the context of predicting multiphase FSI with strongly coupled dynamics. We first review the kinematic descriptions for multiphase FSI problems and justify the selection of the fully Eulerian approach for the current problem. With this approach, we then review the techniques for describing the solid kinematics and capturing the interface in an Eulerian frame of reference, therefore justifying the selections of evolving the left Cauchy-Green tensor and phase-field method.

2.1 Review of multiphase FSI formulations

To begin with, a multiphase system can be defined as a mixture of the phases of liquid, gas and solid. The first and foremost consideration in selecting a proper formulation for a given multiphase system is the length scales of the interacting phases. For cases with extremely large length scale ratios, a homogenized/averaged model can be used, where the contribution from the small-scale phases is modeled as a function of its statistic values such as concentration rather than recognizable individuals. Using the continuum theory of mixtures, one can consider a distribution of different phases in the same physical space at a given time. Examples include the modeling of dilute dispersion of gas bubbles in liquid conducted in [17], cavitating flows [18] and porous media [19]. For intermediate length scale ratio, simplified dynamics or coupling can be applied to small-scale phases in modeling processes, such as the Eulerian-Lagrangian simulation for the particle-laden flow [20], or discrete element method for the ice-ship interaction [21, 22]. When the interacting phases have approximately the same length scale, both of the phases need to be resolved accurately so that the details of the interaction can be captured faithfully. In the context of local load prediction of ship-ice interaction, we consider the extreme load as the result of contact with ice floes which are at the same length scale as the ship. Therefore, a continuum mechanics-based approach is employed for all the phases, including the ship structure, the ice floes, the wind flow and hydrodynamics to capture the fully coupled dynamics.

In the continuum mechanics formulation of multiphase FSI, the key challenges are associated with dissimilar coordinate frames for the fluid and solid domains, the proper treatment of the boundary conditions at the interfaces, and the design of stable and accurate discretizations for the coupled nonlinear PDEs [23, 24]. We will further discuss these aspects in the following paragraphs.

2.1.1 Kinematic descriptions for fluids and solids

In the past several decades, various techniques treating the interfaces have been developed based on different kinematic descriptions for fluids and solids. The kinematic description is a fundamental consideration in the modeling of continuum, which can be classified into Lagrangian and Eulerian descriptions. From a
computational point of view, the selection determines the relationship between the mesh and the deforming continuum. In the Lagrangian description, the grid points move consistently with the motion of material points. On the contrary, the grid points merely represent the spatial location in the Eulerian description. In a solid object, the material points are tightly bounded and highly organized. Therefore, the Lagrangian description can be applied without the concern of distorting the mesh, thus being convenient and accurate. On the other hand, the motion of fluid particles is quite chaotic. And usually, we care more about a fixed control volume where the fluid particles flow through, rather than the trajectory to individual fluid particles. Hence the Eulerian description is more appropriate for fluids. While the reverse is not frequently used, they have their own advantages in certain scenarios. The Lagrangian description for fluids can be used when trajectories of fluid particles are of key importance. The Eulerian description for solids facilitates large topological changes and contact. The kinematic descriptions are summarized and illustrated in Fig. 2.1.

**Figure 2.1:** Illustration of kinematic descriptions for fluids and solids. (Portraits from Wiki)
2.1.2 Interface techniques

Based on different kinematic descriptions for fluids and solids, various techniques for treating the interfaces are applicable. Broadly speaking, they can be classified into four categories: fully Lagrangian approach, arbitrary Lagrangian-Eulerian (ALE) method, hybrid Lagrangian-Eulerian approach, and fully Eulerian approach. They are discussed respectively in the following paragraphs and collectively illustrated in Fig. 2.2.

**Fully Lagrangian approach**

As the name suggests, the fully Lagrangian approach employs Lagrangian description for both fluids and solids. To resolve the mesh distortion on the fluid side, the smoothed-particle hydrodynamics method [25] employed a mesh-free particle-based discretization, where the physical quantities are approximated via integral
interpolation. However, it usually suffers from difficulties in conserving momentum and mass and imposing boundary conditions accurately. Another approach is to continuously remesh the computational domain, as proposed in [26], which is computationally inefficient.

**ALE! method**

One of the most accurate and wildly used approaches is the ALE! method developed in [27, 28]. In the ALE! method, the Lagrangian description is used for solids, which employs a conformal mesh to represent the solid object and the fluid-solid interface. When the fluid-solid interface moves along with the motion and deformation of the solid object, the mesh at the fluid side is governed by partial differential equations (PDEs) which deforms the mesh continuously in a way similar to elastic materials. And the surrounding fluids are solved in this moving frame of reference. With conformal mesh on the fluid-solid interface, the velocity and traction continuities can be accurately imposed [29–31]. Its accuracy and robustness have been demonstrated in several complicated multiphase FSI applications such as vortex-induced vibration for a drilling vessel-riser system [32], internal two-phase flow in pipelines [33, 34] and elastocapillarity phenomenon [35–37]. However, the conformal mesh can generate distorted elements and fail due to large motion and deformation of solids, which requires special treatment such as remeshing strategies. While the remeshing strategies are effective, they can be cumbersome in coding and costly in computation.

**Mixed Lagrangian-Eulerian approach**

The difficulty in mesh motion is further reduced in the mixed Lagrangian-Eulerian approach. This approach allows independent Lagrangian and Eulerian meshes for solids and fluids, respectively. The fluid-solid coupling at the non-matching interface is realized in a relaxed manner. For example, in the immersed boundary method [38, 39], the velocity and force of fluids and solids were projected back and forth at the interface between the Lagrangian grid and the Eulerian grid with a Dirac Delta function. In the front-tracking method [40], a similar treatment was employed for the fluid-fluid interface.
The coupling can also be achieved by a Lagrange multiplier, as conducted in the fictitious domain method [41, 42]. The fictitious domain method assumes a complete computational domain for the background fluid, which is composed of a real fluid domain and a fictitious domain. The latter is in fact occupied by the solid object. By satisfying the condition that the boundary velocity of the fictitious domain is the same as the solid object, the displacement of the solid object is passed to the fluid domain. This process is weakly enforced by a Lagrange multiplier. Then, the fluid load is calculated and passed to the solid object to complete the coupling.

While conducted differently, both the immersed boundary and the fictitious domain methods approximated the interface location in a fixed mesh, which inevitably introduce errors. This drawback is overcome in the extended finite element method, where the interface position is explicitly captured by additional degrees of freedom, which are spent in enriching the function space with discontinuous basis functions in the interface elements. The extended finite element method was initially used to capture the crack growth without remeshing [43, 44], and later used for FSI problems [45]. While the coupling between fluids and solids is performed in a way that is similar to the fictitious domain method, the boundary of the fictitious domain, in other words, the fluid-solid interface, is now explicitly captured, hence improving the accuracy of the coupling and numerical solution.

To summarize, the mixed Lagrangian-Eulerian approach almost eliminates the mesh operation and facilitates the topological changes of fluid-solid interfaces. However, the inconsistency in the kinematic descriptions of solids and fluids cause non-matching grids at fluid-solid interfaces, which may give rise to errors in boundary conditions and fluid-solid coupling. Usually, extra efforts are needed to resolve this issue.

**Fully Eulerian approach**

In the fully Eulerian approach, a consistent Eulerian description is used for both fluids and solids. The governing equations for fluids and solids are unified as a one-field formulation in the Eulerian frame of reference, in which the velocity and stress continuities are naturally satisfied. As a result of the consistency, large motion and
deformation of solids, as well as topological changes of interfaces, can be conveniently described without any extra effort. This merit becomes prominent with the increase in the number of phases and interfaces, and elevation of geometric complexity in multiphase FSI problems. Examples include contact dynamics, fracture, and phase transfer of solids [46–48]. The numerical simulation of FSI problems in a fully Eulerian approach was first demonstrated by [49] and further developed by [50]. While the fully Eulerian approach brings convenience in the formulation and interface motion, there are two major considerations: (i) How to track the displacement and strain of solids in an Eulerian frame of reference? (ii) How to represent and evolve the interface with reasonable accuracy in a fixed mesh? The literature regarding these two problems will be reviewed in the following sections.

2.1.3 Discretization

In discretizing the fully Eulerian formulations, while the particle-based approaches such as the smoothed-particle hydrodynamics [25] or the lattice Boltzmann methods [51] are quite convenient in representing the particles and handling the interfaces, the underlying conservation laws are hard to keep, and accurate implementation of boundary conditions is challenging. It is therefore desirable to consider a mesh-based approach such as finite volume or finite element method. In this thesis, we employ the finite element method, which has the advantages of great robustness, ease in using unstructured mesh for complex domains, and accurate boundary condition implementations. The instability arising from the convection and source term in PDEs is resolved with the Petrov-Galerkin stabilization [52] and positivity preserving variational method [53]. The equations in the formulation are solved in a partitioned iterative manner.

2.2 Review of the solid kinematics in an Eulerian frame of reference

In the Eulerian description, the grid nodes only represent the spatial locations. Therefore, the displacement or strain of solids need to be tracked by additional function fields. In the initial point set method proposed by [49], the material particles are marked by their initial locations, and collectively form a marker field, as
Figure 2.3: Illustration of the marker field for the solid kinematics.

Illustrated in Fig. 2.3. The marker field is specific to material particles, therefore, evolved according to zero total derivatives in the Eulerian frame of reference. Once the current location is known and the initial position is given by the initial point set, the displacement can be calculated. Another issue is that the markers will be entangled in the fluid domain and near the fluid-solid interface. This will cause spurious displacement in the fluid domain and near the fluid-solid interface, which will later contaminate the strain and stress inside the solid domain. To resolve this, instead of using the fluid velocity for the convection of the initial point set in the fluid domain, [49] created an auxiliary velocity field. The auxiliary velocity in the fluid domain is constructed as a harmonic extension of the solid domain, thus fixing the entanglement issue.

The formulations of the initial point set method were further simplified in the reference map technique proposed by [46, 54], in which the initial positions rather than the displacements were directly used to calculate the stress. The harmonic extension was replaced by discrete interpolation. The constitutive relation of solid objects was further generalized by [50] to St. Venant-Kirchhoff material. In [55], the momentum equation was written purely based on the velocity of solids, which simplified the discretization and allowed fully implicit discretization.

While the initial point set and the reference map techniques are effective, second-order differentiation is required from the displacement to the divergence of the solid
stress in the momentum conservation equation, which causes difficulties in linear FEM discretization. Alternatively, the kinematics of solids can be captured by evolving the left Cauchy-Green tensor, as conducted in [56]. With this approach, the second-order differentiation was reduced to first-order. More detailed formulation and discussions regarding the Eulerian description for solids can be found in Chapter 5.

2.3 Review of the interface capturing methods

The volume of fluid, level set and phase-field methods are the state-of-the-art interface capturing techniques for the fully Eulerian description. In these methods, the change of phases at the interface is described via a continuous scalar-valued function serving as a phase indicator. The indicator is almost a constant in the bulk of the continuum, while a rapid variation occurs near the interface. The interface is usually considered as an isoline or isosurface of the phase indicator, as illustrated in Fig. 2.4. The interface capturing methods have became an active area of research owing to its convenience in describing large motion and deformation of continua and interfaces.

One of the earliest and most popular methods is the volume of fluid method developed in [57], where the volume fraction of each fluid was evaluated on grid points and used to approximate the interface position. From the interface capturing perspective, the major drawback of the volume of fluid method is the smearing of the interface caused by the convection effect and numerical diffusion.

This issue is addressed in the level set method [58–61], where a signed distance function was used as the phase indicator, with the zero isoline or isosurface being the interface. Note that this definition not only indicates the interface position, but also poses a constraint on the slope of the phase indicator. As a signed distance function, its slope should be one in the normal direction of the interface. Once the interface is contracted or diffused in the convection, a reinitialization equation, which enforces the constraint on the slope, is solved to reinitialize the phase indicator near the interface. Therefore the smearing of the interface is resolved.

The phase-field method was initially developed for modeling phase separation and formation of interfaces [62, 63]. In the phase field method, the interface be-
Figure 2.4: Illustration of interface capturing in 2D: the interface plotted with red line is captured in the $X-Y$ plane as the zero isoline of the phase indicator $\phi$ visualized by its contour.

tween phases is formed due to the minimization of free energy. The minimum free energy is reached with a phase transition of hyperbolic tangent profile, which is a profile with a smooth yet highly localized transition near the interface. The feature of autonomous evolution towards the hyperbolic tangent profile is particularly desirable to eliminate the smearing of the interface, thus being coupled with the convection effect and naturally applied for interface capturing. Compared to the level set method, the phase-field method integrates the interface convection and the interface regularization in a single equation, thus being more efficient [64].

With the captured interface, the phase transitions and boundary conditions can be imposed in either a sharp or diffuse interface approach. In the sharp interface approach, the interface is explicitly reconstructed. The physical properties at both sides are selected from the corresponding phases, respectively. The boundary condition at the interface, such as the pressure jump due to surface tension force, is implemented according to the interface position. However, the evaluation of normal and curvature can be complex due to the non-smoothness and discontinuity of the reconstructed interface. On the other hand, the diffuse interface approach considers the phase transition as a gradual variation across a transitional region with finite thickness, which can be formulated as a function of the phase indicator. The boundary condition can be implemented in a smeared manner with the Dirac Delta
function. With this approach, the normal and curvature can be easily calculated from the first and second order derivatives of the phase indicator. Based on the review, we employ a phase-field diffuse interface description for interfaces in the current thesis. The details will be further discussed in Chapter 3.

2.4 Summary

In this chapter, we comprehensively reviewed the multiphase FSI formulations. From the perspective of simulating the ice-going ships, the key features of the problem are: (i) interaction between multiphase fluids and multiple solids of distinct properties, (ii) requirement of strict satisfaction of conservation laws and continuities of velocity and stress, (iii) complex topological changes of interfaces such as translational/rotational motion, free surface merging and breaking-up, and contact between solids. Based on these characteristics, we select the fully Eulerian formulation to unify the dynamics of different phases, where the conservation laws and the continuities of velocity and stress are naturally satisfied. To describe the kinematics of solids with Eulerian description, the evolution of the left Cauchy-Green tensor is considered. The complex interface evolution and interaction are realized through phase-field diffuse interface description. The formulation is discretized with the finite element method to facilitates the unstructured mesh for complex domains and accurate implementation of boundary conditions. To the best of our knowledge, there exists no literature on multiphase FSI involving interactions between solid objects using a phase-field diffuse interface approach. As the key to the interface kinematics and dynamics, the phase-field method is introduced in Chapter 3, and applied to multiphase fluids interfaces and fluid-solid interfaces in Chapters 4 and 5, respectively.
Chapter 3

Phase-field diffuse interface description *

In this chapter, we introduce the diffuse interface description using the phase-field method. Generally speaking, the phase-field method indicates the phases of a multiphase system in a fixed Eulerian grid with scalar fields so-called phase indicators or order parameters. Driven by the free energy minimization, the evolution of the phases in a given problem is obtained, which can be considered as the process of interface generation during phase separation. We next describe the dynamics of the convective Allen-Cahn equation for evolving interfaces. Several important features of the dynamics such as the convective distortion, the interface regularization by free energy minimization and the curvature flow are discussed in detail, the insights of which will be reflected throughout the dissertation.

3.1 Review of the phase-field method

The moving interfaces between different continuum fields, such as the air-water interface, or the interface between solid objects and the surrounding air, are encountered frequently. A traditional and intuitive description for the interface is the sharp interface description, which considers the interface as a surface with zero

thickness sharply separating the materials. Later, the observation of microscopic problems, such as the surface tension effect and solidification process, reveals that the interface has its own dynamics arising from the difference between nearby materials. This stimulates the emergence of the diffuse interface description. The idea of the diffuse interface description can be traced back to van der Waals [65], in which the interface was considered as a region with gradual transition from one phase to another. The transition region moved autonomously to minimize the free energy. This understanding and modeling approach were further developed for solving phase separation problems in [62, 63, 66], where the Cahn-Hilliard and the Allen-Cahn phase-field equations were established. Later, the phase-field methods are generalized to interface capturing for multiphysics problems [67–71].

In the phase-field diffuse interface description, an order parameter \( \phi \) is used as the phase-indicator, where \( \phi = 1 \) indicates one phase, and \( \phi = -1 \) indicates the other. The smooth transition between \( \phi = 1 \) and \( \phi = -1 \) forms the diffuse interface description, as shown in Fig. 3.1. The diffuse interface between the two phases is considered as a region where the phases are mixed and store free energy. The free energy functional \( \mathcal{E} \) is defined as:

\[
\mathcal{E} : H^1(\Omega) \cap L^4(\Omega) \rightarrow \mathbb{R}_{\geq 0}, \quad \mathcal{E}(\phi(x,t)) = \int_{\Omega} \left( F(\phi(x,t)) + \frac{\epsilon^2}{2} |\nabla \phi(x,t)|^2 \right) \, d\Omega,
\]

where \( \Omega \) is a bounded fluid domain consisting of spatial points \( x \) at time \( t \), \( H^1(\Omega) \) denotes the space of square-integrable real-valued functions with square-integrable derivatives on \( \Omega \), \( L^4(\Omega) \) denotes the function space in which the fourth power of the function is integrable, \( \mathbb{R}_{\geq 0} \) represents the set of non-negative real numbers, \( \phi(x,t) \) is referred to as the order parameter or the phase-field function which indicates the components of the two-phase mixture. The first term \( F(\phi(x,t)) \) in Eq. (3.1), which is called as the bulk or mixing energy, depends on the local composition of the two-phase mixture indicated by \( \phi \). To invoke the phase separation, a double-well potential is employed: \( F(\phi) = \frac{1}{4} (\phi^2 - 1)^2 \), in which the minimum bulk energy is attained with separated pure phases \( \phi = 1 \) and \( \phi = -1 \), as shown in Fig. 3.2 (a). The second term, which is called as the interfacial or gradient energy, depends on
Figure 3.1: Illustration of (a) diffuse interface representation of a circular interface via the order parameter field, and (b) function value of $\phi$ at the cross section $x = 0$.

The composition of the immediate environment indicated by $\nabla \phi$, as illustrated in Fig. 3.2 (b) and (c). The gradient energy dictates the interaction between the two phases. The ratio between the bulk energy and the interfacial energy is determined by a parameter $\epsilon$.

The evolution of the order parameter is considered as a result of the gradient flow minimizing the free energy functional in the Cahn-Hilliard and the Allen-Cahn phase-field equations [62, 63]. The Cahn-Hilliard equation naturally satisfies the mass conservation [72], therefore facilitating the development of conservative numerical schemes [73, 74]. This brings convenience in describing physical interfaces in mass-conserved problems. For example, the coupled Navier-Stokes-Cahn-Hilliard equations are used to describe immiscible two-component fluid flow with surface tension [71, 75]. However, the Cahn-Hilliard equation is cumbersome to implement due to its fourth-order terms, which require longer stencils or high-order polynomial approximation. When approximated with low-order polynomials, the order needs to be decreased by splitting the equation as two second-order equations with an intermediate variable, which increases the degrees of freedom. In contrast, the Allen-Cahn equation is a second-order convection-diffusion-reaction PDE which has attractive numerical properties from the implementation standpoint. Although the original Allen-Cahn equation is not mass-conservative, the
The conservation property can be realized by adding a Lagrange multiplier \cite{76, 77} or employing an anti-curvature term \cite{78}. The former is more stable, while the latter is more accurate \cite{79}. Concerning the computational efficiency and stability, we employ the Allen-Cahn phase-field equation with a Lagrange multiplier for solving two-phase flow problems in the current study.

In the original Allen-Cahn equation, the evolution of the phase-field function seeks the minimum of the free energy functional:

$$\frac{\partial \phi}{\partial t} = -\gamma \left( \frac{\delta \mathcal{E}(\phi)}{\delta \phi} \right),$$

(3.2)
where $\gamma$ is the mobility coefficient and $\frac{\delta \mathcal{E}(\phi)}{\delta \phi} = (F'(\phi) - \epsilon^2 \nabla^2 \phi)$ represents the variational derivative of the free energy functional. Eq. (3.2) can be formulated as the gradient flow of the free energy functional in $L^2$ space [80]:

$$\frac{\partial}{\partial t} \mathcal{E}(\phi) = -\gamma \int_{\Omega} \left| \frac{\delta \mathcal{E}(\phi)}{\delta \phi} \right|^2 d\Omega.$$

In the free energy minimization, the bulk energy minimization encourages abrupt transition between pure phases, while the interfacial energy minimization prefers a mixed uniform phase without transition. Using the interplay between these two effects, the parameter $\epsilon$ controls the thickness of the transition region, therefore usually referred to as the interface thickness parameter. The mobility coefficient determines the intensity of the gradient flow of the free energy functional and controls the speed at which the interface geometry relaxes to the equilibrium profile and shape with minimum free energy. For a planar interface in equilibrium, which can be considered as a one-dimensional case, the equilibrium interface profile can be solved as: $\phi_{eq} = \tanh \left( \frac{d}{\sqrt{2\epsilon}} \right)$, where $d$ is the signed distance function to the interface. The equilibrium interface profile has a smooth but highly localized phase transition between the phases, where the distance from $\phi = -0.9$ to $\phi = 0.9$ denoted as $\epsilon_d$ happens in $4.164\epsilon$, as shown in Fig. 3.3. As $\epsilon \to 0$, the interface converges to the sharp interface limit.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{diffuse_interface_profile.png}
\caption{Equilibrium hyperbolic tangent interface profile of the phase-field diffuse interface profile.}
\end{figure}
To conserve the mass of each phase, a Lagrange multiplier is employed, which further changes the equation as:

$$\frac{\partial \phi}{\partial t} = -\gamma \left( \frac{\delta \mathcal{E}(\phi)}{\delta \phi} - \beta(t) \sqrt{F(\phi)} \right),$$

(3.3)

where $\beta(t)$ is the time-dependent part of the Lagrange multiplier for mass conservation [77], which is given by $\beta(t) = \frac{\int_\Omega F'(\phi) d\Omega}{\int_\Omega \sqrt{F(\phi)} d\Omega}$.

### 3.2 Dynamics of the convective Allen-Cahn equation

#### 3.2.1 Convective distortion

When used for interface capturing in fully Eulerian description, the convection effect must be incorporated, which gives the convective Allen-Cahn equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = -\gamma \left( \frac{\delta \mathcal{E}(\phi)}{\delta \phi} - \beta(t) \sqrt{F(\phi)} \right).$$

(3.4)

Due to the convection effect, the hyperbolic tangent profile can be distorted. Consider a 1D case where the diffuse interface profile is initialized as a hyperbolic tangent profile shown in Fig. 3.4 (a). In a compressional velocity field, the diffuse interface region becomes thinner, as illustrated in Fig. 3.4 (b). On the other hand, the diffuse interface region can be thickened in an extensional velocity field shown in Fig. 3.4 (c). We refer to the distortion caused by the convection as the convective distortion. The compressed interface region may generate under-resolved high gradients and cause stability issues. The thickened interface further diffuses the interface and reduces the accuracy. Furthermore, when part of the interface is compressed and the others are extended, the inconsistency itself gives rise to false interface dynamics. Therefore, the interface distortion due to convection needs to be suppressed.

#### 3.2.2 Interface regularization

Once the interface is compressed or extended, the interface deviates from the hyperbolic tangent profile where the minimum free energy is attained. In this situa-
Figure 3.4: Illustration of the convective distortion on 1D interface profile: (a) initialized hyperbolic tangent profile, (b) thinned diffuse interface region due to a compressional velocity field, and (c) thickened diffuse interface region due to an extensional velocity field.

...tion, the free energy minimization process formulated by the Allen-Cahn equation will evolve the interface profile back to the hyperbolic tangent profile, as illustrated in Fig. 3.5. This can be used to regularize the diffuse interface profile against the convective distortion. The intensity of the regularization effect is controlled by the mobility coefficient $\gamma$.

3.2.3 Curvature flow

In 2D or 3D cases, the total free energy of the interface is closely related to the perimeter or area of the interface [81]. As a result, the minimization of free energy shortens the interface. The interface shortening effect can be observed as a mean curvature flow that moves the interface in the normal direction, which is illustrated in Fig. 3.6 (a). Under the constraint of the volume conservation, which is the equivalence of the mass conservation of each phase, the free energy minimization will evolve the actual interface contour $\phi_a = 0$ towards the contour with minimum
perimeter or area. Consequently, the interface convected by the convective velocity relaxes towards a circular or spherical shape \[76, 77, 81\]. The flow induced by this process is referred to as the volume-conserved mean curvature flow, as illustrated in Fig. 3.6 (b). The flow velocity can be derived from asymptotic analysis \[76, 77, 82\].

For the current formulation, consider the interface \(\Gamma^\phi(t) = \{x \in \Omega | \phi(x, t) = 0\}\), the velocity of the volume-conserved mean curvature flow at the interface is given by:

\[
\mathbf{v}_\kappa(x, t) = \gamma \varepsilon^2 \left( \kappa(x, t) - \frac{1}{|\Gamma^\phi_I(t)|} \int_{\Gamma^\phi_I(t)} \kappa(x, t) ds \right) \mathbf{n}_L^\phi(x, t), x \in \Gamma^\phi_I(t),
\]

where \(\mathbf{v}_\kappa(x, t)\) is the velocity of the volume-conserved mean curvature flow, \(\kappa(x, t)\) is defined as \(\kappa(x, t) = \sum_{i=1}^{n_{sd}-1} \kappa_i(x, t)\), \(n_{sd}\) being the number of dimensions and \(\kappa_i(x, t)\) being the principle curvatures of the interface, \(|\Gamma^\phi_I(t)|\) is the perimeter or area of the interface, \(\mathbf{n}_L^\phi(x, t) = \nabla \phi / |\nabla \phi|\) is the unit normal vector of the isolines or isosurfaces of \(\phi\), \(\kappa(x, t)\) is defined as positive when \(\mathbf{n}_L^\phi(x, t)\) is pointing to the concave side of

\[\begin{align*}
\Gamma^\phi_I(t) &= \{x \in \Omega | \phi(x, t) = 0\}, \\
\kappa(x, t) &= \sum_{i=1}^{n_{sd}-1} \kappa_i(x, t), \\
\mathbf{n}_L^\phi(x, t) &= \nabla \phi / |\nabla \phi|,
\end{align*}\]
3.3 Summary

To summarize, the convective Allen-Cahn equation involves the dynamics of the convective distortion caused by $\mathbf{v}$, the interface regularization controlled by $\gamma$, and the curvature flow which is proportional to $\gamma \varepsilon^2$. The adaptive control of these dynamics through the related variables and parameters is the key to accurate and robust interface capturing with the phase-field method. This is one of the key objects of this thesis and will be further discussed in Chapters 4 and 5.
Chapter 4

Interface-preserving phase-field for two-phase flow *

In this chapter, we apply the phase-field diffuse interface description to two-phase flow problems. For accurate representation and evolution of the fluid-fluid interface, we develop an interface-preserving phase-field method. The method uses a time-dependent mobility model to adaptively adjust the interface regularization according to the intensity of the convective distortion, and significantly reduces the interface distortion. This is vital to the surface tension effect, the modeling of which is based on the hyperbolic tangent profile. The method is validated for a series of 2D and 3D rising bubble problems.

4.1 Background

Two-phase flow of immiscible fluids is ubiquitous in natural phenomena and engineering applications. Examples include bubbly cavitating flows around marine propellers [83], wake bubbles behind ships [84], and the bubble sweep-down problem of oceanographic vessels [85]. The modeling of immiscible two-phase flows poses well-known difficulties regarding the topological changes during simulating realistic flows, the mass conservation, the discontinuity of properties across the

interface, and sensitive dynamics due to the surface tension effect.

Most of the challenges can be resolved with the phase-field diffuse interface description. The topological changes can be easily handled in the Eulerian frame of reference with interface capturing methods, the mass conservation can be resolved by the Lagrange multiplier, and the discontinuity is smoothed with diffuse interface description, as discussed in Chapter 3. However, the interface parameters need to be selected judiciously to have accurate interface representation and evolution, as discussed in Section 3.2, especially in the presence of sensitive surface tension dynamics.

The surface tension can be imposed in either a sharp or diffuse interface approach. Since the sharp interface approach suffers from the difficulty in interface reconstruction and normal and curvature calculation as reviewed in Section 2.3, we employ the diffuse interface approach. Two popular approaches for surface tension modeling with diffuse interface description are: (i) continuum surface force (CSF) model, which distributes the sharply defined force with a Dirac Delta function to the diffuse interface region [86], (ii) free energy based surface tension model, which imposes the energy balance in the context of the phase-field method [65, 87, 88]. However, both of them are derived based on a prescribed interface profile. Once the interface profile is distorted, surface tension calculation is subjected to errors. The erroneous surface tension will degrade the accuracy of the interface evolution and further distort the interface profile. As a result, mutual dependency between the interface representation and evolution is established due to the surface tension effect, which further increases the sensitivity of the simulation to the interface distortion error. Therefore, preserving the interface profile is vital to the two-phase flow simulations with phase-field diffuse interface description.

The interface preservation can be improved by enhancing the interface regularization from free energy minimization. The competition between the convective distortion and the interface regularization leads to an actual interface profile $\phi$. With the increase in the mobility coefficient, a stronger regularization will be imposed, and the actual interface profile is closer to the hyperbolic tangent profile, as shown in Fig. 4.1 (a). However, we should note that the mobility coefficient is also proportional to the curvature flow, as discussed in Section 3.2. In the context of two-phase flows at the macro scale, where the interface motion should be
Convective distortion

Free energy minimization

Figure 4.1: Illustrations of the interface dynamics of the convective form of the conservative Allen-Cahn equation: (a) one-dimensional equilibrium interface profile \( \phi_{eq} \) and the actual interface profile \( \phi_a \) subjected to an extensional velocity field, and (b) volume-conserved mean curvature flow velocity \( \mathbf{v}_\kappa(x,t) \) and the convective velocity \( \mathbf{v}(x,t) \) of the interface \( \phi(x,t) = 0 \). The free energy minimization described by the equation balances the convective distortion with \( \phi_a \) in (a), and induces \( \mathbf{v}_\kappa(x,t) \) in (b).

dominated by local convective velocities, the curvature flow velocity is an artifact velocity that disturbs the interface geometry, as illustrated in Fig. 4.1 (b). The dilemma between preserving the interface profile through interface regularization and minimizing the artifact curvature flow is the key problem in the current study.

The effect of the phase-field parameters, namely the mobility coefficient \( \gamma \) and the interface thickness \( \varepsilon \), have been discussed in some literature. Jacqmin [87] suggested that the gradient flow minimizing the free energy should properly oppose the convective distortion, while the gradient flow should converge to zero (i.e., the phase-field equation converges to a pure convection equation) as the diffuse interface converges to the sharp interface. According to the order of magnitude analysis, a mobility coefficient varying between \( \mathcal{O}(\varepsilon) \) and \( \mathcal{O}(\varepsilon^2) \) in the Cahn-Hilliard equation was found to be appropriate. In [89], the magnitude of the total free energy is adjusted dynamically to ensure its consistency with the surface tension coefficient viewed as free energy density. The explicit calculation of the interface length or area was required during the adjustment.

In [78], the phase-field propagation equation was formulated for tracking sharp interfaces. The mobility coefficient, the interface thickness parameter, and the maximum convective velocity are combined to form a non-dimensionalized pa-
rameter via a standard explicit finite difference discretization. The parameter was considered purely as a numerical parameter, the impact of which on the interface profile and evolution was studied for stationary and evolving interfaces. It was found that the increase in the mobility coefficient results in better enforcement of the hyperbolic tangent profile and helps to suppress the instabilities at corners. The mobility coefficient was controlled one order of magnitude below its upper limit given by the Courant-Friedrichs-Levy (CFL) condition to avoid significant discretization errors. In [90], an additional free energy functional punishing the deviation from the hyperbolic tangent profile was designed, which provides a correction term in the Cahn-Hilliard equation via the minimization process. The profile correction term enforces the hyperbolic tangent profile, thereby reducing the interface shrinkage effect, the convective distortion, and improving the surface tension calculation. This approach was further developed in the profile-flux correction [91] and applied in the turbulent multi-phase flow problems [92].

In this chapter, we propose a time-dependent mobility coefficient to resolve the dilemma through adaptively interface regularization. When applied to the phase field method, we have an interface-preserving and conservative phase-field method for incompressible two-phase flows with a particular emphasis on accurate surface tension dynamics. A continuum formulation and a systematic approach for determining the phase-field parameters $\gamma$ and $\epsilon$ are presented. The effects of the parameters are analyzed by directly considering the associated terms in the convective form of the Allen-Cahn equation in a non-dimensional moving orthogonal curvilinear coordinate system. The term representing the effect of the convective distortion is identified wherein the convective distortion parameter quantifies the ratio between the convective distortion and the free energy minimization. An interface-preserving condition for the parameter enforcing the free energy minimization dominance over the convective distortion is derived. To fulfill the condition, we propose a time-dependent mobility model for controlling the RMS convective distortion parameter in the diffuse interface region. Direct relationships between the RMS convective distortion parameter and relative interface thickness and surface tension errors are assessed by numerical simulations of the interface convection problems. By establishing a suitable range for the mobility coefficient, excessive gradient flow minimizing the free energy functional and the resulting
spurious volume-conserved mean curvature flow is avoided.

The present study builds upon our previous conservative and energy-stable variational scheme for the Allen-Cahn and Navier-Stokes system proposed in [93]. The scheme was integrated with a mesh adaptivity process in [94], and has been proven to be accurate and stable for a wide range of FSI problems in the inertia dominate regime with high-density ratio [33]. In the current work, we further improve the accuracy of the scheme in the capillary-dominated regime by considering the interface-preserving Allen-Cahn-based phase-field model. We employ the model together with the CSF model, where the surface tension is transformed into a volumetric force spreading over a few layers of elements.

We discretize the incompressible Navier-Stokes and Allen-Cahn equations with the finite element method in a fully implicit manner. We maintain the bounded and stable solution of the Allen-Cahn system via the positivity preserving variational (PPV) technique [53] and the coupling between the Allen-Cahn and the Navier-Stokes systems retaining second-order accuracy in time domain [33, 93]. With the aid of a generic 1D bistable diffusion-reaction system in a stretching flow, we first carry out a systematic convergence and verification study of our 1D steady Allen-Cahn solver based on the PPV technique and implicit discretization. To demonstrate the interface-preserving formulation, we employ the Allen-Cahn solver for the convection of diffuse interfaces in prescribed velocity fields for planar and curved situations.

We examine the proposed formulation in the two- and three-dimensional rising bubble benchmark cases through a systematic convergence study. We compare accuracy and convergence with the sharp interface formulation. Our results show that only when the interface-preserving capability is improved and the volume-conserved mean curvature flow is decreased simultaneously, the simulation results will converge to the accurate solution. This requires the reduction of the RMS convective distortion parameter and the interface thickness parameter at the same time. Finally, we simulate two rising bubbles merging with a free surface with an unstructured mesh to demonstrate the applicability of the proposed model in practical problems, which have complex topological changes of the interface and complex dynamics including bubble-bubble and bubble-free surface interaction.

The organization of this chapter is as follows: Section 2 presents a mathe-
atical analysis of the diffuse interface profile, wherein the convective distortion parameter and the interface-preserving condition are identified. The time-dependent mobility model is proposed according to the interface-preserving condition. Section 3 describes the implementation of the variational formulation for the interface-preserving conservative Allen-Cahn-Navier-Stokes system with the time-dependent mobility model. Section 4 verifies our implementation through a 1D bistable convection-diffusion-reaction system in a stretching flow and provides a numerical assessment of the errors associated with the convective distortion parameter for a planar and a curved interface. Two- and three-dimensional rising bubble cases are investigated in Section 5 to demonstrate the effect of the proposed model on the volume-conserved mean curvature flow and the interface preservation property. Section 6 demonstrates the applicability of the model by solving for two bubbles rising and merging with a free surface. The conclusions are summarized in Section 7.

4.2 Interface-preserving formulation

In this section, we present the continuum formulation of the time-dependent mobility model for preserving the hyperbolic tangent profile. The convective form of the Allen-Cahn equation is directly analyzed in a non-dimensional moving orthogonal curvilinear coordinate system. The term representing the influence of the convective distortion is identified in the governing equation. The magnitude of the term depends on a non-dimensional parameter, which we refer to as the convective distortion parameter. An interface-preserving condition is derived for the convective distortion parameter to preserve the interface profile. The time-dependent mobility model is proposed based on the interface-preserving condition.

4.2.1 Interface profile in curvilinear coordinate system

Following the original work of [63], we describe the evolution of the two-phase interface in an orthogonal curvilinear coordinate system. This allows us to simplify the governing equation utilizing the property that the level sets of the order parameter are parallel to the interface. Consider a physical domain \( \Omega \times [0, T] \) with spatial coordinates \( \mathbf{x} \) and temporal coordinate \( t \). The boundary of the computational do-
main $\Gamma$ is decomposed as $\Gamma = \Gamma_D^\phi \cup \Gamma_H^\phi$, where $\Gamma_D^\phi$ and $\Gamma_H^\phi$ denote the Dirichlet and Neumann boundaries for the order parameter respectively. A diffuse interface that separates the immiscible two-phase fluids defined on $\Omega$ is indicated by the order parameter $\phi(x,t)$. The diffuse interface is convected by a velocity field $v(x,t)$. In the orthogonal curvilinear coordinate system, the spatial coordinates are given by $x = (n, \tau_1, \tau_2)$, where $n$ is the coordinate of the axis normal to the level sets of $\phi$, and the rest two coordinates $\tau_1$ and $\tau_2$ are the coordinates of the axes which are tangential to the level sets of $\phi$. In this coordinate system, the convection of a diffuse interface is given by the following initial boundary value problem based on the Allen-Cahn equation:

$$\frac{\partial \phi}{\partial t} + v \cdot \nabla \phi = -\gamma \left( F'(\phi) - \varepsilon^2 \nabla^2 \phi \right), \quad \text{on } \Omega,$$

$$\begin{aligned}
\phi &= \phi_D, & \forall x \in \Gamma_D^\phi, \\
n^\phi_t \cdot \nabla \phi &= 0, & \forall x \in \Gamma_H^\phi, \\
\phi \big|_{t=0} &= \phi_0, & \text{on } \Omega,
\end{aligned} \quad (4.1)$$

where $F'(\phi) = \phi^3 - \phi$ is the derivative of the double-well potential with respect to $\phi$, $n^\phi_t$ represents the unit vector normal to the boundary of the computational domain and $\phi_0$ represents the initial condition for the order parameter. The velocity in the orthogonal curvilinear coordinate system can be expressed as:

$$v = v_n n^\phi_t + v_{\tau_1} \tau_1 + v_{\tau_2} \tau_2, \quad (4.2)$$

where $n^\phi_t$, $\tau_1$ and $\tau_2$ are the unit vectors in the normal and two tangential directions of the level sets of $\phi$ respectively, and $v_n, v_{\tau_1}, v_{\tau_2}$ are the corresponding velocity components.

Assume that the normal profile of the interface is almost the same everywhere on the interface. Therefore the derivatives of the order parameter in the tangential directions are much smaller than the normal direction, thus being negligible. With this assumption, the spatial derivatives of the order parameter can be calculated as:

$$\nabla \phi = \frac{\partial \phi}{\partial n} n^\phi_t, \quad \nabla^2 \phi = \nabla \cdot \nabla \phi = \frac{\partial^2 \phi}{\partial n^2} + \frac{\partial \phi}{\partial n} \nabla \cdot n^\phi_t. \quad (4.3)$$
Notice that $\nabla \cdot n^\phi_L = -\kappa$, where $\kappa$ is the summation of principle curvatures of the interface. Substituting Eqs. (4.2) and (4.3) into the first equation of Eq. (4.1), the convective form of the Allen-Cahn equation in the orthogonal curvilinear coordinate system is given by:

$$\frac{\partial \phi}{\partial t} + v_n \frac{\partial \phi}{\partial n} = -\gamma \left( F'(\phi) - \varepsilon^2 \left( \frac{\partial^2 \phi}{\partial n^2} - \kappa \frac{\partial \phi}{\partial n} \right) \right).$$  \hspace{1cm} (4.4)

Now we write the convective Allen-Cahn equation in a non-dimensional moving orthogonal curvilinear coordinate system. We non-dimensionalize the coordinate system using the interface thickness parameter. For the convenience of analyzing the interface distortion due to the convective velocity difference in the diffuse interface region, we translate the coordinate system with the interface. As a result, the relative convective velocity to the interface, which leads to the convective distortion, appears explicitly in the governing equation. To begin with, we carry out the non-dimensionalization of the coordinate system by denoting the dimensionless coordinates as $\tilde{n}, \tilde{\tau}_1, \tilde{\tau}_2$, which are non-dimensionalized with respect to $\varepsilon$:

$$\tilde{n} = n / \varepsilon, \quad \tilde{\tau}_1 = \tau_1 / \varepsilon, \quad \tilde{\tau}_2 = \tau_2 / \varepsilon.$$  \hspace{1cm} (4.5)

Non-dimensionalizing the spatial coordinates in Eq. (4.4) accordingly, we obtain:

$$\frac{\partial \phi}{\partial \tilde{t}} + v_n \frac{\partial \phi}{\partial \tilde{n}} = -\gamma \left( F'(\phi) - \left( \frac{\partial^2 \phi}{\partial \tilde{n}^2} - \varepsilon \kappa \frac{\partial \phi}{\partial \tilde{n}} \right) \right).$$  \hspace{1cm} (4.6)

Assume that the principal radii of the interface are large compared to the interface thickness, which leads to $\kappa \ll 1 / \varepsilon$. With this assumption, the last term in Eq. (4.6) can be neglected:

$$\frac{\partial \phi}{\partial \tilde{t}} + v_n \frac{\partial \phi}{\partial \tilde{n}} = -\gamma \left( F'(\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}^2} \right).$$  \hspace{1cm} (4.7)

This completes the non-dimensionalization.

Next, we write Eq. (4.7) in a coordinate system which translates with the interface. We define the coordinates of the interface as $\Gamma^\phi_I(t) = \{(n_0(t), \tau_1, \tau_2) \in \Omega | \phi(n_0, \tau_1, \tau_2, t) = 0\}$. The coordinate transformation to the moving coordinate
Figure 4.2: Schematic diagram of the diffuse interface in non-dimensional moving orthogonal curvilinear coordinate system. The coordinate system \((\tilde{n}_m, \tilde{\tau}_1, \tilde{\tau}_2)\) is attached on the moving interface indicated by \(\phi(x,t)\) convected in the velocity field \(\mathbf{v}(x,t)\). The thickness of the diffuse interface in the coordinate system is \(\sim O(1)\) due to the non-dimensionalization.

The system can be written as:

\[
\begin{align*}
n_m &= n - n_0(t), \\
\tilde{n}_m &= \tilde{n} - \tilde{n}_0(t), \\
\tilde{n}_0(t) &= n_0(t)/\epsilon, \quad (4.8)
\end{align*}
\]

where \(n_m\) represents the normal coordinate in the moving coordinate system, \(\tilde{n}_m\) is the non-dimensionalized \(n_m\) with respect to \(\epsilon\), \(\tilde{n}_0(t)\) is the non-dimensional normal coordinate of the interface. The coordinate system is illustrated in Fig. 4.2.

In the moving coordinate system, the temporal and spatial derivatives of the order parameter become:

\[
\begin{align*}
\frac{\partial \phi}{\partial t} &= \frac{\partial \phi}{\partial t} - \frac{\partial \phi}{\partial \tilde{n}_m} \frac{d \tilde{n}_0(t)}{dt}, \\
\frac{\partial \phi}{\partial n} &= \frac{\partial \phi}{\partial n_m}, \\
\frac{\partial \phi}{\partial \tilde{n}} &= \frac{\partial \phi}{\partial \tilde{n}_m}, \\
\frac{\partial^2 \phi}{\partial \tilde{n}_m^2} &= \frac{\partial^2 \phi}{\partial \tilde{n}^2}. \quad (4.9)
\end{align*}
\]

Replacing the temporal and spatial derivatives in Eq. (4.7) with Eq. (4.9), we have:

\[
\begin{align*}
\frac{\partial \phi}{\partial t} - \frac{\partial \phi}{\partial \tilde{n}_m} \frac{d \tilde{n}_0(t)}{dt} + \frac{v_n(\tilde{n}_m, \tilde{\tau}_1, \tilde{\tau}_2, t)}{\epsilon} \frac{\partial \phi}{\partial \tilde{n}_m} &= -\gamma \left( F'(\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}_m^2} \right). \quad (4.10)
\end{align*}
\]

Notice that \(\tilde{n}_0(t)\) is the non-dimensional normal coordinate of the interface, the time derivative of which in Eq. (4.10) gives the normal velocity of the interface in...
the non-dimensional coordinate system. To get the normal velocity at the interface, we substitute $\phi = 0$ into Eq. (4.7):

$$\left. \frac{\partial \phi}{\partial t} \right|_{\phi=0} + v_n(\tilde{n}_0(t), \tilde{\tau}_1, \tilde{\tau}_2, t) \left. \frac{\partial \phi}{\partial \tilde{n}} \right|_{\phi=0} \frac{1}{\varepsilon} = -\gamma \left( -\frac{\partial^2 \phi}{\partial \tilde{n}^2} \right)_{\phi=0}. \quad (4.11)$$

For the hyperbolic tangent profile, $\frac{\partial^2 \phi}{\partial \tilde{n}^2} = 0$ at $\phi = 0$. Assuming that this is approximately satisfied when the convective distortion is not significant, thus the right-hand side of Eq. (4.11) is negligible:

$$\left. \frac{\partial \phi}{\partial t} \right|_{\phi=0} + v_n(\tilde{n}_0(t), \tilde{\tau}_1, \tilde{\tau}_2, t) \left. \frac{\partial \phi}{\partial \tilde{n}} \right|_{\phi=0} \frac{1}{\varepsilon} = 0. \quad (4.12)$$

The velocity of the interface can be identified from the convection equation (4.12) as:

$$\frac{d\tilde{n}_0(t)}{dt} = \frac{v_n(\tilde{n}_0(t), \tilde{\tau}_1, \tilde{\tau}_2, t)}{\varepsilon}. \quad (4.13)$$

Substituting Eq. (4.13) into Eq. (4.10), rewriting the velocity in the moving coordinate system and non-dimensionalize the equation with respect to $\gamma$, we get the governing equation for the interface profile:

$$\frac{\partial \phi}{\partial \tilde{t}} + \left( \frac{v_n(\tilde{n}_m, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{t}) - v_n(0, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{t})}{\gamma \varepsilon} \right) \frac{\partial \phi}{\partial \tilde{n}_m} = -\left( F'(\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}^2} \right), \quad (4.14)$$

where $\tilde{t} = \gamma t$ is the non-dimensional time. As the second term in Eq. (4.14) goes to zero, the equation recovers to the equation which gives the well-known hyperbolic tangent profile. The assumptions used in the derivation that the normal interface profile is almost identical on the interface and $\frac{\partial^2 \phi}{\partial \tilde{n}^2} = 0$ is approximately satisfied at $\phi = 0$ are valid.

### 4.2.2 Interface-preserving condition

As mentioned earlier, a non-zero second term of Eq. (4.14) causes the deviation from the hyperbolic tangent profile due to convection. We refer to the term as the convective distortion term. Multiplying and dividing the term by $\tilde{n}_m$, Eq. (4.14)
becomes:
\[
\frac{\partial \phi}{\partial \tilde{t}} + \left( \frac{v_n(\tilde{n}_m, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau}) - v_n(0, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau})}{\tilde{n}_m} \right) \frac{1}{\gamma e} \tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} = - \left( F'(\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}_m^2} \right).
\]

(4.15)

Suppose that \(v_n\) is continuous on \([0, \tilde{n}_m]\) and differentiable on \((0, \tilde{n}_m)\) when \(0 < \tilde{n}_m\), or \(v_n\) is continuous on \([\tilde{n}_m, 0]\), and differentiable on \((\tilde{n}_m, 0)\) when \(\tilde{n}_m < 0\), according to the mean value theorem [95], there exists \(\tilde{n}_s \in (0, \tilde{n}_m)\) or \(\tilde{n}_s \in (\tilde{n}_m, 0)\) respectively such that:

\[
\left( \frac{v_n(\tilde{n}_m, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau}) - v_n(0, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau})}{\tilde{n}_m} \right) = \frac{\partial v_n}{\partial \tilde{n}_m}(\tilde{n}_s, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau}).
\]

(4.16)

With Eq. (4.16), Eq. (4.15) can be rewritten as:

\[
\frac{\partial \phi}{\partial \tilde{t}} + \left( \frac{\partial v_n}{\partial \tilde{n}_m}(\tilde{n}_s, \tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau}) \right) \frac{1}{\gamma e} \tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} = - \left( F'(\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}_m^2} \right),
\]

(4.17)

where \(\tilde{n}_s \in (0, \tilde{n}_m)\) when \(0 < \tilde{n}_m\) and \(\tilde{n}_s \in (\tilde{n}_m, 0)\) when \(\tilde{n}_m < 0\). Transform the partial derivative of the normal velocity back to the dimensional spatial coordinate system using Eqs. (4.5) and (4.9):

\[
\frac{\partial \phi}{\partial \tilde{t}} + \left( \frac{\partial v_n}{\partial n}(n_s, \tau_1, \tau_2, \tilde{\tau}) \right) \frac{1}{\gamma e} \tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} = - \left( F'(\phi) - \frac{\partial^2 \phi}{\partial n^2} \right),
\]

(4.18)

where \(n_s \in (0, n_m)\) when \(0 < n_m\) and \(n_s \in (n_m, 0)\) when \(n_m < 0\).

For the convenience of notation, we replace the notation of the non-dimensional time \(\tilde{t}\) with \(t\) and denote the normal velocity gradient in the normal direction as:

\[
\zeta(x, t) = \frac{\partial v_n}{\partial n}(x, t),
\]

(4.19)

which can be considered as the intensity of the convective distortion (see A for detailed explanation).

**Remark 1.** The magnitude of \(\zeta(x, t)\) usually increases with the increase in the principal curvatures of the interface. The reason is that high principal curvatures cause strong surface tension effect. When it is distributed to the diffuse interface
region by a Dirac delta function, the violent variation of the surface tension force term across the diffuse interface gives rise to high velocity gradients, and furthermore causes the large magnitude of \( \zeta(x, t) \).

We next define a non-dimensional parameter, which we refer to as the convective distortion parameter:

\[
\xi(x, t) = \frac{\zeta(x, t)}{\gamma}. \tag{4.20}
\]

With the notations in Eqs. (4.19) and (4.20), the governing equation for the interface profile Eq. (4.18) becomes:

\[
\frac{\partial \phi}{\partial t} + \xi(n_s, \tau_1, \tau_2, t)\tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} = -\left( F' (\phi) - \frac{\partial^2 \phi}{\partial \tilde{n}_m^2} \right), \tag{4.21}
\]

where \( n_s \in (0, n_m) \) when \( n_m > 0 \) and \( n_s \in (n_m, 0) \) when \( n_m < 0 \).

As the convective distortion term goes to zero, the interface profile approaches the hyperbolic tangent profile. Thus, the interface-preserving condition is given by:

\[
\left| \xi(n_s, \tau_1, \tau_2, t)\tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} \right| \leq \eta_1, \tag{4.22}
\]

where \( \eta_1 \) is a desired upper bound for the magnitude of the convective distortion term. Apply the Cauchy-Schwarz inequality for the convective distortion term in the condition (4.22) as:

\[
\left| \xi(n_s, \tau_1, \tau_2, t)\tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} \right| \leq \left| \xi(n_s, \tau_1, \tau_2, t)\right| \left| \tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} \right| \leq \eta_1, \tag{4.23}
\]

where \( n_s \in (0, n_m) \) when \( n_m > 0 \) and \( n_s \in (n_m, 0) \) when \( n_m < 0 \). For the hyperbolic tangent profile \( \phi(\tilde{n}_m) = \tanh(\tilde{n}_m / \sqrt{2}) \), \( |\tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m}| \) approaches zero outside the diffuse interface region, which satisfies the condition (4.23). Inside the diffuse interface region, \( |\tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m}| \) is bounded by a constant. Denoting the constant as \( \eta_2 \), we have:

\[
\left| \tilde{n}_m \frac{\partial \phi}{\partial \tilde{n}_m} \right| \leq \eta_2, \quad x \in \Gamma_D^\phi(t), \tag{4.24}
\]

where \( \Gamma_D^\phi(t) \) represents the diffuse interface region at time \( t \). We assume that
inequality (4.24) is still valid when the interface profile is close to the hyperbolic tangent profile. Thus, the interface-preserving condition becomes:

$$|\xi(x,t)| \leq \eta, \quad x \in \Gamma_{\phi,DI}(t)$$

(4.25)

where $\eta = \eta_1/\eta_2$ is a desired upper bound for the convective distortion parameter. Since $\eta_2$ is a constant once the diffuse interface region is defined, $\eta_1 \to 0$ as $\eta \to 0$. In other words, the magnitude of the convective distortion term solely depends on $\xi$, and decreases with the reduction of the absolute value of the convective distortion parameter, which leads to the convergence of the interface profile to the hyperbolic tangent profile.

**Remark 2.** The diffuse interface region defines the spatial domain where the convective distortion is considered. A large diffuse interface region includes the distortion away from the interface, which may lead to an overestimation of the convective distortion at the interface and the free energy gradient flow required to oppose the convective distortion. The overestimation provides better interface-preserving capability but may induce a larger volume-conserved mean curvature flow velocity. In contrast, a small diffuse interface region may underestimate the interface distortion, thus giving rise to a smaller volume-conserved mean curvature flow velocity but weakening the interface-preserving capability. In the current study, we define the diffuse interface region as the region where 90% of the variation of $\phi$ occurs: $\Gamma_{\phi,DI}(t) = \{(x,t)||\phi(x,t)|| \leq 0.9\}$. For the hyperbolic tangent profile, the thickness of the region in the normal direction is approximately $4.164\varepsilon$.

### 4.2.3 Time-dependent mobility model

To satisfy the interface-preserving condition, one needs to adjust the mobility coefficient dynamically according to the normal velocity gradient in the normal direction. The interface-preserving condition (4.25) can be written as:

$$\gamma \geq \frac{|\zeta(x,t)|}{\eta}, \quad x \in \Gamma_{\phi,DI}(t).$$

(4.26)
We notice that the right-hand side of inequality (4.26) varies in both space and time. To satisfy the inequality, it is natural to consider a mobility model with spatial and temporal dependence. However, a mobility model that prohibits the variation in the normal direction while allows variations in tangential directions poses challenges in its construction. Consequently, we consider a time-dependent mobility model in the current study. The mobility coefficient is taken as a constant throughout the computational domain at each time instance, while it is allowed to change as time evolves. This requires a projection at time $t$ from the spatially varying $|\zeta(x,t)|$ to a real-valued $\gamma(t)$:

$$\mathcal{F}: \Omega \to \mathbb{R}_{\geq 0}, \quad \gamma(t) = \frac{1}{\eta} \mathcal{F}(|\zeta(x,t)|).$$

In the current study, we employ the RMS value in the diffuse interface region for the projection, which relaxes the condition (4.26) in an average sense:

$$\mathcal{F}(\varphi(x,t)) = \sqrt{\frac{\int (\varphi(x,t))^2 d\Omega}{\int 1 d\Omega}}, \quad x \in \Gamma^\phi_D(t).$$

We refer to $\eta$ as the RMS convective distortion parameter in the rest of the thesis, which is a user-defined parameter. The effects of $\eta$ selection on the interface profile and the surface tension modeling are quantified in Section 4.4. The frame independent form of the model (as derived in Appendix B) can be expressed as:

$$\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{\nabla \varphi^T \cdot \nabla v \cdot \nabla \varphi}{|\nabla \varphi|^2} \right),$$

which facilitates its numerical implementation in Cartesian coordinate system presented in the next section.

**Remark 3.** By taking the RMS function to perform the projection, the condition (4.26) is relaxed in an average sense. Because the mobility is calculated according to the RMS value of $|\zeta(x,t)|$, at the location where $|\zeta(x,t)|$ exceeds the RMS value, the condition (4.26) is violated. As mentioned in Remark 1, the violation usually happens in the region with high principle curvatures and singularities of the
interface. This allows the merging and breaking-up of the interface, where keeping the hyperbolic tangent profile is no longer required. Other projection methods can be employed for different considerations and requirements.

4.3 Conservative Allen-Cahn-Navier-Stokes formulation

In this section, we present a variational implementation of the interface-preserving conservative phase-field formulation. For the sake of completeness, we describe the governing equations of the two-phase flow modeling, viz., the incompressible Navier-Stokes equations and the conservative Allen-Cahn equation with the proposed time-dependent mobility model. We begin with the strong form of the equations and then project them into finite element space as the semi-discrete variational form. Specifically, we describe the discretization of the time-dependent mobility model. The section is closed with the coupled linearized matrix form of the variational discretization.

4.3.1 Coupled governing equations

Consider a domain $\Omega \times [0,T]$ consisting of the spatial points $\mathbf{x}$ at time $t$. The boundary of the domain, $\Gamma$ can be decomposed in two ways, $\Gamma = \Gamma_D^\phi \cup \Gamma_H^\phi$ and $\Gamma = \Gamma_D^\phi \cup \Gamma_H^\phi$, where $\Gamma_D^\phi$ and $\Gamma_H^\phi$ denote the Dirichlet and Neumann boundaries for the Navier-Stokes equations respectively, while $\Gamma_D^\phi$ and $\Gamma_H^\phi$ denote the same for the Allen-Cahn counterpart respectively. The diffuse interface region between the two-phases is denoted as $\Gamma_D^\phi(t)$. The one-fluid formulation for the two-phase incompressible and immiscible fluids system with the boundary conditions is given
as:

\[
\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = \nabla \cdot \mathbf{\sigma} + s \mathbf{f} + \mathbf{b}, \quad \text{on } \Omega,
\]

\[
\nabla \cdot \mathbf{v} = 0, \quad \mathbf{v} = \mathbf{v}_D, \quad \mathbf{\sigma} \cdot \mathbf{n}^f = \mathbf{h}, \quad \mathbf{v} = \mathbf{v}_0, \quad \text{on } \Omega,
\]

\[
(4.30)
\]

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = -\gamma(t) \left( F'(\phi) - \epsilon^2 \nabla^2 \phi - \beta(t) \sqrt{F(\phi)} \right), \quad \text{on } \Omega,
\]

\[
\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{(\nabla \phi)^T \cdot \nabla \mathbf{v} \cdot \nabla \phi}{|\nabla \phi|^2} \right), \quad x \in \Gamma^D(t)
\]

\[
\phi = \phi_D, \quad \nabla \phi \cdot \mathbf{n}^f = 0, \quad \phi|_{t=0} = \phi_0, \quad \text{on } \Omega(0),
\]

\[
(4.31)
\]

where Eq. (5.24) and Eq. (4.31) represent the Navier-Stokes and Allen-Cahn equations respectively. In the Navier-Stokes equations, \( \rho \) is the density of the fluid, \( \mathbf{v} \) represents the fluid velocity defined for each spatial point \( x \) in \( \Omega \), \( \mathbf{b} \) is the body force on the fluid such as gravity \( \mathbf{b} = \rho \mathbf{g} \), \( \mathbf{g} \) being the acceleration due to gravity, \( \mathbf{v}_D \) and \( \mathbf{h} \) denote the boundary conditions at the Dirichlet and Neumann boundaries respectively, \( \mathbf{n}^f \) is the unit outward normal to the Neumann boundary and \( \mathbf{v}_0 \) represents the initial velocity field at \( t = 0 \). The Cauchy stress tensor for a Newtonian fluid is given as:

\[
\mathbf{\sigma} = -p \mathbf{I} + \mathbf{T}, \quad \mathbf{T} = 2\mu \mathbf{\varepsilon}(\mathbf{v}), \quad \mathbf{\varepsilon}(\mathbf{v}) = \frac{1}{2} \left[ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right], \quad (4.32)
\]

where \( p \) is the pressure field, \( \mathbf{T} \) and \( \mathbf{\varepsilon} \) represent the shear stress tensor and the fluid strain rate tensor respectively and \( \mu \) denotes the dynamic viscosity of the fluid. The physical parameters of the fluid such as \( \rho \) and \( \mu \) vary with the evolution of the
interface indicated by order parameter $\phi$:

$$
\rho(\phi) = \frac{1 + \phi}{2} \rho_1 + \frac{1 - \phi}{2} \rho_2, \quad (4.33)
$$

$$
\mu(\phi) = \frac{1 + \phi}{2} \mu_1 + \frac{1 - \phi}{2} \mu_2, \quad (4.34)
$$

where $\rho_i$ and $\mu_i$ are the density and dynamic viscosity of the $i$th phase of the fluid respectively. The surface tension $sf$ is modeled by the CSF model [86], in which it is reformulated as a volumetric source term with a Dirac Delta function utilizing the gradient of the phase indicator $\phi$. Several forms of $sf(\phi)$ have been used in the literature which are reviewed in [96, 97]. In this study, we employ the following definition [98]:

$$
sf(\phi) = \kappa n^\phi \delta_S
$$

$$
= \sigma \nabla \cdot \left( \left( I - n^\phi \otimes n^\phi \right) \delta_S \right)
$$

$$
= \sigma \alpha_{sf} \varepsilon \nabla \cdot \left( |\nabla \phi|^2 I - \nabla \phi \otimes \nabla \phi \right) \quad (4.35)
$$

where $\sigma$ is the surface tension coefficient, $\delta_S = \varepsilon \alpha_{sf} |\nabla \phi|^2$ is the Dirac delta function at the interface, $\alpha_{sf} = 3\sqrt{2}/4$ is a constant derived by the property of the Dirac delta function, $\kappa$ being the summation of the principle curvatures of the interface and $n^\phi_L = \nabla \phi / |\nabla \phi|$ denotes the normal vector of the level sets of $\phi$.

On the other hand, in Eq. (4.31), $\varepsilon$ is the interface thickness parameter, $\gamma(t)$ is the time-dependent mobility, $F(\phi)$ is the double-well potential, $\eta$ is the RMS convective distortion parameter and $n^\phi_L$ is the unit normal vector of the level sets of the order parameter $\phi$. The value of the order parameter at the Dirichlet boundary is denoted by $\phi_D$, the initial condition is represented by $\phi_0$ and $n^\phi_E$ denotes the unit outward normal to the Neumann boundary where a zero flux condition is satisfied. The mass conservation is enforced in the Allen-Cahn equation by a Lagrange multiplier $\beta(t) \sqrt{F(\phi)}$ where $\beta(t) = \int_\Omega F'(\phi) d\Omega / \int_\Omega \sqrt{F(\phi)} d\Omega$. $F'(\phi)$ is the derivative of the energy potential with respect to the order parameter. The Allen-Cahn equation can be transformed into a convection-diffusion-reaction equation as follows:

$$
\partial_t \phi + v \cdot \nabla \phi - \gamma(t)(\hat{k} \nabla^2 \phi - \hat{s} \phi + \hat{f}) = 0 \text{ on } \Omega^f, \quad (4.36)
$$
where $\mathbf{v}$, $\mathbf{k}$, $s$ and $f$ are the convective velocity, modified diffusion coefficient, modified reaction coefficient and modified source respectively which are defined in [93].

### 4.3.2 Semi-discrete equations

In this subsection, we present the semi-discrete variational form of the Navier-Stokes-Allen-Cahn (NS-AC) system, which has been described earlier. We employ the generalized-$\alpha$ technique [99] for the temporal discretization which enables a user-controlled high frequency damping desirable for coarse discretizations in space and time. The following expressions are employed for the temporal discretization of the Navier-Stokes equations:

\begin{align}
\mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta t \partial_t \mathbf{v}^n + \zeta \Delta t (\partial_t \mathbf{v}^{n+1} - \partial_t \mathbf{v}^n), \\
\partial_t \mathbf{v}^{n+\alpha_m} &= \partial_t \mathbf{v}^n + \alpha_m (\partial_t \mathbf{v}^{n+1} - \partial_t \mathbf{v}^n), \\
\mathbf{v}^{n+\alpha} &= \mathbf{v}^n + \alpha (\mathbf{v}^{n+1} - \mathbf{v}^n),
\end{align}

where $\alpha$, $\alpha_m$ and $\zeta$ are the generalized-$\alpha$ parameters which are dependent on the user-defined spectral radius $\rho_\infty$. The time step size is denoted by $\Delta t$ and $\partial_t$ denotes the partial differentiation with respect to time. Similar expressions can be written for the Allen-Cahn equation as well.

Suppose $\mathcal{S}_\mathbf{V}^h$, $\mathcal{S}_p^h$ and $\mathcal{S}_\phi^h$ denote the space of trial solution such that:

\begin{align}
\mathcal{S}_\mathbf{V}^h &= \{ \mathbf{v}_h \mid \mathbf{v}_h \in (H^1(\Omega))^d, \mathbf{v}_h = \mathbf{v}_D \text{ on } \Gamma_D \}, \\
\mathcal{S}_p^h &= \{ p_h \mid p_h \in L^2(\Omega) \}, \\
\mathcal{S}_\phi^h &= \{ \phi_h \mid \phi_h \in H^1(\Omega), \phi_h = \phi_D \text{ on } \Gamma_D \},
\end{align}

where $(H^1(\Omega))^d$ denotes the space of square-integrable $\mathbb{R}^d$-valued functions with square-integrable derivatives on $\Omega$ and $L^2(\Omega)$ is the space of the scalar-valued functions that are square-integrable on $\Omega$. Similarly, we define $\mathcal{V}_\mathbf{W}^h$, $\mathcal{V}_q^h$ and $\mathcal{V}_\phi^h$ as the
space of test functions such that:

\[
\begin{align*}
\mathcal{V}_h^b & = \{ \psi_h \mid \psi_h \in (H^1(\Omega))^d, \psi_h = 0 \text{ on } \Gamma_D^e \}, \\
\mathcal{V}_q^b & = \{ q_h \mid q_h \in L^2(\Omega) \}, \\
\mathcal{V}_\phi^b & = \{ \hat{\phi}_h \mid \hat{\phi}_h \in H^1(\Omega), \hat{\phi}_h = 0 \text{ on } \Gamma_D^e \}.
\end{align*}
\]  

(4.43)

(4.44)

(4.45)

The variational statement of the combined NS-AC system can be written as:

\[
\begin{align*}
\int_{\Omega} \rho(\phi)(\partial_t \mathbf{v}_h + \mathbf{v}_h \cdot \nabla \mathbf{v}_h) \cdot \mathbf{v}_h d\Omega & + \int_{\Omega} \sigma_h : \nabla \mathbf{v}_h d\Omega + \int_{\Omega} \alpha_{ef} \sigma_e \left( |\nabla \phi_h|^2 I - \nabla \phi_h \otimes \nabla \phi_h \right) : \nabla \mathbf{v}_h d\Omega \\
& + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \frac{\tau_m}{\rho(\phi)} (\rho(\phi) \mathbf{v}_h \cdot \nabla \mathbf{v}_h + \nabla q_h) \cdot \mathcal{R}_m d\Omega \\
& + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nabla \cdot \mathbf{v}_h \tau_e \rho(\phi) \mathcal{R}_c d\Omega \\
& - \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_m \mathbf{v}_h \cdot (\mathcal{R}_m \cdot \nabla \mathbf{v}_h) d\Omega - \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nabla \mathbf{v}_h \cdot \frac{\tau_m}{\rho(\phi)} (\tau_m \mathcal{R}_m \otimes \tau_m \mathcal{R}_m) d\Omega \\
& = \int_{\Gamma_D^e} \mathbf{b}(t^{n+\alpha}) \cdot \mathbf{v}_h d\Gamma \\
& + \int_{\Gamma_D^f} h \cdot \mathbf{v}_h d\Gamma,
\end{align*}
\]

(4.46)

and for the Allen-Cahn equation:

\[
\begin{align*}
\int_{\Omega} \left( \hat{\theta}_h \partial_t \phi_h + \hat{\theta}_h (\mathbf{v}_h \cdot \nabla \phi_h) + \gamma(t^{n+\alpha}) \left( \nabla \hat{\theta}_h \cdot (\hat{k} \nabla \phi_h) + \hat{\theta}_h \hat{k} \hat{\phi}_h - \hat{\theta}_h \hat{\phi}_h \hat{f} \right) \right) d\Omega \\
& + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \left( \mathbf{v}_h \cdot \nabla \hat{\phi}_h \right) \tau_e \left( \partial_t \phi_h + \mathbf{v}_h \cdot \nabla \phi_h - \gamma(t^{n+\alpha}) \left( \nabla \cdot (\hat{k} \nabla \phi_h) - \hat{k} \phi_h + \hat{\phi}_h \hat{f} \right) \right) d\Omega \\
& + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \chi \left[ \mathcal{R}_m(\hat{\phi}_h) \right] \kappa_{\text{add}} \nabla \hat{\theta}_h \cdot \left( \frac{\mathbf{v}_h \otimes \mathbf{v}_h}{|\mathbf{v}_h|^2} \right) \cdot \nabla \phi_h d\Omega \\
& + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \chi \left[ \mathcal{R}_c(\hat{\phi}_h) \right] \kappa_{\text{add}} \nabla \hat{\theta}_h \cdot \left( I - \frac{\mathbf{v}_h \otimes \mathbf{v}_h}{|\mathbf{v}_h|^2} \right) \cdot \nabla \phi_h d\Omega = 0,
\end{align*}
\]

(4.47)

where the terms with under brackets representing the fluid-fluid interface dynamics are central to the current study, \( \mathcal{R}_m, \mathcal{R}_c \) and \( \mathcal{R}(\hat{\phi}_h) \) denote the element-wise resid-
uals for the momentum, continuity and the Allen-Cahn equations, respectively.

In Eq. (4.46), the terms in the first line represent the Galerkin projection of the momentum equation in the test function space $\psi_h$ and the second line comprises of the Petrov-Galerkin stabilization term for the momentum equation. The third line denotes the Galerkin projection and stabilization terms for the continuity equation and the terms in the fourth line are derived via approximation of fine scale velocity on the element interiors based on multi-scale argument [100, 101]. The terms in the final line are the Galerkin projection of the body force and Neumann boundary condition. On the other hand, in Eq. (4.47), the first line is the Galerkin projection of the transient, convection, diffusion, reaction and source terms, the second line represents the Streamline-Upwind Petrov-Galerkin stabilization and the third line depicts the PPV terms that are derived for the multi-dimensional convection-diffusion-reaction equation via satisfaction of the positivity condition at the element matrix level [53]. Several test cases have been performed to assess the effectiveness of this PPV technique in [53]. The details of the derivation of the added diffusions $k_{s}^{\text{add}}$, $k_{c}^{\text{add}}$ and $\chi$ can be found in [53], which are given for the present context by [93]:

\begin{equation}
\chi = \frac{2}{|\hat{s}|h + 2|\psi_h|}, \tag{4.48}
\end{equation}

\begin{equation}
k_{s}^{\text{add}} = \max \left\{ \frac{|\psi_h - \tau_{\phi}|\psi_h|\hat{s}|h}{2} - (\hat{k} + \tau_{\phi}|\psi_h|^2) + \frac{\hat{s}h^2}{6} , 0 \right\}, \tag{4.49}
\end{equation}

\begin{equation}
k_{c}^{\text{add}} = \max \left\{ \frac{|\psi_h|h}{2} - \hat{k} + \frac{\hat{s}h^2}{6} , 0 \right\}, \tag{4.50}
\end{equation}

where $|\psi_h|$ is the magnitude of the convective velocity and $h$ is the characteristic element length defined in [53]. The stabilization parameters $\tau_m$, $\tau_c$ and $\tau_{\phi}$ in Eqs. (4.46) and (4.47) are given by [52, 102]:

\begin{align}
\tau_m &= \left[ \left( \frac{2}{\Delta t} \right)^2 + \mathbf{v}_h \cdot \mathbf{G} \mathbf{v}_h + C_l \left( \frac{\mu(\phi)}{\rho(\phi)} \right)^2 \mathbf{G} : \mathbf{G} \right]^{-1/2}, \quad \tau_c = \frac{1}{\text{tr}(\mathbf{G}) \tau_m}, \tag{4.51}
\end{align}

\begin{align}
\tau_{\phi} &= \left[ \left( \frac{2}{\Delta t} \right)^2 + \mathbf{v}_h \cdot \mathbf{G} \mathbf{v}_h + 9\hat{k}^2 \mathbf{G} : \mathbf{G} + \hat{s}^2 \right]^{-1/2}. \tag{4.52}
\end{align}

where $C_l$ is a constant derived from the element-wise inverse estimates [103], $\mathbf{G}$ is
the element contravariant metric tensor and $\text{tr}(G)$ is the trace of the contravariant metric tensor. This stabilization in the variational form circumvents the Babuška-Brezzi condition that is required to be satisfied by any standard mixed Galerkin method [104].

### 4.3.3 Discrete form of time-dependent mobility model

We present the discrete form of the time-dependent mobility model in this subsection. The strong form of the time-dependent mobility model is given by Eq. (4.29):

$$\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{(\nabla \phi)^T \cdot \nabla v \cdot \nabla \phi}{|\nabla \phi|^2} \right),$$  \hspace{1cm} (4.53)

where $\mathcal{F}(\varphi(x,t)) = \sqrt{\int_{\Omega} (\varphi(x,t))^2 \, d\Omega}$, $x \in \Gamma_{DI}(t)$. In Eq. (4.53), $\mathcal{F} \left( \frac{(\nabla \phi)^T \cdot \nabla v \cdot \nabla \phi}{|\nabla \phi|^2} \right)$ can be approximated as the RMS of $|\nabla \phi|^T \cdot \nabla v \cdot \nabla \phi / |\nabla \phi|^2$ at all the nodes located inside the diffuse interface region $\Gamma_{DI}^p(t)$. The nodal value of $|\nabla \phi|^T \cdot \nabla v \cdot \nabla \phi / |\nabla \phi|^2$ is calculated as follows.

The nodal value of $v_{h}(t^{n+\alpha})$, $\phi_{h}(t^{n+\alpha})$ is used to interpolate the $\nabla v_{h}(t^{n+\alpha})$ and $\nabla \phi_{h}(t^{n+\alpha})$ at the quadrature points, and $L^2$-projection is used to project the value on the quadrature points back to the nodes inside the diffuse interface region [105]. If the node lies outside the diffuse interface region, the value is assigned to be zero. For example, for the node $p$, we have:

$$\left| \frac{(\nabla \phi_{h})^T \cdot \nabla v_{h} \cdot \nabla \phi_{h}}{|\nabla \phi_{h}|^2} \right|_p = \begin{cases} \sum_e \int_{\Omega_e} N_p((\nabla \phi_{h})^T \cdot \nabla v_{h} \cdot \nabla \phi_{h})/|\nabla \phi_{h}|^2 \, d\Omega_e & \text{if } |\phi_p| \leq 0.9, \\ 0 & \text{if } |\phi_p| > 0.9, \end{cases}$$

where $N_p$ represents the shape function at node $p$. The discrete form of the time-dependent mobility model is given by:

$$\gamma(t^{n+\alpha}) = \frac{1}{\eta} \left( \frac{1}{n_{DI}} \sum_{p=1}^{n_{DI}} \left| \frac{(\nabla \phi_{h})^T \cdot \nabla v_{h} \cdot \nabla \phi_{h}}{|\nabla \phi_{h}|^2} \right|_p \right)^2, $$  \hspace{1cm} (4.54)

where $n_{DI}$ denotes the number of the nodes lying inside the diffuse interface region.
4.3.4 Coupled partitioned matrix formulation

In this subsection, we present the coupled linearized matrix form of the variationally discretized two-phase flow equations. Employing the Newton-Raphson linearization technique, the coupled two-phase fluid system can be expressed in terms of the solution increments for velocity, pressure and order parameter ($\Delta \mathbf{v}$, $\Delta p$ and $\Delta \phi$ respectively) as:

$$
\begin{bmatrix}
  \mathbf{K}_\Omega & \mathbf{G}_\Omega & \mathbf{D}_\Omega \\
  -\mathbf{G}_\Omega^T & \mathbf{C}_\Omega & 0 \\
  \mathbf{G}_{\text{AC}} & 0 & \mathbf{K}_{\text{AC}}
\end{bmatrix}
\begin{bmatrix}
  \Delta \mathbf{v} \\
  \Delta p \\
  \Delta \phi
\end{bmatrix}
= -
\begin{bmatrix}
  \mathbf{R}_m \\
  \mathbf{R}_c \\
  \mathbf{R}(\phi)
\end{bmatrix}
$$

(4.55)

where $\mathbf{K}_\Omega$ is the stiffness matrix of the momentum equation consisting of transient, convection, viscous and Petrov-Galerkin stabilization terms, $\mathbf{G}_\Omega$ is the gradient operator, $-\mathbf{G}_\Omega^T$ is the divergence operator for the continuity equation and $\mathbf{C}_\Omega$ is the stabilization term for cross-coupling of pressure terms. On the other hand, $\mathbf{D}_\Omega$ consists of the terms in the momentum equation which depend on the phase-indicator $\phi$, $\mathbf{G}_{\text{AC}}$ is the velocity coupled term in the Allen-Cahn equation and $\mathbf{K}_{\text{AC}}$ is the left-hand side stiffness matrix for the Allen-Cahn equation comprising of transient, convection, diffusion, reaction and positivity preserving stabilization terms. Here, $\mathbf{R}_m$, $\mathbf{R}_c$ and $\mathbf{R}(\phi)$ represent the weighted residuals of the variational forms in Eqs. (4.46-4.47).

The two-phase flow system in Eq. (4.55) is decoupled into two subsystems: Navier-Stokes and Allen-Cahn solves, for which the linear system of equations can be summarized as:

$$
\begin{bmatrix}
  \mathbf{K}_\Omega & \mathbf{G}_\Omega \\
  -\mathbf{G}_\Omega^T & \mathbf{C}_\Omega
\end{bmatrix}
\begin{bmatrix}
  \Delta \mathbf{v} \\
  \Delta p
\end{bmatrix}
= -
\begin{bmatrix}
  \mathbf{R}_m \\
  \mathbf{R}_c
\end{bmatrix}
$$

(4.56)

$$
\mathbf{K}_{\text{AC}} \left\{ \Delta \phi \right\} = -\left\{ \mathbf{R}(\phi) \right\}
$$

(4.57)

Note that the cross-coupling terms between the Navier-Stokes and the Allen-Cahn equations ($\mathbf{D}_\Omega$ and $\mathbf{G}_{\text{AC}}$) are not present in the decoupled form. We solve the decoupled system in a partitioned-block iterative manner which leads to flexibil-
ity and ease in its implementation to the existing variational solvers. The linear systems (Eqs. (4.56) and (4.57)) are solved by the Generalized Minimal Residual (GMRES) algorithm proposed by [106]. The algorithm relies on Krylov subspace iteration and modified Gram-Schmidt orthogonalization. Instead of construction of the left-hand side matrices explicitly, we only construct the required matrix-vector products of each block matrix in the GMRES solver. Detailed algorithmic steps for the partitioned coupling of the fully implicit solutions of the conservative Allen-Cahn and the incompressible Navier-Stokes equations can be found in [93]. The stability and robustness of the partitioned decoupled system have been demonstrated for a broad range of problems involving high-density and viscosity ratios, high Reynolds number and complex topological changes over unstructured meshes [33, 93].

4.4 Interface convection problem

In this section, we first verify the convergence and accuracy of our fully-implicit finite element solver by simulating a bistable steady convection-diffusion-reaction system in a one-dimensional stretching flow. We then turn our attention to the convection of a planar interface and a curved interface in prescribed velocity fields. The convective distortion of the diffuse interface is quantified by the relative interface thickness and surface tension errors. The dependence of the errors on the convective distortion parameter $\xi$ is assessed systematically.

4.4.1 Verification of steady Allen-Cahn phase-field solver

For simplification, we consider the interface profile given by the 1D steady-state solution of Eq. (4.21) for constant convective distortion parameter:

$$\tilde{x} \frac{d\phi}{d\tilde{x}} = -\left(\phi^3 - \phi - \frac{d^2\phi}{d\tilde{x}^2}\right),$$

where $\tilde{x} = x/\varepsilon$ is the non-dimensionalized coordinate. The above equation can be considered as a special case of a generic bistable steady convection-diffusion-
reaction system in a stretching flow, which can be written as:

$$-S \frac{d\phi}{dx} = D \frac{d^2\phi}{dx^2} + R\phi(\phi - 1)(A - \phi), \quad (4.59)$$

where $S$ is the stretching rate, $D$ is the diffusion coefficient, $R$ is the reaction rate, and $A$ is a parameter determining the unstable equilibrium phase separating the two stable equilibrium phases with minimum bulk energy. In [107], Eq. (4.59) has been solved semi-analytically in the large Damköhler number limit defined as $Da = R/S \gg 1$ with a fixed stretching rate $S = 1$. The solutions of Eq. (4.59) include the plateau-like solution and the pulse-like solution. Since the plateau-like solution can be considered as a solution composed of two diffuse interfaces subjected to the convective distortion (as shown in Fig. 4.4 (a)), it is used for the verification of our implicit finite element Allen-Cahn solver. The plateau-like solution takes the form:

$$\phi(x) = \frac{1}{2} f \left[ \tanh \left( w \left( x + v \right) \right) - \tanh \left( w \left( x - v \right) \right) \right],$$

where $f$ represents the height of the “plateau”, $w$ is referred to as the inverse width of the diffuse interface which is inversely proportional to the width of the diffuse interface, and $v$ is the half-width of the “plateau”. They are given semi-analytically by:

$$f \sim 1, \quad w \sim \sqrt{\frac{Da}{8D}} v \sim \sqrt{2DDa(0.5 - A)}.$$

To form a discrete system which is consistent with Eq. (4.59), we directly prescribe the velocity as $u = -Sx$ without solving the Navier-Stokes equations. The Lagrange parameter is set to be zero and the reaction term is adjusted accordingly.

We consider a one-dimensional computational domain $x \in [-L, L]$. The computational domain is discretized by a uniform mesh of grid size $h$. A zero flux boundary condition is applied on the left and the right boundaries. The initial condition is specified as:

$$\phi(x) = \frac{1}{2} \left( \tanh \left( \frac{1}{\sqrt{2}} (x + 5) \right) - \tanh \left( \frac{1}{\sqrt{2}} (x - 5) \right) \right). \quad (4.61)$$

The stretching rate and the diffusion coefficient are taken as $S = 1$ and $D = 1$.
respectively. The reaction rates $R \in [20, 140]$ corresponding to $Da \in [20, 140]$ are considered for the verification purpose. The unstable equilibrium phase is set to be $A = 0.2$ and the time step is taken as $\Delta t = 0.1$ for marching the solution till the steady state solution is reached.

We perform a systematic convergence study for the final time when the steady state solution is reached, the length of the computational domain and the grid size. In the convergence study, we set the convergence tolerance to $10^{-5}$ for both the linear GMRES and the nonlinear Newton solvers. To quantify the error in the convergence study, we define the relative error in $L^2$ norm as $e_2 = \frac{||\phi - \phi_{\text{ref}}||_2}{||\phi_{\text{ref}}||_2}$, where $|| \cdot ||_2$ denotes the $L^2$ norm of the vector. We first study the final time for the case $Da = 140, h = 0.01$ and $L = 15$. Considering the solution at $t = 40$ as the reference, the error at $t = 36$ reaches $e_2 = 1.3 \times 10^{-8}$. Hence we consider the solution at $t = 40$ as the fully-converged steady state solution. We next investigate the domain length $L$ to ensure that the zero flux boundary condition is far enough so that its influence on the solution is negligible. The solution of $Da = 140$, which has the wildest “plateau” according to Eq. (4.60), is analyzed at $t = 40$ with $h = 0.01$ and various $L$. The variation of the derivative of $\phi$ at the left boundary with respect to the change in $L$ is shown in Fig. 4.3 (a). When $L = 15$, $d\phi/dx \ (x = -L) = 5.1 \times 10^{-7}$. As a result, $L = 15$ is considered as the converged domain length. We further investigate the convergence with respect to the grid size $h$. While keeping $t = 40$ and $L = 15$, $Da = 20$ is selected for the mesh convergence study. Because the solution of $Da = 20$ has the smallest width of the diffuse interface according to Eq. (4.60), which leads to the highest gradient of $\phi$ among all the cases and needs the finest mesh to resolve the gradient effects. By considering the solution at $h = 0.0025$ as the reference, the error $e_2$ is plotted in Fig. 4.3 (b). It shows that our implementation is spatially second-order accurate. The relative $L^2$ error reduces to $2.2 \times 10^{-6}$ when $h = 0.005$, which is considered to be converged. To summarize, $t = 40, L = 15$ and $h = 0.005$ are taken as the converged parameters for the numerical simulation used in the verification.

After establishing the convergence of our phase-field solver, we verify our solver with respect to Eq. (4.60) and numerical results from [107]. The plateau-like solution at $Da = 100$ and the change of $h, v, w$ with respect to $Da$ are shown in Fig. 4.4 (a)-(d), respectively. The comparisons clearly show excellent agreements
of our numerical results against previously reported analytical and numerical data. Our fully implicit variationally discretized solver for computing the bistable steady convection-reaction-diffusion system in a stretching flow is successfully verified.

4.4.2 Convection of a planar interface

Following the verification of our Allen-Cahn phase-field solver, we now turn our attention to the solution of Eq. (4.58), which can be considered as another scenario of parameter specifications of Eq. (4.59) describing the convective distortion of the diffuse interface. To form a constant $\xi$ used in Eq. (4.58), the velocity field and the mobility coefficient are explicitly prescribed without solving the Navier-Stokes equations and the time-dependent mobility model.

In the numerical simulation, the one-dimensional computational domain is taken as $\tilde{x} \in [-L,L]$, where $\tilde{x} = x/\varepsilon$ is the non-dimensional coordinate. The interface thickness parameter is set to be $\varepsilon = 1$. The computational domain is discretized by uniform mesh of grid size $h = \Delta \tilde{x}$. A zero flux boundary condition is imposed for the order parameter $\phi$ on the left and the right boundaries. The planar interface is initialized as $\phi(\tilde{x}) = \tanh(\tilde{x}/\sqrt{2})$. The mobility coefficient of the Allen-Cahn equation is chosen as $\gamma = 1$. The velocity is prescribed as $v_x(\tilde{x}) = a\tilde{x}$,
Figure 4.4: Accuracy assessment of fully-implicit finite element formulation for a generic bistable convection-diffusion-reaction system: (a) steady state plateau-like solution as a function of distance $x$, and (b) the height of the solution $f$, (c) half-width of the solution $v$, (d) inverse width of the diffuse interface $w$ as a function of Damköhler number $Da$.

where $a \in [-0.25, 0.25]$ is a constant selected according to the desired convective distortion parameter. From the problem setup, the convective distortion parameter can be calculated as $\xi = a$. The time step is taken as $\Delta t = 0.1$. The problem setup with the illustration of an extensional velocity field is shown in Fig. 4.5.

We carry out a convergence study to minimize the discretization error so that the effect of $\xi$ can be accurately captured. To ensure that the discretization error is negligible, the convergence of the final time when the steady state is achieved, the length of the computational domain and the mesh resolution at the diffuse interface
Figure 4.5: Schematic diagram showing the computational domain for the convection of a one-dimensional planar interface in a prescribed extensional velocity field. $\Omega_1$ and $\Omega_2$ are domains of the two phases. A zero flux boundary condition for the order parameter is applied on the left and the right boundaries.

are studied with the tolerance of $10^{-8}$ for the linear GMRES and the nonlinear Newton solvers. The final time is examined for the values of $\xi = -0.25$ and $\xi = 0.25$, at which the steady state solution deviates the most from the initial condition among all the cases. The grid size $h = 0.01$ and the size of the computational domain $L = 10$ are used. By considering $t = 20$ as the reference, we check the relative $L^2$ norm of the solution at $t = 18$. For $\xi = -0.25$ and $\xi = 0.25$, the errors reduce to $e_2 = 3.4 \times 10^{-8}$ and $e_2 = 7.6 \times 10^{-11}$, respectively. Hence the solution at $t = 20$ is considered to be fully converged.

We proceed to the investigation of $L$ to check whether the zero flux boundary condition is far enough so that its influence on the solution is negligible. The solution at $\xi = 0.25$, which leads to the maximum extensional distortion and the widest diffuse interface among all the cases, is analyzed at $t = 20$ with $h = 0.01$. The derivative of the order parameter on the right boundary $d\phi/d\bar{x}$ ($\bar{x} = L$) is plotted as a function of $L$ in Fig. 4.6 (a). When $L = 12$, the derivative reduces to $d\phi/dx$ ($\bar{x} = L$) = $8.7 \times 10^{-7}$, which indicates an error of $\phi$ at the order of $10^{-9}$ (with $h = 0.01$). Therefore it is considered as the converged domain length.

The convergence of the mesh resolution in the diffuse interface region is studied
at $t = 20$ with $L = 12$. The solution at $\xi = -0.25$ is investigated, which results in the maximum compressional distortion and the highest gradient among all the cases requiring the finest mesh to resolve. By taking the solution at $\varepsilon/h = 1600$ as the reference, the relative $L^2$ error as a function of the mesh resolution $\varepsilon/h$ is plotted in Fig. 4.6 (b). The plot confirms the second-order spatial accuracy of our implementation. When $\varepsilon/h = 800$, the error reduces to $e_2 = 6.9 \times 10^{-9}$. The resolution is deemed to be converged. To summarize, $t = 20, L = 12$ and $\varepsilon/h = 800$ are employed to minimize the discretization error in the investigation of the effect of $\xi$.

![Figure 4.6](image)

**Figure 4.6:** Convergence of a convecting planar diffuse interface with a prescribed velocity: (a) the variation of the derivative of $\phi$ with respect to domain length $L$, and (b) the relative $L^2$ error ($e_2$) as a function of mesh resolution $\varepsilon/h$.

With the converged numerical parameters, we first consider the effect of the convective distortion parameter on the interface profile. As shown in Fig. 4.7, when $\xi = 0$, the interface profile from the numerical simulation tends to the hyperbolic tangent profile. When $\xi > 0$, an extensional distortion is observed. The extensional distortion increases with an increase in $\xi$. Compressional distortion is noted when $\xi < 0$ whereby the compressional distortion increases with the decrease in $\xi$. To quantify the deviation of the interface profile from the hyperbolic tangent profile,
we define the relative interface thickness error as:

\[ e_\varepsilon = \left| \frac{\tilde{\varepsilon}_d - \tilde{\varepsilon}_{eq}}{\tilde{\varepsilon}_{eq}} \right|, \quad (4.62) \]

where \( \tilde{\varepsilon}_d \) and \( \tilde{\varepsilon}_{eq} \) denote the non-dimensionalized distance with respect to \( \varepsilon \) from \( \phi = -0.9 \) to \( \phi = 0.9 \) of the distorted interface, and of the hyperbolic tangent profile respectively. The coordinates of \( \phi = 0.9 \) and \( \phi = -0.9 \) are linearly interpolated from the numerical solution. The relative interface thickness error as a function of \( \xi \) is shown in Fig. 4.10 (a).

![Figure 4.7: Convection of a planar interface in a prescribed velocity field: the interface profiles corresponding to various distortion parameter \( \xi \).](image)

Furthermore, we examine the error in surface tension modeling due to the convective distortion. In the CSF model, the singular surface tension at the interface is distributed to the diffuse interface region by a Dirac delta function at the interface. In the current model, the function is given by 

\[ \delta_S = \alpha_{sf} \varepsilon \left| \nabla \phi \right|^2, \]

which should satisfy:

\[ \int_{-\infty}^{\infty} \alpha_{sf} \varepsilon \left( \frac{\partial \phi}{\partial n} \right)^2 \, dn = 1, \quad (4.63) \]

where \( \alpha_{sf} \) is a constant parameter. For the hyperbolic tangent profile \( \phi = \tanh(n/\sqrt{2}\varepsilon) \),
the constant parameter can be calculated as \( \alpha_{sf} = \frac{3\sqrt{2}}{4} \). When the interface profile is affected by the convective distortion, its deviation from the hyperbolic tangent profile leads to the violation of Eq. (4.63). This gives rise to a relative surface tension error quantified as:

\[
e_\sigma = \left| \int_{-\infty}^{\infty} \alpha_{sf} \left( \frac{\partial \phi}{\partial \hat{n}} \right)^2 d\hat{n} - 1 \right|.
\]

(4.64)

The error is evaluated numerically in the current study. The derivative is calculated by the central difference method at the interior points and the forward or backward difference technique at the boundary points of the computational domain. The integral is calculated by the standard trapezoidal rule. The surface tension error as a function of \( \dot{\xi} \) is plotted in Fig. 4.10 (b).

### 4.4.3 Convection of a curved interface

To demonstrate the extensional and compressional distortion in an incompressible fluid flow, we consider the convection of a curved interface in a prescribed divergence-free 2D velocity field. The computational domain is in the shape of an arch with \( r \times \theta \in [R_1, R_3] \times [0, \pi/2] \). A zero flux Neumann boundary condition is imposed for \( \phi \) on all the boundaries. The curved interface is initialized as a circular arc centered at \( r = 0 \) with radius \( R_2 \):

\[
\phi(x, y, 0) = -\tanh \left( \frac{R_2 - \sqrt{x^2 + y^2}}{\sqrt{2}\varepsilon} \right).
\]

(4.65)

The curved interface is convected by a divergence-free velocity field \( \mathbf{v}(x, y) \). The horizontal and vertical components of the velocity are given by \( v_x(x, y) = x \) and \( v_y(x, y) = -y \) respectively. The mobility coefficient in the range of \( \gamma = b \in [4, 20] \) are investigated, where \( b \) is a constant parameter. From the problem setup, the convective distortion parameter can be calculated as \( \dot{\xi}(r, 0) = 1/b \) at the bottom boundary and \( \dot{\xi}(r, \pi/2) = -1/b \) at the left boundary. In the present cases, we use \( R_1 = 0.1, R_2 = 0.25 \) and \( R_3 = 0.55 \). A structured mesh of grid size \( \Delta r = 6.25 \times 10^{-5} \) and \( \Delta \theta = \pi/2400 \) is used for the spatial discretization. The interface thickness parameter is chosen as \( \varepsilon = 6.25 \times 10^{-4} \). The mesh resolution can be calculated...
as $\varepsilon/h = 10$, which leads to a relative $L^2$ convergence error at the order of $10^{-5}$. The computational domain and the initial condition are illustrated in Fig. 4.8. The time step size is taken as $\Delta t = 1.25 \times 10^{-4}$. The numerical solutions at $t = 0.75$ are analyzed, when the interface thickness at $\theta = 0$ and $\theta = \pi/2$ reaches a constant value.

![Figure 4.8](image_url)

**Figure 4.8:** Schematic diagram showing the computational domain for the convection of a curved interface in a prescribed incompressible velocity field illustrated with streamlines. $\Omega_1$ and $\Omega_2$ are domains of the two phases. A zero flux Neumann boundary conditions for the order parameter is applied on all the boundaries.

The volume-conserved mean curvature flow is another source of error in the convection of a curved interface. To isolate the effect of the convective distortion from the effect of the volume-conserved mean curvature flow, the latter is minimized utilizing a small interface thickness parameter $\varepsilon$. From Eq. (3.5), the maximum $v_\kappa(x,t)$ occurs at $\gamma = 100$, $t = 0.75$, which can be calculated as $\max |v_\kappa(x,t)| = 0.0013$. It is negligible compared to the convective velocity in the computational domain which is $O(0.1)$. On the other hand, the minimum radius of curvature at $t = 0.75$ can be calculated as $\min R = 0.028$. Since $\varepsilon \ll R$, the normal velocity gradient in the normal direction introduced by the volume-conserved mean curvature flow being $O\left((\varepsilon/R)^2\right)$ (by taking the derivative of $v_\kappa(x,t)$ with respect to $R$) is negligible. Consequently, the effect of the volume-conserved mean curvature flow
is negligible in these cases.

The case at $\xi = 0.1$ is used to illustrate the simulation results. The contour of the order parameter from $t = 0$ to $t = 0.75$ are shown in Figs. 4.9 (a)-(d). The time history of $\tilde{\varepsilon}_d$ on $\theta = 0$ and $\theta = \pi/2$, which are the bottom boundary and the left boundary respectively, are shown in Fig. 4.9 (e). It can be observed that due to the convective distortion, the interface is expanded at $\theta = 0$ and compressed at $\theta = \pi/2$. The distortion increases during the convection of the curved interface. On the other hand, as the interface deviates further from the equilibrium interface profile, the effect of the free energy minimization increases. When the free energy minimization opposes the convective distortion, the deviation will stop increasing, which leads to a constant $\tilde{\varepsilon}_d$. Following similar definitions of the errors in Eqs. (4.62), (4.64) and similar calculation techniques, the relative interface thickness error and the relative surface tension error are calculated at $\theta = 0$ and $\theta = \pi/2$. The results are shown in Fig. 4.10 (a)-(b) respectively.

### 4.4.4 Relationship between errors and convective distortion

In Fig. (4.10), the relative interface thickness error and the relative surface tension force error are plotted as a function of $\xi$ for the convection of the planar and the curved interfaces. It is worth mentioning that the errors vary continuously with respect to $\xi$, while the singularities at $\xi = 0$ is merely a result of taking the absolute value of the errors. When the effect of the volume-conserved mean curvature flow is minimized by reducing $\varepsilon/R$ in the curved cases, the dependency of the errors on the convective distortion parameter $\xi$ is almost identical for both the cases. It shows that the relationship is consistent in one and two dimensions with different problem setup. Considering the numerical results and the analysis of the interface-preserving condition (4.25), we can further infer that the relationship between the errors and a constant $\xi$ is general. As shown in the figure, the errors decrease with the decrease in $|\xi|$. For the current cases with a constant $\xi$, at the discussed location, the RMS convective distortion parameter $\eta = |\xi|$. Hence a small $\eta$ can be used to reduce the error due to the convective distortion and to improve the interface-preserving capability. In Fig. 4.10, the interface errors $e_\varepsilon$ and $e_\sigma$ can be fitted as functions which are proportional to $\eta$ with the corresponding coefficients.
Figure 4.9: Convection of a curved interface with $\xi = 0.1$: the contours of $\phi$ at (a) $t = 0$, (b) $t = 0.25$, (c) $t = 0.5$, (d) $t = 0.75$, and (e) the time history of the non-dimensional interface thickness $\tilde{\varepsilon}_d$ on the bottom boundary $\theta = 0$ and the left boundary $\theta = \pi/2$ with the comparison to the equilibrium interface thickness $\tilde{\varepsilon}_{eq}$. 
Figure 4.10: Dependence of the interface errors on the convective distortion parameter $\xi$: (a) the relative interface thickness error $e_\varepsilon$, and (b) the relative surface tension error $e_\sigma$.

$k_\varepsilon$ and $k_\sigma$:

$$e_\varepsilon = k_\varepsilon \eta, \quad e_\sigma = k_\sigma \eta,$$

where the coefficients $k_\varepsilon = 0.7371$ and $k_\sigma = 0.6352$. The simple correlations are shown in Fig. 4.11. When diffuse interface is subjected to complex motions, there can be the loss of accuracy or the unresolved gradients due to the extensional and compressional distortions. In that case, there is a need to minimize the interface thickness error $e_\varepsilon$. Furthermore, the control of $e_\sigma$ is critical when the surface tension force and the interface dynamics play an important role. The RMS convective distortion parameter $\eta$ can be selected as:

$$\eta = \min \left\{ \frac{e_\varepsilon}{k_\varepsilon}, \frac{e_\sigma}{k_\sigma} \right\}$$

for desired thresholds of the relative interface thickness and surface tension force errors.

4.5 Rising bubble problem

After analyzing the selection of the RMS convective distortion parameter, we assess the effectiveness of our Navier-Stokes Allen-Cahn system with the time-dependent
Figure 4.11: Correlations of the interface errors as a function of RMS convective distortion parameter $\eta$: (a) the relative interface thickness error $e_{\varepsilon}$, and (b) the relative surface tension error $e_{\sigma}$.

mobility model by simulating 2D and 3D rising bubble benchmark cases. A systematic convergence study is performed for the volume-conserved mean curvature flow and the interface-preserving capability. We assess the accuracy of the current formulation by comparing the diffuse interface solution with the sharp interface counterpart. We will show that the interface-preserving capability is necessary to guarantee an accurate solution from the diffuse interface formulation. The international system of unit is used in all the cases by default.

4.5.1 Two-dimensional rising bubble benchmark

In this subsection, we present a well-known two-dimensional rising bubble benchmark case for assessing the role of the time-dependent mobility model on the accurate surface tension dynamics. The benchmark case considers the rising and deforming of an initially circular bubble immersed in a quiescent fluid. A rectangular computational domain $[0, 1] \times [0, 2]$ is considered for the benchmark case. The initial condition for the circular bubble is given by:

$$
\phi(x, y, 0) = -\tanh \left( \frac{R - \sqrt{(x-x_c)^2 + (y-y_c)^2}}{\sqrt{2\varepsilon}} \right), \quad (4.68)
$$
where $R = 0.25$ is the radius of the bubble with its center at $(x_c, y_c) = (0.5, 0.5)$. The quiescent fluid is initialized with zero velocity and pressure. The slip boundary condition is satisfied on the left and the right boundaries, while the no-slip boundary condition is prescribed on the top and the bottom boundaries. A zero flux Neumann boundary condition is imposed on all the boundaries for the order parameter. The density and the dynamic viscosity of the fluid and the bubble are selected as $\rho_1 = 1000$, $\rho_2 = 100$ and $\mu_1 = 10$, $\mu_2 = 1$. The surface tension coefficient is set to be $\sigma = 24.5$. The gravitational acceleration is taken as $g = (0, -0.98)$. The problem setup is illustrated in Fig. 4.12 (a). The benchmark problem has been studied by several research groups employing various numerical techniques in [108]. In the current study, we consider the data from the first group in [108] for comparison purposes, which employs the finite element method for spatial discretization and the sharp level-set method for the interface capturing.

Because the problem has a symmetric axis $x = 0.5$, we conduct the simulation with the right half of the computational domain. A symmetric boundary condition is imposed on the axis of symmetry. The contour of the order parameter in the computational domain at $t = 0$ is shown in Fig. 4.12 (b). The computational domain is discretized with a uniform structured mesh of grid size $\Delta x = \Delta y = h$. The grid size is selected according to the mesh resolution at the interface as $\varepsilon/h = 1$. The time step size is chosen as $\Delta t = 0.00125$. Similar to our earlier study in [94], the divergence free condition (i.e., incompressibility constraint) is approximately satisfied within the convergence tolerance of the linear GMRES and the nonlinear Newton solvers in the current case and the cases presented hereafter.

To quantify the mass conservation and the rising bubble dynamics, the mass of the order parameter $m$, the circularity of the bubble $\zeta$, the rise velocity of the
bubble $V_b$ and the center of mass of the bubble $Y_b$ are defined as follows:

\[
m = \int_{\Omega} \phi \, d\Omega,
\]

\[
\phi' = \frac{P_a}{P_b},
\]

\[
V_b = \frac{\int_{\Omega_2} v_y \, d\Omega}{\int_{\Omega_2} 1 \, d\Omega},
\]

\[
Y_b = \frac{\int_{\Omega_2} y \, d\Omega}{\int_{\Omega_2} 1 \, d\Omega},
\]

where $P_a$ is the perimeter of the circle which has the same area as the deformed bubble, $P_b$ denotes the perimeter of the bubble, $v$ is the velocity in the Y direction and $y$ is the Y coordinate. The defined variables and the bubble shape at $t = 3$ are compared in the convergence study.
Convergence of the volume-conserved mean curvature flow

The volume-conserved mean curvature flow velocity disturbs the convection of the two-phase interface according to the fluid flow velocity. Therefore we perform a convergence study to make sure that the disturbance is negligible. With the time-dependent mobility, the velocity is given by:

\[
v_{\kappa}(x,t) = \gamma(t) \varepsilon^2 \left( \kappa(x,t) - \frac{1}{|I_{\phi}^0(t)|} \int_{I_{\phi}^0} \kappa(x,t) ds \right) n_L^\phi(x,t)
\]

\[
= \frac{1}{\eta} \mathcal{F}(|\zeta(x,t)|) \varepsilon^2 \left( \kappa(x,t) - \frac{1}{|I_{\phi}^0(t)|} \int_{I_{\phi}^0} \kappa(x,t) ds \right) n_L^\phi(x,t), \quad x \in I_{\phi}^0(t).
\]

(4.69)

We refer to the quantity \( \gamma(t) \varepsilon^2 \) as the scaling factor of the volume-conserved mean curvature flow. According to Eq. (4.69), the scaling factor is affected by the user-defined parameters \( \eta \) and \( \varepsilon \). In the present convergence study, we decrease \( \varepsilon \) by a factor of 2 from \( \varepsilon = 0.01 \) to \( \varepsilon = 0.00125 \), while keeping \( \eta = 0.1 \). Thus, the volume-conserved mean curvature flow is reduced while the RMS convective distortion parameter is kept the same. The resulting scaling factor \( \gamma(t) \varepsilon^2 \) at \( t = 3 \) at various \( \varepsilon \) is summarized in Table 4.1. The circularity \( \mathcal{C} \), the bubble shape \( \phi = 0 \) at \( t = 3 \), the rise velocity \( V_b \), the center of mass \( Y_c \), and their comparison with the data in [108] are shown in Fig. 4.13.

To further quantify the results, we define the mass conservation error and the convergence errors as follows:

\[
e_m = \frac{|m_{t=0} - m_{t=3}|}{m_{t=0}},
\]

\[
e_\mathcal{C} = \frac{||\mathcal{C} - \mathcal{C}_{\text{ref}}||_2}{||\mathcal{C}_{\text{ref}}||_2},
\]

\[
e_{V_b} = \frac{||V_b - V_{b,\text{ref}}||_2}{||V_{b,\text{ref}}||_2},
\]

\[
e_{Y_b} = \frac{||Y_b - Y_{b,\text{ref}}||_2}{||Y_{b,\text{ref}}||_2},
\]

where \( | \cdot | \) denotes the absolute value and \( || \cdot ||_2 \) denotes the \( L^2 \) norm of the vector.
Figure 4.13: volume-conserved mean curvature flow convergence study for 2D rising bubble benchmark case: (a) circularity of the bubble, (b) interface shape at $t = 3$, (c) rise velocity, and (d) center of mass.

The simulation results from the case with $\epsilon = 0.00125$ are taken as the reference. The errors including the relative interface thickness and surface tension errors estimated by Eq. (4.66) are summarized in Table 4.1.

It can be observed from Table 4.1 that the mass conservation error is below 1% and it decreases with the reduction of $\epsilon$. The total mass is well conserved. The decrease in the scaling factor $\gamma(t)\epsilon^2$ at $t = 3$ along with the reduction in $\epsilon$ reflects the diminishing of the volume-conserved mean curvature flow. Since the flow directly affects the topology of the bubble, its influence is shown clearly in the convergence of the circularity and the bubble shape. As shown in Fig. 4.13 (a),
Table 4.1: Quantification of the errors for 2D rising bubble case: convergence with respect to $\varepsilon$ at a constant $\eta$.

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$\varepsilon$</th>
<th>$e_\varepsilon$</th>
<th>$e_\sigma$</th>
<th>$\gamma(t)e^2$</th>
<th>$e_m$</th>
<th>$e_\varepsilon$</th>
<th>$e_{V_b}$</th>
<th>$e_{Y_b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.01</td>
<td>0.074</td>
<td>0.064</td>
<td>$1.1 \times 10^{-3}$</td>
<td>0.0082</td>
<td>0.0105</td>
<td>0.0279</td>
<td>0.0048</td>
</tr>
<tr>
<td>0.1</td>
<td>0.005</td>
<td>0.074</td>
<td>0.064</td>
<td>$3.1 \times 10^{-4}$</td>
<td>0.0047</td>
<td>0.0061</td>
<td>0.0172</td>
<td>0.0029</td>
</tr>
<tr>
<td>0.1</td>
<td>0.0025</td>
<td>0.074</td>
<td>0.064</td>
<td>$9.1 \times 10^{-5}$</td>
<td>0.0025</td>
<td>0.0034</td>
<td>0.0089</td>
<td>0.0014</td>
</tr>
<tr>
<td>0.1</td>
<td>0.00125</td>
<td>0.074</td>
<td>0.064</td>
<td>$2.7 \times 10^{-5}$</td>
<td>0.0013</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

the circularity is reduced with the reduction of $\varepsilon$. This indicates that the bubble experiences larger deformation and higher curvature due to the reduction of the volume-conserved mean curvature flow. This is consistently observed in the convergence of the bubble shape shown in Fig. 4.13 (b). However, the bubble shape deviates from the data in [108]. The deviation can be observed in the rise velocity plotted in Fig. 4.13 (c) as well. This deviation is due to the error in the surface tension calculation introduced by the convective distortion. To conclude, the decreasing of the volume-conserved mean curvature flow with the decreasing of $\varepsilon$ cannot guarantee the accuracy of the solution, which leads to the investigation of the interface-preserving property.

Convergence of the interface-preserving property

Following the convergence study of the volume-conserved mean curvature flow, we study the convergence of the interface-preserving capability. From the discussion in Section 4, we know that by decreasing the RMS convective distortion parameter $\eta$, the convective distortion error will decrease. However, as shown in Eq. (4.69), a decrease in $\eta$ will increase the volume-conserved mean curvature flow. Thus we need to decrease both $\eta$ and $\varepsilon$ to improve the interface-preserving capability and decrease the volume-conserved mean curvature flow simultaneously. Considering this, we conduct studies with the following parameter combinations: $\eta = 0.1, \varepsilon = 0.005$; $\eta = 0.05, \varepsilon = 0.0025$ and $\eta = 0.025, \varepsilon = 0.00125$. The scaling factor of the volume-conserved mean curvature flow $\gamma(t)e^2$ at $t = 3$ for each combination is shown in Table 4.2. The circularity $\varepsilon$, the bubble shape at $t = 3$, the rise velocity $V_b$, the center of mass of the bubble $Y_b$ and the comparison with the data in [108] are shown in Fig. 4.14. Taking $\eta = 0.025, \varepsilon = 0.00125$ as the reference case, the
errors including the relative interface thickness and surface tension errors estimated by Eq. (4.66) are shown in Table 4.2.

It can be observed from Table 4.2 that the mass is well conserved. The scaling factor of the volume-conserved mean curvature flow decreases with the decreasing of $\varepsilon$ and $\eta$ in the test cases. The decreasing of the RMS convective distortion parameter $\eta$ reduces the errors from the convective distortion and improves the interface preservation property. As shown in Fig. 4.14, with the decrease in the volume-conserved mean curvature flow and the enforcement of the interface preservation capability, the simulation results converge and match well with the data in [108].

![Graphs showing convergence study](image)

**Figure 4.14:** The interface-preserving capability convergence study for 2D rising bubble benchmark case: (a) circularity of the bubble (b) interface shape at $t = 3$ (c) rise velocity, and (d) center of mass.
Table 4.2: Quantification of the errors for 2D rising bubble case: variation of $\varepsilon$ and $\eta$

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$\varepsilon$</th>
<th>$e_{\varepsilon}$</th>
<th>$e_{\sigma}$</th>
<th>$\gamma(t)e^{\varepsilon}$</th>
<th>$e_m$</th>
<th>$e_t$</th>
<th>$e_{V_b}$</th>
<th>$e_{Y_b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.005</td>
<td>0.074</td>
<td>0.064</td>
<td>$3.1 \times 10^{-4}$</td>
<td>0.0047</td>
<td>0.0051</td>
<td>0.0130</td>
<td>0.0070</td>
</tr>
<tr>
<td>0.05</td>
<td>0.0025</td>
<td>0.037</td>
<td>0.032</td>
<td>$1.8 \times 10^{-4}$</td>
<td>0.0027</td>
<td>0.0017</td>
<td>0.0047</td>
<td>0.0033</td>
</tr>
<tr>
<td>0.025</td>
<td>0.00125</td>
<td>0.018</td>
<td>0.016</td>
<td>$1.2 \times 10^{-4}$</td>
<td>0.0016</td>
<td>- - - -</td>
<td>- - - -</td>
<td>- - - -</td>
</tr>
</tbody>
</table>

Error due to insufficient interface-preserving capability

We further emphasize the importance of the interface-preserving capability by comparing the results of the 2D rising bubble benchmark case simulated by the constant mobility model with $\gamma = 1$ and the time-dependent mobility with $\eta = 0.1$. The complete computational domain $[0,1] \times [0,2]$ is used in the simulations. The interface thickness parameter is set to be $\varepsilon = 0.01$ and a uniform structured mesh $\Delta x = \Delta y = h$ of grid size $\varepsilon/h = 1$ is employed for the spatial discretization via linear finite elements. The time step size is taken as $\Delta t = 0.005$.

The contour of the order parameter at $t = 3$ superimposed on the mesh simulated by the constant and the time-dependent mobility are shown in Figs. 4.15 (a) and (b), respectively. As observed in Fig. 4.15 (a), when $\gamma = 1$, the interface-preserving capability is not sufficient to keep the interface profile against the convective distortion. Therefore, at the bottom of the bubble, the interface is subjected to an observable extensional distortion, which leads to an excessively low Laplace pressure. This changes the shape of the bubble, decreases the buoyancy force, and further reduces the rise velocity as shown in Fig. 4.15 (c). On the contrary, when the time-dependent mobility model with $\eta = 0.1$ is used, the interface profile is preserved well as shown in Fig. 4.15 (b), which gives a correct bubble shape and surface tension modeling. To further justify the above statements, we quantify the convective distortion by calculating the RMS convective distortion parameter as $\eta = F(|\zeta(x,t)|)/\gamma$. As shown in Fig. 4.15 (d), a larger $\eta$ representing insufficient interface-preserving capability is observed in the simulation with the constant mobility compared to the time-dependent mobility. The comparison shows that the proposed time-dependent model provides an approach to estimate as well as control the convective distortion.

74
Figure 4.15: Comparison of the constant and the time-dependent mobility model in 2D rising bubble case: contour of the order parameter at $t = 3$ simulated with (a) constant mobility coefficient $\gamma = 1$, (b) time-dependent mobility model at $\eta = 0.1$, and the difference in (c) rise velocity, and (d) the time history of the RMS convective distortion parameter $\eta$. 

75
4.5.2 Three-dimensional rising bubble benchmark

The 3D rising bubble benchmark case is a generalization of the 2D rising bubble case with increasing complexity and practicality due to the 3D topology and motion of the bubble. We use the benchmark case to further assess the Navier-Stokes Allen-Cahn CSF system with the time-dependent mobility model. The benchmark case considers the rising and deforming of an initially spherical bubble in a cuboid tank occupying the spatial domain \( \Omega \in [0, 1] \times [0, 2] \times [0, 1] \). The phase-field function describing the bubble is initialized as:

\[
\phi(x, y, z, 0) = -\tanh\left(\frac{R - \sqrt{(x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2}}{\sqrt{2} \epsilon}\right),
\]

where \( R = 0.25 \) is the radius of the bubble with its center at \((x_c, y_c, z_c) = (0.5, 0.5, 0.5)\). The no-slip boundary condition and the zero flux Neumann boundary condition are imposed on all the boundaries for the velocity and the order parameter respectively. The density and the viscosity of the fluid and the bubble are taken as \( \rho_1 = 1000, \rho_2 = 100, \mu_1 = 10, \mu_2 = 1 \). The surface tension coefficient is taken as \( \sigma = 24.5 \). The gravitational acceleration is set to be \( g = (0, -0.98, 0) \). The problem setup is illustrated in Fig. 4.16 (a). The 3D rising bubble benchmark case is investigated in [109] by several research groups. We consider the data from the second group in [109] for comparison purposes, in which the finite difference method and the sharp level-set method are employed for the discretization and the interface capturing respectively. As the case is symmetric with respect to planes \( x = 0.5 \) and \( z = 0.5 \), we simulate one quarter of the computational domain, as shown in Fig. 4.16 (b) with the symmetric boundary condition imposed on the symmetric planes. The computational domain is discretized with a uniform structured mesh of grid size \( \Delta x = \Delta y = \Delta z = h \). The mesh resolution at the interface is selected as \( \epsilon/h = 1 \), while the time step is taken as \( \Delta t = 0.005 \).

We define the following variables to assess the simulation results quantitatively: the total mass of the order parameter \( m \), the sphericity of the bubble \( \hat{s} \), the diameter of the bubble in X direction \( D_x \) and Y direction \( D_y \), the rise velocity
of the bubble $V_b$ and the center of mass of the bubble $Y_b$, which are given by:

\[
\begin{align*}
    m &= \int_{\Omega} \phi d\Omega, \\
    \dot{s} &= \frac{A_a}{A_b}, \\
    D_x &= \max(\{x|x \in \Omega_2\}) - \min(\{x|x \in \Omega_2\}) , \\
    D_y &= \max(\{y|y \in \Omega_2\}) - \min(\{y|y \in \Omega_2\}) , \\
    V_b &= \frac{\int_{\Omega_2} v_y d\Omega}{\int_{\Omega_2} 1 d\Omega}, \\
    Y_b &= \frac{\int_{\Omega_2} y d\Omega}{\int_{\Omega_2} 1 d\Omega},
\end{align*}
\]

where $A_a$ is the area of the sphere which has the same volume as the deformed
bubble. $A_b$ denotes the surface area of the bubble, $x$ and $y$ are the coordinates in X and Y directions respectively, and $v$ is the velocity in the Y direction. The defined variables are compared in the convergence study.

Similar to the convergence study of the 2D rising bubble case, we decrease $\eta$ and $\varepsilon$ to improve the interface preservation capability and decrease the volume-conserved mean curvature flow simultaneously. The following combinations are tested: $\eta = 0.1, \varepsilon = 0.01$; $\eta = 0.05, \varepsilon = 0.005$ and $\eta = 0.025, \varepsilon = 0.0025$. The scaling factor of the volume-conserved mean curvature flow $\gamma(t)e^2$ at $t = 3$ for each combination is tabulated in Table 4.3. The defined variables and their comparison to the data in [109] are shown in Fig. 4.17.

To further quantify the results, we define the mass conservation error and convergence errors as:

$$e_m = \frac{|m_{t=0} - m_{t=3}|}{m_{t=0}},$$
$$e_f = \frac{||f - f_{ref}||_2}{||f_{ref}||_2},$$
$$e_{D_x} = \frac{||D_x - D_{x,ref}||_2}{||D_{x,ref}||_2},$$
$$e_{D_y} = \frac{||D_y - D_{y,ref}||_2}{||D_{y,ref}||_2},$$
$$e_{V_b} = \frac{||V_b - V_{b,ref}||_2}{||V_{b,ref}||_2},$$
$$e_{Y_b} = \frac{||Y_b - Y_{b,ref}||_2}{||Y_{b,ref}||_2}.$$  

The simulation results of $\eta = 0.025, \varepsilon = 0.0025$ are taken as the reference. The errors including the relative interface thickness and surface tension errors estimated by Eq. (4.66) are tabulated in Table 4.3.

It can be observed that the total mass is well conserved with less than 1% relative error. The relative interface thickness and surface tension errors decreases with the decrease in the RMS convective distortion parameter $\eta$. The reduction of the volume-conserved mean curvature flow is reflected by the reduction of its scaling factor $\gamma(t)e^2$ at $t = 3$ in current cases. As a result, lower sphericity representing
larger deformation and higher curvature is observed in Fig. 4.17 (a). This is further confirmed in Fig. 4.17 (b), where a larger $D_x$ and a smaller $D_y$ representing more deviation from the spherical shape are observed. With both the improvement of the interface-preserving capability and the decrease in the volume-conserved mean curvature flow, the converged simulation results agree well with the data in [109].

### 4.6 Two rising bubbles merging with a free surface

In this section, we demonstrate the applicability of the proposed model in the case of two rising bubbles merging with a free surface, in which complicated topological changes of the interface and dynamics of the bubble-bubble and bubble-free surface interaction occur in an unstructured finite element mesh. The case considers the rising of two vertically aligned spherical bubbles driven by gravitational force and the merging of bubbles with the free surface in a cuboid tank. The computational domain is taken as $\Omega \in [0,1] \times [0,2] \times [0,1]$. The no-slip boundary condition and the zero flux Neumann boundary condition are applied on all the boundaries for the velocity and the order parameter, respectively. The order parameter is initialized...
Figure 4.17: Convergence study for the 3D bubble rising problem: (a) sphericity of the bubble, (b) bubble diameters in X and Y directions, (c) rise velocity, and (d) center of mass.

for the bubbles and the free surface as:

\[
\phi(x, y, z, 0) = -\tanh\left(\frac{R_l - \sqrt{(x-x_{lc})^2 + (y-y_{lc})^2 + (z-z_{lc})^2}}{\sqrt{2}\epsilon}\right) - \tanh\left(\frac{R_u - \sqrt{(x-x_{uc})^2 + (y-y_{uc})^2 + (z-z_{uc})^2}}{\sqrt{2}\epsilon}\right) - \tanh\left(\frac{y-y_{wl}}{\sqrt{2}\epsilon}\right) - 2,
\]

(4.71)
where $R_l = 0.25$ is the radius of the lower bubble with its center at $(x_{lc}, y_{lc}, z_{lc}) = (0.5, 0.5, 0.5)$, $R_u = 0.2$ is the radius of the upper bubble with its center at $(x_{uc}, y_{uc}, z_{uc}) = (0.5, 1, 0.5)$, $y_{wl} = 1.5$ is the water level of the free surface. The density and viscosity of the fluid and the bubbles are taken as $\rho_1 = 1000$, $\rho_2 = 100$, $\mu_1 = 10$, $\mu_2 = 1$.

The surface tension coefficient is chosen as $\sigma = 24.5$. The gravitational acceleration is set to be $g = (0, -0.98, 0)$. The problem definition is illustrated in Fig. 4.18 (a). The interface thickness parameter is selected as $\epsilon = 0.005$ to reduce the volume-conserved mean curvature flow. In the time-dependent mobility model, the RMS convective distortion parameter $\eta = 0.05$ is used to get an accurate surface tension modeling. The above combinations of $\epsilon$ and $\gamma$ have been proven to be accurate in the simulation of the 3D rising bubble case, which uses the same physical parameters. A non-uniform unstructured mesh consisting of 7,077,043 nodes and 45,078,392 tetrahedrons is employed for spatial discretization. The mesh at the plane $x = 0.5$ is shown in Fig. 4.18 (b). The time step size is selected as $\Delta t = 0.0025$. The evolution of the interface $\phi = 0$ is shown in Fig. 4.19. The complex topological changes including the rising of the bubbles, the merging of the bubbles with the free surface and the wave formation at the free surface in the merging process can be observed clearly using our 3D phase-field Navier-Stokes solver with the unstructured mesh.

### 4.7 Summary

In this chapter, a variational interface-preserving Allen-Cahn phase-field formulation relying on a novel time-dependent mobility model has been developed for accurate surface tension calculation. By writing the convective Allen-Cahn equation in a non-dimensional moving orthogonal curvilinear coordinate system, we have derived the governing equation for the interface profile. We have identified the convective distortion term and the effective parameter determining the deviation of the diffuse interface profile from the hyperbolic tangent profile in the governing equation. A time-dependent mobility model to control the convective distortion parameter in the diffuse interface region and to preserve the hyperbolic tangent profile has been constructed accordingly. Following the verification of our im-

81
For Figure 4.18: Two rising bubbles merging with a free surface problem: (a) schematic diagram showing the computational domain, and (b) unstructured finite element mesh at the plane $x = 0.5$.

With a generic bistable convection-reaction-diffusion system, we established the correlation between the convective distortion parameter and the interface errors through numerical simulations of the planar and curved interface convection problems. We then assessed the solutions of the proposed model in two- and three-dimensional rising bubble benchmark cases against the sharp interface counterparts. Through the assessment, it has been shown that the interface preservation achieved by the proposed model and the minimization of the volume-conserved mean curvature flow realized by decreasing the interface thickness parameter is essential for accurate surface tension dynamics.
Finally, by simulating two rising bubbles merging with a free surface, we have shown that the proposed technique is applicable in a practical problem involving complex topology changes of the interface in an unstructured mesh and complex dynamics involving bubble-bubble and bubble-free surface interactions.
Chapter 5

Geometry-preserving phase-field for fluid-structure interaction *

In this chapter, we present the phase-field diffuse interface description for fluid-solid interface in FSI problems. The geometry of solid objects is usually featured by large aspect ratios and sharp corners. In such cases, the curvature flow of the phase-field method becomes the major issue for accurate interface evolution. To resolve this issue, we develop an interface and geometry preserving phase-field method. The method constructs an auxiliary velocity field, which aims to decrease the convective distortion and further the need for interface regularization. With less interface regularization, the curvature flow is reduced. The auxiliary velocity is constructed such that the normal velocity gradient in the normal direction is reduced inside the diffuse interface region, therefore referred to as the gradient-minimizing velocity field. The interface and geometry preserving method is examined in FSI problems such as channel flow passing a fixed block and Turek’s benchmark, which significantly reduces the curvature flow.

5.1 Background

Fluid-structure interaction is a coupled highly-nonlinear multiphysics problem that can be found in various natural phenomena and industrial processes. Examples include from traditional aeroelasticity and flow-induced vibration problems in aerospace [110], marine/offshore [24], and biomedical engineering [111], to the emerging fields of energy harvesting devices [112], muscular hydrostat [113, 114] and soft robotics [115].

The interface between fluids and solids poses significant challenges in mathematical modeling and numerical simulation [23, 24], especially for cases where the interface experiences large topological changes such as large displacement/rotational motion and interface contact. While the phase-field diffuse interface description facilitates the interface motion, it induces two new issues: (i) additional function fields are required to capture the solid kinematics in the Eulerian frame of reference, (ii) keeping an accurate interface geometry of solid objects is considerably challenging. Because geometric features such as large aspect ratio or sharp corners of solid objects can induce significant curvature flow as discussed in Section 3.2. While (i) can be resolved by evolving the left Cauchy-Green tensor as reviewed in Section 2.2, (ii) is rarely discussed in the literature and becomes the bottleneck of applying the phase-field diffuse interface description to fluid-structure interface in FSI problems. To address this problem, it is necessary to revisit and clarify the relationship between the convective distortion, time-dependent mobility, and curvature flow in the interface-preserving phase-field method proposed in Chapter 4.

5.2 Review of interface-preserving parameters

In Section 4.2.3, the convective distortion is quantified by the normal velocity gradient in the normal direction:

$$\frac{\partial v_n}{\partial n} = \frac{(\nabla \phi)^T \cdot \mathbf{v} \cdot \nabla \phi}{|\nabla \phi|^2}.$$  \hspace{1cm} (5.1)
The convective form of the Allen-Cahn phase-field equation with a Lagrange multiplier for the mass conservation \[77\] is given by:

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = -\gamma(t) \left( \frac{\delta \mathcal{E}(\phi)}{\delta \phi} - \beta(t) \sqrt{F(\sigma)} \right),
\]

where \( \mathbf{v} \) is the convection velocity, \( \gamma(t) \) is the time-dependent mobility model controls the intensity of the free energy minimization, and \( \beta(t) = \frac{\int_\Omega F'(\phi)|d\Omega}{\int_\Omega \sqrt{F(\phi)}|d\Omega} \) is a Lagrange multiplier to ensure the mass conservation. As mentioned previously, the interface profile evolves towards the hyperbolic tangent profile as the free energy is minimized. The required free energy minimization to regularize the hyperbolic tangent profile against the convective distortion is given by:

\[
\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{(\nabla \phi)^T \cdot \nabla \mathbf{v} \cdot \nabla \phi}{|\nabla \phi|^2} \right), \quad -\delta < \phi < \delta,
\]

where \( \mathcal{F}(\cdot) \) is a RMS function and \( \eta \) is a positive user-controlled parameter termed as the RMS interface distortion number \[116\]. When the value of \( \eta \) decreases, the ratio between the free energy minimization and the convective distortion increases and the interface distortion is reduced. A detailed explanation of the effect and the selection of the interface distortion number \( \eta \) can be found in Chapter 4.

While the time-dependent mobility model is effective in reducing the interface distortion, the free energy minimization induces an undesired interface displacement. The velocity associated with the undesired interface displacement is proportional to the local curvature, which can be written as:

\[
\mathbf{v}_\kappa = \gamma(t) \epsilon^2 (\kappa - \overline{\kappa}) \mathbf{n},
\]

where \( \kappa \) is the local curvature, \( \overline{\kappa} \) is the average curvature along the interface and \( \mathbf{n} \) is the normal vector of the interface. We refer to this as the volume-conserved mean curvature flow. The volume-conserved mean curvature flow can be significantly large in a fully Eulerian FSI model when: (i) the solid moves at a relatively high speed, which induces significant convective distortion and requires large \( \gamma(t) \) to regularize the hyperbolic tangent profile; (ii) the solid object has sharp geometry features, where the curvature is ill-defined and becomes a drastically large value in
numerical simulations.

The difficulty can be eased by directly modifying the reinitialization or the free energy minimization process. In [117], the location of the interface is considered explicitly and the displacement caused by the reinitialization process is minimized. In [78], an anti-curvature term is suggested to nullify the curvature flow induced by the phase-field method. Recently in [118], the authors introduced sub-iterations to correct the undesired interface displacement within the iteration of the reinitialization process.

In the current work, instead of directly working on the reinitialization and free energy minimization processes, we preserve the interface geometry by minimizing the convective distortion. Inspired by the harmonic extension of the velocity in the fluid domain to avoid the entanglement of the initial point set [49], we propose an auxiliary gradient-minimizing velocity field for the convection of the order parameter in the phase-field method. The GMV retains the solid velocity in the solid domain and extends the solid velocity along the normal direction throughout the diffuse interface region. The stability of this process is enhanced by a diffusion term. By this construction, the normal velocities of isosurfaces of the order parameter are maintained the same inside the diffuse interface region. As a result, the convective distortion decreases, reducing the need for the free energy minimization process to regularize the interface profile, therefore inducing less interface displacement. Hence the solid geometry is better preserved. In the context of the fully Eulerian FSI, the GMV keeps the velocity of the diffuse interface region close to the velocity of the solid bulk so that the diffuse interface region better conforms to the geometry of the solid. When the GMV is integrated with the Lagrange multiplier for the mass conservation [77] and the time-dependent mobility coefficient for the interface profile preservation [116], the resulting phase-field method better preserves the diffuse interface profile as well as the interface geometry. In this thesis, we refer to this as the interface and geometry preserving phase-field method. The concept of the IGP method is illustrated in Fig. 5.1

**Remark 1.** In short, we introduce a gradient-minimizing velocity field to reduce $\partial v_n / \partial n$, thus decreasing the mobility coefficient $\gamma(t)$ and the curvature flow velocity $v_\kappa$ during the interface evolution. While the mobility coefficient is adaptively...
reduced, the desired traits of the phase-field method are maintained, such as the well-posedness arising from the variational minimization of the free energy.

The order parameter solve by the IGP method is then used to unify the coupled dynamics of the incompressible fluid and the incompressible neo-Hookean solid via phase-dependent interpolation. The stabilized finite element technique is employed for the variational discretization while the generalized-α method is used for fully implicit time marching [24, 52, 119]. We first analyze the effectiveness of the IGP method in maintaining the interface profile and geometry in a prescribed velocity field. We examine the evolution of circular and square interfaces when convected by a velocity field that is extensional in the horizontal direction and compressional in the vertical direction. After investigating the IGP method alone, the IGP method is integrated into a variational fully Eulerian FSI formulation. The variational framework is examined with the deformation of a solid block under lid-driven cavity flow. We then consider a fixed deformable block subjected to incoming channel flow, where the convective distortion is relatively strong and the geometry-preserving effect can be clearly observed. Finally, we demonstrate the proposed framework for an unsteady FSI application of the cylinder-flexible plate problem, where a flexible plate attached behind a stationary cylinder vibrates sub-
jected to a channel flow.

The organization of this chapter is as follows: Section 3 presents the construction of the GMV. The GMV is integrated into the phase-field method in Section 4. The resulting IGP method and its implementation in our fully Eulerian FSI solver is discussed. Section 5 describes the variational discretization of the proposed formulation. Section 6 presents the test cases of increasing complexity, including the convection of circular and square interfaces in a prescribed velocity field, the deformation of a solid block under lid-driven cavity flow, the channel flow passing a fixed deformable block, and the cylinder-flexible plate problem. This chapter is summarized in Section 7.

5.3 Gradient-minimizing velocity field

In this subsection we discuss the volume-conserved mean curvature flow, which disturbs the geometry of the interface. Lastly, we introduce the construction of the gradient-minimizing velocity field and explain how it reduces the volume-conserved mean curvature flow.

The fundamental proposition of the gradient-minimizing velocity field is to convect the isosurfaces of the order parameter with approximately the same normal velocity in the normal direction. By employing such a velocity field, the distortion on the hyperbolic tangent profile or, equivalently, the thickening or thinning effect on the diffuse interface region can be reduced. Moreover, there is a need for the normal diffuse interface velocity to be tied to the velocity of the solid bulk such that the diffuse interface region conforms to the solid bulk. To achieve these kinematic constraints, we construct the GMV in the diffuse interface region such that it follows the velocity field in the solid bulk. Consequently, the solid velocity field along the periphery of the solid bulk is propagated in the normal direction throughout the diffuse interface region. Denoting the GMV as \( \mathbf{w} \), the governing equation can be constructed as:

\[
\alpha(\phi)(\mathbf{w} - \mathbf{v}) + (1 - \alpha(\phi))( - \varepsilon \nabla \phi \cdot \nabla) \mathbf{w} = \mathbf{0},
\]

(5.5)

where \( \alpha(\phi) \) is the weight function mentioned previously. The construction of the gradient-minimizing velocity field is further illustrated in Fig. 5.2.
In the current work, we select $\alpha(\phi) = (1/2)(1 + \phi)$. In evaluating $\alpha(\phi)$, we let $\alpha(\phi) = 1$ when $\alpha(\phi) > 1$ and $\alpha(\phi) = 0$ when $\alpha(\phi) < 0$ to ensure the boundness of the phase-dependent interpolation. The first term assigns the solid velocity to the GMV in the solid bulk, which we refer to as the Dirichlet term. The second term can be considered as a convection term, which propagates the velocity at the periphery of the solid bulk along the normal direction throughout the diffuse interface region. Since $\nabla \phi \sim O(1/\varepsilon)$, we premultiply $\varepsilon$ to keep the magnitude of the convection velocity $\varepsilon \nabla \phi \sim O(1)$. This ensures that the ratio between the convection and the Dirichlet term is only affected by the phase-dependent interpolation regardless of $\varepsilon$. Without the scaling by $\varepsilon$, the convection term dominates when $\varepsilon \to 0$. As a result, $\mathbf{w} = \mathbf{v}$ is only enforced when $\alpha(\phi) \to 1$, which goes interior of the solid domain. On the contrary, with relatively large $\varepsilon$, $\mathbf{w} = \mathbf{v}$ is imposed even at the fluid side.

![Diagram](image)

**Figure 5.2:** Illustration on the construction of the gradient-minimizing velocity field. Streamlines of $-\varepsilon \nabla \phi$ which passes $\mathbf{w}$ in the normal direction throughout the diffuse interface region are shown as the blue arrows in the left figure, while the magnitude of the velocity in the normal direction $-\varepsilon \nabla \phi \cdot \mathbf{n}$ is shown in the right figure.

To enhance the stability of the GMV construction, we add a diffusion term to ensure that $Pe = |v|h/2\nu \leq 1$. We approximate the maximum magnitude of the propagation velocity $|v|_{\text{max}}$ as $|v|_{\text{max}} = | -\varepsilon \partial \phi / \partial n |_{\phi=0} = 1/\sqrt{2}$, as shown in Fig. 5.2. The grid size is approximated as $h = \varepsilon$, where the diffuse interface region is well resolved by four elements [93]. With these approximations, the diffusion coefficient can be selected as $\nu = \varepsilon/2\sqrt{2}$, and the governing equation for the GMV
is finally given by:

\[ \alpha(\phi)(w - v) + (1 - \alpha(\phi)) \left( -\varepsilon \nabla \phi \cdot \nabla w - \frac{\varepsilon}{2\sqrt{2}} \Delta w \right) = 0. \quad (5.6) \]

The boundary condition are taken as \( w = 0 \) on the wall and \( \nabla w \cdot n^\Gamma = 0 \) otherwise, where \( n^\Gamma \) is the outer normal of the computational domain.

With the constructed GMV, the interface and geometry preserving phase-field method can be written as:

\[ \frac{\partial \phi}{\partial t} + w \cdot \nabla \phi = -\gamma(t) \left( \frac{\delta E(\phi)}{\delta \phi} - \beta(t) \sqrt{F(\phi)} \right), \quad (5.7) \]

where

\[ \gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{(\nabla \phi)^T \cdot \nabla w \cdot \nabla \phi}{|\nabla \phi|^2} \right), \quad -\delta < \phi < \delta. \quad (5.8) \]

In the current work, we use \( \delta = 0.9 \) as boundaries of the diffuse interface region, within which 90% of the variation of \( \phi \) occurs.

**Remark 2.** The GMV reduces the convective distortion \( \partial w_n / \partial n = (\nabla \phi)^T \cdot \nabla w \cdot \nabla \phi / |\nabla \phi|^2 \) compared to that of flow field velocity \( \partial v_n / \partial n \), which further decreases the dynamic mobility coefficient \( \gamma(t) \) in Eq. (5.8), and the resulting curvature flow \( \nu_\kappa = \gamma(t) \varepsilon^2 (\kappa - \bar{\kappa}) n \).  

### 5.4 FSI dynamics and solid kinematics in Eulerian frame

In this section, we present the formulations for FSI dynamics and solid kinematics in Eulerian frame of reference. We start with the mass and momentum conservation equations of the underlying coupled fluid-structure system. After that, we describe the evolution of the left Cauchy-Green tensor for calculating the solid stress. Finally, we summarize the fully Eulerian FSI formulation with the IGP method.

#### 5.4.1 Conservation laws for the fully Eulerian FSI

Consider a physical domain \( \Omega \times [0, T] \) with spatial coordinates \( x \) and temporal coordinate \( t \). The domain comprises the solid domain \( \Omega^s_t \) and the surrounding fluid domain \( \Omega^f_t \). The momentum balance law for the solid and the fluid can be written
\[\rho^s (\partial_t v^s + v^s \cdot \nabla v^s) = \nabla \cdot \sigma^s + b^s, \quad \rho^f (\partial_t v^f + v^f \cdot \nabla v^f) = \nabla \cdot \sigma^f + b^f, \quad (5.9)\]

where \(v^s, \rho^s, \sigma^s, b^s\) represent the velocity, the density, the Cauchy stress and the body force of the solid respectively, and \(v^f, \rho^f, \sigma^f, b^f\) represent the corresponding physical properties of the fluid. In terms of the stresses, we restrict the material properties to the incompressible fluid and the incompressible neo-Hookean solid. With the incompressible conditions in both the solid and the fluid domains, the mass conservation equation reduces to a divergence-free condition for both the solid and the fluid velocity fields:

\[\nabla \cdot v^s = 0, \quad \nabla \cdot v^f = 0. \quad (5.10)\]

The mass and momentum conservation equations can be integrated through a phase-dependent interpolation as follows:

\[\alpha(\phi)\rho^s (\partial_t v^s + v^s \cdot \nabla v^s) + (1 - \alpha(\phi)) \rho^f (\partial_t v^f + v^f \cdot \nabla v^f) = \nabla \cdot (\alpha(\phi) \sigma^s + (1 - \alpha(\phi)) \sigma^f) + \alpha(\phi)b^s + (1 - \alpha(\phi))b^f, \]

\[\alpha(\phi)\nabla \cdot v^s + (1 - \alpha(\phi)) \nabla \cdot v^f = 0, \]

where \(\alpha(\phi)\) is a weight function satisfying \(\alpha(\phi(x,t)) = 1, x \in \Omega^s_t; \alpha(\phi(x,t)) = 0, x \in \Omega^f_t\), and \(\phi(x,t)\) being the order parameter in the phase-field method which indicates the local phase compositions. A unified and continuous velocity field can be used to simplify the coupled fluid-solid equations as follows:

\[\rho(\phi) (\partial_t v + v \cdot \nabla v) = \nabla \cdot \sigma(\phi) + b(\phi), \quad (5.11)\]

\[\nabla \cdot v = 0, \quad (5.12)\]

where \(v\) is the unified velocity field subjected to the density, the stress and the body force interpolations: \(\rho(\phi) = \alpha(\phi)\rho^s + (1 - \alpha(\phi))\rho^f, \sigma(\phi) = \alpha(\phi)\sigma^s + (1 - \alpha(\phi))\sigma^f\) and \(b(\phi) = \alpha(\phi)b^s + (1 - \alpha(\phi))b^f\).
5.4.2 Evolution of the left Cauchy-Green tensor

Following the convention of the continuum mechanics [120], a solid \( \mathcal{B} \) can be defined as a collection of particles. A one-to-one correspondence can be established between each particle \( P \) and its spatial coordinates in the Euclidean space \( x \in \mathbb{R}^3 \). The correspondence is referred to as a configuration of the body, which can be denoted as \( \chi : x = \chi(P) \), where \( P \in \mathcal{B}, x \in \mathbb{R}^3 \). To describe the deformation of the solid, we need to define a reference configuration. The reference configuration is usually selected as the initial configuration when the solid is undeformed and in a stress-free state. Mathematically, this can be denoted as:

\[
\chi(P) = \chi_{\text{ref}}(P, t = 0) = x(P, t = 0),
\]

(5.13)

where \( \chi \) is the spatial coordinates of the particle \( P \) in the reference configuration. Note that the one-to-one correspondence between \( \chi \) and \( P \) established by Eq. (5.13) is invariant in time. In other words, the initial position of the particle \( \chi \) can serve as a unique marker for the solid particle. From this perspective, \( \chi \) can be considered as the material coordinates of the solid.

With the definition of the reference configuration, we now consider the deformation of a solid and the resulting restoring force. In the constitutive relation of solids, stretch or compression of a line element between any two particles causes restoring normal stress. In contrast, the angle change between two line elements causes restoring shear stress. Consequently, the solid particles take an orderly arrangement in a continuously deformed configuration without rupture [47] or wrinkling [121]. From the computational point of view, this facilitates the description of a solid in a Lagrangian frame of reference, where the grid points follow the moving particles without entangling the mesh. The current positions of the solid particles can be written as follows in the Lagrangian description:

\[
x(\chi, t) = \chi(P, t = 0) = x(P, t = 0) + u(\chi, t).
\]

(5.14)

Computationally, \( \chi(P) \) plays multiple roles in describing the motion of particles. It is the material coordinates of the particle \( P \) and the position of the particle in the initial configuration. Since the same grid point is used for the particle in the
Lagrangian description, $X(P)$ is directly used as the coordinates of the grid points. The displacement of the particle represented by $u(X,t)$ is stored at the grid node located at $X$.

While the mesh is well-behaved in the Lagrangian description for the solid due to the orderly arrangement of the solid particles, the surrounding mesh for the fluid domain can be stretched extensively and fail when following the motion of the solid, especially when the solid experiences large deformation or contact with another. In such cases, the Eulerian description for the solid can be used to circumvent this difficulty. In the Eulerian description of a solid, the correspondence between the particles and the grid points is implicit, hence allowing large deformation of solids and topological changes of interfaces. Specifically, the solid particles move through an Eulerian mesh fixed in space. As a result, the coordinates of a grid point merely represent its spatial location but no longer provide the initial positions of solid particles. Without the reference from the initial positions, the relative displacements of the solid particles cannot be calculated. This poses difficulties in the calculation of the solid strain and stress. Therefore, we need an intermediate vector field to indicate the initial position of the particle located at the grid point. We denote the intermediate or supplementary vector field as $\xi$. Since $\xi$ gives the initial positions of the particles, at $t = 0$, we have:

$$\xi(x,t = 0) = x(P,t = 0).$$

For a solid particle, its initial position is time-invariant. In other words, $\xi$ can serve as unique markers to specify the solid particles, which essentially becomes the material coordinates of the solid in the Eulerian description. As markers of the solid particles, they should move along with the particles at the solid velocity. Therefore, the evolution of the material coordinates in the Eulerian description is given by:

$$\frac{\partial \xi(x,t)}{\partial t} + (v^s \cdot \nabla) \xi(x,t) = 0.$$  

Furthermore, the initial positions can be backtracked as:

$$x(\xi,0) = \xi(x,t).$$
The complete process of the mapping for the solid material coordinates in the Eulerian description is illustrated in Fig. 5.3.

\[ \frac{d\xi}{dt} = 0 \]

Figure 5.3: Illustration of the material coordinates of a deformable solid in an Eulerian mesh.

With the material coordinates, we can calculate the strain and stress of the deformed solid. The deformation of the solid relative to its reference configuration can be expressed as: \( F = \frac{\partial x}{\partial \xi} \), where \( F \) is referred to as the deformation gradient tensor. Using \( \frac{\partial \xi}{\partial x} = I \), one can write \( \nabla \xi = \frac{\partial \xi}{\partial x} = F^{-1} \), where \( \xi \) at fixed Eulerian mesh nodes represent the markers of the particles. For the incompressible neo-Hookean solid, the constitutive relation is given by [122]:

\[
\sigma^s = -p^s I + \mu_L^s (FF^T - I) + \mu^s \left( \nabla v^s + (\nabla v^s)^T \right) \\
= -p^s I + \mu_L^s (\left( \nabla \xi \right)^{-1} (\nabla \xi)^{-T} - I) + \mu^s (\nabla v^s + (\nabla v^s)^T) ,
\]

(5.18)

where \( p^s, \mu_L^s \) and \( \mu^s \) are the hydrostatic pressure, the shear modulus and the viscosity of the solid, respectively. However, the calculation of the inverse of the gradient of the material coordinates is complex. To avoid this issue, we directly evolve the left Cauchy-Green tensor \( B = FF^T \). To derive the evolution equation, we start from the total derivative of the deformation gradient tensor by taking the gradient
of Eq. (5.16):

\[
D(F^{-1}) = -F^{-1} \nabla v^s,
\]

(5.19)

where \( D(A) = \partial A / \partial t + (v^s \cdot \nabla)A \) denotes the material derivative, the velocity gradient \( \nabla v^s_{i,j} = \partial v^s_i / \partial x_j \) and the inner product of tensors is defined as \((AB)_{i,j} = A_{i,k}B_{k,j} \). Using \( FF^{-1} = I \) and \( D(F)F^{-1} + FD(F^{-1}) = 0 \), we have:

\[
D(F) = \nabla v^s F,
\]

(5.20)

and further:

\[
D(B) = D(FF^T) = D(F)F^T + FD(F^T) = \nabla v^s FF^T + FF^T (\nabla v^s)^T = \nabla v^s B + B (\nabla v^s)^T.
\]

(5.21)

For the current FSI model, the stress of the incompressible Newtonian fluid used is given by:

\[
\sigma^f = -p^f I + \mu^f \left( \nabla v^f + (\nabla v^f)^T \right),
\]

(5.22)

where \( p^f \) is the hydrostatic pressure of the fluid and \( \mu^f \) is the dynamic viscosity.

In the fully Eulerian FSI model, the material coordinates \( \xi \) need to be convected inside the solid bulk and in the vicinity of the diffuse interface region. This is particularly required for the smoothness of the material coordinates and the solid stress. However, the unified velocity field in the diffuse interface region is a composition of the fluid and the solid velocities. When the fluid velocity is involved, the material coordinates may be convected further downstream. This can violate the underlying physics of the solid, leading to spurious errors and instability in the stress calculation. One can see similar situations for the evolution of the left Cauchy-Green tensor. To address this problem, we employ a phase-dependent interpolation to increase the robustness in the stress calculation. In the fluid-solid domain, the left Cauchy-Green tensor is evolved as

\[
\frac{\partial B}{\partial t} = \alpha(\phi) \left( - (v \cdot \nabla)B + \nabla v B + B (\nabla v)^T \right),
\]

(5.23)
which provides smooth attenuation across the diffuse interface.

5.4.3 Summary for the Eulerian FSI formulation

Integrating all above equations, the fully Eulerian FSI formulation with the IGP method can be summarized as:

\[
\begin{align*}
\rho(\phi)(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) &= \nabla \cdot \mathbf{\sigma}(\phi) + \mathbf{b}(\phi), \\
\nabla \cdot \mathbf{v} &= 0, \\
\alpha(\phi)(\mathbf{w} - \mathbf{v}) + (1 - \alpha(\phi)) \left( (-\varepsilon \nabla \phi \cdot \nabla) \mathbf{w} - \frac{\varepsilon}{2\sqrt{2}} \Delta \mathbf{w} \right) &= 0, \\
\partial_t \phi + \mathbf{w} \cdot \nabla \phi &= -\gamma(t) \left( F(\phi)' - \varepsilon^2 \Delta \phi - \beta(t) \sqrt{F(\phi)} \right), \\
\frac{\partial \mathbf{B}}{\partial t} &= \alpha(\phi) \left( -(\mathbf{v} \cdot \nabla) \mathbf{B} + \nabla \mathbf{v} \mathbf{B} + \mathbf{B} (\nabla \mathbf{v})^T \right),
\end{align*}
\] (5.24)

with

\[
\begin{align*}
\rho(\phi) &= \alpha(\phi)\rho^s + (1 - \alpha(\phi))\rho^f, \\
\mathbf{\sigma}(\phi) &= \alpha(\phi)\mathbf{\sigma}^s + (1 - \alpha(\phi))\mathbf{\sigma}^f, \\
\mathbf{b}(\phi) &= \alpha(\phi)b^s + (1 - \alpha(\phi))b^f, \\
\alpha(\phi) &= (1/2)(1 + \phi), \\
\gamma(t) &= \frac{1}{\eta} \frac{\mathcal{F}}{\Phi} \left( \frac{|\nabla \phi|^2}{|\nabla \phi|^2} \right), \quad -\delta < \phi < \delta, \\
\mathbf{\sigma}^s &= -p^s I + \mu^s_L (\mathbf{B} - I) + \mu^s (\nabla \mathbf{v}^s + (\nabla \mathbf{v}^s)^T), \\
\mathbf{\sigma}^f &= -p^f I + \mu^f (\nabla \mathbf{v}^f + (\nabla \mathbf{v}^f)^T).
\end{align*}
\]

Generally speaking, the GMV can reduce the convective distortion in diffuse interface methods (where the interface is resolved by three to four elements) independent of the time-dependent mobility and the phase-field method. For example, the GMV should be able to reduce the convective distortion of the diffuse interface region in the level set method, thus reducing the frequency and iteration number of the reinitialization process, furthermore the undesired interface displacement introduced by the reinitialization. The discretization of the continuum formulation will be introduced in the following section.
5.5 Variational implementation

In this section, we present the variational implementation of our fully Eulerian FSI formulation. We start with temporal discretization, which applies to each of the partitioned implicit solvers when required. We then present the semi-discrete form of each component of the framework. Specifically, we provide a detailed description of the Jacobian matrix of the solid stress required in the variational minimization of the momentum conservation equations. Finally, we present the linearized matrix form of the proposed variational framework.

5.5.1 Temporal discretization

We employ the generalized-\(\alpha\) technique \[123\] for the temporal discretization which enables a user-controlled high-frequency damping desirable for coarse discretizations in space and time. For a first-order system of variable \(\varphi\), the generalized-\(\alpha\) method is given by:

\[
\partial_t \varphi^{n+\alpha_m} = f(\varphi^{n+\alpha}),
\]

\[
\varphi^{n+1} = \varphi^n + \Delta t \partial_t \varphi^n + \Delta t \zeta (\partial_t \varphi^{n+1} - \partial_t \varphi^n),
\]

\[
\partial_t \varphi^{n+\alpha_m} = \partial_t \varphi^n + \alpha_m (\partial_t \varphi^{n+1} - \partial_t \varphi^n),
\]

\[
\varphi^{n+\alpha} = \varphi^n + \alpha (\varphi^{n+1} - \varphi^n),
\]

where \(\alpha, \alpha_m\) and \(\zeta\) are the generalized-\(\alpha\) parameters depending on the user-defined spectral radius \(\rho_\infty\):

\[
\alpha = \frac{1}{1 + \rho_\infty}, \quad \alpha_m = \frac{1}{2} \left(\frac{3 - \rho_\infty}{1 + \rho_\infty}\right), \quad \zeta = \frac{1}{2} + \alpha_m - \alpha.
\]

The temporal evolution works in a predictor-multicorrector manner. In every non-linear iteration, we first predict the solution at \(n + 1\), interpolate the solution to \(n + \alpha\) and solve the first order system. After that, we correct the solution at \(n + 1\) according to the solution at \(n + \alpha\). In the current work, the spectral radius is selected as \(\rho_\infty = 0\).
5.5.2 Semi-discrete form of equations

In this subsection, we present the semi-discrete form of all the components of the formulation, including the momentum and mass conservation equations, the gradient-minimizing velocity field, the Allen-Cahn equation and the evolution equation for the material coordinates.

Momentum and mass conservation

Suppose $S_h^v$ and $S_h^p$ denote the space of trial solution such that:

$$S_h^v = \{ v_h \mid v_h \in (H^1(\Omega))^d, v_h = v_D \text{ on } \Gamma_D \},$$

$$S_h^p = \{ p_h \mid p_h \in L^2(\Omega) \},$$

where $(H^1(\Omega))^d$ denotes the space of square-integrable $\mathbb{R}^d$-valued functions with square-integrable derivatives on $\Omega$, $L^2(\Omega)$ is the space of the scalar-valued functions that are square-integrable on $\Omega$ and $\Gamma_D$ represents the Dirichlet boundaries with the value of $v_D$. Similarly, we define $V_h^\psi$ and $V_h^q$ as the space of test functions such that:

$$V_h^\psi = \{ \psi_h \mid \psi_h \in (H^1(\Omega))^d, \psi_h = 0 \text{ on } \Gamma_D \},$$

$$V_h^q = \{ q_h \mid q_h \in L^2(\Omega) \}. $$

The variational statement of the momentum and mass conservation equations can be written as:

find $[v_h^{n+1}, p_h^{n+1}] \in S_h^v \times S_h^p$ such that $\forall [\psi_h, q_h] \in V_h^\psi \times V_h^q$,

$$\int_\Omega \rho(\phi_h^{n+\alpha})(\partial_t v_h^{n+\alpha} + v_h \cdot \nabla v_h) \cdot \psi_h d\Omega + \int_\Omega \sigma_h(\phi_h^{n+\alpha}) : \nabla \psi_h d\Omega$$

$$+ \sum_{e=1}^{n_e} \int_{\Omega_e} \frac{\tau_m}{\rho(\phi_h^{n+\alpha})} (\rho(\phi_h^{n+\alpha}) v_h \cdot \nabla \psi_h + \nabla q_h) \cdot \mathcal{R}_m d\Omega^e$$

$$+ \int_\Omega q_h (\nabla \cdot v_h) d\Omega + \sum_{e=1}^{n_f} \int_{\Omega_e} \nabla \cdot \psi_h \tau_c \rho(\phi_h^{n+\alpha}) \mathcal{R}_c d\Omega^e$$

$$= \int_\Omega b(\phi_h^{n+\alpha}) \cdot \psi_h d\Omega + \int_{\Gamma_W} h \cdot \psi_h d\Gamma,$$  

(5.34)
where $A : B = A_{i,j} B_{i,j}$. $R_m$ and $R_c$ denote the element-wise residuals of the momentum and mass conservation equations respectively, $n_{el}$ is the number of elements and $\Gamma_H$ represents the Neumann boundaries with fluxes of $h$. In Eq. (5.34), the terms in the first line represent the Galerkin projection of the momentum conservation equation in the test function space $\psi_h$ and the second line comprises of the Petrov-Galerkin stabilization term for the momentum conservation equation. The third line denotes the Galerkin projection and stabilization terms for the mass conservation equation. The terms in the last line are the Galerkin projection of the body force and the Neumann boundary condition. The stabilization parameters $\tau_m$ and $\tau_c$ in Eq. (5.34) are given by [52, 102]:

$$
\tau_m = \left( \frac{2}{\Delta t} \right)^2 + v_h \cdot G_v h + C_I \left( \frac{\mu(\phi)}{\rho(\phi)} \right)^2 G : G \right)^{-1/2}, \\
\tau_c = \frac{1}{\mathrm{tr}(G) \tau_m}, 
$$

where $C_I$ is a constant derived from the element-wise inverse estimates [103], $G$ is the element contravariant metric tensor and $\mathrm{tr}(G)$ is the trace of the contravariant metric tensor. This stabilization in the variational form circumvents the Babuška-Brezzi condition which needs to be satisfied by any standard mixed Galerkin method [104].

**Gradient-minimizing velocity field**

For the gradient-minimizing velocity field, we define the space of trial solution $S^h_w$ and test functions $V^h_\psi$ as:

$$
S^h_w = \{ w_h \mid w_h \in (H^1(\Omega))^d, w_h = w_D \text{ on } \Gamma_D^w \}, \\
V^h_\psi = \{ \psi_h \mid \psi_h \in (H^1(\Omega))^d \},
$$

where $\Gamma_D^w$ denotes the Dirichlet boundaries for the GMV with the boundary value of $w_D$. The variational statement of constructing the gradient-minimizing velocity
field can be written as: find $w_h(t^{n+\alpha}) \in \mathcal{S}^h_w$ such that $\forall \psi_h \in \mathcal{V}^h_\psi$

\[
\int_\Omega \alpha \left( \phi_h^{n+\alpha} w_h - \phi_h^{n+\alpha} \cdot \psi_h \right) d\Omega + \int_\Omega (1 - \alpha \phi_h^{n+\alpha}) \left( - \varepsilon \nabla \phi_h^{n+\alpha} \cdot \nabla w_h \right) \cdot \psi_h d\Omega \\
+ \int_\Omega (1 - \alpha \phi_h^{n+\alpha}) \frac{\varepsilon}{2\sqrt{2}} \nabla w_h : \nabla \psi_h d\Omega = 0.
\]

(5.38)

Note that the generalized-\(\alpha\) method does not apply to this elliptic equation. Instead, the equation for the GMV is solved via Newton-Raphson sub-iterations until convergence within every nonlinear iteration. The constructed GMV is subsequently passed to the Allen-Cahn equation.

**Allen-Cahn equation**

Suppose $\mathcal{S}^h_\phi$ and $\mathcal{V}^h_\psi$ denote the space of trial solution and test functions such that:

\[
\mathcal{S}^h_\phi = \{ \phi_h | \phi_h \in H^1(\Omega), \phi_h = \phi_D \text{ on } \Gamma^0_D \},
\]

(5.39)

\[
\mathcal{V}^h_\psi = \{ \psi_h | \psi_h \in H^1(\Omega), \psi_h = 0 \text{ on } \Gamma^0_D \},
\]

(5.40)

where $\Gamma^0_D$ denotes the Dirichlet boundaries for the order parameter with boundary value of $\phi_D$. The variational statement of the Allen-Cahn equations can be written as: find $\phi_h(t^{n+\alpha}) \in \mathcal{S}^h_\phi$ such that $\forall \psi_h \in \mathcal{V}^h_\psi$ for the Allen-Cahn equation:

\[
\int_\Omega \left( \partial_t \phi_h^{n+\alpha} + \psi_h \left( w_h^{n+\alpha} \cdot \nabla \phi_h \right) + \gamma(t^{n+\alpha}) \left( \nabla \psi_h \cdot (\hat{k} \nabla \phi_h) + \psi_h \hat{s} \phi_h - \psi_h \hat{f} \right) \right) d\Omega \\
+ \sum_{e=1}^{n_{\text{el}}} \int_{\Omega_e} \left( w_h^{n+\alpha} \cdot \nabla \psi_h \right) \tau_\phi \mathcal{R}_\phi d\Omega_e = 0,
\]

(5.41)

where $w$, $\hat{k}$, $\hat{s}$ and $\hat{f}$ are the GMV, the modified diffusion coefficient, modified reaction coefficient and modified source respectively which are defined in [93]. $\mathcal{R}_\phi$ denotes the element-wise residuals for the Allen-Cahn equation with the GMV $w$ and time-dependent mobility $\gamma(t^{n+\alpha})$. The implementation details of the time-dependent mobility model can be found in [116]. In Eq. (5.41), the first line is the Galerkin projection of the transient, convection, diffusion, reaction and source terms, the second line represents the Petrov-Galerkin stabilization terms where the
stabilization parameters \( \tau \) are given by \([52, 102]\):

\[
\tau = \left( \frac{2}{\Delta t} \right)^2 + w_h \cdot Gw_h + 9k^2G:G + s^2 \right)^{-1/2}.
\] (5.42)

**Evolution of the left Cauchy-Green tensor**

Similarly, we define the space of trial solution \( \mathcal{S}^h \) and test functions \( \mathcal{V}^h \) as:

\[
\mathcal{S}^h = \{ B_h \mid B_h \in (H^1(\Omega))^d \},
\] (5.43)

\[
\mathcal{V}^h = \{ \psi_h \mid \psi_h \in (H^1(\Omega))^d \}.
\] (5.44)

The variational statement of the Cauchy-Green tensor can be written as: find \( B_h(t_{n+\alpha}) \in \mathcal{S}^h \) such that \( \forall \psi_h \in \mathcal{V}^h \)

\[
\int_\Omega \left( \partial_t B_h^{n+\alpha} + \alpha(\phi^{n+\alpha})(\nabla B_h - \nabla v_h^{n+\alpha} B_h - B_h(\nabla v_h^{n+\alpha})^T) : \psi_h \right) d\Omega
\]

\[
+ \sum_{e=1}^{n_{el}} \int_{\Omega^e} \tau_B \left( (v_h^{n+\alpha} \cdot \nabla) \psi_h \right) : \mathcal{R}_B d\Omega^e = 0,
\] (5.45)

where \( \mathcal{R}_B \) denotes the element-wise residuals for the evolution equation of the left Cauchy-Green tensor. In Eq. (5.45), the first line is the Galerkin projection, the second line represents the Petrov-Galerkin stabilization term. The stabilization parameter is selected as \( \tau_B = \left( (2/\Delta t)^2 + v_h^{n+\alpha} \cdot Gv_h^{n+\alpha} \right) \).

**5.5.3 Linearization of the solid stress**

We employ Newton-Raphson iterations to find the solution of the momentum conservation equation. Therefore, the residuals and directional derivatives associated with the solid stress are needed. While the discretizations of the hydrostatic pressure and viscous terms are quite standard, the shear components \( \mu_s L (B - I) \), as a function of the left Cauchy-Green tensor, need to be handled carefully. In the calculation of the residuals associated with the left Cauchy-Green tensor, \( B_{h}^{n+\alpha} \) is directly used. The directional derivatives are calculated following \([55]\), where
\( B_h^{n+\alpha} \) is written as a function of the velocity utilizing the evolution equation of the left Cauchy-Green tensor. Hence, the Jacobian terms can be derived naturally. Furthermore, the momentum conservation equation and the evolution equation of the left Cauchy-Green tensor are decoupled with this treatment. According to the generalized-\( \alpha \) discretization, the left Cauchy-Green tensor at \( t^{n+\alpha} \) can be derived as:

\[
B^{n+\alpha} = B^n + \alpha (B^{n+1} - B^n),
\]

\[
= B^n + \alpha \Delta t \left( \partial_t B^n + \zeta \left( \partial_t B^{n+1} - \partial_t B^n \right) \right),
\]

\[
= B^n + \alpha \Delta t \left( \partial_t B^n + \frac{\zeta}{\alpha_m} \left( \partial_t B^{n+\alpha_m} - \partial_t B^n \right) \right),
\]

\[
= B^n + \alpha \Delta t \left( 1 - \frac{\zeta}{\alpha_m} \right) \partial_t B^n + \frac{\zeta}{\alpha_m} \partial_t B^{n+\alpha_m}. \tag{5.46}
\]

Note that Eq. (5.46) is merely used for the derivation of the Jacobian matrix rather than the calculation of the residuals. To eliminate \( \partial_t B^{n+\alpha_m} \), we consider the evolution equation of the left Cauchy-Green tensor:

\[
\partial_t B^{n+\alpha_m} = \phi^{n+\alpha} \left( -(v^{n+\alpha} \cdot \nabla) B^{n+\alpha} + \nabla v^{n+\alpha} B^{n+\alpha} + B^{n+\alpha} (\nabla v^{n+\alpha})^T \right). \tag{5.47}
\]

The Jacobian terms can be calculated as:

\[
\frac{\delta B^{n+\alpha}}{\delta v^{n+\alpha}} = \alpha (\phi^{n+\alpha}) \frac{\alpha \zeta \Delta t}{\alpha_m} \left( -(N \cdot \nabla) B^{n+\alpha} + \nabla N B^{n+\alpha} + B^{n+\alpha} (\nabla N)^T \right), \tag{5.48}
\]

where \( N \) is a vector composed of the shape functions.

To avoid confusions arise from the tensor notation, the component form of the residuals and Jacobian terms associated with the solid stress is shown in Appendix C. Lastly, the residuals and Jacobian terms of the stress via phase-dependent interpolation in the unified momentum conservation equation can be derived as:

\[
\sigma = \phi \sigma^s + (1 - \alpha(\phi)) \sigma^f, \tag{5.49}
\]

\[
\frac{\delta \sigma}{\delta v} = \alpha(\phi) \frac{\delta \sigma^s}{\delta v} + (1 - \alpha(\phi)) \frac{\delta \sigma^f}{\delta v}. \tag{5.50}
\]
5.5.4 Implementation details

In this subsection, we present the implementation details of our variational framework. The fully Eulerian FSI framework is decoupled and solved in a partitioned-block iterative manner which leads to flexibility and ease in its implementation to existing variational solvers. The root finding process of each block employs the Newton-Raphson method, which can be expressed in terms of the solution increments of the velocity, the pressure, the order parameter and the left Cauchy-Green tensor ($\Delta u, \Delta p, \Delta \phi$ and $\Delta B$ respectively). We start with the increment of the velocity and pressure:

\[
\begin{bmatrix}
K_{\Omega} & G_{\Omega} \\
-G_{\Omega}^T & C_{\Omega}
\end{bmatrix}
\begin{bmatrix}
\Delta v \\
\Delta p
\end{bmatrix} = -\begin{bmatrix}
\mathcal{R}_m \\
\mathcal{R}_c
\end{bmatrix},
\tag{5.51}
\]

where $K_{\Omega}$ is the stiffness matrix of the momentum conservation equation consisting of transient, convection, viscous and Petrov-Galerkin stabilization terms, $G_{\Omega}$ is the gradient operator, $G_{\Omega}^T$ is the divergence operator for the mass conservation equation and $C_{\Omega}$ is the stabilization term for the cross-coupling of pressure terms. $\mathcal{R}_m$ and $\mathcal{R}_c$ represent the weighted residuals of the variational forms of the momentum and mass conservation equations. The updated velocity is used to construct the gradient-minimizing velocity field. Noting that the governing equation of GMV is an elliptic PDE, the generalized-$\alpha$ method is not applied. We solve the elliptic equation of GMV for multiple sub-iterations within the nonlinear iteration until convergence is reached:

\[
\begin{bmatrix}
K_w
\end{bmatrix}
\begin{bmatrix}
\Delta w
\end{bmatrix} = -\begin{bmatrix}
\mathcal{R}(w)
\end{bmatrix},
\tag{5.52}
\]

where $K_w$ is the stiffness matrix for the construction equation of GMV and $\mathcal{R}(w)$ is the weighted residual of the governing equation of GMV. After that, the constructed GMV is passed to the Allen-Cahn equation:

\[
\begin{bmatrix}
K_{\phi}
\end{bmatrix}
\begin{bmatrix}
\Delta \phi
\end{bmatrix} = -\begin{bmatrix}
\mathcal{R}(\phi)
\end{bmatrix},
\tag{5.53}
\]

\[
\tag{5.54}
\]
where $K_\phi$ and $R(\phi)$ are the stiffness matrix and the weighted residual of the Allen-Cahn equation. Lastly, we evolve of the left Cauchy-Green tensor:

$$
\begin{bmatrix}
K_B \\
\end{bmatrix}
\begin{bmatrix}
\Delta B \\
\end{bmatrix}
= -\left\{R(B)\right\},
$$

(5.55)

where $K_B$ and $R(B)$ are the stiffness matrix and the weighted residual of the evolution equation for the left Cauchy-Green tensor. This finishes one nonlinear iteration. The nonlinear iteration stops when the ratio between the $L^2$ norm of the increment and the current solution is less than $5 \times 10^{-4}$ for all the blocks, or the nonlinear iteration number exceeds the upper limit, which is set as 10 in the current work.

## 5.6 Test cases

In this section, we examine the accuracy and robustness of the IGP method in cases with increasing complexity. We first demonstrate the interface and geometry-preserving effect of the IGP method with the convection of circular and square interfaces in a prescribed velocity field. After that, we verify our fully Eulerian FSI framework with the deformation of a solid block under lid-driven cavity flow. We then highlight the geometry-preserving effect in FSI problems with the case of channel flow passing a fixed deformable block. Finally, we consider the cylinder-flexible plate problem to showcase the framework for the unsteady FSI problems. The international system of unit is used in all the cases by default.

### 5.6.1 Convection of square and circular interfaces

In this subsection, we demonstrate the interface and geometry-preserving effect of the IGP method. The evolution of circular and square interfaces is considered because they cover the geometries of a planar interface, curved interface and sharp corner, which can serve as building blocks for complex geometries. To quantitatively specify the convection and distortion of the interfaces, the velocity is prescribed such that the interfaces are thickened in the $X$-direction and thinned in the $Y$-direction.

The computational domain is defined as $[0, 2] \times [0, 1.5]$. We first examine a
circular interface, the order parameter field of which is initialized as:

\[ \phi(x, y) = \tanh \left( \frac{R - \sqrt{(x-x_c)^2 + (y-y_c)^2}}{\sqrt{2}\epsilon} \right), \]  

(5.56)

where \( R = 0.25 \) and \((x_c, y_c) = (0.5, 0.85)\) are the radius and the center of the circular interface given by \( \phi = 0 \). The circular interface is convected in an incompressible velocity field \( v_x = x, v_y = -y \). In this velocity field, the location of the interface can be calculated analytically by solving ordinary differential equations \( dx/dt = v \).

In the \( X \)-direction, the velocity gradient \( \partial v_x / \partial x = 1 > 0 \), which means that the relative velocity between the isolines of the order parameter is positive. Therefore, the isolines will move far away from each other and the diffuse interface region is thickened in the \( X \)-direction. Similarly, due to the negative velocity gradient in the \( Y \)-direction \( \partial v_y / \partial y = -1 < 0 \), the diffuse interface region is thinned in the \( Y \)-direction. The zero Neumann boundary condition is used for \( \phi \) and \( w \) on all the boundaries. To visualize the resulting interface distortion due to the convection, we use \( \phi = \delta \) and \( \phi = -\delta \) to illustrate the diffuse interface region with \( \delta = 0.9 \).

The interface is convected until \( t = 0.8 \). The diffuse interface region at the initial and last time steps are plotted in Fig. 5.4 (a). With the same setup, the interface distortion of a square interface whose diagonal points of \( \phi = 0 \) are initially located at \((0.25, 0.6)\) and \((0.75, 1.1)\) are shown in Fig. 5.4 (b).

**Comparison between IP method and IGP methods**

We solve the problems numerically with the IP method, where the original velocity \( v \) is used in the Allen-Cahn equation, and the IGP method, where the constructed velocity \( w \) is employed. The diffuse interface parameters are selected as \( \epsilon = 0.02 \) and \( \eta = 0.1 \). The computational domain is discretized with a structured triangular mesh, the size of which is taken as \( h = 0.02 \). The time step is taken as \( \Delta t = 0.002 \). The diffuse interface regions of the circular and square interfaces calculated from the IP method and the IGP method are shown in Fig. 5.5 (a) and (b). The time histories of the mobility coefficient are plotted in Fig. 5.5 (c) and (d), respectively.

As shown in Fig. 5.5 (a) and (b), in the pure convection cases, the diffuse interface regions are thickened and thinned in \( X \)- and \( Y \)-directions, respectively. In
Figure 5.4: The interface distortion of the circular and square interfaces in the velocity field $v_x = x, v_y = -y$ until $t = 0.8$. The diffuse interface region is shown as the space between $\phi = 0.9$ (solid line) and $\phi = -0.9$ (dashed line).

contrast, both the IP and IGP methods can maintain the thickness of the diffuse interface region for both the circular and square interfaces. While the geometry-preserving effect of the IGP method is not obvious in the circular interface case, it is shown clearly in the square interface case. Because in the latter case, the sharp corners lead to significant differences between the local curvature and the average curvature along the interface, thus larger volume-conserved mean curvature flow. Quantitatively, we can measure the reduction of the volume-conserved mean curvature flow by the mobility coefficient ($\kappa \gamma(t) \epsilon^2 (\kappa - \bar{\kappa}) n$). As seen in Fig. 5.5 (c) and (d), reductions at factors of around 5 and 9 are attained in the mobility coefficient through the IGP method.

Spatial and temporal convergence study

We then inspect the spatial and temporal convergence of the numerical discretization for the IGP method. The numerical error is quantified through the $L^2$ error of the order parameter field over the entire domain at $t = 0.8$. The $L^2$ error is calculated as:

$$e_2 = \frac{||\phi - \phi_{ref}||_2}{||\phi_{ref}||_2}.$$  \hspace{1cm} (5.57)
Figure 5.5: Diffuse interface regions at $t = 0.8$ given by purely convection, the IP method and the IGP method in the convection of circular and square interfaces, and the corresponding time histories of the mobility coefficient for quantifying the volume-conserved mean curvature flow.

where $\phi$ is the solution vector of the order parameter at $t = 0.8$, $\phi_{\text{ref}}$ is the solution vector from the finest resolution, and $\| \cdot \|_2$ is the $L^2$ norm. Both $\phi$ and $\phi_{\text{ref}}$ are interpolated to the coarsest mesh to have the same dimension. The diffuse interface parameters are selected as $\varepsilon = 0.02$ and $\eta = 0.1$. In the mesh convergence study, we vary the grid size from $h/\varepsilon = 4/3$ to $h/\varepsilon = 4/7$ corresponding to around 3 to 7 elements across the diffuse interface region. For temporal convergence study, we keep the grid size at $h/\varepsilon = 1$ and bisect the time step from $\Delta t = 0.008$ to $\Delta t = 0.001$. As shown in Fig. 5.6, the current spatial and temporal discretization are both second-order accurate.
5.6.2 Deformation of a solid block under lid-driven cavity flow

In this subsection, we consider the deformation of an elastic solid block under lid-driven cavity flow for the verification of the fully Eulerian FSI framework. In the benchmark case, the geometry of the interface is close to a planar interface. The volume-conserved mean curvature flow is almost negligible. Therefore while the GMV is used for the order parameter, the geometry-preserving effect is not discussed. To be consistent with the work of [124, 125], the convection term in the momentum conservation equation is omitted. A rectangular computational domain \([0, 2] \times [0, 2]\) is considered in this problem. The order parameter field representing the solid block is given by \(\phi(x, y, 0) = -\tanh \left( \frac{(y - T)}{\sqrt{2} \epsilon} \right)\), where \(T = 0.5\) is the height of the solid block. The no-slip boundary condition is applied on the left, right and bottom boundaries. A prescribed velocity in the X-direction is applied on the top boundary to drive the lid-driven cavity flow which deforms the solid block:

\[
v_x(x, 2) = 0.5 \begin{cases} 
\sin^2(\pi x/0.6), & x \in [0, 0.3], \\
1, & x \in [0.3, 1.7], \\
\sin^2(\pi(x - 2)/0.6), & x \in [1.7, 2.0]. 
\end{cases}
\]
The pressure at the right bottom corner is set to be zero. The order parameter $\phi$ is kept as its initial value on all the boundaries. The value of $w$ is assigned as 0 at all the boundaries. The left Cauchy-Green tensor $B$ is evolved in the entire computational domain with the zero Neumann boundary condition on all the boundaries. The densities of the solid and the fluid are selected as $\rho^s = 1$, $\rho^f = 1$. The dynamic viscosity of the fluid is chosen as $\mu^f = 0.2$. The shear modulus and the viscosity of the solid are taken as $\mu_s^s = 0.2$ and $\mu^s = 0$. The problem setup is illustrated in Fig. 5.7.

**Figure 5.7:** Schematic diagram of an elastic solid block under lid-driven cavity flow.

**Mesh convergence study**

We first conduct a systematic mesh convergence study for our fully Eulerian FSI framework employing the IGP method. The interface thickness parameter is selected as $\varepsilon = 0.04$. The RMS interface distortion parameter is taken as $\eta = 0.1$. The computational domain is discretized with a uniform structured triangular mesh. The grid size is bisected from $h/\varepsilon = 1$ to $h/\varepsilon = 1/4$. For $h/\varepsilon = 1/8$, the structured mesh is only used between $y = 0.4$ and $y = 0.6$ with unstructured mesh covering the rest of the computational domain. The time step is chosen as $\Delta t = 0.005$ and
the solution at $t = 20$ is used for the analysis. The resulting interface locations are shown in Fig. 5.8 (a). To demonstrate the order of convergence for the current framework, we quantify the error as discussed in Eq. (5.57). The results in Fig. 5.8 (b) illustrate the second-order accuracy. The difference between the current solution and the reference is due to the lack of convergence in the diffuse interface model.

**Figure 5.8**: Mesh convergence study for the deformation of a solid block under lid-driven cavity flow: (a) interface position, and (b) relative $L^2$ error of the order parameter field.

**Sensitivity study of diffuse interface model**

After the mesh convergence study, we perform a sensitivity study for the diffuse interface model. In the phase-field diffuse interface method, the diffuse interface profile should be close to the hyperbolic tangent profile so that the transition of physical properties across the diffuse interface region is uniform. Furthermore, the thickness of the diffuse interface region should be small compared to the bulk region such that the sharp jump in the physical properties across the fluid-solid interface can be properly represented. Moreover, the volume-conserved mean curvature flow should be small enough so that the geometry of the interface is not severely disturbed. We consider the satisfaction of the aforementioned conditions as the desensitization of the physical problem to the diffuse interface model. Next, we discuss how this can be achieved by scaling down $\varepsilon$ and $\eta$ proportionally in the
current IGP method.

We first consider a group of diffuse interface parameters $\eta_0$ and $\varepsilon_0$ for the flow field velocity $v$. The interface distortion is controlled by $\eta_0$. The volume-conserved mean curvature flow is given by:

$$v_{\kappa_0}(v) = \frac{1}{\eta_0} \mathcal{F} \left( \left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_0} \right) \varepsilon_0^2 (\kappa - \overline{\kappa}) n. \quad (5.58)$$

Now we consider the diffuse interface parameters $\eta_1 = (1/2) \eta_0$, $\varepsilon_1 = (1/2) \varepsilon_0$. The convergence of the interface profile is relatively straightforward. The interface distortion is proportional to $\eta$. For example, since $\eta_1 = (1/2) \eta_0 < \eta_0$, the interface distortion is decreased at $\eta_1$. Similarly, we denote the characteristic size of the solid bulk as $L$. Since $\varepsilon_1/L = (1/2) \varepsilon_0/L < \varepsilon_0/L$, the diffuse interface model converges towards the shape interface limit. For the volume-conserved mean curvature flow, the current velocity can be derived as:

$$v_{\kappa_1}(v) = \frac{1}{\eta_1} \mathcal{F} \left( \left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_1} \right) \varepsilon_1^2 (\kappa - \overline{\kappa}) n. \quad (5.59)$$

Note that in FSI problems, the physical properties vary rapidly across the diffuse interface region, which leads to large velocity gradients. As we reduce the interface thickness by $\varepsilon_1 = (1/2) \varepsilon_0$, the transition in physical properties happen in a shorter distance. The resulting velocity change occurs in a shorter distance as well, which leads to increased velocity gradients. We approximate this increment through:

$$\left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_1} \approx 2 \left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_0}. \quad (5.60)$$

Substituting $\eta_1 = (1/2) \eta_0$, $\varepsilon_1 = (1/2) \varepsilon_0$ and $\left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_1} \approx 2 \left| \frac{\partial v_n}{\partial n} \right|_{\varepsilon_0}$ into Eq. (5.59), we have:

$$v_{\kappa_1}(v) \approx v_{\kappa_0}(v). \quad (5.61)$$

Now we consider the gradient-minimizing velocity field $w$. Since $w$ is a constructed velocity field based on the solid velocity, which is independent of the
transition at the fluid-solid interface, we can expect:

\[
\left| \frac{\partial w_n}{\partial n} \right|_{\eta_1} \approx \left| \frac{\partial w_n}{\partial n} \right|_{\eta_0},
\]

(5.62)

Substituting \( \eta_1 = (1/2)\eta_0, \varepsilon_1 = (1/2)\varepsilon_0 \) and \( |\partial w_n/\partial n|_{\eta_1} \approx |\partial w_n/\partial n|_{\eta_0} \), we have:

\[
v_{x_1}(w) \approx (1/2)v_{x_0}(w) \leq v_{x_0}(w),
\]

(5.63)

where the reduction of the volume-conserved mean curvature flow is realized. Together with the interface profile convergence ensured by \( \eta_1 \leq \eta_0 \), and the convergence towards the sharp interface limit ensured by \( \varepsilon_1/L < \varepsilon_0/L \), the desensitization from the diffuse interface model is further accomplished via the refinement approach of scaling down \( \eta \) and \( \varepsilon \) simultaneously with the same factor.

As discussed above, in the current sensitivity study, we bisect \( \eta \) and \( \varepsilon \) simultaneously from \( \eta_0 = 0.1, \varepsilon_0 = 0.04 \) to \( \eta_3 = 0.00125, \varepsilon_3 = 0.005 \), where the subscripts denote the times of bisection. The meshes are refined accordingly to maintain the interface resolution as \( h/\varepsilon = 1 \). The time step is selected as \( \Delta t = 0.005 \) and the solution at \( t = 20 \) is analyzed. The converged interface position is shown in Fig. 5.9, which matches well with the reference data.

5.6.3 Channel flow passing a fixed deformable block

In this subsection, we examine the interface-preserving effect in the case of channel flow passing a fixed deformable block, which involves interface with sharp corners and severe convective distortion. The computational domain \([0,2.5] \times [0,0.4]\) is considered for the case. The diagonal points of the rectangular block are located at \((0.2, 0)\) and \((0.3, 0.2)\). The bottom of the block is fixed at the wall. The order parameter field representing the block is initialized by calculating the signed distance to the left, top and right boundaries of the block \( d \) (the bottom boundary is not included because there is no fluid-solid interface). Then \( d \) is composed by a hyperbolic tangent function, which results in \( \phi(x,0) = \tanh(d/\sqrt{2}\varepsilon) \). An inflow velocity is prescribed at the left boundary, whose \( X \)-component is prescribed as a
Figure 5.9: Convergence of the diffuse interface model in the deformation of a solid block under lid-driven cavity flow. The subscripts denote the times of bisection ($\eta_n = (1/2)^n \eta_0, \epsilon_n = (1/2)^n \epsilon_0$).

The parabolic function with ramping in time:

\[
v_x(0,y,t) = \begin{cases} 
0.5 (1 - \cos(2\pi t)) y(H - y)/(0.5H)^2, & t \leq 0.5, \\
y(H - y)/(0.5H)^2, & t > 0.5, 
\end{cases}
\]

(5.64)

where $H = 0.4$ represents the height of the computational domain. While the no-slip boundary condition is specified on the top and bottom boundaries, an outflow boundary condition is applied on the right boundary with a reference pressure $p = 0$ at the right bottom corner. The order parameter $\phi$ is kept as its initial value on all the boundaries. The value of $w$ is assigned as $0$ on the bottom wall, while the zero Neumann boundary condition is used for the rest of the boundaries. The left Cauchy-Green tensor $B$ is evolved in the entire computational domain with the zero Neumann condition on all the boundaries. The densities of the solid and the fluid are chosen as $\rho^s = 1000, \rho^f = 1000$, the dynamic viscosity of the fluid is $\mu^f = 1$, the shear modulus and the viscosity of the solid are $\mu^s_L = 2 \times 10^6$ and $\mu^s = 0$ respectively. A marker is placed at the midpoint of the top boundary of the block to quantify the displacement. To avoid the influence of the fluid velocity, the marker is set inside the solid domain at $(0.25, 0.2 - 2\epsilon)$. The marker is convected explicitly.
with the velocity of $v^{n+\alpha}$ at every time step. The problem setup is illustrated in Fig. 5.10 (a).

![Figure 5.10: Channel flow passing a fixed deformable block: (a) schematic diagram showing the computational domain, and (b) structured finite element mesh covering the block and the surrounding unstructured mesh.](image)

**Comparison between the IP method and the IGP method**

To begin with, we perform a comparison between the IP method and the IGP method. The diffuse interface parameters are selected as $\varepsilon = 0.01$ and $\eta = 0.1$. The computational domain near the block $[0.15, 0.4] \times [0, 0.25]$ is discretized with a structured triangular mesh at the size of $h/\varepsilon = 1$, while the rest of the computational domain is discretized with an unstructured triangular mesh. The mesh is illustrated in Fig. 5.10 (b). The time step is selected as $\Delta t = 0.005$. The diffuse interface regions at $t = 5$ are shown in Fig. 5.11 (a), and the time histories of the mobility coefficient are depicted in Fig. 5.11 (b). As observed, the IGP method preserves the geometry of the block substantially. The mobility coefficient, which is proportional to the volume-conserved mean curvature flow, is reduced at around two orders of magnitude.

**Spatial and temporal convergence study**

We then perform a systematic numerical convergence study for this problem. The diffuse interface parameters are selected as $\eta = 0.0025$ and $\varepsilon = 0.025$. The mesh size varies from $h/\varepsilon = 4/3$ to $h/\varepsilon = 4/6$ corresponding to around 3 elements to 6 elements across the diffuse interface region. The time steps are bisected from
$\Delta t = 0.04$ to $\Delta t = 0.005$. The $X$-displacement of the marker point is used for the comparison. The spatial and temporal convergence study are shown in Fig. 5.12. As shown in the figure, the improvements from refining the mesh and time step below $h/\varepsilon = 1$ and $\Delta t = 0.005$ are not significant. Therefore these two values are considered as the converged discretization parameters.
Sensitivity study of diffuse interface model

We next turn our attention to the sensitivity to the diffuse interface model. In the current study, we bisect $\eta$ and $\varepsilon$ simultaneously from $\eta_0 = 0.01$, $\varepsilon_0 = 0.1$ to $\eta_3 = 0.00125$, $\varepsilon_3 = 0.0125$, where the subscripts denote the times of bisection. The meshes are refined accordingly to maintain the interface resolution around the block as $h/\varepsilon = 1$. The time step is taken as $\Delta t = 0.005$ and the solution at $t = 5$ is analyzed. The same problem is solved by employing a monolithic ALE solver [126], with an implementation of the incompressible neo-Hookean constitutive model. In the simulation with the monolithic ALE solver, the solid is discretized with a structured triangular mesh at the size of $h = 0.01$ and the time step is chosen as $\Delta t = 0.01$. The resulting convergence and comparison of the interface position represented by $\phi = 0$ are shown in Fig. 5.13 (a). The convergence of the $X$-displacement of the marker points is shown in Fig. 5.13 (b). As observed, with the reduction of $\varepsilon$ and $\eta$, the solution converges and the converged solution closely matches the result from the monolithic ALE solver. It is worth noting that the reduction in $\varepsilon$ gives two benefits: (i) sharpening the diffuse interface and reducing the curvature flow as discussed earlier, and (ii) restricting the oscillation of $B$ caused by its evolution in the fluid domain to a smaller region, which improves the accuracy of the stress field in the bulk of the solid. The block depicted by $\phi > 0$ and the flow field velocity $v_x$ at $t = 5$ in the finest case are shown in Fig. 5.14. In the contour, we can observe that the flow is blocked by the solid and squeezes through the top gap, which forms a high-velocity region. The negative velocity behind the block shows the formation of a recirculation zone.

Large deformation solutions

Next, we demonstrate the channel flow passing a fixed deformable block with larger deformations due to reduced shear modulus. To further eliminate the instability caused by the evolution of $B$ in the fluid domain, we truncate the evolution at nodes where $\phi < -0.95$. This is realized by using a truncated phase-dependent interpolation: $\alpha(\phi) = \frac{1+\phi}{2}H(\phi + 0.95)$, where $H$ denotes the heaviside function. At the same time, the left Cauchy-Green tensor on these nodes is reset as $B = I$. The solid viscosity is selected as $\mu^s = 1$. The shear modulus of $\mu^s_L = 2 \times 10^5$.
Figure 5.13: Convergence of the diffuse interface model in the channel flow passing a fixed deformable block. The subscripts denote the times of bisection \((\eta_n = (1/2)^n\eta_0, \epsilon_n = (1/2)^n\epsilon_0)\): (a) interface position represented by \(\phi = 0\), and (b) time histories of the X-displacement of the marker point.

and \(\mu_s^L = 2 \times 10^4\) are examined. The diffuse interface parameters are selected as \(\epsilon = 0.0025\) and \(\eta = 0.025\). \(h/\epsilon = 1\) and \(\Delta t = 0.005\) are used for the numerical discretization. The interface position given by \(\phi = 0\) and the time histories of the X-displacement of the marker point are shown in Fig. 5.15 (a) and (b) respectively. The block depicted by \(\phi > 0\) and the flow field velocity \(v_x\) at \(t = 5\) are shown in Fig. 5.16.

5.6.4 Application to the cylinder-flexible plate problem

For further demonstration, we consider a cylinder-flexible plate problem, which is modified from the FSI3 case in [127]. The computational domain \([0, 2.5] \times [0, 0.41]\) is considered for the case. The center of the rigid cylinder of radius \(r = 0.05\) is located at \((0.2, 0.2)\). The flexible plate of thickness \(T = 0.02\) and length \(L = 0.35\) is attached in the downstream direction of the rigid cylinder, the right bottom corner of which is located at \((0.6, 0.19)\). The order parameter field representing the plate is initialized by generating the signed distance \(d\) of each grid point to the top, right and bottom boundaries and then calculating \(\phi(x, 0) = \tanh(d/\sqrt{2\epsilon})\). The inflow
velocity at the left boundary is prescribed as a parabolic function with ramping in time, whose $X$-component is given by:

\[
v_x(0, y, t) = \begin{cases} 
0.5 (1 - \cos(2\pi t)) & t \leq 0.5, \\
3.0y(H - y)/(0.5H)^2, & t > 0.5, 
\end{cases}
\]

where $H = 0.41$ represents the height of the computational domain. While the no-slip boundary condition is applied on the top and bottom boundaries, the outflow condition is applied on the right boundary with a reference pressure $p = 0$ at the right bottom corner of the computational domain. The value of $\phi$ is kept the same with the initial condition on all the boundaries. The value of $w$ is assigned as
Figure 5.15: Channel flow passing a fixed block with different shear modulus: (a) interface position represented by $\phi = 0$, and (b) the $X$-displacement of the marker point

0 on the circular cylinder, while the zero Neumann boundary condition is used for the rest of the boundaries. The left Cauchy-Green strain tensor $B$ is evolved in the entire computational domain with the treatment discussed in Section 5.6.3 while zero Neumann conditions are specified on all the boundaries. The densities of the solid and the fluid are chosen as $\rho^s = 1000$ and $\rho^f = 1000$, respectively. The dynamic viscosity of the fluid is taken as $\mu^f = 1$. The shear modulus and viscosity of the solid are selected as $\mu^s = 2 \times 10^6$ and $\mu^s = 1$. A marker initialized at $(0.6 - 2\varepsilon, 0.2)$ is used to quantify the vibration of the plate. The problem setup is illustrated in Fig. 5.17 (a).

We first look into the comparison between the IP method and the IGP method. The diffuse interface parameters are selected as $\varepsilon = 7.5 \times 10^{-4} \times \sqrt{2}$ and $\eta = 0.1 \times \sqrt{2}$. An unstructured triangular mesh locally refined in the region where the flat plate sweeps through is used for the spatial discretization, as shown in Fig. 5.17 (b). The mesh resolution around the plate is selected as $h/\varepsilon = 4/3$. The time step is chosen as $\Delta t = 5 \times 10^{-3}$ and the flow-induced vibration is simulated until $t = 5$. The displacements of the marker point in the $Y$-direction are shown in Fig. 5.18 (a). The time histories of the mobility coefficient are depicted in Fig. 5.18 (b). As
observed, the mobility coefficient is reduced approximately at a factor of two. Note that if one would like to achieve the same amount of reduction in the curvature flow with the IP method by refining the mesh, the grid size needs to be reduced at a factor of two, which can be derived by going through Eqs. (5.58) ∼ (5.61) assuming the same \( \eta \) and \( h/\varepsilon \). The computational cost of this is significantly higher than using the IGP method. In addition, a temporal oscillation can be observed clearly in the time histories of the mobility coefficient. To further examine this oscillation, we plot the normalized mobility coefficient and the normalized \( Y \)-velocity from the IGP method together to analyze their phases in Fig. 5.19. As observed, the \( Y \)-velocity of the plate is in phase with the mobility coefficient and they reach their peaks almost at the same time. This observation is consistent with our idea in Section 5.2 that when the solid bulk moves at a relatively high speed, a significant
convective distortion will be introduced, thus requiring larger mobility to preserve the interface profile.

Lastly, we examine the sensitivity to the diffuse interface model. Starting from $\varepsilon_0 = 7.5 \times 10^{-4} \times \sqrt{2}$ and $\eta_0 = 0.1 \times \sqrt{2}$, we scale down the diffuse interface parameters by a factor of $\sqrt{2}$ until $\varepsilon_2 = 7.5 \times 10^{-4} / \sqrt{2}$ and $\eta_2 = 0.1 / \sqrt{2}$, where the subscripts denote the times of scaling. The meshes are refined accordingly to maintain the interface resolution around the flexible plate as $h/\varepsilon = \ldots$
The time step is chosen as $\Delta t = 5 \times 10^{-3}$ and the vibration is simulated until $t = 5$. The displacement of the marker point in the $Y$-direction is shown in Fig. 5.20. As observed, the results from $\varepsilon_1, \eta_1$ and $\varepsilon_2, \eta_2$ are close to each other, which shows that the solution is insensitive to the diffuse interface model below $\varepsilon_2, \eta_2$. In the converged solution, we consider $t = 4$ to $t = 5$ as the time period where the steady state vibration has reached. The steady-state vibration is further quantified by the neutral position calculated as $(1/2)(\max(u_y) + \min(u_y))$ and the vibration amplitude calculated as $(1/2)(\max(u_y) - \min(u_y))$, which results in $(0.34 \pm 30.3) \times 10^{-3}$. Qualitatively, the predicted vibration is comparable with the reference value $(1.48 \pm 34.38) \times 10^{-3}$ in [127]. The under-predicted vibration amplitude may arise from the increased Poisson’s ratio and viscosity of the solid ($\nu = 0.5, \mu^s = 1$) in the current case compared to the reference case ($\nu = 0.4, \mu^s = 0$). The interaction between the fluid flow and the flexible plate is illustrated through two snapshots at $t = 3.1$ and $t = 3.2$, where the flexible plate is depicted by $\phi > 0$ and the flow field is demonstrated through the contour of $v_x$.

As being a PDE-based technique, the proposed phase-field-based IGP method can be easily extended to three-dimension with parallel implementation. The effectiveness and efficiency of the IGP method have the potential to be improved by reducing the weights of the Dirichlet term in the diffuse interface region and
Figure 5.20: Convergence of the diffuse interface model in the cylinder-flexible plate problem. The subscripts denote the number of times of scaling down by the factor of \(1/\sqrt{2}\). \(\eta_n = (1/\sqrt{2})^n \eta_0, \epsilon_n = (1/\sqrt{2})^n \epsilon_0\). The mesh resolution is kept as three elements across the diffuse interface region by taking \(h = 4/3 \varepsilon\).

Figure 5.21: Cylinder-flexible plate problem: demonstration of the flow field \(v_x\) and the flexible plate depicted by \(\phi > 0\) at (a) \(t = 3.1\), and (b) \(t = 3.2\).

restrict the generation of the GMV near the diffuse interface region, respectively. The generalization of the current method to multiphase and flexible multibody FSI problems needs to be further investigated.
5.7 Summary

In this chapter, we proposed an interface and geometry preserving phase-field method for fully Eulerian FSI problems. The key innovation is to convect the isosurfaces of the order parameter with approximately the same normal velocity in the normal direction such that the convective distortion is reduced. This is achieved by a novel PDE-based construction of an auxiliary gradient-minimizing velocity field. This treatment significantly reduces the time-dependent mobility coefficient associated with free energy minimization in the phase-field formulation. Consequently, there is a lesser volume-conserved mean curvature flow. Furthermore, the GMV is constructed by extending the solid velocity, which excludes the fluid velocity involved in the unified velocity field. Hence the GMV guarantees that the diffuse interface region conforms to the solid bulk. As a result, the description of the fluid-solid interface geometry is substantially improved in geometric details and global conformity behavior in the newly developed IGP formulation. The improvement is demonstrated through the convection of circular and square interfaces, and the channel flow passing a fixed deformable block. Finally, as demonstrated by the cylinder-flexible plate problem, the IGP method is of practical usage for fully Eulerian FSI problems. The proposed IGP method can be employed by other interface-capturing methods, such as the level set method, where the interface region is resolved with around three to four elements. Since the proposed IGP method relies on the partial differential equation, it can be easily extended to three-dimension with parallel implementation for complex geometries.
Chapter 6

Combined multiphase flow and fluid-structure interaction

In this chapter, we present a combined formulation for multiphase flow and fluid-structure interaction using our interface and geometry preserving method for unstructured meshes. We consider a 3D finite element discretization in a general computational domain with given boundary conditions. In practical multiphase FSI problems, solid objects can have complex geometries which cannot be generated through simple analytical expressions. In these cases, the initialization of the hyperbolic tangent profile needs to be achieved in a general and robust manner during the pre-processing stage. Therefore, we first introduce a grid cell based algorithm to initialize the order parameter fields for given discrete interface mesh. With the geometries of the phases readily available, we integrate the techniques developed in Chapters 4 and 5 with multiple order parameters to evolve the interfaces accurately. The resulting order parameters are used to unify the mass and momentum conservation equations via phase-dependent interpolation, hence completing the Eulerian multiphase FSI framework. The capability of the framework is demonstrated for cases of increasing complexity, namely a rotating disk and a sphere in a lid-driven cavity flow, falling and bouncing back of elastic ball, and collision of two elastic balls. Finally, we demonstrate the simulation framework for a simplified situation of ship-ice interaction.
6.1 Background

Multiphase FSI involving the structural dynamics with contact are pervasive in many natural phenomena and engineering applications. Examples include the offshore riser array in proximity [105] and subsea pipelines near the seabed [128] in marine engineering and soft robotics [129].

For real-world applications, multiphase FSI problems can involve solid objects with complex geometries. To perform numerical simulations, the domain and the interface are usually given in a discrete form: the computational domain is discretized by fixed Eulerian mesh, while the interface usually takes the form of a 2D interface mesh from computer-aided design software. In other words, the initialization of the phase-field variable in a 3D Eulerian mesh according a 2D interface mesh is required for the actual implementation. Considering that the Eulerian mesh can have millions of nodes, and the interface mesh is usually at the order of thousands, the efficiency of the calculation is critical.

In addition to the complexity of geometry aspects, the multiphase and multi-physics dynamics give rise to significant challenges in mathematical modeling and numerical simulation. Except for the common issues encountered in two-phase problems, such as the discontinuity of physical properties across the interface and the inherent difference in kinematic descriptions between fluid and solid, specific issues arise from the multiphase nature of the problem. The phases should not overlap each other, nor should they create any void in between. During the interaction between multiphase fluids on the solid interface, the cross-point between the three phases should slide freely along the solid interface. Ideally, contact and bouncing back should occur naturally due to the non-penetration constraint on the surface and the build-up of internal stress without phenomenological models.

In this chapter, we start with the techniques for initializing the order parameter for complex geometries. After that, we bring the techniques introduced in Chapters 4 and 5 together combined with multiple order parameters to form the unified Eulerian variational framework for multiphase FSI. We intend to satisfy the non-penetration condition via dynamics of the continuum field instead of modifying phase-field equations. While the no-void condition is not imposed explicitly, we consider any void space created as a source of dynamics that drives the interface
to move and fill in the gap. The collision between solids is facilitated by a linear interpolation of densities and stresses which relaxes the collision as a gradual process. While a side effect of artificial interface adhesion appears on solid-multiphase fluids intersection points due to the linear interpolation, the error arising from this effect can be reduced by decreasing the diffuse interface thickness parameter. With a parallel finite element implementation using unstructured meshes, we can perform a fully 3D simulation for multiphase FSI problems.

6.2 Initialization of the phase-field variable

In the phase-field diffuse interface description, the order parameter takes the form of a hyperbolic tangent profile. To initialize the hyperbolic tangent profile, we need the signed distance function \( d \) to the target interface. This can be further decomposed into two sub-problems: (i) calculate the distance function to the interface and (ii) decide the sign of the distance according to the relative position of the current location to the interface. In the current work, we adopt a grid cell based method [130] to reduce the computational cost.

6.2.1 Calculation of the distance function

We first introduce the calculation of the distance function. As discussed previously, the variation of the order parameter is highly localized. For example, for points which are \( 3\varepsilon \) away from the interface, \( \phi(d = 3\varepsilon) = 0.9717 \), while \( \phi(d = \infty) = 1 \). At the same time, the phase-field method is inherently energy stable due to the free energy minimization. Therefore, we can safely truncate the calculation of the distance at points that are \( 3\varepsilon \) away from the interface without the concern of inaccuracy or instability, and assign values of \( |d| = 1 \), such that the distance calculation is restricted to positions which are close to the interface.

The algorithm starts by decomposing the domain into a series of grid cells. Then, we identify the grid cells which contain the interface elements and associate these interface elements with the grid cell. Lastly, the calculation of the distance is restricted to the nodes in the grid cell and the associated interface elements.

In dividing the grid cells, we employ the approach of [130]. Denote the coordinates of the Eulerian mesh as \((x_p, y_p, z_p)\) where \(x, y, z\) are the coordinates in the
$X$, $Y$ and $Z$ directions, and the subscript $p = 1, 2, \cdots, n$ denotes the index of the node with $n$ being the total number of nodes. We can define a bounding box for the Eulerian mesh $[x_{\text{min}}, x_{\text{max}}] \times [y_{\text{min}}, y_{\text{max}}] \times [z_{\text{min}}, z_{\text{max}}]$, where $x_{\text{min}} = \min_{p=1,2,\cdots,n} \{x_p\}$ and the rest values are defined in a similar manner. If $n_x, n_y, n_z$ grid cells are needed in each of the directions, the size of the grid cells will be $h_x = (x_{\text{max}} - x_{\text{min}}) / n_x$.

To determine the grid cell index $(i, j, k)$ of a point $(x_p, y_p, z_p)$ where $i, j, k$ are grid cell indices in the $X$, $Y$ and $Z$ directions, one just need to calculate $i = \lfloor x_p / h_x \rfloor$, $j = \lfloor y_p / h_x \rfloor$, $k = \lfloor z_p / h_x \rfloor$, where $\lfloor \cdot \rfloor$ denotes the floor calculation which takes the integer part of a positive real number.

After the division, we need to build up the relevance between the grid cells and the surface elements. For a given surface mesh, we first decompose the surface elements as triangle elements by rewriting the connectivity to unify the calculation for all the surface elements. For each triangle element, we create a bounding box around it and assign the element to the grid cells where the bounding box spans through. For example, for a triangular element with vertices $(x_v, y_v, z_v), v = 1, 2, 3$, we define the bounding box as $[x_{\text{min}}, x_{\text{max}}] \times [y_{\text{min}}, y_{\text{max}}] \times [z_{\text{min}}, z_{\text{max}}]$, where the minimum and the maximum are picked among the three vertices. We further expand the bounding box by $3\varepsilon$, which ends up with $[x_{\text{min}} - 3\varepsilon, x_{\text{max}} + 3\varepsilon] \times [y_{\text{min}} - 3\varepsilon, y_{\text{max}} + 3\varepsilon] \times [z_{\text{min}} - 3\varepsilon, z_{\text{max}} + 3\varepsilon]$ so that all the nodes within $3\varepsilon$ distance from the surface element can be involved. The index of the corresponding grid cells can be denoted as $[i_{\text{min}}, i_{\text{max}}] \times [j_{\text{min}}, j_{\text{max}}] \times [k_{\text{min}}, k_{\text{max}}]$, where $i_{\text{min}} = \lfloor (x_{\text{min}} - 3\varepsilon) / h_x \rfloor$ and rests are defined similarly. The surface elements are then assigned to these grid cells.

Once the grid cells and the associated nodes and surface elements are identified, we can restrict the scope of the calculation to each grid cell. For a given node belonging to the grid cell, the distance to the interface is taken as the shortest $L_2$ distance to the vertices of the surface elements assigned to the current grid cell. After the distance function is acquired, we composite the distance function by hyperbolic tangent function $\phi = \tanh(|d| / \sqrt{2}\varepsilon)$ to form the value of the order parameter field. For grid cells that do not contain any surface elements, we assign the unsigned function value as $\phi = 1$.  

129
6.2.2 Determination of the sign on a node

Following the calculation of the magnitude for the order parameter value, we need to determine the sign on each node according to its relative position to the surface mesh. To be more specific, whether the point is inside or outside the given 2D interface mesh. This is a well-known topic in planar geometry problems which can be solved by the ray-casting algorithm [130]. In short, we cast a semi-infinite ray from the node in the positive X direction. Then, we count how many times the ray crosses the surface. Once the ray crosses the surface, the cross number shifts between even and odd. Accordingly, we know that the point is located inside/outside the interface according to the odd/even cross number.

With the domain decomposition as grid cells, we can restrict the calculation to the grid cells where the ray passes through. Since the projection in the position X-direction is used, for a node \((x_p, y_p, z_p)\) located at grid cell \((i, j, k)\), we only need to consider an array of the grid cells \([i, n_x] \times j \times k\). In the grid cell \((i, j, k)\), only the surface elements with at least one vertex located at the positive X-direction of the node can be crossed by the ray. For triangle surface elements, this condition can be expressed as \(\forall (x_v, y_v, z_v), v = 1, 2, 3, \exists x_v > x_p\). For grid cells \([i+1, n_x] \times j \times k\), all the surface elements need to be considered.

After restricting the scope of computation to the node and these triangle elements, we now need to determine whether the ray crosses these triangle elements or not. We first project the node and the triangle elements to the \(Y-Z\) plane of \(x = x_{\text{max}}, x_{\text{max}} = \max_{p=1,2,\ldots,n} \{x_p\}\). As shown in Fig. 6.1, we denote the area of the projected triangle from the surface element as \(A_0\). The areas of the three triangles, which are formed by the projected node and the projected edges of the triangle element, are denoted as \(A_1, A_2, A_3\), where \(A_i\) denotes the area of the triangle formed by the projected node and the opposite edge of vertex \(v = i\). If the point lies inside the triangle, we have \(A_0 = \sum_{i=1}^{3} A_i\), which indicates that the ray crosses the surface element. For triangle elements that the ray does not cross through, \(A_0 < \sum_{i=1}^{3} A_i\) is satisfied. This is illustrated in Fig. 6.1.

However, the criteria of \(A_0 = \sum_{i=1}^{3} A_i\) can be problematic in implementation. The issue arises from the numerical error introduced in the calculation of the areas,
Figure 6.1: Illustration of ray casting algorithm: conditions for ray (a) crossing and (b) missing the surface element.

which fails to satisfy the equality exactly. Therefore, we relax the condition as:

$$A_1 + A_2 + A_3 - A_0 \leq 2\chi,$$

(6.1)

When the condition is satisfied, we consider that the ray crosses the elements, and the cross number adds one.

The relaxation introduces new errors. For example, as illustrated in Fig. 6.2 (a), where the projected node is close to but located outside the projected triangle element. For all positions where $A_1 \leq \chi$ is satisfied, $A_1 + A_2 + A_3 - A_0 = 2A_1 + A_0 - A_0 \leq 2\chi$ is true. While the ray does not cross the element, the condition is satisfied and falsely adds one to the cross number. A similar situation happens when the ray is close to the vertices. To resolve this repeated counting issue, we classify the cross into three types: element cross, edge cross and node cross. If all the areas $A_1, A_2, A_3$ are larger than $\chi$, the projected node are far away from the edges, and the cross is classified as an element cross. If there exists only one area which is smaller than $\chi$, the cross is classified as an edge cross. If there are two areas that are smaller than $\chi$, the cross is classified as a node cross. These situations are illustrated in Fig. 6.2 (b). Once the cross type is identified, we store the relevant vertex indices. Thus three, two, and one indices are recorded for element cross, edge cross, and node cross, respectively. The cross number adds one only for non-repeated vortex indices combinations, therefore avoiding the repeated counting problem. Finally,
the total cross number equals the summation of these three types of crosses.

![Illustration of ray casting algorithm](image)

**Figure 6.2:** Illustration of ray casting algorithm: (a) case where the relaxed condition is satisfied but the ray doesn’t cross the surface element (b) classification of cross types.

For grid cells that do not contain any surface element, all the nodes inside the grid cell lie on the same side of the interface. In such cases, we only judge the sign for a single node in the grid cell, then assign this sign for all the rest nodes inside the grid cell.

### 6.3 Examples of order parameter initialization

In this section, we examine the algorithm with multiple examples. We first verify the calculation of the signed distance function in a single grid cell for sphere and cubic interfaces to establish the order of convergence. Then, we test the algorithm for multiple grid cells with the cubic interface case. Finally, we demonstrate the algorithm for the complex geometry of a ship hull.

#### 6.3.1 Interface meshes for sphere and cube

We start by verifying the calculation of the signed distance function. A domain of $[0, 1] \times [0, 1] \times [0, 1]$ is considered in this problem. A sphere interface is located
at the center of the domain \((0.5,0.5,0.5)\) with a radius of \(r = 0.25\). The signed distance function needs to be generated with the definition of a positive sign inside the sphere. A single grid cell is used for the calculation so that the signed distance is calculated throughout the domain.

The computational domain is discretized with uniform structured cubic elements with an edge length of \(h_E = 0.02\) and \(h_E = 0.01\), where \(E\) denotes the Eulerian background mesh. The sphere interface is discretized with unstructured triangular mesh, whose edge length is denoted as \(h_S\). The interface mesh is shown in Fig. 6.3 (a). We vary the ratio of the surface mesh size to the Eulerian background mesh from \(h_S/h_E = 2\) to \(h_S/h_E = 0.5\). The error is quantified with the \(L_2\) norm of the difference between the computational and analytical results as 
\[
e^2 = \frac{||\phi - \phi_{ref}||}{||\phi_{ref}||}.
\] The results are shown in Fig. 6.4 (a), where a second-order convergence is observed. We further test the algorithm with a cubic interface mesh, which contains sharp edges and corners. A cubic interface mesh spans through \([0.25,0.75] \times [0.25,0.75] \times [0.25,0.75]\) is used as shown in Fig. 6.3 (b), the rest of the numerical setup are kept the same. The second-order convergence is confirmed in Fig. 6.4 (b).

![Illustration of the interface meshes for two simple geometries: (a) sphere and (b) cube.](image-url)
6.3.2 Calculation with multiple grid cells

We then examine the algorithm with multiple grid cells. The cubic interface mesh case discussed in Subsection 6.3.1 is used. The domain is discretized with a uniform structure mesh of size $h_E = 0.02$, and an unstructured triangle mesh of size $h_S = 0.005$ is used for the cubic interface. The domain is decomposed as 9 grid cells in the $X$, $Y$ and $Z$ directions, respectively. The slice of $Y-Z$ plane at $x = 0.5$ is shown in Fig. 6.5 (a). As observed, the calculation of the signed distance function is restricted to grid cells that are close to the interface. In the grid cells which are far from the interface, the calculation is omitted, and the values of 1 and $-1$ are assigned to the order parameter for nodes located inside and outside of the interface, respectively. The last step is to composite the signed distance function with the hyperbolic tangent function. As a result, an order parameter field in which the variation is highly localized to the interface is generated, as shown in Fig. 6.5 (b).

6.3.3 Demonstration with ship hull

Lastly, we demonstrate the algorithm for complex interfaces with the ship hull of a tug boat. We employ the vessel STAN TUG 1004 for which the vessel geometry is available online [https://grabcad.com/library/stan-tug-1004-1]. The domain and the interface are discretized with unstructured meshes of size $h_E = h_S = 0.02$ The
interface mesh is shown in Fig. 6.6 (a), while the isosurface of $\phi = 0$ of the generated order parameter field representing the interface in the Eulerian mesh is shown in Fig. 6.6 (b). As observed, the current algorithm can successfully generate the order parameter field for complex interfaces. The generated field will be further used as the initial condition for demonstrating the ship-ice interaction problem.

Figure 6.6: An illustration of a tugboat represented by (a) interface mesh and (b) isosurface of $\phi = 0$. 
6.4 **Fully Eulerian formulation for multiphase FSI**

In this section, we present the continuum formulation for the fully Eulerian multiphase FSI framework. We start with the unified mass and momentum conservation equations for the continuum. Then we describe the interface equations and the constitutive relation for the fluid phases. Finally, we introduce the interface equations, the constitutive relation, and the kinematic equations for the solid phases.

6.4.1 **Conservation laws for the multiphase FSI system**

Consider a physical domain \( \Omega \times [0,T] \) with spatial coordinates \( x \) and temporal coordinate \( t \). The domain comprises subdomains \( \Omega_i, i = 1, 2, \ldots, n \), where \( i \) and \( n \) are the index and the total number of the subdomains. Each subdomain is considered to be an incompressible Newtonian fluid or Neo-Hookean solid of particular physical properties. The subdomains are distinguished by a fraction function \( \alpha^i(\phi^i(x,t)) \), where \( \phi^i(x,t) \) being the order parameter in the phase-field method. Both \( \alpha^i(\phi^i) \) and \( \phi^i \) are used to indicate a binary system that the current location \( (x,t) \) is or is not phase \( i \), which leads to \( \alpha^i(\phi^i(x,t)) = 1, x \in \Omega_i \) and \( \alpha^i(\phi^i(x,t)) = 0, x \in \Omega \setminus \Omega_i \).

Through phase-dependent interpolation, the density, viscosity, stress, and the body force of the continua can be calculated as:

\[
\rho = \sum_{i=1}^{n} \alpha^i(\phi^i) \rho^i,
\nu = \sum_{i=1}^{n} \alpha^i(\phi^i) \nu^i,
\mathbf{b} = \sum_{i=1}^{n} \alpha^i(\phi^i) \mathbf{b}^i \quad \text{and} \quad \sigma = \sum_{i=1}^{n} \alpha^i(\phi^i) \sigma^i.
\]

Along with the incompressible constraint, the momentum and mass conservation can be written as:

\[
\rho (\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = \nabla \cdot \sigma + \mathbf{b}, \quad \text{(6.2)}
\]

\[
\nabla \cdot \mathbf{v} = 0. \quad \text{(6.3)}
\]

where \( \mathbf{v} \) is a unified velocity field for the continua.
6.4.2 Equations for the fluid phases

For each component of a Newtonian fluid, we employ the interface-preserving phase-field method introduced in Chapter 4, which is given as:

\[
\frac{\partial \phi^i}{\partial t} + \mathbf{v} \cdot \nabla \phi^i = -\gamma(t) \left( F'(\phi^i) - \epsilon^2 \nabla^2 \phi^i - \beta(t) \sqrt{F(\phi^i)} \right)
\]

\[
\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{\left| (\nabla \phi^i)^T \cdot \nabla \mathbf{v} \cdot \nabla \phi^i \right|}{|\nabla \phi^i|^2} \right)
\]

where \( F(\phi^i) = \left( 0.25 \left( \left( \phi^i \right)^2 - 1 \right)^2 \right) \) is the bulk energy, \( \beta(t) = \frac{\int_{\Omega} F(\phi^i) d\Omega}{\int_{\Omega} \sqrt{F(\phi^i)} d\Omega} \) is the Lagrange multiplier for mass conservation [77], and \( \mathcal{F}(\phi(x,t)) = \sqrt{\frac{\int_{\Omega} \left( |(\phi(x,t)|^2 \right) d\Omega}{\int_{\Omega} |d\Omega} \right), -\delta < \phi < \delta \) is the RMS value of the function field \( \phi(x,t) \) in the interface region, where the boundaries of the region are selected as \( \delta = 0.9 \).

6.4.3 Equations for the solid phases

For each component of the incompressible solid, we employ the interface and geometry preserving phase-field method introduced in Chapter 5, which is given as:

\[
\alpha'(\phi^i)(\mathbf{w}^i - \mathbf{v}) + \left( 1 - \alpha'(\phi^i) \right) \left( -\epsilon \nabla \phi^i \cdot \nabla \mathbf{w}^i \right) = 0,
\]

\[
\frac{\partial \phi^i}{\partial t} + \mathbf{w}^i \cdot \nabla \phi^i = -\gamma'(t) \left( F'(\phi^i) - \epsilon^2 \nabla^2 \phi^i - \beta(t) \sqrt{F(\phi^i)} \right)
\]

\[
\gamma'(t) = \frac{1}{\eta} \mathcal{F} \left( \frac{\left| (\nabla \phi^i)^T \cdot \nabla \mathbf{w} \cdot \nabla \phi^i \right|}{|\nabla \phi^i|^2} \right)
\]

To further enhance the stability of the left Cauchy-Green tensor near the interface and recover \( \mathbf{B} = \mathbf{I} \) at regions where the solid passes through, we employ an approach that is similar to [56]:

\[
\alpha'(\phi^i) \left( \frac{\partial \mathbf{B}^i}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{B}^i - \nabla \mathbf{v} \mathbf{B} - \mathbf{B}(\nabla \mathbf{v})^T \right) + (1 - \alpha'(\phi^i)) (\mathbf{B}^i - \mathbf{I}) = 0
\]

The solid stress is given as \( \sigma^i = -p \mathbf{I} + \mu_L^i (\mathbf{B}^i - \mathbf{I}) + \mu^i (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \), where \( \mu_L^i \) and \( \mu^i \) are the shear modulus and the viscosity, respectively.
6.4.4 Remarks on implementation details

1. The semi-discrete form and spatial and temporal discretization are identical to the corresponding sections introduced in Chapters 4 and 5.

2. For continua with \( n_f \) number of fluid phases and \( n_s \) number of solid objects, the current PDE system is comprised by a unified mass and momentum conservation equation, \( n_f \) set of equations in Subsection 6.4.2 and \( n_s \) set of equations in Subsection 6.4.3.

3. The left Cauchy-Green tensor is solved as a symmetry tensor with six degrees of freedom. The equation is linearized via the Newton-Raphson iteration. In forming the block matrices, the solution vector is organized as \([\Delta B_{11}, \Delta B_{22}, \Delta B_{33}, \Delta B_{12}, \Delta B_{23}, \Delta B_{13}]^T\). The subsequent linear system is solved with the GMRES method.

4. The fraction function is chosen as linear interpolation given by \( \alpha^i(\phi^i) = (1/2)(1 + \phi^i) \).

6.5 Test cases

In this section, we validate and demonstrate the framework with cases of increasing complexity. We start with verifying the framework with a rotational disk in lid-driven cavity flow. Then, we demonstrate the solver with a series of 3D cases that are hard to be solved by the traditional ALE framework. Through the solid sphere rotating in lid-driven cavity flow, the ability of the framework to handle rotational motion is demonstrated. The large transnational displacement, deformation, and contact dynamics are resolved by the framework in the solid ball falling and bouncing back case and the collision of two solid balls. The international system of unit is used in all the cases by default.

6.5.1 Rotating disk in lid-driven cavity flow

In this section, we examine the fluid-solid interaction aspect of our solver in the case of a rotating disk in lid-driven cavity flow. Consider the computational domain of \([0, 1] \times [0, 1] \). A circular disk of radius \( r = 0.2 \) is centered at \((0.6, 0.5)\). The
no-slip boundary condition is applied to the left, right, and bottom boundaries, with a prescribed velocity at the top boundary as $v_\text{c} = 1$. The order parameter and the left Cauchy-Green tensor on the boundaries are evolved according to the prescribed velocity. The zero Neumann boundary condition is applied for $w$ on all the boundaries. The densities of the solid and fluid are selected as $\rho^s = \rho^f = 1$. The dynamic viscosity is taken as $\mu^s = \mu^f = 0.02$. The shear modulus of the solid is chosen as $\mu^s_L = 0.1$. The problem setup is illustrated in Fig. 6.7.

![Figure 6.7: Schematic diagram of a rotating disk in lid-driven cavity flow.](image)

We first perform a time convergence study. The interface parameters are selected as $\eta = 0.2, \varepsilon = 0.02$. A uniform structured triangle mesh with edge length $h = 0.01$ is used to discretize the computational domain. The time steps are bisected from $\Delta t = 0.004$ to $\Delta t = 0.001$, and the case is simulated until $t = 20$. Defining the center of mass of the solid as $x_c = \int x d\Omega^s / \int 1 d\Omega^s$, where the solid domain is identified through the corresponding order parameter $d\Omega^s = \alpha^s(\phi^s) d\Omega$. The trajectories of the center of mass with different time steps are plotted in Fig. 6.8 (a). As observed, the solution has converged at $\Delta t = 0.001$.

After that, we perform an interface convergence study. With the converged
time step $\Delta t = 0.001$, we bisect $\eta$ and $\varepsilon$ simultaneously from $\eta = 0.2, \varepsilon = 0.02$ to $\eta = 0.05, \varepsilon = 0.005$. The meshes are refined according to maintain the interface resolution at $h/\varepsilon = 1$. The trajectories of the center of mass are plotted in Fig. 6.8 (b). As shown by the figure, the solution converges to the reference solution.

![Figure 6.8](image)

**Figure 6.8**: Rotating disk in lid-driven cavity flow: (a) temporal and (b) interface convergence study for the center of mass of the disk.

### 6.5.2 Rotating sphere in lid-driven cavity flow

We generalize the rotating disk case as a rotating sphere case to demonstrate the 3D aspect of the solver. A computational domain of $[0, 1] \times [0, 1] \times [0, 1]$ is considered. A solid sphere of radius $r = 0.2$ is initially centered at $(0.6, 0.5, 0.5)$. The no-slip boundary condition is applied to the side and bottom walls, while a constant velocity of $v_x = 1$ is applied at the top boundary. The order parameter and the left Cauchy-Green tensor on the boundaries are evolved according to the prescribed velocity. The zero Neumann boundary condition is applied for $w$ on all the boundaries. The densities of the fluid and the solid are chosen as $\rho^s = \rho^f = 1$. The dynamic viscosity is taken as $\mu^s = \mu^f = 0.01$. The shear modulus of the solid is selected as $\mu^I_s = 5$. The case setup is illustrated in Fig. 6.9.

Similarly, we perform a temporal and interface convergence study. The inter-
Figure 6.9: Schematic of a rotating sphere in lid-driven cavity flow.

Figure 6.10: Rotating sphere in lid-driven cavity flow: (a) temporal and (b) interface convergence study for the center of mass of the sphere in $X-Z$ plane.

face parameters are selected as $\eta = 0.2, \varepsilon = 0.02$. The time steps are bisected from $\Delta t = 0.04$ to $\Delta t = 0.01$, and the case is simulated until $t = 20$. The trajectory of the center of mass on the $X-Y$ plane is plotted in Fig. 6.10 (a). As shown by the figure, the solution has converged at $\Delta t = 0.01$. With the converged time step, we perform an interface convergence study. The interface parameters $\eta$ and $\varepsilon$ are scaled with $1/\sqrt{2}$ simultaneously from $\eta = 0.2, \varepsilon = 0.02$ to $\eta = 0.1, \varepsilon = 0.01$. The
6.5.3 Falling and bouncing back of an elastic sphere

In this subsection, we demonstrate the ability of the framework in handling solid contact and resulting elastic deformation. The case of falling and bouncing back
Figure 6.12: Schematic of the case setup for falling and bouncing back of an elastic sphere.

Figure 6.13: Falling and bouncing back of an elastic sphere: (a) temporal and (b) interface convergence study for the center of mass of the sphere.

of a solid sphere is considered in a computational domain of $[-1,1] \times [-1,1] \times [-1,1]$. The sphere with a radius of $R = 0.4$ is initially centered at $(0,0,0)$. The no-slip boundary condition is applied to all the boundaries. The order parameter on the boundaries is fixed as $\phi = -1$ so that the solid phase can not penetrate the bottom boundary. The zero Neumann boundary condition is applied for $w$ on all the boundaries. The density of the sphere is selected as $\rho_s = 5000$, while the rest of the domain is filled with fluid of density $\rho_f = 1000$. The shear modulus of the solid is $\mu_s = 1 \times 10^4$, and the viscosity of the fluid is $\mu_f = 10$. The gravitational
force of \( \mathbf{b} = (0, -0.98, 0) \) is applied. The problem setup is shown in Fig. 6.12.

Figure 6.14: Falling and bouncing back of an elastic sphere: the evolution of the interface \( \phi = 0 \) at different time instants \( t = (a) 0.1, (b) 2, (c) 2.9, (d) 3.8, (e) 3.9, (f) 4.7 \).

Herein we perform a temporal and interface convergence study of our implementation. The interface parameters are selected as \( \eta = 0.2, \varepsilon = 0.04 \). The time steps are bisected from \( \Delta t = 0.004 \) to \( \Delta t = 0.001 \), and the case is simulated until \( t = 5 \). The \( Y \) coordinate of the center of mass of the sphere is plotted in Fig. 6.13 (a). As shown, the solution has converged at \( \Delta t = 0.001 \). With the converged time step, we examine the interface convergence. The interface parameters \( \eta \) and \( \varepsilon \) of \( \eta = 0.2, \varepsilon = 0.04 \) and \( \eta = 0.141, \varepsilon = 0.0141 \) are tested. The meshes are refined according to maintain the interface resolution at \( h/\varepsilon = 1 \). The \( Y \) coordinate of the center of mass is plotted in Fig. 6.13 (b). As observed, the solutions do not vary much, which shows that the solution has converged. To better visualize the field, we show the interface of \( \phi = 0 \) and \( v_y \) at the slice of \( z = 0 \) at \( t = 0.1, 2, 2.9, 3.8, 3.9, 4.7 \) in Fig. 6.14. As observed, the sphere falls due to the gravitational force. At \( t = 2 \), it reaches the lowest position and starts to bounce.
back. At $t = 3.8$, the solid sphere reaches the peak and starts to fall again. This cycle repeats at $t = 3.8, 3.9$ and $t = 4.7$. As demonstrated, the large elastic deformation and contact can be handled naturally in the current framework.

### 6.5.4 Collision of two elastic spheres

We next showcase the deformation due to contact between two elastic solids by collision of solid spheres. The computational domain of $[0, 1] \times [0, 1] \times [0, 1]$ is considered. Two solid balls with radius of $R = 0.15$ are initially centered at $(0.5, 0.3, 0.5)$ and $(0.5, 0.7, 0.5)$. The slip boundary condition is applied to all the boundaries. For the order parameters of the two solid phases, the boundary condition is set to be $\phi = -1$ on all the boundaries. The zero Neumann boundary conditions for the left Cauchy-Green tensors and the gradient-minimizing velocities are applied to all the boundaries of the computational domain. The solid spheres have the same physical properties. Their density, viscosity and shear modulus are $\rho^s = 5000, \mu^s = 10$ and $\mu_L^s = 1 \times 10^4$, respectively. The surrounding fluid has the density and viscosity of $\rho^f = 1000$ and $\nu^f = 10$. The gravitational force of $\mathbf{b} = (0, -0.98, 0)$ is applied. Fig. 6.15 shows the case setup and the associated details.

![Figure 6.15: Schematic diagram of collision of two elastic spheres.](image)

The interface parameters are selected as $\varepsilon = 0.03, \eta = 0.2$. The computational domain is discretized with cubic elements of edge length $h = 0.02$. The time step is selected as $\Delta t = 0.001$. The case is simulated until $t = 10$. The simulation results are visualized in Fig. 6.16 with the interface of $\phi = 0$ and $v_y$ at $x = 0.5$.
at $t = 0.1, 0.9, 1.1, 1.8, 2.8, 6.8$. As observed, the two spheres start to fall under gravity. The lower ball hit the ground at $t = 0.9$. Later the upper ball collides with the lower ball and becomes stagnant at $t = 1.1$. The upper ball bounces back and reaches the peak at $t = 1.8$. It falls again and causes the flow towards the top of the domain at $t = 2.8$. Later they reach the bottom, and the flow velocity is reduced to almost zero at $t = 6.8$. As discussed, the contact dynamics is reasonably captured by the current framework.

Figure 6.16: Collision of two elastic spheres: superposition of the interfaces $\phi^i = 0$ at different time instants $t =$ (a) 0.1, (b) 0.9, (c) 1.1, (d) 1.8, (e) 2.8, (f) 6.8.

### 6.6 Demonstration on ship-ice interaction

Lastly, we demonstrate our fully Eulerian 3D finite element solver for a simplified case whereby a moving ship interacts with ice floes. We employ the vessel STAN TUG 1004 for which the vessel geometry is available online [https://grabcad.com/library/stan-tug-1004-1]. The domain of $[-9.81, 17.44] \times [-5.45, 5.45] \times [-5.45, 5.45]$ is considered. The free water level is the $X - Y$ plane of $z = 0$. The leading point
of the cross-plane of the ship and the free water level is placed at \((-1.1157, 0, 0)\). Six pieces of ice floes in total are posed in front of the boat. They are formed by extruding the cross section from \(z = 0\) to \(z = -0.3\). The geometries of the ice floes cross-sections are listed in Table 6.1.

**Table 6.1: Geometry of the ice floes**

<table>
<thead>
<tr>
<th>Index</th>
<th>shape of cross section</th>
<th>coordinate of cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>triangle</td>
<td>((-1.1, 0.6), (-1.7, 0.2), (-1.7, 0.9))</td>
</tr>
<tr>
<td>2</td>
<td>quadrilateral</td>
<td>((-1.6, -0.2), (-2.1, -0.6), (-1.8, -1), (-1, -0.6))</td>
</tr>
<tr>
<td>3</td>
<td>quadrilateral</td>
<td>((-3.1, 1.3), (-3.7, 1), (-3.2, 0.3), (-2.7, 0.7))</td>
</tr>
<tr>
<td>4</td>
<td>quadrilateral</td>
<td>((-4, -0.4), (-4.4, -0.9), (-3.8, -1.7), (-3.2, -0.7))</td>
</tr>
<tr>
<td>5</td>
<td>quadrilateral</td>
<td>((-4.8, 1), (-5.4, 0.6), (-4.7, 0.4), (-4.1, 0.5))</td>
</tr>
<tr>
<td>6</td>
<td>quadrilateral</td>
<td>((-5.3, -0.4), (-6, -0.7), (-5.9, -1.2), (-5.1, -1))</td>
</tr>
</tbody>
</table>

**Figure 6.17:** Schematic diagram of an ice-going ship with free surface and ice floes.

The boat is sailing in the negative \(X\) direction at the speed of \(v_x = -1\). This is realized by finding the nodes inside the boat and specifying the velocity on these nodes. The nodes are identified by \(-0.2 - tv_x \leq x \leq 0.2 - tv_x, |y| \leq 0.2, |z| \leq 0.2\). The slip boundary condition is applied to all the boundaries. The zero Neumann boundary condition is applied for all the order parameters, extended velocities, and left Cauchy-Green tensors on all the boundaries. The densities of the ship, ice,
water, and air phases are selected as $\rho^s = 600, \rho^i = 800, \rho^w = 1000, \rho^a = 100$. The viscosities of the phases are selected as $\nu^s = \nu^i = \nu^w = \nu^a = 1$. The shear modulus of the ship and the ice are selected as $\nu^s_L = \nu^i_L = 1 \times 10^6$. The gravitational acceleration is chosen as $g = (0, -0.98, 0)$. The case is simulated until $t = 11.25$. The case setup is illustrated in Fig. 6.17.

![Figure 6.17](image)

**Figure 6.17**: Representative results of ship-ice interaction: superposition of the interfaces $\phi^i = 0$ at different time instants $t = (a) 0.25, (b) 2.5, (c) 5, (d) 7.5, (e) 10, (f) 11.25.

The computational domain is discretized with tetrahedron elements of size $h = 0.04$ around the interacting phases. The diffuse interface thickness is chosen as $\varepsilon = h$. $\eta = 1$ is used to further reduce the curvature flow. The time step is selected as $\Delta t = 0.0025$. The simulation results are visualized at $t = 0.25, 2.5, 5, 7.5, 10, 11.25$ in Fig. 6.18. As observed, the rich physics of interactions between the ship and free surface, the ship-ice interaction, the coupling of ice floes and free surface are captured. An interesting dynamics of ship-ice interaction at the bow area can be observed qualitatively. It is worth mentioning that the ice mechanics model
is very simplified without considering detailed aspects of constitutive modeling and fracture mechanics. Further parametric investigations and validation should be carried out for more realistic modeling of ice mechanics for the ship-ice interaction with nonlinear hydrodynamics effects.

6.7 Summary

By integrating the diffused interface techniques for the fluid-fluid and fluid-solid couplings, we completed the development of a unified Eulerian variational FSI framework in this chapter. We achieved the target to simulate the ship-ice interaction using a fully coupled continuum mechanics formulation. Some of the key features of the computational framework are:

- Grid cell based initialization of the hyperbolic tangent profile for complex interface mesh;
- Unified momentum and mass conservation equations for the dynamics of multiphase FSI problems;
- Improved accuracy in interface evolution and representation with phase-field diffuse interface description via IP and IGP methods;
- High robustness in handling interface motion, including large translation/rotational motion, interface merging/breaking-up and contact;
- 3D parallelized implementation for large-scale simulation.

The framework is verified by a rotating disk problem and further demonstrated in cases such as a rotating sphere in lid-driven cavity flow, falling and bouncing back of a sphere, and collision of two spheres. Finally, the framework is demonstrated with a representative case of ship-ice interaction.
Chapter 7

Conclusion

In this chapter, we provide a concluding summary of the present dissertation and suggest some recommendations for future work in the present area of research.

7.1 Concluding remarks

The present thesis has focused on the development of a general-purpose three-dimensional unified Eulerian variational framework for multiphase FSI. The thesis introduced and analyzed novel diffuse interface methods for the phase-field modeling of evolving fluid-fluid and fluid-solid interfaces. The study began with the phase-field diffuse interface description, which diffuses the sharp interface between phases as a hyperbolic tangent profile that can be captured by a volumetric solution field termed as the order parameter. This allows large topological changes of interfaces in a fixed Eulerian mesh via order parameter evolution instead of complex mesh manipulation.

We first looked into the application of the diffuse interface description to the fluid-fluid interface with the surface tension effect. Since the surface tension effect is modeled assuming a hyperbolic tangent profile, any distortion on the profile induces errors in surface tension dynamics, which contaminates the interface evolution and stretches the interface profile further. The coupled interface representation and evolution due to the surface tension effect is very sensitive and error-prone, therefore demanding the preservation of the interface profile. To achieve this, we
developed an *interface-preserving* phase-field method. The method quantifies the convective distortion and adaptively regularizes the hyperbolic tangent profile with free energy minimization through a *time-dependent mobility coefficient*. The model was tested in 1D and 2D fields of prescribed convective velocity to show its second-order convergence and effectiveness in preserving the hyperbolic tangent interface profile. Then, the model is applied to 2D and 3D rising bubble problems to confirm the improvement in surface tension modeling, and further the accuracy of two-phase flow simulations.

We then focused on the phase-field diffuse interface description for the fluid-solid interface. In this scenario, the disturbance from the curvature flow to the geometry of solid objects is especially severe for objects with sharp corners and large aspect ratios, which becomes the bottleneck of the accuracy. In the analysis of the curvature flow in the IP method, we found that it is proportional to the free energy minimization, which further correlates with the convective distortion. Based on this understanding, an *interface and geometry preserving* phase-field method has been developed to suppress the curvature flow. In this method, we evolve the order parameter with an auxiliary velocity field instead of the original velocity field. The auxiliary velocity field attains the solid velocity in the solid phase and extends the velocity along the normal direction throughout the diffuse interface region. With this treatment, the interface conforms to the solid object, while the velocity gradient which distorts the interface profile is reduced. As a result, the auxiliary velocity field is referred to as the *gradient-minimizing velocity field*, which reduces the convective distortion and hence, the curvature flow. Thus the geometry of the interface is better preserved. The model is tested and proven to be effective in preserving the geometry of 2D circular and square interfaces and numerically being second-order accurate spatially and temporally. It is then coupled with fully Eulerian FSI dynamics and examined in channel flow passing a fixed deformable block and cylinder-flexible plate problem.

With the improved interface representation and evolution, we generalized the framework to 3D multiphase FSI problems. To efficiently handle complex geometries of solid objects in practical application, we implemented a *grid cell based* algorithm to initialize the order parameter field according to given interface meshes. The method restricts the calculation close to the interface, therefore significantly
reducing the computational cost. As the interface mesh is refined, a second-order convergence in the signed distance function calculation is observed. The generated order parameter fields indicate the initial positions of the interfaces in the computational framework. In terms of the dynamics of the multiphase FSI framework, we solve a unified momentum and mass conservation equation through phase-dependent interpolation. For each fluid phase, the interface-preserving phase-field equation is solved, while the interface and geometry preserving phase-field method and a left Cauchy-Green tensor are solved for each solid object. The framework is verified with a rotational disk in lid-driven cavity flow, then the 3D solver is demonstrated with the cases of a rotational sphere, falling and bouncing back of a sphere and two deformable spheres colliding with each other. Finally, we demonstrate our 3D fully Eulerian framework for an ice-going ship.

To summarize, the developed multiphase FSI framework is featured by consistent formulation for fluids and solids, which facilitates the generalization to a wide range of applications. It has excellent robustness in handling complex interface motions and dynamics, therefore allowing the simulations of multiphase FSI in most complex scenarios. The framework based on variational finite element discretization is implemented with the capability of parallel computing for large-scale 3D problems. To the best of our knowledge, the development of this 3D phase-field based unified Eulerian continuum mechanics framework is the first-of-its-kind and will push the boundaries of computational multiphysics simulations to the next level.

7.2 Future recommendations

The current work can lead to several future extensions. They are summarized as follows:

- In the current thesis, most of the cases belong to the small to medium mass ratio of around 1 to 10. The stability and accuracy of the framework at large density and viscosity ratios need to be systematically assessed. Introducing the consistent formulation [131], improving the interface resolution by adaptive refinement, developing novel coupling algorithms, and employing a better pre-conditioner for GMRES linear solver are all possible directions.
that can further improve the performance of the framework.

- In Chapter 6, we have demonstrated the collision of solid spheres and contact between ice and ship hull. While the dynamics is qualitatively correct, more rigorous investigation and validation of the solid-solid interaction and the strain due to contact dynamics are needed. Accurate post-process and visualization tools are to be further developed to facilitate the analysis and validation of the coupled mechanics effects, such as extracting the local stress at the interface and calculating force coefficients.

- In the current framework, the interacting solids must be represented by different phases. However, this approach becomes quite tedious when the number of interacting objects increases and does not apply to cases involving self-contact of the same phase. New contact formulations or order parameter reassignment based on the four color theorem [132, 133] can be considered to overcome these drawbacks.

- The modeling of full-scale ship-ice interaction is a complex task, which requires a fundamental understanding of ice mechanics and an accurate constitutive model for ice behavior. As for future work, the proposed framework with proper ice modeling should be considered for ice-going ships to predict local and global performance.

- The failure modeling of the ice is not considered in the current framework, which might be of interest for detailed dynamics. Fortunately, the simulation for crack propagation with the phase-field method has been developed in literature such as [70, 134], where the void introduced by the crack is simply considered as another phase. Therefore, it is possible to introduce a phase-field-based crack model for ice-breaking mechanics, which can be integrated seamlessly with the current unified formulation.

- Beyond the application of the ice-going ships, the proposed framework can be further developed to explore phase transfer problems such as the ice melting problem [67], the boiling process [68], phase transfer in alloy [69], and the cavitation process [135]. Inclusion of contact angle boundary condition [136] helps to handle elastocapillaity phenomenon [35]. Concerning
the modeling marine propeller cavitation, one can incorporate the thermo-
dynamically consistent potential to model the formation of vapor cavities
which subsequently can be integrated within the fully Eulerian framework.
Bibliography


158


161


163


164


165


[132] Kenneth Appel and Wolfgang Haken. Every planar map is four colorable. 1976. → page 153


Appendix A

Quantification of the convective distortion intensity

In this appendix, we demonstrate the quantification of the intensity of the convective distortion by the normal velocity gradient in the normal direction $\zeta$. Consider two level sets of $\phi = \phi_1$ and $\phi = \phi_2$. Due to the finite thickness of the region, the convective velocity of the two level sets can be different. The tangential velocities are ignored since they do not affect the propagation of level sets. The normal velocity of the level sets are denoted as $v_n(x_1, t)$ and $v_n(x_2, t)$, where $x_1$ and $x_2$ are in the same normal axis with identical tangential coordinates. Suppose $\phi$ is continuous and differentiable with respect to $x \in (x_1, x_2)$, we want to quantify the convective distortion intensity at $x$.

Consider the initial distance between the two level sets at the discussed normal axis as $\varepsilon_i = ||x_2 - x_1||$. After a small time increment $\Delta t$, the thickness is distorted due to the difference in the normal velocity, which can be linearly approximated as:

$$\varepsilon_e = \varepsilon_i + (v_n(x_2, t) - v_n(x_1, t))\Delta t,$$

where $\varepsilon_e$ represents the distance between the two level sets at the end of the time increment, as shown in Fig. A.1. The intensity of the convective distortion at $x \in (x_1, x_2)$ can be considered as the relative change of the thickness per unit time due
Figure A.1: Schematic diagram of the convective distortion of the thickness between the level sets of $\phi = \phi_1$ and $\phi = \phi_2$ due to different normal velocities.

to the difference in the convective velocity:

$$\lim_{\varepsilon_i \to 0} \lim_{\Delta t \to 0} \frac{\varepsilon_f - \varepsilon_i}{\varepsilon_i \Delta t} = \lim_{\varepsilon_i \to 0} \lim_{\Delta t \to 0} \frac{v_n(x_2, t) - v_n(x_1, t)}{\varepsilon_i} = \frac{\partial v_n}{\partial n}(x, t) = \zeta(x, t)$$ (A.2)
Appendix B

Frame independent form of time-dependent mobility

The normal velocity gradient in the normal direction \( \zeta(x, t) \) in Eq. (4.27) can be written in a frame independent form:

\[
\zeta(x, t) = \nabla (v \cdot n_L^\phi) \cdot n_L^\phi. 
\] (B.1)

To simplify the equation, we expand the normal velocity gradient in the normal direction as:

\[
\nabla (v \cdot n_L^\phi) \cdot n_L^\phi = (n_L^\phi)^T \cdot \nabla v \cdot n_L^\phi + (v)^T \cdot \nabla n_L^\phi \cdot n_L^\phi + v \times (\nabla \times n_L^\phi) \cdot n_L^\phi + n_L^\phi \times (\nabla \times v) \cdot n_L^\phi
\]

where the second, the third and the fourth terms are zero. For example, the second term:

\[
(v)^T \cdot \nabla n_L^\phi \cdot n_L^\phi = v \cdot (\nabla n_L^\phi \cdot n_L^\phi) = v \cdot \frac{1}{2} \nabla (n_L^\phi \cdot n_L^\phi) = 0
\]

and the third term \( \nabla \times n_L^\phi = \nabla \times \left( \frac{\nabla \phi}{|\nabla \phi|} \right) = \nabla \left( \frac{1}{|\nabla \phi|} \right) \times \nabla \phi + \frac{1}{|\nabla \phi|} \nabla \times \nabla \phi \). Notice that with the assumption of uniform interface profile along the interface, \( 1/|\nabla \phi| \) is a constant on the level sets of \( \phi \). Thus both \( \nabla (1/|\nabla \phi|) \) and \( \nabla \phi \) are normal to the level sets of \( \phi \), which leads to \( \nabla (1/|\nabla \phi|) \times \nabla \phi = 0 \). The curl of gradient of a scalar field is identically zero. As a result, the third term vanishes. The last term equals to zero since for arbitrary vectors \( \mathbf{a} \) and \( \mathbf{b} \), \( (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{a} = 0 \). As a result, the normal velocity gradient
in the normal direction can be simplified as:

\[
\zeta(x,t) = (n^\phi_L)^T \cdot \nabla v \cdot n^\phi_L. \tag{B.2}
\]

and by substituting \( n^\phi_L = \nabla \phi / |\nabla \phi| \), we get the frame-independent form of the normal velocity gradient in the normal direction:

\[
\zeta(x,t) = \left( \nabla \phi \right)^T \cdot \nabla v \cdot \nabla \phi \left/ |\nabla \phi|^2 \right.. \tag{B.3}
\]

Finally, the frame independent form of the time-dependent mobility model is given by:

\[
\gamma(t) = \frac{1}{\eta} \mathcal{F} \left( \left| \left( \nabla \phi \right)^T \cdot \nabla v \cdot \nabla \phi \right| / |\nabla \phi|^2 \right), \tag{B.4}
\]

where \( \mathcal{F}(\phi(x,t)) = \sqrt{ \frac{\int_{\Gamma_D(t)} (\phi(x,t))^2 \, d\Omega}{\int_{\Gamma_D(t)}} }, \ x \in \Gamma_D(t) \). The frame independent form facilitates its numerical implementation in Cartesian coordinate system.
Appendix C

Jacobian terms of the solid stress

In this appendix, we present the 2D component form of the Jacobian terms of the solid stress in the momentum conservation equation with the focus on the shear component. We start from the convection of the left Cauchy-Green tensor:

\[
\frac{\partial B_{11}}{\partial t} = \alpha(\phi) \left( -v_x \frac{\partial B_{11}}{\partial x} - v_y \frac{\partial B_{11}}{\partial y} + \left( \frac{\partial v_x}{\partial x} B_{11} + \frac{\partial v_y}{\partial y} B_{21} \right) + \left( B_{11} \frac{\partial v_x}{\partial x} + B_{12} \frac{\partial v_y}{\partial y} \right) \right),
\]

\[
\frac{\partial B_{12}}{\partial t} = \alpha(\phi) \left( -v_x \frac{\partial B_{12}}{\partial x} - v_y \frac{\partial B_{12}}{\partial y} + \left( \frac{\partial v_x}{\partial x} B_{12} + \frac{\partial v_y}{\partial y} B_{22} \right) + \left( B_{11} \frac{\partial v_y}{\partial x} + B_{12} \frac{\partial v_y}{\partial y} \right) \right),
\]

\[
\frac{\partial B_{21}}{\partial t} = \alpha(\phi) \left( -v_x \frac{\partial B_{21}}{\partial x} - v_y \frac{\partial B_{21}}{\partial y} + \left( \frac{\partial v_x}{\partial x} B_{11} + \frac{\partial v_y}{\partial y} B_{21} \right) + \left( B_{21} \frac{\partial v_x}{\partial x} + B_{22} \frac{\partial v_y}{\partial y} \right) \right),
\]

\[
\frac{\partial B_{22}}{\partial t} = \alpha(\phi) \left( -v_x \frac{\partial B_{22}}{\partial x} - v_y \frac{\partial B_{22}}{\partial y} + \left( \frac{\partial v_x}{\partial x} B_{12} + \frac{\partial v_y}{\partial y} B_{22} \right) + \left( B_{21} \frac{\partial v_y}{\partial x} + B_{22} \frac{\partial v_y}{\partial y} \right) \right).
\]

To keep the symmetry of the left Cauchy-Green tensor, we let $B_{21} = B_{12}$ in the practical implementation. Using the generalized-$\alpha$ method, $B^{\alpha+\alpha}$ can be written
as a function of $\psi^{n+\alpha}$ as follows:

\[
B_{11}^{n+\alpha} = B_{11}^n + \alpha \Delta t \left( 1 - \frac{\gamma}{\alpha_m} \right) \frac{\partial B_{11}^n}{\partial t} + \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -v_x^{n+\alpha} \frac{\partial B_{11}^{n+\alpha}}{\partial x} - v_y^{n+\alpha} \frac{\partial B_{11}^{n+\alpha}}{\partial y} + 2 \frac{\partial v_x^{n+\alpha}}{\partial t} B_{11}^{n+\alpha} + 2 \frac{\partial v_y^{n+\alpha}}{\partial t} B_{12}^{n+\alpha} \right),
\]

\[
B_{12}^{n+\alpha} = B_{12}^n + \alpha \Delta t \left( 1 - \frac{\gamma}{\alpha_m} \right) \frac{\partial B_{12}^n}{\partial t} + \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -v_x^{n+\alpha} \frac{\partial B_{12}^{n+\alpha}}{\partial x} - v_y^{n+\alpha} \frac{\partial B_{12}^{n+\alpha}}{\partial y} \right) + \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( \frac{\partial v_x^{n+\alpha}}{\partial x} B_{12}^{n+\alpha} + \frac{\partial v_y^{n+\alpha}}{\partial y} B_{22}^{n+\alpha} + \frac{\partial v_y^{n+\alpha}}{\partial y} B_{12}^{n+\alpha} \right),
\]

\[
B_{21}^{n+\alpha} = B_{12}^{n+\alpha},
\]

\[
B_{22}^{n+\alpha} = B_{22}^n + \alpha \Delta t \left( 1 - \frac{\gamma}{\alpha_m} \right) \frac{\partial B_{22}^n}{\partial t} + \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -v_x^{n+\alpha} \frac{\partial B_{22}^{n+\alpha}}{\partial x} - v_y^{n+\alpha} \frac{\partial B_{22}^{n+\alpha}}{\partial y} + 2 \frac{\partial v_x^{n+\alpha}}{\partial t} B_{22}^{n+\alpha} + 2 \frac{\partial v_y^{n+\alpha}}{\partial t} B_{12}^{n+\alpha} \right).
\]

Finally, the Jacobian terms of the shear components in the solid stress are given by:

\[
\mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_x^{n+\alpha}} = \mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_y^{n+\alpha}} = \mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_x^{n+\alpha}} = \mu_L N_x \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{11}^{n+\alpha}}{\partial x} + 2 N_x B_{11}^{n+\alpha} + 2 N_y B_{12}^{n+\alpha} \right),
\]

\[
\mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_y^{n+\alpha}} = \mu_L N_y \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{12}^{n+\alpha}}{\partial y} + N_x B_{12}^{n+\alpha} + N_y B_{22}^{n+\alpha} \right),
\]

\[
\mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_x^{n+\alpha}} = \mu_L N_x \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{12}^{n+\alpha}}{\partial y} + N_x B_{12}^{n+\alpha} + N_y B_{22}^{n+\alpha} \right),
\]

\[
\mu_L \frac{\partial (N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha})}{\partial v_y^{n+\alpha}} = \mu_L N_y \alpha \left( \phi^{n+\alpha} \right) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{22}^{n+\alpha}}{\partial x} \right),
\]
\[
\mu_L \frac{\delta(N_x B_{12}^{n+\alpha} + N_y B_{22}^{n+\alpha})}{\delta \alpha} = \mu_L N_x \alpha (\phi^{n+\alpha}) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{12}^{n+\alpha}}{\partial y} + N_x B_{11}^{n+\alpha} + N_y B_{12}^{n+\alpha} \right) \\
+ \mu_L N_y \alpha (\phi^{n+\alpha}) \frac{\Delta \alpha \gamma}{\alpha_m} \left( -N \frac{\partial B_{22}^{n+\alpha}}{\partial y} + 2 N_x \partial B_{22}^{n+\alpha} + 2 N_y B_{12}^{n+\alpha} \right).
\]
Appendix D

Parallel implementation of particle tracking method

In an Eulerian frame of reference, tracking a solid particle may be required to know the exact motion of the solid. To achieve this, we need to search for the solid particle in the entire domain according to its coordinates, interpolate the velocity at the particle position, and evolve the particle accordingly. This procedure is repeated at each time step, which can become a large overhead without efficient implementation.

To avoid this issue, we adopt a parallelized implementation. We first broadcast the particle position to all the processors. In each processor, we split the elements into tetrahedrons. Then the particle is searched in all the tetrahedrons.

Inside each tetrahedron, assuming linear basis function, we have four basis functions corresponding to the four vertices \( N_i(x, y, z) = a_i x + b_i y + c_i z + d_i, i = 1, 2, 3, 4 \). According to the definition of the shape function, \( N_i(x, y, z) \) takes the value of 1 at the node \( i \), and takes the value of 0 at the rest nodes. Due to the linearity, for all the points \( (x, y, z) \) inside the tetrahedron, \( N_i(x, y, z) \in [0, 1], i = 1, 2, 3, 4 \).

With this in mind, we solve for the coefficients \( a_i, b_i, c_i, d_i, i = 1, 2, 3, 4 \). Considering the first shape function, which takes the value of 1 at the first node, and
becomes zero at the rest nodes:

\[
\begin{bmatrix}
  x_1 & y_1 & z_1 & 1 \\
  x_2 & y_2 & z_2 & 1 \\
  x_3 & y_3 & z_3 & 1 \\
  x_4 & y_4 & z_4 & 1 \\
\end{bmatrix}
\begin{bmatrix}
  a_1 \\
  b_1 \\
  c_1 \\
  d_1 \\
\end{bmatrix}
= \begin{bmatrix}
  1 \\
  0 \\
  0 \\
  0 \\
\end{bmatrix}.
\]

(D.1)

Considering all the four nodes, we have:

\[
\begin{bmatrix}
  x_1 & y_1 & z_1 & 1 \\
  x_2 & y_2 & z_2 & 1 \\
  x_3 & y_3 & z_3 & 1 \\
  x_4 & y_4 & z_4 & 1 \\
\end{bmatrix}
\begin{bmatrix}
  a_1 & a_2 & a_3 & a_4 \\
  b_1 & b_2 & b_3 & b_4 \\
  c_1 & c_2 & c_3 & c_4 \\
  d_1 & d_2 & d_3 & d_4 \\
\end{bmatrix}
= \begin{bmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 1 & 0 \\
  0 & 0 & 0 & 1 \\
\end{bmatrix}.
\]

(D.2)

The coefficients can be solved as:

\[
\begin{bmatrix}
  a_1 & a_2 & a_3 & a_4 \\
  b_1 & b_2 & b_3 & b_4 \\
  c_1 & c_2 & c_3 & c_4 \\
  d_1 & d_2 & d_3 & d_4 \\
\end{bmatrix}
= \begin{bmatrix}
  x_1 & y_1 & z_1 & 1 \\
  x_2 & y_2 & z_2 & 1 \\
  x_3 & y_3 & z_3 & 1 \\
  x_4 & y_4 & z_4 & 1 \\
\end{bmatrix}^{-1}.
\]

(D.3)

After getting the coefficients, the value of the shape function on the particle position \((x,y,z)\) can be calculated as:

\[
\begin{bmatrix}
  N_1(x,y,z) \\
  N_2(x,y,z) \\
  N_3(x,y,z) \\
  N_4(x,y,z) \\
\end{bmatrix}
= \begin{bmatrix}
  a_1 & a_2 & a_3 & a_4 \\
  b_1 & b_2 & b_3 & b_4 \\
  c_1 & c_2 & c_3 & c_4 \\
  d_1 & d_2 & d_3 & d_4 \\
\end{bmatrix}^T \begin{bmatrix}
  x \\
  y \\
  z \\
  1 \\
\end{bmatrix}.
\]

(D.4)

if \(\forall i = 1,2,3,4, \; N_i(x,y,z) \in [0,1]\), the particle is inside the tetrahedron. Once the particle is found, its velocity can be interpolated as \(\mathbf{v} = \sum_{i=1}^{4} N_i(x,y,z) \mathbf{v}_i\). The solid particle is then updated and passed back to the root processor.
Appendix E

Parallel implementation for backward projection

In the implementation of time-dependent mobility model, we need to calculate the first-order derivatives of velocities and order parameters at nodes. A shape function based weighted average is used to achieve this, which is referred to as the backward projection. It projects the first-order derivatives from quadrature points to nodes. For node point $p$ and the shape function on this point $N_p$, the formulation is given as:

$$ (\nabla \varphi)_p = \frac{\int N_p \nabla \varphi d\Omega}{\int N_p d\Omega} \quad (E.1) $$

This step takes the information from all directions for nodes inside the domain. However, the information can only come from a single side for nodes located at boundaries. This will cause inconsistency in the order of accuracy.

For example, consider the domain of $x \in [0, 2]$ with three nodes $x = 0, 1, 2$. Denote the domain of $x \in [0, 1]$ as $\Omega_L$ and $x \in [1, 2]$ as $\Omega_R$. Piece-wise linear shape function is used for Galerkin projection. We test the backward projection for the function of $\varphi = x^2$, the analytical solution of the first order derivative is $\frac{d\varphi}{dx} = 2x$, which is a linear function. When multiplied with linear shape function at the numerator of Eq. E.1, the integrated function is a second-order polynomial, which can be calculated exactly with first-order quadrature. As a result, the first-
order derivative values calculated from the backward projection are:

$$
\frac{\partial \phi}{\partial x} \bigg|_{x=0} = \frac{\int (1-x) 2x d\Omega_L}{\int (1-x) d\Omega_L} \approx \frac{\sum_{qp=1}^{2} w_{qp}(1-x_{qp}) 2x_{qp}}{\sum_{qp=1}^{2} w_{qp}(1-x_{qp})} \approx 0.667 \quad \text{(E.2)}
$$

$$
\frac{\partial \phi}{\partial x} \bigg|_{x=1} = \frac{\int (x) 2x d\Omega_L + \int (2-x) 2x d\Omega_R}{\int (x) d\Omega_L + \int (2-x) d\Omega_R} \approx \frac{\sum_{qp=1}^{2} w_{qp}(x_{qp}) 2x_{qp} + \sum_{qp=1}^{2} w_{qp}(2-x_{qp}) 2x_{qp}}{\sum_{qp=1}^{2} w_{qp}(x_{qp}) + \sum_{qp=1}^{2} w_{qp}(2-x_{qp})} \approx 2 \quad \text{(E.3)}
$$

$$
\frac{\partial \phi}{\partial x} \bigg|_{x=2} = \frac{\int (x-1) 2x d\Omega_R}{\int (x-1) d\Omega_R} \approx \frac{\sum_{qp=1}^{2} w_{qp}(x_{qp}-1) 2x_{qp}}{\sum_{qp=1}^{2} w_{qp}(x_{qp}-1)} \approx 3.333 \quad \text{(E.4)}
$$

As observed, while the result at the interior node $x = 1$ is identical with the exact value, errors are introduced at the boundary points of $x = 0$ and $x = 2$. This can be further clarified by expanding the domain to $x \in [-1, 3]$. Following the same procedures, the first order derivatives can be calculated as: $\frac{\partial \phi}{\partial x} \bigg|_{x=-1} = -1.333, \frac{\partial \phi}{\partial x} \bigg|_{x=0} = 0, \frac{\partial \phi}{\partial x} \bigg|_{x=1} = 2, \frac{\partial \phi}{\partial x} \bigg|_{x=2} = 4, \frac{\partial \phi}{\partial x} \bigg|_{x=3} = 5.333$. As we can see, the error only occurs at the boundaries of the domain.

When the backward projection is implemented in parallel, the computational grid will be decomposed as multiple subgrids. At the boundary of subgrids, the error mentioned in previous paragraphs is introduced. To fix this issue, we first calculate the numerator $\int N_p \nabla \phi d\Omega$ and the denominator $\int N_p d\Omega$ of Eq. E.1 at each subgrid. Then we add the values at the subgrid boundary nodes together to take information from all directions. After this synchronization, we perform a node-wise division to complete the backward projection.