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An Immersed Finite Element Method and its Application to Multiphase Problems

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Abstract

Multiphase flows are frequently encountered in many important physical and industrial applications. These flows are usually characterized by very complicated structure that involves free moving surfaces inside the fluid domain and discontinuous or even singular material properties of the flow. The application range for the multiphase flow phenomena is extremely wide, ranging from processing industry to environmental problems, from biological applications to food industry and so on. Unfortunately, due to the inherent complexity of these problems, their solution proved to be a considerable challenge. Thus, in the many applications, the predictive capability and physical understanding must rely heavily on numerical models.

In this thesis we develop and analyze a finite element based method for the solution of multiphase problems. This thesis consists of four papers. In paper 1 we develop our finite element based method for the elliptic interface problems. The interface jump conditions that are present due to the discontinuity of the coefficients and presence of the singular forces are derived. Using these jump conditions, we enrich the finite element spaces in order to account for the irregularities in the flow. The resulting method was applied to the interface Stokes problem, modeling a thin elastic rubber band immersed in the homogeneous fluid. In order to apply the introduced method, the interface Stokes problem was rewritten as a sequence of three Poisson problems, one for the pressure and two for the velocity components. Paper 2 is an extension of the ideas used in paper 1. Namely, third order Hermitian polynomials are used as basis functions, their modification according to the interface jump conditions is presented and analyzed, both theoretically and numerically. The rigorous error analysis of the introduced method for two-dimensional elliptic problems is presented in paper 3. The results imply that our method is second order accurate in the L^2 norm. Finally, paper 4 concerns with the extension of our method to a coupled interface Stokes problem, that contains both singular forces and discontinuities in the material properties. An application to the Rayleigh-Taylor instability problem is presented.

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Preface

This thesis consists of four papers and an introduction.

Paper I: A.Loubenets, B.Engquist and M.Hanke. *A Non Body-fitted Finite Element Method for Elliptic Interface Problems*, Proceedings of the International Conference on Numerical Analysis and Applied Mathematics, Greece, WILEY-VCH.

The author of this thesis contributed to the ideas, performed the numerical computations and wrote the manuscript.

This paper is also part of the licentiate thesis [3].

Paper II: A.Loubenets, T.Ali and M.Hanke, *Highly accurate finite element method for one-dimensional elliptic interface problems*, Technical Report, TRITA-NA 2007:1, NADA, KTH, 2007. Submitted to Applied Numerical Mathematics, 2007.

The development of the method was done in close cooperation between the authors, all of them contributing in an equal amount. The author of this thesis had the main responsibility for the theoretical derivations and writing the manuscript.

Paper III: M.Hanke and A.Loubenets, *An immersed finite element method and its convergence for elliptic interface problems with discontinuous coefficients and singular sources*, Technical Report, TRITA-NA 2007:3, NADA, KTH, 2007. Submitted to Numerishe Matematiken, 2007.

The author of this thesis contributed to the ideas, performed the mathematical derivations and wrote the manuscript.

Paper IV: A.Loubenets and M.Hanke, *A non-conforming finite element method for interface Stokes problems and its application to two-phase Rayleigh-Taylor instability with solid obstacles*, Technical Report, TRITA-NA 2007:4, NADA, KTH, 2007. In preparation for publication.

The author of this thesis contributed to the ideas, performed the simulations and wrote the manuscript.

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Contents

Chapter 1

Introduction

Multiphase flows are frequently encountered in many important physical and industrial applications. These flows are usually characterized by very complicated structure that involves free moving surfaces inside the fluid domain and discontinuous or even singular material properties of the flow. Almost every processing technology must deal with multiphase flow, from cavitating pumps and turbines to electro-photographic processes, to paper-making, to the pellet form of almost all raw plastics. Multiphase flows are also a ubiquitous feature of our environment whether one considers rain, snow, fog, avalanches, mud slides, sediment transport, debris flows and countless other natural phenomenas. Very critical biological and medical flows are also multiphase, including blood flow, bends, lithotripsy, laser surgery, cavitation and so on.

A persistent theme throughout the study of multiphase flows is the need to model and predict the detailed behavior of those flows and the phenomenas that they manifest. There are three ways in which models are explored: experimentally, theoretically and numerically. Clearly there are some applications in which full scale experimental or theoretical investigation is possible. But, in the many instances, the predictive capability and physical understanding must rely heavily on numerical models and here the inheritent complexity of most multiphase flows presents a major challenge. Consequently, any numerical method designed for the multiphase problems has to include an accurate description of the moving and deforming interface between the phases and has to account for the complex dynamics and the properties of the flow.

This thesis work was motivated by the need in the robust numerical method for the simulation of the multiphase problems that models moving inner boundaries in the incompressible flow of a highly viscous fluid. These equations are a limit case of Navier-Stokes equations where the Reynolds number tends to zero and both convective and the inertial terms are dropped. We will concentrate on the two-dimensional problems in which the interface between the phases exerts a singular force on the fluid.

In paper 1 we develop our finite element based method for the elliptic interface problems. The interface jump conditions that are present due to the discontinuity of the coefficients and presence of the singular forces are derived. Using these jump conditions, we enrich the finite element spaces in order to account for the irregularities in the flow. The resulting method was applied to the interface Stokes problem, modeling a thin elastic rubber band immersed in the homogeneous fluid. In order to apply the introduced method, the interface Stokes problem was rewritten as a sequence of three Poisson problems, one for the pressure and two for the velocity components. Paper 2 is an extension of the ideas used in paper 1. Namely, third order Hermitian polynomials are used as basis functions, their modification

according to the interface jump conditions is presented and analyzed, both theoretically and numerically. The theoretical analysis of the introduced method for two-dimensional elliptic problems is presented in paper 3. The results imply that our method is second order accurate in L^2 norm. Finally, paper 4 concerns with the extension of our method to a coupled interface Stokes problem, that contains both singular forces and discontinuities in the material properties. An application to the Rayleigh-Taylor instability problem is presented.

The initial chapters of this thesis gives a brief background to the topics of these four papers. In Chapter 2 a review of major numerical methods used for the multiphase problems is given. Special attention is given to the immersed interface method (IIM) since it had inspired our work. In Chapter 3, the Rayleigh-Taylor instability problem is introduced. The literature available on this problem is vast, a brief list of references on experimental and theoretical investigations is given. Most popular numerical methods that were applied to the Rayleigh-Taylor instability problem are also discussed. Finally, Chapter 4 contains a short summary of the included four papers. The summaries are a bit more extensive than the corresponding abstracts and are included for the readers convenience.

Chapter 2

Existing numerical methods for the Multiphase problems

In this chapter we review some of the existing numerical methods for multiphase problems and discuss in particular the immersed interface method (IIM).

One of the main difficulties arising when dealing with multiphase problems is the fact that the solution itself is usually non-smooth or discontinuous across the moving inner boundaries. Due to this fact many classical numerical methods designed for smooth solutions perform poorly or do not work at all for this kind of problems. One has also to take care of the topological changes that can occur near the interface between the phases. To summarize, a numerical scheme developed particularly for the multiphase problems should be able to handle the following:

- Discontinuity in the coefficients of the differential equation/system;
- Singularity of the source terms of differential equation/system (Dirac delta function as an example);
- One or several internal moving boundaries, with a changing topology.

Over the years, several approaches have been proposed for this purpose, which can be divided into Eulerian, Lagrangian and mixed Eulerian-Lagrangian methods. With Lagrangian methods, the mesh moves and is distorted as the interface moves. Unfortunately, the topological changes in the interface (merger and break-up) cannot be well captured by this method, unless some re-meshing strategy is employed, which lead to increased computational costs. In the case of the mixed Eulerian-Lagrangian methods, the mesh is updated in the vicinity of the moving interface, with the rest of the mesh being generally kept fixed. The Eulerian approach, makes use of a fixed mesh, together with some additional structure representing the interface.

In this thesis we will consider the Eulerian approach. The first Eulerian models, introduced over 50 year ago are the PIC (particle-in-cell) [20] and the MAC (marker-in-cell) methods [21]. In both methods, marker particles are used to represent the interface.

Those numerical methods that belong to Eulerian family can be further classified as interface tracking or an interface capturing methods. In interface tracking (examples include the immersed boundary method, the immersed interface method, the volume-of-fluid method and the front tracking method) the interfaces are then represented as codimension 1 surfaces moving relative to the fixed grid. In interface capturing methods, such as level-set and phase-field methods, the interface is implicitly represented by a contour of a

particular scalar function, defined over the computational domain. The evolution of the interface is governed by the level set PDE's discretized on fixed, uniform grids. Recently, a large number of hybrid methods that combine interface tracking and interface capturing methods together have appeared as well.

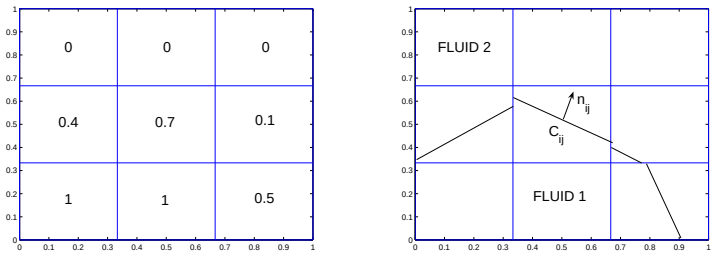
2.1 Interface tracking methods

The volume-of-fluid method

The volume-of-fluid (VOF) method was first reported in Nichols and Hirt [7] and [11]. In this approach, a volume fraction function c is defined. The value of the volume fraction in each grid cell is equal to the ratio of the volume of one of the fluids in this cell, called fluid 1, to the total volume of the grid cell. Thus, c is unity in a cell that lies completely in fluid 1, and is zero if the cell lies completely in the other fluid, called fluid 2. For cells that include an interface (called the interfacial cells), and thus contain both fluid 1 and fluid 2, $0 < \ c \ < 1$, see Figure 2.1. Conversely, given the volume fraction in each grid cell, one can reconstruct an approximate interface, which is called "interface reconstruction". The field c is advected by the flow field, that is

$$c_t + \mathbf{u} \cdot \nabla c = 0.$$

However, due to the discontinuity of the volume fraction function c, a meaningful solution of this equation is not easy. The standard numerical schemes such as for example an upwind finite difference method can easily diffuse the interface, which should remain sharp. One way to overcome this problem is to advect c based on a reconstructed interface determined by the c field. Thus interface reconstruction is a key part of any VOF method. Over the past years, these reconstruction schemes have improved significantly, starting from simple line (piecewise constant) interface reconstruction (SLIC), to piecewise linear (PLIC), piecewise circle [49], piecewise parabolic [23] and piecewise spline interface reconstruction methods [28].



(a) Volume fraction function c_{ij}

(b) Reconstructed interface using PLIC. Here, c_{ij} denotes the volume of fluid 1 in the computational cell Ω_{ij}.

Figure 2.1: Volume of fluid representation of interface

VOF methods are popular and have been used in commercial multiphase flow codes. The principal advantage of VOF methods is their inherent volume conserving property. Unfortunately, spurious bubbles or drops may be created. Because of the discontinuity of the volume fraction c, the computation of geometric quantities such as curvature and

reconstruction of the interfaces from the volume fractions tends to be less accurate compared to other methods. By now, the method has seen larger improvements by many authors, see [48],[57] for a recent reviews of the VOF methods.

The immersed boundary method

The immersed boundary method (IBM) was introduced to study flow patterns around heart valves [9] and has evolved into a generally useful method for multiphase problems. It has been used for many applications, examples include modeling of swimming organisms, platelet aggregation in blood clotting, cochlea dynamics, wood pulp fiber dynamics and many more. See a recent paper of Peskin [8] for a thorough review on the immersed boundary method.

The key idea is to employ a mixture of Eulerian and Lagrangian variables. These are related by interaction equations in which the Dirac delta function plays a prominent role. Numerically, the Eulerian variables are defined on a fixed Cartesian mesh, and the Lagrangian variables are defined on a curvilinear mesh, represented by a set of discrete control points $\{\mathbf{X}_k^n\}$ for $1 \leq k \leq N$ and $t = t^n$. These points move freely through the fixed Cartesian mesh without being constrained to adapt to it in any way at all. The interaction between two meshes comes from the singular force that is exerted by the interface. Namely, the singular force of each control point $\mathbf{F}_k^n$ is spread to the nearby Cartesian grid points near the interface by a discrete delta function so that it yields nonzero force term $\mathbf{F}_k^n$ at grid points near the interface. A typical example of the discrete one-dimensional delta function is

$$\delta_h(x) = \begin{cases} (h - |x|)/h^2, & \text{if} \quad |x| \leq h \\ 0, & \text{otherwise} \end{cases} \tag{2.1}$$

or Peskin's original discrete cosine delta function

$$\delta_h(x) = \begin{cases} (1 + \cos(\pi x/2h)/4h, & \text{if} \quad |x| \leq 2h \\ 0, & \text{otherwise} \end{cases} \tag{2.2}$$

where h is a grid size parameter. The first one is not smooth but the solution obtained using it gives second order accuracy for some one-dimensional problems [46]. The discrete cosine delta function is smooth but the solution is only first order accurate. In higher dimensions, the discrete delta function is often taken as a product of one dimensional discrete delta functions. Then, the numerical approximation of the singular force is given in the form of a sum over the interface elements

$$\mathbf{F}_{ij}(\mathbf{x}) = \sum_k \mathbf{f}_k(t)\delta_h(\mathbf{x}_{ij} - \mathbf{X}_k^n) \tag{2.3}$$

where $\mathbf{f}_k$ is the discrete force density at the point $\mathbf{X}_k^n$ and $\mathbf{x}_{ij}$ is an Eulerian mesh grid point.

After the singular force is approximated the fluid equations can be solved on the Cartesian mesh by a simple finite difference method. The same discrete delta function is used to interpolate the resulting velocity to the control points

$$\mathbf{U}_k^n = \sum_{ij} \mathbf{u}_{ij}(\mathbf{x})\delta_h(\mathbf{x}_{ij} - \mathbf{X}_k^n) \tag{2.4}$$

Finally, the control points are advected by solving

$$\frac{\partial \mathbf{X}_k}{\partial t} = \mathbf{U}_k(\mathbf{X}_k, t) \tag{2.5}$$

by an appropriate method. To summarize, the immersed boundary method involves the following steps

- Given the location of the interface $\mathbf{X}_k^n$ at time t^n compute the force densities $\mathbf{f}_k^n$ at the immersed points.
- Spread the forces $\mathbf{f}_k^n$ to values $\mathbf{F}_{ij}(\mathbf{x})$ on the background grid using (2.3).
- Solve the fluid equations on the regular grid with appropriate boundary conditions to obtain $\mathbf{u}_{ij}^{n+1}$.
- Interpolate the resulting velocities $\mathbf{u}_{ij}^{n+1}$ to the immersed boundary using (2.4) to obtain $\mathbf{U}_k^{n+1}$.
- Move the boundary points $\mathbf{X}_k^n$ to $\mathbf{X}_k^{n+1}$ using the velocities $\mathbf{U}_k^n$ and/or $\mathbf{U}_k^n$ and some discrete approximation to the ODE (2.5).
- Repeat all the steps for next timestep.

The immersed boundary method is fast and simple to implement. Additionally, it is a flexible method that can deal with complex geometries. However, as a trade off the original method is at most first-order accurate (except for a few special cases), due to the smearing effect of the discrete delta function [46] (though some recent work [4] uses adaptive gridding to overcome this limitations). Immersed boundary computations have also been demonstrated to suffer from a high degree of stiffness. In [10] Tu and Peskin recognized the necessity of handling the singular force calculation implicitly and several implicit and semi-implicit schemes were proposed. Unfortunately, in practice, schemes based on the fully implicit equations are extremely expensive since it requires the solution of the nonlinear coupled interface-fluid equations at each time step. Due to their simplicity, the semi-explicit and "approximate implicit" schemes perform much better than the implicit ones, but the time-step restrictions are still severe.

The front-tracking method

This method was introduced by Richtmyer and Morton [40] and further developed by Glimm [32]. For most recent advances see Unverdi and Tryggvason [25] and [51]. The front-tracking method has its roots in the immersed boundary method of Peskin and McQueen [9] and marker-and-cell (MAC) method [21]. The basic idea is very similar to Peskin's approach, that is to use of two grids, see Figure 2.2. One standard, Eulerian finite difference mesh is used to solve the fluid equations. The other is a set of Lagrangian markers, the disretized interface mesh, that is used to explicitly track the interface and compute the singular force which is then transferred to the finite difference mesh via discrete delta-functions. Similar to the immersed boundary method, the interface is represented by a given ordered list of marker particles $\{\mathbf{X}_k^n\}$. The first step in this algorithm is to reconstruct the interface by a list of connected polynomials using the marker list. This gives a parametric representation of the interface. Since both lists are ordered the topology of the interface is uniquely identified. Next, one computes the singular forces defined only along the interfaces. This is done using Peskin's immersed boundary technique. That is, one uses discrete functions (2.1) or (2.2) to distribute the singular forces over the grid points nearest to the interface via (2.3). The same discrete delta functions are used to interpolate the velocity field from the stationary grid to the interface using (2.4).

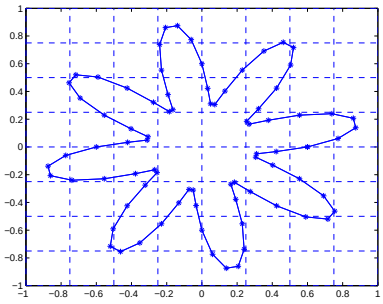


Figure 2.2: Example of the stationary and moving meshes for the front-tracking method. Here the stationary mesh is shown with the dashed lines. The stars mark the positions of the markers and the solid line represents the piecewise linear reconstruction of the interface.

The major novelty in the front-tracking method is the construction of the indicator function $I(\mathbf{x})$ which enables computations with discontinuous material properties. This is done by solving the Poisson equation

$$\Delta I = \nabla \cdot \mathbf{G}$$

where $\mathbf{G}(\mathbf{x})$ is a grid-gradient field generated by spreading the jump in the indicator function by the discrete delta function to the stationary grid. The indicator function is constant within each material region. The primary advantage of this approach is that closed interfaces can interact in a natural way since the gradients simply add or cancel as the grid distribution is constructed from the information carried by the tracked front. Then the fluid properties are easily determined via $\rho(\mathbf{x}) = \rho_1 + (\rho_2 - \rho_1)I(\mathbf{x})$, etc.

The next step is to solve the resulting fluid equations on the Eulerian mesh and interpolate the velocity field on the marker positions. Finally, the advection of the particles is performed by solving equation (2.5).

Front-tracking methods give the precise location and geometry of the interfaces. These algorithms are considered to be very accurate since they can use a large number of grid points on the interface. In addition, front-tracking permits more than one interface to be present in one computational cell without coalescence, which can be important in some applications. Another crucial property of the front tracking method is the ability to handle topological changes. During the computations the interface usually moves and deforms, thus markers tend to deplete in some regions and cluster in other regions. Thus, one has to add or delete some of these markers to maintain regularity. Namely, the distance between the adjacent points, d, is maintained on the order of the stationary grid spacing, h (for example $0.4 < d/h < 0.6$). To accommodate topology changes, interfaces are allowed to reconnect when either parts of the same interface or parts of two separate interfaces come close together. The instantaneous change in topology is, of course, only an approximation of what happens in reality. Since it is not well known at what distance the interfaces will merge, we artificially reconnect the interface when two points come closer than some small distance, l. This distance is chosen rather arbitrarily for lack of a better physical model. But here the advantage of front-tracking is evident since we can control the distance at which the interfaces merge and study the effect of varying l, unlike in some other methods where there is no control over topology changes.

The major disadvantages of front-tracking methods is the difficulty in handling topological changes for three-dimensional simulations and the relative complexity in implementation.

2.2 Interface capturing methods

The level set method

The level set method was first introduced by Osher and Sethian [50] and is a popular computational technique for tracking moving interfaces. The main idea is to rely on a implicit representation of the interface as the zero set of an auxiliary function (level-set function). The first application of this method to incompressible multiphase flows was done by Sussman [39] and Chang [58]. A review of level set method with an emphasis on applications to multiphase problems was given by Smereka and Sethian [29].

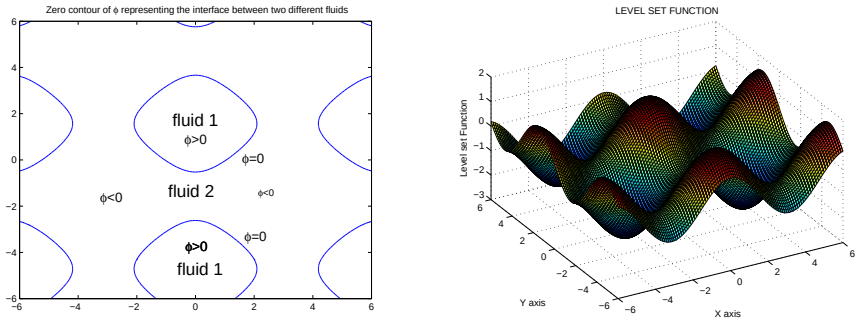
The level set function $\phi(\mathbf{x}, t)$ is defined as follows

$$\phi(\mathbf{x},t) = \begin{cases} > 0, & \text{if } \mathbf{x} \in \text{ fluid 1} \\ = 0, & \text{if } \mathbf{x} \in \Gamma \text{ (the interface between fluids)} \\ < 0, & \text{if } \mathbf{x} \in \text{ fluid 2} \end{cases}$$

and the evolution of ϕ is given by the level set PDE

$$\phi_t + \mathbf{u} \cdot \nabla \phi = 0,$$

meaning that the interface moves with the fluid (see Figure 2.3 for an example of the level set function). To keep the interface geometry well resolved, the level-set function is required to



(a) Zero contour of ϕ representing the interfaces. (b) Level set function $\phi = \cos(x) + \sin(y) - 0.5$

Figure 2.3: Example of the level set function

be a distance function near the interface. However, under the evolution ϕ will not necessary remain as such. Typically, a reinitilization step (solving a Hamilton-Jacobi type equation) is performed to keep ϕ as a distance function near the interface while keeping the original zero level set unchanged. Namely, given ϕ at time t, the contours are redistributed by finding the steady state solution of the equation

$$\frac{\partial d}{\partial \tau} = S_\epsilon(\phi)(1 - |\nabla d|), \quad d(\mathbf{x}, 0) = \phi(\mathbf{x})$$

where S_ϵ is the smoothed sign function defined as

$$S_\epsilon(\phi) = \frac{\phi}{\sqrt{\phi^2 + \epsilon^2}},$$

where ϵ is usually equal to one or two grids lengths. After solving the above equations to steady state $\phi(\mathbf{x}, t)$ is then replaced by $d(\mathbf{x}, \tau_{\text{steady}})$. The density and viscosity are defined as

$$\rho(\phi) = \rho_2 + (\rho_1 - \rho_2)H_\epsilon(\phi) \quad \text{and} \quad \mu(\phi) = \mu_2 + (\mu_1 - \mu_2)H_\epsilon(\phi)$$

where $H_\epsilon(\phi)$ is the smoothed Heaviside function given by

$$H_\epsilon(\phi) = \begin{cases} 0 & \text{if } \phi < -\epsilon \\ 0.5(1 + \phi/\epsilon + \sin(\pi\phi/\epsilon)/\pi) & \text{if } |\phi| \leq \epsilon \\ 1 & \text{if } \phi > -\epsilon \end{cases}$$

The mollified delta function is $\delta_\epsilon(\phi) = dH_\epsilon/d\phi$. The surface tension force is given as

$$\mathbf{F}_{\text{sing}} = -\tau\nabla \cdot \Big(\frac{\nabla\phi}{|\nabla\phi|}\Big)\delta_\epsilon(\phi)\frac{\nabla\phi}{|\nabla\phi|}$$

Finally, the fluid equations are solved with some appropriate method.

Advantages of the level-set algorithm include the simplicity of implementation, the inherited ability to capture topological changes of interfaces and ease with which the intrinsic properties of the interface (such as curvature, normal, etc.) can be obtained from the level-set function. A well-known drawback of the level set method is that mass is not conserved.

The phase-field method

Phase field, or diffuse-interface, models are another popular technique that belongs to the family of interface capturing methods. For a recent review see [19]. The main idea is to replace sharp fluid interfaces by thin but nonzero thickness transition regions where the interfacial forces are smoothly distributed. The idea is to introduce a conserved order parameter, for example mass concentration, that varies continuously over thin interfacial layers and is mostly uniform in the bulk phases.

The phase field is governed by the following advective Cahn-Hilliard equation

$$\begin{aligned} \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot \Big(M(c)\nabla\mu\Big), \\ \mu = F'(c) - \epsilon^2\Delta c \end{aligned} \tag{2.6}$$

where $M(c) = c(1-c)$ is the mobility, $F(c) = 0.25c^2(1-c)^2$ is a Helmholtz free energy that describe the coexistence of immiscible phases, and ϵ is a measure of interface thickness. It can be shown that in the sharp interface limit $\epsilon \Rightarrow 0$, the classical Navier-Stokes equations and jump conditions are recovered [35]. The singular surface tension force is $\mathbf{F}_{sing} = -6\sqrt{2}\tau\epsilon\nabla \cdot (\nabla c \otimes \nabla c)$, where τ is the surface tension coefficient [35].

The main advantages of the phase-field method are: topological changes are automatically described and the composition field c has a physical meaning both in the bulk phases and near the interface. It is also easy to incorporate complex physics into the framework, thus the phase-field methods are straightforwardly extended to multicomponent systems, where miscible, immiscible and partially miscible phases can be modeled. Unfortunately, for some case the numerical solution can be computationally expensive to obtain.

2.3 Hybrid methods

Recently, a number of hybrid methods that combine good features of each algorithm, have been developed. These include coupled particle level-set methods, level-set VOF algorithms, marker and VOF methods.

In the particle level-set method [15], Lagrangian disconnected marker particles are randomly positioned near the interface and are passively advected by the flow in order to rebuild the level set function in underresolved zones, such as high curvature regions. In these regions, the standard non-adaptive level-set method regularizes excessively the interface structure and mass is lost. The use of the Lagrangian markers significantly decreases these difficulties.

VOF and level-set methods have been combined in [38] and [37]. The level-set function is used to describe the geometry of the interface while VOF is used to maintain volume conservation properties. Both functions are made compatible after every time step. The coupling between the volume fraction function c_{ij} and level-set function ϕ occurs through the normal of the reconstructed interface and through the fact that the level-set function is reset to the exact signed normal distance to the reconstructed interface.

The hybrid method that uses both VOF and marker particles is developed in [1]. As usual, the volume fraction function is used to assure mass conservation while marker particles are used to reconstruct and move the interface. As a result, one achieves a smooth motion of the interface, typical for all marker methods, together with volume conservation, which is standard for VOF methods. Thus, this approach increases both the accuracy of interface tracking, when compared to standard VOF methods, and the conservation of mass, with respect to original marker method.

2.4 Immersed interface method and its extensions

The immersed interface method (IIM) was first introduced by LeVeque and Li in [42] as a finite difference type method for elliptic equations

$$\nabla \cdot (\beta(x,y)\nabla u) + k(x,y)u = f \quad (x,y) \in \Omega$$

with the interface Γ being an arbitrary piecewise smooth curve such that $\Omega = \Omega^+ \cup \Omega^- \cup \Gamma$, discontinuous coefficients $\beta(x,y)$, $k(x,y)$ across the interface

$$\beta(x,y) = \begin{cases} \beta^+(x,y) & \in \Omega^+ \quad \text{(outer part)} \\ \beta^-(x,y) & \in \Omega^- \quad \text{(inner part)} \end{cases} \qquad k(x,y) = \begin{cases} k^+(x,y) & \in \Omega^+ \\ k^-(x,y) & \in \Omega^- \end{cases}$$

and a singular force f.

Similar to IBM and front-tracking methods, the immersed interface method employs two different meshes: a fixed mesh for the fluid equations and a moving one for the interface representation. However, it seemed unlikely [46] that the discrete delta function approach can achieve second order or higher accuracy in two or three dimensional problems (except for a few special situations when the grid is aligned with the interface). Thus, the key idea of the IIM is to avoid the discretisation of the delta function by introducing the explicitly calculated jump conditions directly into the finite difference stencil. To do that, the finite difference stencil was modified, such that the grid points on either side of the interface are used. Namely, the standard finite difference approximation was rewritten as

$$\sum_k \gamma_k u_{i+i_k, j+j_k} + k_{ij} u_{ij} = f_{ij} + C_{ij}$$

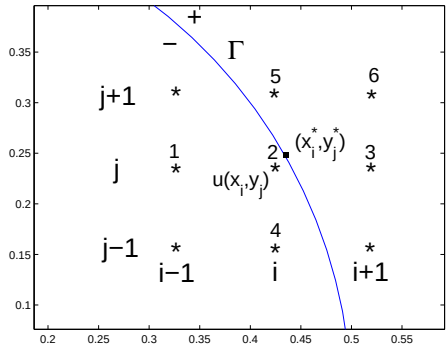


Figure 2.4: The geometry near the modified stencil. The coefficients γ_1 through γ_6 will be determined in the labeled points.

for every grid point (x_i, y_j). The sum over k involves a finite numbers of points neighboring (x_i, y_j) (at most six in the derived formula). So each i_k, j_k will take a value in the set $\{-1, 0, 1\}$. If the interface does not lie between any points in the standard 5-point stencil centered in (x_i, y_j) no modification is needed for γ_k and $C_{ij} = 0$. For the rest of the grid points the modified coefficients γ_k are determined by requiring truncation error at these points to be of order $O(h)$. It turns out to be sufficient to require $O(h)$ truncation error since the interface forms a lower dimensional set.

To obtain γ_k , the functions $u_{x_i,y_{j\pm1}}$,$u_{x_{i\pm1},y_j}$ and u_{x_i,y_j} were expanded in Taylor series at some point (x_i^*, y_j^*) on the interface (which is usually the closest point to (x_i, y_j)). Extra attention is paid in order to use the limiting values of derivatives of u from the correct side of the interface. As an example, in the configuration shown on Figure 2.4, one would obtain

$$u(x_i, y_j) = u^- + u_x^-(x_i - x^*) + u_y^-(y_j - y^*) + \frac{1}{2}u_{xx}^-(x_i - x^*)^2 + \frac{1}{2}u_{yy}^-(y_j - y^*)^2 + u_{xy}^-(x_i - x^*)(y_j - y^*) + O(h^3)$$

and

$$u(x_{i+1}, y_j) = u^+ + u_x^+(x_{i+1} - x^*) + u_y^+(y_j - y^*) + \frac{1}{2}u_{xx}^+(x_{i+1} - x^*)^2 + \frac{1}{2}u_{yy}^+(y_j - y^*)^2 + u_{xy}^+(x_{i+1} - x^*)(y_j - y^*) + O(h^3)$$

After inserting this expansions at each point in the difference equation one can express the local truncation error as a linear combination of the values $u^\pm$, $u_x^\pm$, $u_y^\pm$, $u_{xx}^\pm$, $u_{yy}^\pm$ and $u_{xy}^\pm$. The idea now is to eliminate all values on one side, say the values on $+$, in terms of the values on the other side, say $-$ side. That is done with the help of interface jump conditions

$$[u] = u^+ - u^- = G(x, y) \quad \text{and} \quad \left[\beta\frac{\partial u}{\partial n}\right] = \beta^+\frac{\partial u^+}{\partial n} - \beta^-\frac{\partial u^-}{\partial n} = H(x, y)$$

where $\partial/\partial n$ represents a differentiation in normal direction. Differentiating these jump conditions and manipulating the results allows to perform the desired elimination. In order

to do this, it turns out to be very convenient to perform a local coordinate transformation into normal and tangential directions to the interface.

Once the local truncation error is expressed as a linear combination of the values $u^{\pm}$, $u_x^{\pm}$, $u_y^{\pm}$, $u_{xx}^{\pm}$, $u_{yy}^{\pm}$ and $u_{xy}^{\pm}$, we must require that the coefficient of each of these terms vanish in order to achieve an $O(h)$ truncation error. This gives a system of six equations to determine the unknown coefficients γ_k. Thus, we require six points in the stencil: a 5-point stencil together with one additional point. To summarize, in order to determine a modified stencil we need to do the following

- Select a point $(x_i^*, y_j^*) \in \Gamma$ near (x_i, y_j).
- Apply a local coordinate transformation in directions normal and tangential to Γ at (x_i^*, y_j^*).
- Derive the jump conditions relating u^+ and u^- (and their derivatives) at (x_i^*, y_j^*) in the local coordinates.
- Choose an additional point to form a 6-point stencil.
- Set up and solve a linear system of six equations for the coefficients γ_k. The value of C_{ij} is also obtained.

Finally, the resulting linear system is solved then with some appropriate method. The method has been successfully used in several applications and extended in different directions, notably to hyperbolic and parabolic problems. Li applied the IIM idea to heat equations in 2D with fixed interfaces, followed by his dissertation [61] where IIM was applied to some 3D partial differential equations. LeVeque and Li used IIM for Stokes interface problem in 2D [42]. In [62] and [6] the method was extended to treat nonlinear problems.

However, the original method suffered from lack of fast solvers and strong dependence of the error on the relative position of interface and grid even for moderate contrast in the coefficients. In the original paper [43], the discontinuities in the coefficient were always "mild" (the quotient between β's on different sides of the interface was always $0.1 \leq \beta^+/\beta^- \leq 10$).

In [63] Li introduced a Fast Iterative IIM (FIIIM). Li used the observation that for piecewise constant coefficients, the equation can be written as a Poisson equation by dividing through the coefficient, if in addition one observes the jump condition across the interface. This leads naturally to the idea of splitting the finite differences near the interface into standard differences and corrections to the standard differences, and brings the FIIIM closer to Peskin's immersed boundary method. The jumps in the function and its derivatives (not jumps in the flux $[\beta u_n]$) turn out to be crucial quantities. Given the jumps, the FIIIM needed only corrections to the right hand side. Li chose to do that in the spirit of the original IIM, by selecting a point on the interface and developing Taylor expansions about it on both sides of the interface. Another question was how to find the jumps. To do that, Li used the equations for the jumps based on local properties of the solution derived in [42]. The jumps were computed only at the fixed set of control points and then interpolated.

It was shown in [26] and [2] that stability of the original algorithm depends on the choice of one or more extra grid points in addition to the standard five-point stencil. In other words, it is not always guaranteed that the original IIM will converge and satisfy the maximum principle. To eliminate this problem, Li and Ito proposed a modification to the original approach [66]. The new method was to guarantee that the discrete maximum principle is satisfied.

The original spline representation of the interface was replaced with a level set method by Hou, Li, Osher and Zhao which allowed to compute moving interface problems with

topological changes [54]. This formulation was used to study electron migration in [67] and applied to Stefan problems in [65]. IIM was combined with a multigrid approach by Adams in [34]. LeVeque and Zhang used IIM for hyperbolic systems of partial differential equations with discontinuous coefficients arising from acoustic or elastic problems in heterogeneous media [44],[12]. Calhoun [14] and LeVeque and Calhoun [45] extended the IIM to a stream-function vorticity formulation of incompressible flow in 2D.

The recent advances include a finite element formulation of IIM for 1D and 2D elliptic interface problems with discontinuous coefficients [64], [68]. For complete review on IIM and its applications see [66].

Chapter 3

The Rayleigh-Taylor instability problem

The flow situation considered in paper IV of this thesis is a variation of the classical viscous Rayleigh-Taylor (RT) flow problem that is often used in the literature to evaluate the performance of different interface tracking numerical methods. Physically, the RT problem is a fingering instability of an interface between two or more stratified fluids of different density subjected to acceleration, or in a vertical gravitational field. The interface becomes unstable for certain perturbations and these perturbations evolve into spikes of heavy fluid and bubbles of light fluid which penetrate into both fluids. This type of instability occurs in diverse applications, including mantle and lithosphere dynamics, diapirism, post-glacial rebound and many others. The experimental and analytical investigations of this instability were performed by, among others, Lewis [17], Chang and Watson [27], Daff, Harlow and Hirt [41], Popil and Curzon [47], Gertsenstein and Cherniavskii [53], Danilov and Omelyanov [55],[56] , and Barnes [30]. It has been shown that the evolution of a RT instability is a complex phenomenon that involves formation and detachment of droplets, development of a Helmholtz instability on the side of the penetrating spikes, competition and amalgamation among the rising bubbles and etc. The behavior of the classical RT instability problem (without solid obstacles) is usually divided into four separate stages [16]. The first stage is dominated by the small growth of the perturbations. As analyzed by the linear stability theory, the growth rate depends on the fluids density gradient, viscosities, surface tension and compressibility (if applicable). The linear theory is no longer applicable after the perturbation grows to more than $10 - 40\%$ of its original size. The second stage is characterized by the nonlinear perturbation growth, formation of the bubbles of light fluid threading through heavy fluid and emergence of the spikes of the heavy fluid that falls into the light fluid. During this stage, the nonlinear growth of perturbations is strongly influenced by the density ratio and three-dimensional effects. Interactions and amalgamations among the bubbles and the mushroom-shaped spikes are characteristics of this stage. Finally, this interaction evolves into a turbulent or chaotic mixing which dominates the fourth stage of the instability. In this final stage, phenomena such as the penetration of a bubble through a slab of fluid of finite thickness, necking, breakup of the spikes by various mechanism, and other complicated, topology related effects take place.

Since then, many numerical methods have also been developed and applied to study this phenomena. Fraigneau *et al.* [59] developed an Eulerian method for simulating variable density incompressible viscous flows. They compared the finite element method and finite volume method for the RT problem in the viscous regime for two different Reynolds numbers. It was shown that, even at moderate Reynolds numbers, this problem is very sensitive to the numerical method used and, in particular, to the mesh refinement algorithm.

Rudman [36] used an algorithm for volume tracking based on the concept of flux-corrected transport (FCT) to solve the RT flow problem. He also compared his method with three other techniques: the simple line interface calculation (SLIC) method, the VOF method of Hirt and Nichols [11] and Young's method [18].

Zhao *et al.* [60] solved the incompressible Navier-Stokes equations for two superimposed viscous fluids on unstructured grids with the finite volume method. The free surface was computed with the VOF method and the surface tension was taken into account. The motion of the characteristic RT mushroom shape of the interface was studied at $Re = 283$. See [48] and [57] for the further references on VOF methods applied to RT instability.

Popinet and Zaleski in [52] revisited the work of Puckett *et al.* [22] and solved the RT flow problem with the front-tracking technique. A source term was added to account for the surface tension forces as well. Glimm *et al.* have successfully applied front-tracking method to three dimension, as well as extending the front tracking capabilities to deal with the topological changes in the interface [31]. Similar work has been done by Tryggvason and Unverdi in [25], [51] and [24].

Level set method has also been extensively used in the simulation of the RT flow problems, see [5] and [33] for further references.

Chapter 4

Summary of Papers

4.1 Paper I: A Non Body-fitted Finite Element Method for Elliptic Interface Problems

In this paper, we present a new finite element method for two-dimensional elliptic interface problems. Due to the presence of these interfaces the problem will contain discontinuities in the coefficients and singular source terms that are represented by delta functions along the interface. As a result, the solution to the interface problem and its derivatives may have jump discontinuities. The new method is specifically designed to handle this feature of the solution in the context of non-interface fitted grids.

Our method is based on the Immersed Interface Method (IIM) that was first introduced by LeVeque and Li in [42] as a second order accurate finite difference type method for solving elliptic equation whose solution is not smooth across the interface, due to discontinuous coefficients or singular source terms in the equation. The main idea of the original IIM was to incorporate the known jumps in the solution or its derivatives into the finite difference scheme, obtaining a scheme with the modified stencil whose solution is second order accurate at all points on the uniform Cartesian mesh even for arbitrary interfaces. This approach has been extended to parabolic and hyperbolic equations, and successfully applied to many applications, see Chapter 2 for a brief review. Most important for us are Li's papers [64] and [68] where he presented a finite element immersed interface method for one and two-dimensional elliptic problems involving discontinuities in the coefficients. As a consequence of the discontinuity in the coefficients, the solution to those problems is a continuous function that has a jump in the flux. To account for this discontinuity, Li proposed to construct specific basis functions such that the interface jump conditions for the solution and its flux are satisfied either exactly or approximately.

However, in the case of most general elliptic interface problem with both discontinuities in the coefficients and singularities in the source terms, i.e. delta functionals and its derivatives, the solution itself is discontinuous. Thus the original finite element IIM proposed by Li cannot be applied. To improve the capabilities of the method, we use the fact that the problems we are dealing with are linear and that we can always identify the source of the discontinuity in the solution or its derivative. In other words, all information that is needed to evaluate the jump conditions is extracted from the position of the interface together with the equations itself. Using these explicitly known values of the jumps we can calculate the solutions to the simple problems and thus the solution to the original problem. The discretization of the method is based on simple piecewise-linear polynomials on a uniformly triangulated domain. Note that the mesh is not aligned with the interface. Thus there

is almost no cost for such grid generation, which is very significant for moving interface problems. This simple modification allows us to extend Li's approach to a much broader class of interface problems. Numerical results are presented, showing that the method is capable of second order convergence in L^2.

The modified method has also been applied to the Stokes interface problem, modeling an elastic band immersed in the homogeneous fluid. We rewrite Stokes equations as a sequence of three Poisson problems, one for each variable. Namely, by applying the divergence operator to the momentum equations, adding them together and using the incompressibility condition we get the Poisson equation for the pressure p. Once the pressure is known, the momentum equations become independent Poisson problems for u and v. Thus the techniques developed for the elliptic interface problems can be applied directly.

Since the flow is considered to be homogeneous, the jumps in the solution result only from the singularity of the source function, which represent an elastic force along the interface. This singular force leads to jumps in derivatives of u and v. The Poisson problem for the pressure involves derivatives of this source term, and hence a dipole. As a result, the pressure will be discontinuous along with its derivatives. Similar to the model elliptic interface problems, the magnitude of the jump conditions is derived solely from the equations and the location of the interface, without a-priori knowledge of the solution.

The interface is described by a given set of discrete control points $\{\mathbf{X}_i(s,t)\}$, together with a parametric description connecting them. Time evolution of the interface is accomplished by moving these control points using an additional constraint that the interface must move with the fluid.

Our approach differs from that of Li in several ways. The fundamental difference is our treatment of the interface problem via the superposition principle. This improves the applicability of the method greatly by allowing to treat both singular source terms and discontinuous coefficients at the same time. There are other differences as well. Our derivation of the jump conditions is based on comparing the variational formulation obtained from the classical formulation of the problem with the one obtained from the distributional formulation. To our knowledge, it is also first time that finite element IIM was applied to the interface Stokes problem.

4.2 Paper II: Highly accurate finite element method for one-dimensional elliptic interface problems

In paper II, we present and investigate a finite element method based on cubic Hermitian basis functions that takes into account the non-smoothness of the solution and thus does not suffer from the presence of discontinuities/singularities in the problem. The main idea is to calculate the jump conditions at the interface point explicitly and modify the basis functions in the vicinity of the interface such that these jumps are being accounted for. By using the cubic Hermitian polynomials, we do not only obtain a higher order of convergence but also maintain continuity in the first derivative of the numerical solution. Derivation of jump conditions and modification of cubic basis functions is done in the spirit of paper I.

The theoretical investigation of the proposed method has been carried out. It has been proven that the method is forth order accurate in L_2 norm. The strategy of the proof resembles the idea behind the proov of smooth solutions. Namely, we determine the order in the case of approximation of the interpolant of the solution in given finite element space and apply the Cea's lemma and Galerkin orthogonality condition to find the order of the convergence in H_0^1. Finally, we apply the Nitsche's trick to gain one order of convergence in L^2. The critical point in the proof is that, in the present case, the solution

does not fulfill the necessary regularity conditions. Therefore, it is crucial to use the details of the construction of our finite element space. For simplicity, the both theoretical and numerical results are presented only for the case of one interface point α, but the approach is easily extended to any number of the interface points. Note, that the proposed method uses a simple uniform Cartesian mesh, which is a very desirable property if we consider a multidimensional interface problem. The presented numerical results agree well with the theoretical analysis.

4.3 Paper III: An immersed finite element method and its convergence for elliptic interface problems with discontinuous coefficients and singular sources

This paper is concerned with the analysis of an immersed finite element method for two dimensional elliptic interface problems. The elements of the partition are separated in two classes, the one that are intersected by the interface and the rest. On the non-intersected elements we use the standard linear polynomials. On the intersected elements we use the strategy similar to that of the Hsieh-Clough-Tocher macro-element [13]. That is, each intersected element is subdivided by the interface in two subdomains. Then, we construct a C^0 function consisting of piecewise linear polynomials such that the element has a total of 4 degrees of freedom. At the vertices of the original element, we specify the function values. The additional degrees of freedom are satisfied by the approximation of the jump conditions. Since this procedure involves subpartition of the original triangle, we can regard the intersected elements as macro-elements. The resulting immersed finite element space is, in general, non-conforming. It is shown that the presented method is second order accurate in L^2 norm. This investigation should be regarded as a critical step towards analyzing the error of the immersed finite element method applied to the Stokes and Navier-Stokes problems. Numerical results are also presented, showing good agreement with the theoretical findings.

4.4 Paper IV: A non-conforming finite element method for interface Stokes problems and its application to two-phase Rayleigh-Taylor instability with solid obstacles

In paper IV we aim at extending the capabilities of the immersed interface finite element method that was developed and analyzed for the elliptic interface problems (Papers I-III and [64] ,[68],[3]). This extension should allow our method to handle the Stokes interface problems. In addition, solid obstacles are included in the computational domain. That should be regarded as a first step in a practical direction of having suspensions in the flow. Note, that in reference [3] the interface Stokes problem is solved by decoupling the equations into three separate Poisson problems, one for pressure and two for the velocity components. That was possible due to the periodic boundary conditions that were used and homogeneity of the physical fields. In the present work, the Stokes equations are not decoupled, the physical fields are discontinuous and singular source terms are present.

The capability of the method is illustrated in the case of a Rayleigh-Taylor two-phase flow instability problem with solid obstacles governed by the Stokes equations. It has been shown that the method can handle well both the discontinuity of the physical fields and singular forces. The method proved to be of second order accuracy and mass conservative. Based on the numerical experiments, a qualitive description of the interface dynamics for the

considered test cases has been given. The numerical results suggested that the discretization errors are systematically amplified by the instability of the problem at hand, and thus affect, in the long run, both the convergence results and the symmetry of the solution. The symmetry preserving version of the method has also been proposed and successfully tested.

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