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Numerical Methods for the Navier– Stokes Equations applied to Turbulent Flow and to Multi-Phase Flow

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Stokes Equations applied to Turbulent
Flow and to Multi-Phase Flow**

BY
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December 2009

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UPPSALA UNIVERSITY
UPPSALA
SWEDEN

Dissertation for the degree of Licentiate of Philosophy in Scientific Computing with
specialization in Numerical Analysis
at Uppsala University 2009

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Stokes Equations applied to Turbulent
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ISSN 1404-5117

Printed by the Department of Information Technology, Uppsala University, Sweden

Abstract

This thesis discusses the numerical approximation of flow problems, in particular the large eddy simulation of turbulent flow and the simulation of laminar immiscible two-phase flow. The computations for both applications are performed with a coupled solution approach of the Navier–Stokes equations discretized with the finite element method.

Firstly, a new implementation strategy for large eddy simulation of turbulent flow is discussed. The approach is based on the variational multiscale method, where scale ranges are separated by variational projection. The method uses a standard Navier–Stokes model for representing the coarser of the resolved scales, and adds a subgrid viscosity model to the smaller of the resolved scales. The scale separation within the space of resolved scales is implemented in a purely algebraic way based on a plain aggregation algebraic multigrid restriction operator. A Fourier analysis underlines the importance of projective scale separations and that the proposed model does not affect consistency of the numerical scheme. Numerical examples show that the method provides better results than other state-of-the-art methods for computations at low resolutions.

Secondly, a method for modeling laminar two-phase flow problems in the vicinity of contact lines is proposed. This formulation combines the advantages of a level set model and of a phase field model: Motion of contact lines and imposition of contact angles are handled like for a phase field method, but the computational costs are similar to the ones of a level set implementation. The model is realized by formulating the Cahn–Hilliard equation as an extension of a level set model. The phase-field specific terms are only active in the vicinity of contact lines. Moreover, various aspects of a conservative level set method discretized with finite elements regarding the accuracy of force balance and prediction in jump of pressure between the inside and outside of a circular bubble are tested systematically. It is observed that the errors in velocity are mostly due to inaccuracies in curvature evaluation, whereas the errors in pressure prediction mainly come from the finite width of the interface. The error in both velocity and pressure decreases with increasing number of mesh points.

List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

- I V. Gravemeier, M. W. Gee, M. Kronbichler, and W. A. Wall (2009) An algebraic variational multiscale–multigrid method for large eddy simulation of turbulent flow. Accepted for publication in *Computer Methods in Applied Mechanics and Engineering*. doi:10.1016/j.cma.2009.05.017.
Contributions: Initial implementation of the method together with the first and second author. Preparation of a draft of the manuscript, in particular section 2. Ideas were developed in close cooperation between the authors.
- II V. Gravemeier, M. Kronbichler, M. W. Gee, and W. A. Wall (2009) An algebraic variational multiscale–multigrid method for large-eddy simulation: generalized- α time integration, Fourier analysis and application to turbulent flow past a square-section cylinder. Submitted to *Computers and Fluids*.
Contributions: Ideas and analysis in section 3. Preparation of a draft of the manuscript and final work in close cooperation between the authors.
- III M. Kronbichler and G. Kreiss (2008) A Hybrid Level–Set–Cahn–Hilliard Model for Two-Phase Flow. In *Proceedings of the 1st European Conference on Microfluidics*, Bologna, Italy.
Contributions: Implementation of the method and computations. Preparation of the manuscript. Ideas were developed in discussion with the co-author.
- IV S. Zahedi, M. Kronbichler, and G. Kreiss (2009) Evaluation of inaccuracies in two-phase flow simulations with level set methods using finite element discretizations. Technical Report 2009-026, Department of Information Technology, Uppsala University, 2009. Submitted to *Computers and Fluids*.
Contributions: Implementation of and experiments with the coupled two-phase flow solver. First draft of the manuscript. Ideas were developed by close cooperation between the first and the second author in discussion with the third author.

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1. Introduction

The numerical simulation of fluid dynamics is one of the main fields in computational mathematics. Simulation is today both an alternative and a complement to experiments in many engineering disciplines as it helps in predicting the behavior of fluids. Moreover, simulation permits to systematically improve the design and material properties of products by means of optimization algorithms. Such a procedure would be tremendously expensive if it had to be done by prototyping and other experimental means. Simulation is thus a tool that renders technical processes more effective.

One interesting area of research in fluid dynamics is the behavior of turbulent incompressible flow. Turbulent flows often occur in engineering applications, for example, in the air flow around a vehicle, the water flow in turbines of hydroelectric power plants as well as in water networks and oil pipelines with high throughput. For instance, relevant issues are the determination and the control of aerodynamic drag as well as efficiency of engines.

Another area of active research is multiphase flow, a setting that involves two or more different fluids. There is a wide range of applications that involve multiple fluids and where numerical simulation is extensively used. An exceptionally challenging problem is computational combustion, where different fluids and flame fronts need to be represented. Often, the flows occurring in combustion are turbulent. But there are also a lot of multi-phase settings where the flow field is laminar and thus more regular. One such application is intravenous therapy in medicine. The objective of numerical simulations is to understand how bubbles consisting of oleaginous substances are transported and resolved in the circulation of blood. These processes are often strongly driven by surface tension, a force that strives after keeping different fluids separated. A similar application is the modeling of the absorption of air in the blood circulation in human lungs.

Multiphase flow is a phenomenon that is particularly relevant also in subsurface flow. In this area, it is often assumed that the individual fluids are well-separated, that is, the fluids do not mix and there are no additional particles resolved in the fluids. This thesis contributes to the simulation of such laminar well-separated two-phase flows. For subsurface flows, an additional difficulty arises, namely the interaction of systems consisting of different fluids with solids, called capillarity. This interaction takes place on so-called contact lines, locations where the interface (separating two fluids) meets a solid. The properties of the solid and the composition of the fluid give rise to a phenomenon called wetting, indicating which fluid preferably is in contact with the solid. Applications of this kind are the modeling of groundwater basins and oil extraction

from subsurface reservoirs driven by water injection. The pores of rock where the fluid moves are often of the order of a few millimeters or less, whereas the actual simulation region can extend over thousands of square kilometers. In order to tackle problems with such an enormously wide range of scales, simplifications need to be applied. One example is to perform small-scale flow simulations with detailed rock structures in order to determine the permeability of various stone configurations. Such effective parameters are then used as input to a large scale simulation, usually based on Darcy's law [17]. Other applications of multiple fluids in contact with solids are found in industrial processes like sintering, where mixtures of different fluids and their solidification are tracked; lab-on-a-chip processes, which form the basic component for microsystem design in the biomedical industry; and inkjet printing.

This thesis consists of five chapters. First, we discuss the equations that describe the flow of individual fluids, the Navier–Stokes equations. Next, an introduction to turbulence is given, which is followed by a presentation of numerical models for the simulation of laminar two-phase flow. Chapter 5 gives a short summary of the papers included in this thesis, and Chapter 6 identifies possible directions of future research.

2. Numerical Methods for the Navier–Stokes Equations

The motion of fluids at low and medium velocities in a connected computational domain $\Omega \subset \mathbb{R}^d$ (spatial dimension $d = 2, 3$) is given by the *incompressible Navier–Stokes equations* [35], [62], [73],

$$\rho (\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) - \nabla \cdot (2\mu \boldsymbol{\varepsilon}(\mathbf{u})) + \nabla p = \rho \mathbf{f}, \quad (2.1)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (2.2)$$

The vector \mathbf{u} denotes the d components of fluid velocity and p denotes the fluid's (dynamic) pressure. The rank-2 tensor $\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ represents the viscous stress tensor for a Newtonian fluid. The fluid density is denoted by ρ , and the fluid's (dynamic) viscosity by μ . In single-phase fluids, density is constant due to the incompressibility assumption. The term \mathbf{f} specifies external forces acting on the fluid.

The system of Navier–Stokes equations (2.1)–(2.2) is completed by a divergence-free initial velocity field,

$$\mathbf{u}(\cdot, 0) = \mathbf{u}_0, \quad \text{with} \quad \nabla \cdot \mathbf{u}_0 = 0, \quad (2.3)$$

and application-specific boundary conditions (cf. Gresho and Sani [32] for a discussion of various possibilities). In this thesis, we consider flow subject to no-slip boundary conditions

$$\mathbf{u} = 0 \quad \text{on} \quad \Gamma_g \subset \partial\Omega, \quad (2.4)$$

and natural (inflow/outflow) boundary conditions

$$\mathbf{n} \cdot \boldsymbol{\varepsilon}(\mathbf{u}) + p \mathbf{n} = \mathbf{h} \quad \text{on} \quad \Gamma_h \subset \partial\Omega, \quad (2.5)$$

where \mathbf{n} denotes the unit outer normal on the domain boundary Γ_h and \mathbf{h} is some external traction boundary force. The boundary subdomains Γ_g and Γ_h are assumed to be non-overlapping and to span the whole boundary $\partial\Omega$.

For the numerical approximation of the equations of fluid flows, there are various methods available. The most popular ones are the finite volume method, the finite difference method, and the finite element method. A comparative introduction of these methods can be found in Quartapelle [74].

The algorithms developed in this thesis are based on the finite element method (FEM). There is a vast literature discussing various aspects of the finite element discretization of system (2.1)–(2.2). Mathematical aspects are

discussed, e.g., in Glowinski [28] and Gunzburger [35]. The book by Gresho and Sani [32] focuses on practical issues for implementation such as boundary conditions, discretization schemes, and stabilization. The work by Elman, Silvester & Wathen [23] and Turek [88] put special emphasis on algorithmic matters like efficient numerical linear algebra for the flow equations.

2.1 Weak form and spatial discretization

The Navier–Stokes equations (2.1)–(2.2) depend on both space and time. Most discretization approaches split the approximation into separate approximations for spatial and temporal part.

For setting up the spatial FE approximation, the first step is to rewrite the system of equations (2.1)–(2.2) in variational form. To this end, we define the space of admissible velocity solutions at a certain time instant by $\mathcal{V}_{\mathbf{u}} = \{\mathbf{u} \in H^1(\Omega); \mathbf{u} = 0 \text{ on } \Gamma_w\}$, and the space of admissible pressure solutions by $\mathcal{V}_p = L_2(\Omega)$. The variational problem corresponding to (2.1)–(2.2) is to find, at each instant in time, a pair $(\mathbf{u}(\cdot, t), p(\cdot, t)) \in \mathcal{V}_{\mathbf{u}} \times \mathcal{V}_p$ such that

$$(\mathbf{v}, \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}))_{\Omega} + (\varepsilon(\mathbf{v}), \mu \varepsilon(\mathbf{u}))_{\Omega} - (\nabla \cdot \mathbf{v}, p)_{\Omega} - (q, \nabla \cdot \mathbf{u})_{\Omega} = (\mathbf{v}, \mathbf{f})_{\Omega} + (\mathbf{v}, \mathbf{h})_{\Gamma_h} \quad (2.6)$$

holds for all test functions $(\mathbf{v}, q) \in \mathcal{V}_{\mathbf{u}} \times \mathcal{V}_p$. The form $(\cdot, \cdot)_{\Omega}$ denotes the standard L_2 inner product.

The spatial discretization of system (2.6) replaces the (infinite-dimensional) solution function spaces $\mathcal{V}_{\mathbf{u}}$ and \mathcal{V}_p by finite-dimensional subspaces $\mathcal{V}_{\mathbf{u}}^h$ and \mathcal{V}_p^h . Then, only the projection of the Navier–Stokes equations onto finite dimensional test function spaces $\mathcal{V}_{\mathbf{u}}^h \times \mathcal{V}_p^h$ is considered, resulting in numerical approximations \mathbf{u}^h and p^h . The discretizations considered in this thesis use a decomposition of the computational domain into small subsets of characteristic size h , called elements. We mainly focus on quadrilateral elements in 2D and hexahedral (brick) elements in 3D. The basis functions that span $\mathcal{V}_{\mathbf{u}}$ and \mathcal{V}_p are chosen to be piecewise polynomials within the elements, and continuous over the whole domain Ω . For the representation of the velocity \mathbf{u} , equally shaped basis functions are used for each spatial component. For instance, we will denote a finite element approximation with quadratic basis functions for velocity and linear basis functions for pressure on the elements by $\mathcal{Q}_2^d \mathcal{Q}_1$. On each element, the basis functions for \mathbf{u} are defined as a tensor product of Lagrangian interpolation polynomials of degree two in each coordinate direction [43], and the pressure basis functions as tensor product of linear Lagrangian interpolants. Globally, the basis functions are nonzero in exactly one node, and zero on all the others. The support of the basis functions is confined to a patch of elements around the respective nodes.

2.2 Stability of spatial discretization

For the spatial discretization to be stable, a compatibility condition between the approximation of velocity and pressure must be satisfied, namely

$$\inf_{q \in \mathcal{V}_p^h} \sup_{\mathbf{v} \in \mathcal{V}_u^h} \frac{(q, \nabla \cdot \mathbf{v})_\Omega}{\|q\|_{L_2} \|\mathbf{v}\|_{H^1}} \geq \beta > 0, \quad (2.7)$$

where the constant β does not depend on the mesh size parameter h . This condition was independently derived by Ladyzhenskaya [58], Babuška [4], and Brezzi [12] and is called *LBB condition* or *inf-sup condition*. The condition ensures that the divergence matrix discretizing the term $(q, \nabla \cdot \mathbf{u})_\Omega$ is of full rank, and hence the discretized system has a unique solution for velocity and pressure.

The element combination $\mathcal{Q}_2^d \mathcal{Q}_1$, the so-called Taylor–Hood element pair, satisfies the LBB condition [82], whereas the element combination $\mathcal{Q}_1^d \mathcal{Q}_1$ does not. We refer to Donea & Huerta [18] and Gresho & Sani [32] for an extensive discussion of LBB-stable elements. However, an element pair that does not satisfy the LBB condition (2.7) can yet be modified so that stability of discretization is obtained. Papers I and II investigate flow problems with the element pair $\mathcal{Q}_1^d \mathcal{Q}_1$. For stabilization, an artificial diffusion on the pressure space is introduced in a systematic way, so that consistency is preserved. This approach [38], [45], [84] modifies the test functions in the discrete variational form (2.6), resulting in a Petrov–Galerkin type scheme. Similar stabilization approaches have been developed to avoid unphysical oscillations in velocity that otherwise appear in convection-dominated regimes for the standard central difference approximations introduced by the Galerkin FEM [18], [31], [32]. We refer to Braack et al. [10] for a review of various commonly used stabilization techniques.

2.3 Time discretization

For discretization in time, it is usual to use some standard procedure developed for ordinary differential equations and differential–algebraic equations, see Donea & Huerta [18] and Hairer et al. [36], [37] for derivation and analysis of numerical schemes. For schemes that treat both convection and diffusion explicitly, linear stability theory sets a restrictive limit on the time step Δt in terms of the spatial mesh size Δx , namely

$$\Delta t_{\max} \propto \frac{\Delta x}{\|\mathbf{u}\|_\infty} + \frac{\rho \Delta x^2}{\mu},$$

see, e.g., the discussion in [52]. For applications where the viscosity is not too small compared to the velocity, (semi-)implicit time stepping schemes are often preferred in order to avoid the diffusive stability constraint. Popular schemes are variants of the one-step theta method [51] and the BDF-2 method. For a

coupled solution approach, stability requires implicit time discretization of the (differential–algebraic) terms $(\nabla \cdot \mathbf{v}, p)_\Omega$ and $(q, \nabla \cdot \mathbf{u})_\Omega$. These terms enforce the divergence-free condition on the velocity in Lagrangian multiplier form, see, e.g., Gunzburger [35] and Lions [62].

Harlow and Welch [39] proposed to implement time propagation of the Navier–Stokes equations by *fractional time stepping strategy*, and which was then recast as a projection scheme by Chorin [15] and Temam [83]. This concept has been mathematically justified for the finite element method by Guermond and Quartapelle [33], [34]. Projection schemes first advance velocities subject to the momentum equation with pressure extrapolated from the old time step. The resulting velocity is in general not divergence-free, so a pressure Poisson equation is solved with forcing given by the divergence of the medium-step velocity in a second step, in order to correct the velocity. Projection schemes are to date the most popular variant for the numerical approximation of the Navier–Stokes equations [74]. The subsystems resulting from fractional time stepping are of easier structure than the original saddle-point system. However, each of the subproblems needs to be equipped with suitable boundary conditions for well-posedness, which are usually not the physical ones. This can yield a non-consistent approximation close to the boundary. We refer to Gresho & Sani [32] and Quartapelle [74] for discussion, and to the articles [13] and [52] for recent developments.

The work presented in this thesis applies an alternative approach where the system remains coupled. Coupled schemes solve for pressure and velocity as one algebraic system, with boundary conditions set according to physical reasoning. However, the algebraic system is in general more challenging because of its saddle point nature, and puts high demands on numerical linear algebra.

2.4 Numerical linear algebra for coupled discretizations

The introduction of spatial and temporal discretization schemes for the Navier–Stokes system (2.6) results in a nonlinear system to be solved. For resolving the non-linearity, fixed point methods or Newton-type iterations are usually applied, finally yielding a system of linear equations. The Lagrangian basis functions are localized, so the final coefficient matrix is sparse. For the solution of the saddle-point Navier–Stokes system, different techniques have been proposed. Efficient schemes employ multigrid methods with suitably defined smoothing schemes (see Trottenberg, Oosterlee & Schüller [85] and John [48]), or use preconditioners based on the Schur complement of the block 2×2 matrix system defined by velocity and pressure matrices (cf. [55], [53], [22], see also the books by Turek [88] and Elman, Silvester & Wathen [23]). Papers I and II use an algebraic multigrid scheme for the coupled system, and the numerical method used in Papers III and IV is based on a preconditioner constructed from a Schur complement.

3. Computational methods for turbulence

This chapter discusses basics of the simulation of turbulent flow for a single-phase fluid, which is the context of Papers I and II. The modeling equations are the Navier–Stokes equations (2.1)–(2.2), where the viscous stresses are small compared to the inertial stresses. The ratio between inertial and viscous stresses is measured by the so-called Reynolds number,

$$Re = \frac{\rho l u}{\mu}, \quad (3.1)$$

where l is a reference length and u a reference velocity. A situation where inertial stresses dominate is characterized by high Reynolds numbers.

3.1 Basics on turbulence and large eddy simulation

A physical characterization of flow is to distinguish vortex structures by their size relative to the flow domain. A flow field consists of vortices of different size. These vortices are instationary and fluctuating — a phenomenon called *turbulence*. Fig. 3.1 depicts a typical pressure field in a turbulent flow. Vortex structures of different sizes as well as the irregular pattern of the flow can clearly be seen.

For flow at high Reynolds numbers, instabilities lead to a breakup of larger structures into smaller ones. This induces an energy transport from larger scales to smaller scales. The breakup process continues to create smaller and smaller structures until the scale is sufficiently small for viscous dissipation to become dominant, see Dubois et al. [19], Pope [73], and Sagaut [77]. In the Navier–Stokes equations, the interaction between different scales is driven by the nonlinear convective term $\mathbf{u} \cdot \nabla \mathbf{u}$.

The transfer of energy that takes place in the model of fluid motion is schematically depicted as a Kolmogorov scale spectrum in Figure 3.2. The diagram shows the region of active scales in a flow, ranging from the energy-containing scales l_0 (scale range of external forcing \mathbf{f} and \mathbf{h}) to the regime where viscosity becomes dominant at a scale level η , the so-called Kolmogorov scale [73]. The Kolmogorov scale η depends on the Reynolds number based on the production length scale l_0 as

$$\frac{\eta}{l_0} \propto Re_{l_0}^{-3/4}. \quad (3.2)$$

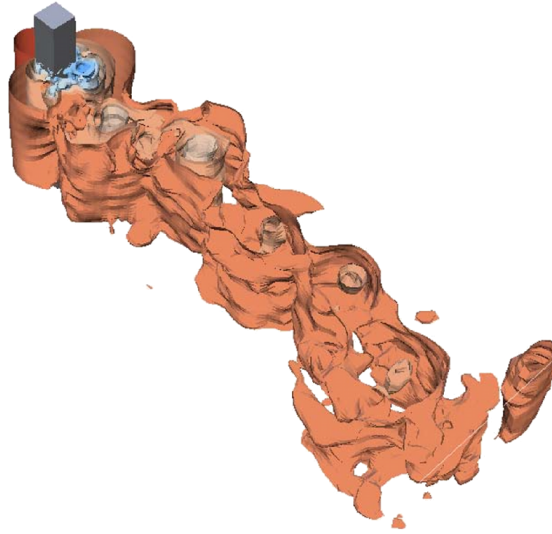


Figure 3.1: Pressure iso-surfaces for turbulent flow around a square obstacle (cf. Paper II).

Kolmogorov [56] noticed a self-similarity between the eddies in the inertial regime, as opposed to large-scale eddies, which depend mainly on geometry. Kolmogorov formulated the hypothesis that the energy content at scales in the inertial subrange, i.e., the range between energy production and viscous flow, is proportional to $\kappa^{-5/3}$, where κ is the scale length.

All the scales in incompressible flows are coupled with one another. Hence, a numerical method approximating the Navier–Stokes equations (2.1)–(2.2) needs to *resolve all* the scales in the flow in order to *represent any* scale correctly. A numerical approach that aims at resolving all necessary scales is called a direct numerical simulation (DNS) [63]. For three-dimensional instationary flow, a DNS requires to resolve a scale range according to (3.2) in each spatial direction as well as in the temporal dimension, which amounts in a number of degrees of freedom that is proportional to Re^3 , often even with a rather large proportionality constant. Many technically relevant flows are described by Reynolds numbers within the range $10^4 - 10^6$, so the requirements in computational effort exceed the capabilities of state-of-the-art schemes for a DNS by far, necessitating other techniques.

Since a full resolution of all flow features is not feasible, at least a fraction of these features needs to be modeled. The so-called large eddy simulation (LES) is one such modeling strategy. It aims at resolving the larger scales (large eddies), and to model the effect of unresolved scales on the large scales, see Pope [73] and Sagaut [77]. This idea is depicted in Fig. 3.2. The large scales in the range between

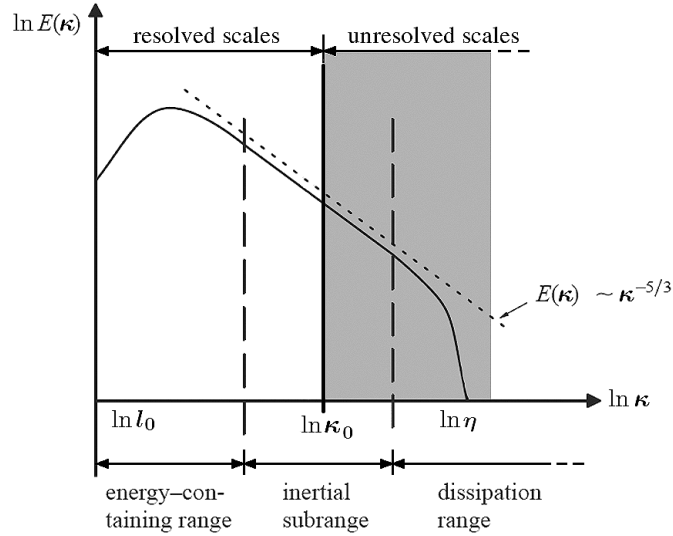


Figure 3.2: Kolmogorov energy spectrum in a double logarithmic plot. The wave length κ_0 denotes the resolution limit of the discretization. All the scales beyond that level will not be captured by the numerics and their effect needs to be modeled in order to correctly describe the physics of turbulence.

l_0 and κ_0 are resolved by the numerical discretization, whereas all scales beyond κ_0 are not resolved and need to be included by some modeling.

A simple, yet very powerful approach is the Smagorinsky model [80]. It is based on the observation that the insufficient resolution within a LES leads to under-resolved viscous effects. Hence, Smagorinsky introduced an artificial *subgrid* or *eddy* viscosity μ_T with the aims of representing the effect of viscosity on the level of the computational mesh size. The eddy viscosity is defined through a non-linear coefficient, based on the magnitude of the viscous stress tensor $\varepsilon(\mathbf{u})$, the square of the mesh size, and a proportionality constant [77].

3.2 A multiscale approach to large eddy simulation

The definition of a LES needs to distinguish between resolved and unresolved scales in order to formulate the subgrid viscosity term. Traditional methods use low-pass filters to extract the large-scale information from the Navier–Stokes equations and introduce the subgrid viscosity [77]. However, this spatial filtering is problematic close to domain boundaries. These problems can be traced back to so-called commutation errors [7], [20]. Moreover, finding appropriate boundary conditions for the averaged large scales is to date an open problem.

An alternative approach to LES is based on the variational multiscale method [44], introduced by Hughes, Mazzei, and Jansen [46]. The ideas are closely related to the concept of dynamic multilevel methods, described in Dubois, Jauberteau & Temam [19], and the multiscale turbulence analysis in Collis [16]. In this framework, filters are replaced by variational projections onto appropriate subspaces. The space for admissible velocity solutions is decomposed into

$$\mathcal{V}_{\mathbf{u}} = \mathcal{V}_{\mathbf{u}}^{3h} \otimes \mathcal{V}_{\mathbf{u}}^{\delta h} \otimes \widehat{\mathcal{V}}_{\mathbf{u}}, \quad (3.3)$$

where $\mathcal{V}_{\mathbf{u}}^{3h}$ is a space associated with mesh size $3h$, representing large resolved scales, $\mathcal{V}_{\mathbf{u}}^{\delta h}$ is the space spanned by $\mathcal{V}_{\mathbf{u}}^h$ except $\mathcal{V}_{\mathbf{u}}^{3h}$, representing small resolved scales, and finally, the space of unresolved scales $\widehat{\mathcal{V}}_{\mathbf{u}}$. We choose a resolution of $3h$, however, different definitions of large resolved scales are common as well, see the review article by Gravemeier [30]. Applying an equivalent decomposition for pressure, we get (following Harten's notation [40])

$$\mathbf{u} = \underbrace{\mathbf{u}^{3h} + \delta \mathbf{u}^h}_{\mathbf{u}^h} + \hat{\mathbf{u}}, \quad p = p^h + \hat{p}. \quad (3.4)$$

Let us denote by

$$\mathcal{B}_{\text{NS}}(\mathbf{v}, q; \mathbf{u}, p) = (\mathbf{v}, \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}))_{\Omega} + (\varepsilon(\mathbf{v}), \mu \varepsilon(\mathbf{u}))_{\Omega} - (\nabla \cdot \mathbf{v}, p)_{\Omega} - (q, \nabla \cdot \mathbf{u})_{\Omega}$$

the form that contains all the left-hand-side terms of the weak form of the Navier–Stokes equations (2.6). The aim of any numerical method is to find numerical approximations \mathbf{u}^h, p^h in the resolved subspace $\mathcal{V}_{\mathbf{u}}^h \otimes \mathcal{V}_p$ according to the direct sum decomposition (3.3). A systematic way of doing so is to insert the decomposition (3.4) into the weak form (2.6), and to restrict the test functions to the space of resolved variables. Then, the nonlinear convective term is linearized and resorted in terms of resolved and unresolved quantities [46]. Hence, we search for (\mathbf{u}^h, p^h) , such that

$$\mathcal{B}_{\text{NS}}(\mathbf{v}^h, q^h; \mathbf{u}^h, p^h) = (\mathbf{v}^h, \mathbf{f})_{\Omega} + (\mathbf{v}^h, \mathbf{h})_{\Gamma_h} - \mathcal{B}_{\text{NS}}^1(\mathbf{v}^h, q^h; \mathbf{u}^h; \hat{\mathbf{u}}, \hat{p}) - \mathcal{B}_{\text{NS}}^2(\mathbf{v}^h, \hat{\mathbf{u}}) \quad (3.5)$$

holds for all test functions $(\mathbf{v}^h, q^h) \in \mathcal{V}_{\mathbf{u}}^h \times \mathcal{V}_p^h$. The term $\mathcal{B}_{\text{NS}}^1(\mathbf{v}^h, q^h; \mathbf{u}^h; \hat{\mathbf{u}}, \hat{p})$ contains linear terms in $(\hat{\mathbf{u}}, \hat{p})$ and the linearized convection around \mathbf{u}^h , and the term $\mathcal{B}_{\text{NS}}^2(\mathbf{v}^h, \hat{\mathbf{u}})$ contains the quadratic convection term. For the numerical approximation to be computable, these two terms need to be substituted by some modeling that eliminates the unresolved variables.

The variational multiscale large eddy simulation with a subgrid viscosity model constructs the approximation as

$$\begin{aligned} \mathcal{B}_{\text{NS}}^1(\mathbf{v}^{3h}, q^{3h}; \mathbf{u}^h; \hat{\mathbf{u}}, \hat{p}) + B_{\text{NS}}^2(\mathbf{v}^{3h}, \hat{\mathbf{u}}) &\approx 0, \\ \mathcal{B}_{\text{NS}}^1(\delta \mathbf{v}^h, \delta q^h; \mathbf{u}^h; \hat{\mathbf{u}}, \hat{p}) + B_{\text{NS}}^2(\delta \mathbf{v}^h, \hat{\mathbf{u}}) &\approx (\varepsilon(\delta \mathbf{v}^h), 2\nu_T \varepsilon(\delta \mathbf{u}^h))_{\Omega}. \end{aligned} \quad (3.6)$$

Note that the subgrid viscosity is only applied to the smaller of the resolved scales, as discussed, e.g., in the review articles by Gravemeier [30] and John [49]. A physical explanation for application of eddy viscosity only on small resolved scales is that energy transport occurs mainly on neighboring scale groups, so that the effect of a not adequately resolved viscosity is best modeled on the fine resolved scales [66].

The implementation of a method according to the framework (3.5) with approximation (3.6) needs to distinguish between coarse and fine resolved scales. Standard methods for doing this are based on different polynomial orders for the FE basis functions, or two different grid levels as used, e.g., in geometric multigrid. Such methods have been presented by John & Kaya [50] and Gravemeier [29]. Papers I and II discuss an implementation where this separation is performed on the algebraic equation system by using routines from algebraic multigrid.

4. Simulation of Two-Phase Flow

We consider the dynamics of two immiscible incompressible fluids separated by an interface Γ as displayed in Fig. 4.1. By Ω_1 we denote the region occupied by the first fluid, and by Ω_2 the region occupied by the second. We assume that the flow is laminar, i.e., the Reynolds number is low for the considerations in this chapter.

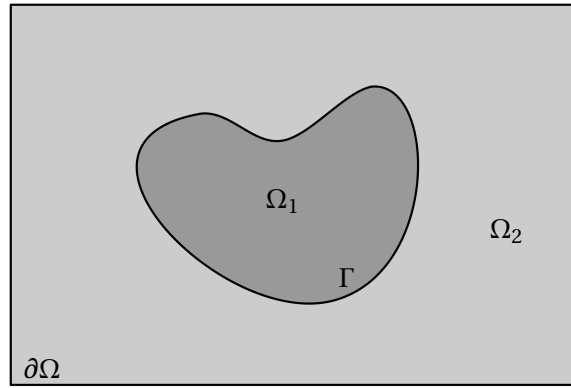


Figure 4.1: Schematic view of a two-phase flow problem. Fluid 1 occupies region Ω_1 , and fluid 2 occupies Ω_2 . The interface Γ separates the two fluids.

The motion of each fluid is described by the Navier–Stokes equations (2.1)–(2.2) using the variables \mathbf{u}_i and p_i , $i = 1, 2$. Extra conditions are necessary to describe the behavior on the interface Γ . A widespread formulation is to pose the two-phase flow problem on the whole domain $\Omega = \Omega_1 \cup \Gamma \cup \Omega_2$ with variables \mathbf{u} and p that take the respective velocity and pressure values in the individual domains. Generally, the fluid densities ρ_i and viscosities μ_i are different for the two fluids. Hence, the material parameters ρ and μ in the global momentum equation have a discontinuity on the interface. In addition, interfacial tension enters the formulation as a forcing of the form

$$\mathbf{f}_{\text{st}} = \sigma \kappa \mathbf{n} \delta_\Gamma. \quad (4.1)$$

Here, σ is a constant specifying the relative strength of the surface tension, κ denotes the interface curvature, \mathbf{n} the direction normal to the interface (pointing into Ω_2), and δ_Γ is a delta function that localizes the force to the interface. The interface Γ is transported by the local fluid motion $\mathbf{u}|_\Gamma$.

The variables in a single-domain formulation comprise kinks and discontinuities due to changes in material parameters and forces: The discontinuous viscosity introduces a discontinuity in the symmetric gradient $\varepsilon(\mathbf{u})$. Similarly, due to the distributional character of the delta function δ_Γ there is a jump in pressure proportional to $\sigma\kappa$. Any change in curvature tangential to the interface gives rise to a discontinuity in the pressure derivative normal to the interface as well as the viscous stress tensor. The conditions describing the irregularities in velocity and pressure over the interface Γ are called *jump conditions*, see Edwards, Brenner & Wasan [21] and Lee & LeVeque [59].

Because of different fluid densities, gravitational forces are often essential for the dynamics of two-phase flow. The gravity force is modeled as

$$\mathbf{f}_g = \rho g \mathbf{e}_g, \quad (4.2)$$

where g is the gravitational acceleration and \mathbf{e}_g denotes the direction of gravity. The total forcing in the momentum equation (2.1) for two-phase flow is hence given by $\mathbf{f} = \mathbf{f}_{st} + \mathbf{f}_g$.

4.1 Overview of numerical models

The two main challenges in the numerical simulation of two-phase flow are the representation of the interface as it evolves in time, and the evaluation of the distributional force term (4.1). Several discrete approaches have been proposed during the last decades. There are two main strategies to couple the interface evolution problem to the Navier–Stokes equations discretized on a fixed grid as discussed in Chapter 2.

The first strategy is to explicitly track the interface position by introducing an additional discrete set of marker points or marker elements that describe the interface. These methods are called front tracking and were introduced in different variants by Peskin [71] and Glimm et al. [27], and reviewed in the articles [78], [86], and [89]. A special class of front tracking schemes are the immersed boundary method by Peskin (see Peskin’s [72] review paper) and a more accurate variant, the immersed interface method, by LeVeque and co-workers [59], [60], [61]. The evolution of the interface in front tracking schemes is accomplished by Lagrangian advection of the marker points, and the surface tension force is generally evaluated based on a discrete approximation of the delta function around the interface. Normal vectors and curvatures can be calculated using the interface points by straight-forward geometric identities. Explicit descriptions are very powerful because they allow to include general models of the interface, like elastic forces in immersed boundary and interface implementation [72]. However, the methods are quite difficult to implement because the marker points need to interact with the fluid grid in order to describe advection and interface forces. Straight-forward implementations are also prone to unphysical changes of the area/volume of the respective fluid. To retain an accurate interface repre-

sensation, the marker points need to be redistributed when the interface is deformed.

The second strategy is front-capturing, where the interface is implicitly defined. Historically, the first scheme of this kind was the marker-and-cell method proposed by Harlow and Welch [39], and can be considered to be a volume-tracking method. Here, one fluid is colored by marker particles whose location is advected with the flow field. The position of the interface can then be reconstructed from this particle field. An extension of this approach is to replace the marker particles by a marker function. This approach has been pursued by Noh & Woodward [65] and Hirt & Nichols [42], who introduced the volume-of-fluid (VOF) method. VOF includes an additional variable that stores the fraction of the first fluid on the total fluid for each cell. From the volume fractions, the position of the interface can be reconstructed, e.g., by defining line segments. For details of the reconstruction, including higher order schemes, we refer to Scardovelli & Zaleski [78] and Sethian [79], and references therein. The advection of the interface is usually implemented by increasing or decreasing the volume fraction depending on the composition of neighboring cells and the velocity field. To put surface tension force in VOF into practice, several different approaches are common. One is to use discrete delta functions in combination with the reconstructed interface, and another employs the continuous surface tension approach by Brackbill, Kothe, and Zemach [11], see also the review by Tryggvason et al. [86]. The advantage of VOF methods is the volume conservation and a natural mechanism for breakup and fusion of bubbles. However, the reconstruction of the interface and the interface motion are considerably more complicated to implement here than for front tracking methods.

While VOF methods operate on the discrete level, a continuous front capturing framework is provided by the level set method, introduced by Osher & Sethian [70] and first applied to two-phase incompressible flow by Sussman, Smereka & Osher [81]. Yet another method is provided by the phase field method, formulated by Jacqmin [47] for the simulation of two-phase flow. The methods discussed in Paper III and IV are based on the latter two approaches, which are discussed in detail in the following two sections.

4.2 Level set models

The basic idea of level set methods is to define the interface implicitly as the zero contour line of a function ϕ that is defined in Ω . Level set methods allow for a straight-forward evaluation of normal vectors by setting $\mathbf{n}(\phi) = \nabla\phi/|\nabla\phi|$, and curvature, $\kappa(\phi) = \nabla \cdot \mathbf{n}(\phi)$. Both these quantities can be computed locally from ϕ on the same computational mesh as the equations of fluid flow. The mechanism for moving the interface in level set methods is advection of the function ϕ with local fluid velocity, i.e.,

$$\phi_t + \mathbf{u} \cdot \nabla\phi = 0. \quad (4.3)$$

This is an additional partial differential equation coupled to the Navier–Stokes equations. The advection equation (4.3) can be solved with standard tools for hyperbolic transport equations, like upwind finite difference/volume schemes or stabilized finite element methods. The advection can be implemented so that the volume is conserved, since the velocity is divergence-free, i.e., $\nabla \cdot \mathbf{u} = 0$.

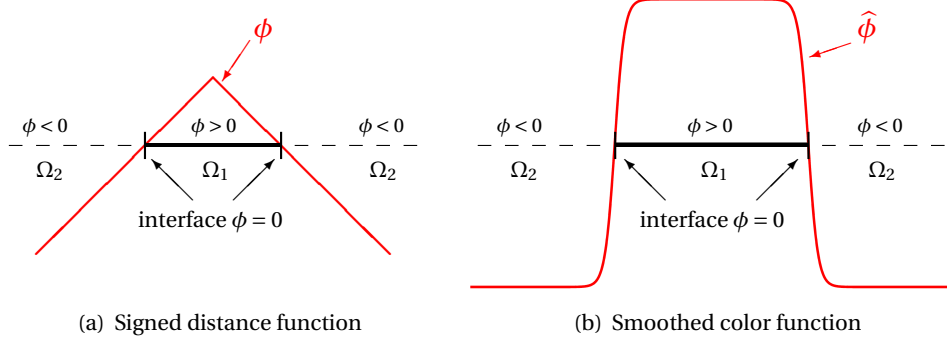


Figure 4.2: Representing an interface by level set functions ϕ .

The most popular choice for a level set function is the signed distance function ϕ , depicted in Fig. 4.2(a). We refer to the books by Sethian [79] as well as Osher and Fedkiw [69] for an extensive discussion of these methods. A signed distance function encodes the distance of a particular point to the interface, and different signs identify the two fluids. A signed distance function has the property $|\nabla\phi| = 1$ almost everywhere. A benefit of this choice is that the integral in the surface tension force can be simplified to a one-dimensional discrete delta function as

$$\int_{\Gamma} \delta(\mathbf{x} - \mathbf{y}(s)) ds \approx \delta_h(\phi(\mathbf{x})),$$

where \mathbf{x} denotes an arbitrary point in the computational domain and $\mathbf{y}(s)$ is the image of a parametrization of the interface, see, e.g., [79]. However, it has been shown by Engquist, Törnberg, and Tsai [24] that such an approximation can lead to $\mathcal{O}(1)$ errors in the force unless the width h of the delta function is varied. Recent implementations therefore reconstruct the interface position from ϕ and apply a d -dimensional discrete delta function that does not show these consistency problems. Since the information from ϕ is only needed in a region around the interface, so-called narrow-band level set implementations are widely used. These methods calculate ϕ only on a few grid cells around the interface, often in combination with high-resolution grids. We refer to Adalsteinsson and Sethian [1] for details. To start a level set calculation, an initial profile $\phi(\cdot, 0)$ needs to be generated given a certain interface position. Moreover, the flow field as well as inaccuracies in the numerical scheme deform the signed distance function in the course of the simulation. Therefore, algorithms have been proposed to (re-

)initialize the signed distance function. These algorithms enforce the property $|\nabla\phi| = 1$, for example, by solving the partial differential equation

$$\phi_\tau + S(\phi_0)(|\nabla\phi| - 1) = 0, \quad (4.4)$$

to steady state, where $S(\phi_0)$ is a sign function with value 1 in the first fluid and value -1 in the other (see, e.g. [69]). However, discretizations of the reinitialization scheme do not preserve mass, so that the overall level set implementation based on signed distance functions may suffer from unphysical volume changes in the fluid phases.

Another choice is to use a smoothed color/indicator function as depicted in Fig. 4.2(b). Such a function is (almost) constantly 1 or -1 away from the interfaces, with positive value in one region and negative value in the other. Around the interface, there is a transition region where the function smoothly switches from one value to the other. This function ϕ can be calculated from the reinitialization equation (cf. Olsson and co-workers [67], [68])

$$\phi_\tau + \nabla \cdot (\mathbf{n}(1 - \phi^2)) - \nabla \cdot (\mathbf{n}\epsilon\nabla\phi \cdot \mathbf{n}) = 0. \quad (4.5)$$

In this equation, diffusion in direction normal to the interface is balanced by a compressive flux. The parameter ϵ is typically chosen to be of similar size as the computational mesh. In one spatial dimension with an interface located at $x = \alpha$, the steady-state value of (4.5) is given by

$$\phi(x) = \tanh\left(\frac{x - \alpha}{\epsilon}\right). \quad (4.6)$$

Since the reinitialization equation (4.5) is posed as a conservation law, a conservative implementation of the method is possible [68]. A smoothed color function also avoids the introduction of an additional discrete delta function and the problems associated with that procedure, since it approximately holds

$$\nabla\phi \approx 2\mathbf{n}\delta_\Gamma. \quad (4.7)$$

The factor two comes from the fact that the function switches from -1 to $+1$. This scheme for evaluating the interface force corresponds to the continuous surface tension model proposed by Brackbill, Kothe, and Zemach [11]. A disadvantage of the formulation with a smoothed color function is that the evaluation of curvature is potentially less accurate because it is calculated from a steep profile. This generally increases resolution requirements compared to the signed distance function approach. Another drawback of the smoothed indicator function is that the function needs to be defined on the whole domain in order to conserve volume. This can be alleviated by the use of adaptive meshes that have low resolution away from the interface, though. Moreover, the discrete delta function underlying (4.6) has support on the whole domain Ω , which necessitates evaluating the discrete version of the force (4.1) everywhere.

4.3 Phase field models

All the methods discussed above are based on the mathematical model (4.1) for interfacial tension, assuming a continuous PDE model for fluid dynamics that does not take processes on the level of atoms and molecules into account. The numerical approximations aim at discretely reproducing the effect of a delta function, and evaluating the curvature to determine the strength of the surface tension. A different approach takes chemical considerations of the interface into account. The so-called van der Waals hypothesis [90] states that immiscible fluids actually mix on molecular level, forming a diffuse interface. The profile of the interface is given by a balance of random molecular motion and molecular attraction, as devised by Cahn and Hilliard [14]. The considerations are based on the free energy of a molecule, given by

$$f(C) = \beta\Psi(C) + \frac{\alpha}{2}|\nabla C|^2, \quad (4.8)$$

where C denotes the concentration and $\Psi(C) = (C + 1)^2(C - 1)^2$. Similar to the smoothed color function (4.6), the function seeks to attain the two equilibrium values $C = \pm 1$, which is driven by the double-well potential $\Psi(C)$. The gradient term ∇C on the other hand enforces a smooth transition. The system seeks to minimize the energy (4.8). This process is described by the Cahn–Hilliard equation

$$C_t = \nabla \cdot (M\nabla\psi) = \nabla \cdot (M\nabla(\beta\Psi'(C) - \alpha\nabla^2 C)) = 0, \quad (4.9)$$

with the chemical potential ψ and the mobility factor M .

The phase field method, formulated by Anderson et al. [2] and Jacqmin [47], includes transport of the interface by convection, i.e., a term $\mathbf{u} \cdot \nabla C$, and formulates an interface force

$$\kappa\mathbf{n}\delta_\Gamma \approx -C\nabla\psi + \nabla P, \quad (4.10)$$

where $P = C\psi$. Equation (4.10) can be rewritten as

$$\kappa\mathbf{n}\delta_\Gamma \approx \psi\nabla C,$$

which is the same form as for the continuous surface tension model, that is, equation (4.7) multiplied by curvature κ . Boyer [9] extended the phase field model to describe motion of fluids with different densities and viscosities.

The phase field model can be augmented in order to include contact forces of the interface with solid walls [47], which results in flux-boundary conditions on the chemical potential ψ . This approach allows for setting static contact angles that correspond to physical wetting properties. The direct inclusion of contact line dynamics is different from the other approaches in computational multi-phase dynamics, where additional mechanisms as slip-velocities and near-wall interface diffusion need to be added, cf. [76], [92].

A considerable challenge in the simulation of phase field models are the high resolution requirements. Even though the interface width α/β can be chosen considerably larger than molecular dynamics would suggest (see Villanueva and Amberg [91]), accurate results require sophisticated numerical approximations and fine computational meshes. Furthermore, the equations are nonlinear and contain fourth order derivatives. Several attempts have been made to make this approach more competitive, see for example the work by Kay and Welford [54].

5. Summary of Papers

5.1 Paper I

Paper I proposes a particular implementation for the scale separation in the variational multiscale large eddy simulation. Our method uses a plain aggregation scheme that is part of an aggregation-based algebraic multigrid implementation [26], [87]. Unlike for geometric multigrid approaches that have been used earlier, no grid hierarchy is needed in our implementation. This makes the method also applicable for discretizations based on fully unstructured grids. The subgrid viscosity term is implemented within a parallel fluid flow solver based on linear interpolation finite elements and uses Trilinos solver algorithms [41]. The focus of the method is the improvement of LES at low resolutions.

The method is tested for some standard sample problems for turbulent flow. A grid refinement study is performed for a turbulent channel flow with DNS data as reference [64]. This study shows that our implementation of the variational multiscale LES model provides better results than other state-of-the-art LES schemes.

5.2 Paper II

Paper II extends and analyzes the method presented in Paper I. In this paper it is proposed to use a second-order accurate generalized-alpha time integration scheme (instead of the Crank–Nicholson scheme in Paper I). The generalized-alpha scheme is a variant of the one-step theta schemes that includes approximations of the first temporal derivative as variables and enables control of the dissipation for high frequencies, which is favorable in low-resolution computations.

The analysis considers details of the subgrid viscosity implementation based on plain aggregation scale separation, showing that the additional model does not affect consistency of the overall Navier–Stokes scheme. Moreover, a clear difference between projective and non-projective scale separations is identified, as was previously observed in numerical computations [29]. Projective implementations retain low frequencies, whereas non-projective implementations also damp low frequencies. We apply our method to turbulent flow around a square cylinder, where the results are better than those of other LES schemes at low resolutions, even though a high sensitivity of the results on stabilization parameters is observed.

5.3 Paper III

The paper is based on the observation that level set methods enable efficient implementations of two-phase flow physics at relatively coarse meshes because they are based on simple advection schemes together with a reinitialization. However, a standard level set method fails in predicting phenomena relevant in wetting where the fluid-fluid interface aligns at some oblique angle with solid walls. Such a simulation is, however, possible with a phase field model.

As the discussion in Section 4.3 suggests, the conservative level set method [68] and the Cahn–Hilliard model have a similar equation structure. Therefore, the paper formulates the Cahn–Hilliard-specific terms as an extension of the level set model, but restricts that additional phase description to a region close to contact points. A continuous switch function is used in order to retain a consistent model. The model is discretized with the finite element method and implemented based on the deal.II library [5]. A test on a channel flow driven by inflow illustrates the beneficial effects of the equation coupling.

5.4 Paper IV

This paper analyzes inaccuracies of the numerical implementation of the conservative level set model [68]. A circular bubble at rest is considered as a model problem. In this case the force due to surface tension should ideally be balanced by a jump in pressure. The study is performed by applying a complete Navier–Stokes/two-phase flow solver to the problem and recording spurious velocities, see, e.g. [3], [25].

We observe that the velocity errors can be traced back to inaccuracies in the numerically calculated curvature that enter the continuous surface tension model. If the exact curvature is prescribed, there are no imbalances in the scheme, in case equal order elements are chosen for approximating pressure and the level set function. Choosing the element order of the level set function higher than the one for pressure introduces an additional imbalance. However, the use of higher order elements for the level set function has beneficial impact on the accuracy of curvature, so that the numerical model is still more accurate. Moreover, we study the effect of the continuous representation of surface tension on the prediction of the jump in pressure between the inside and the outside of the bubble. This showed that the variation of the curvature along the finite width of the interface has the largest impact on pressure accuracy.

We perform the tests using two different flow solvers, in order to further evaluate the accuracy of the force balance for finite element discretizations. The results for a fully coupled implicit method and a decoupled (projection) solver are similar, which shows that choice of the solver does not affect the balance of forces.

6. Future Work

The method proposed in Paper III aims at providing phase-field-like features without having to use all its terms everywhere. This is done so that the phase field method is reduced to a level set formulation in regions far away from contact lines. It will be necessary to perform an in-depth convergence study of level set models and phase field models on several test cases in two-phase flow dynamics. In particular, the resolution requirements of the two methods should be quantified in order to identify the precise benefits of the hybrid method. In our hybrid model, the equations have been coupled by a smoothly varying switch function. The influence of the switch function needs to be considered in an energy estimate in order to ensure stability of the coupling of the equations, which has up to date only been verified numerically. Since the numerical implementation of the equations is based on a system of two equations to avoid the direct appearance of fourth derivatives, the analysis needs to be performed in a way to correctly reflect the discretized state of the equations.

We also aim at using our models for larger problems, especially three-dimensional simulations. For this purpose, parallel implementations of the flow solver and the coupled level-set/Navier–Stokes system are necessary. Within the deal.II software that was used in Papers III and IV, it is possible to use parallel assembly and linear algebra routines. For a Stokes problem coupled to an advection equation, a parallel version for up to about 50 processors has already been implemented by the author of this thesis.¹ The objective is to apply this implementation framework to the coupled Navier–Stokes/level-set system and to eventually extend it to a massively parallel implementation for even larger systems.

The hybrid level-set/phase-field method is a potential tool for improving the simulation of multi-phase flow in porous media [17]. A first step in that direction is to apply the new model to more complicated geometries, like, e.g., channels with oscillating walls or flow around small obstacles. Small scale results are a helpful tool in the simulation of subsurface flow like the prediction of the flow in oil and gas reservoirs. The imposition of a pressure gradient on a small-scale material configuration induces a flow field, which can be used to determine values for the permeability of that configuration. The permeability tensor is one of the main input parameter in coarse-scale simulations based on Darcy’s law.

In Paper IV, a study regarding error sources in the discrete approximation with the conservative level set implementation is presented. These results point out directions where the method needs to be improved. One such direction concerns

¹See the deal.II tutorial program http://www.dealii.org/developer/doxygen/deal.II/step_32.html

the accuracy in the curvature calculations. A particularly easy approach is to use higher order finite elements for representing the level set function. When keeping the interface width constant, increasing the order of approximation considerably increases resolution of the interface, and thus, accuracy of normals and curvature that rely on the interface representation. This improvement should be advantageous for the overall accuracy, even though a small imbalance in the force representation is introduced. Such a strategy increases the costs for the level set portion of the algorithm if the same mesh is used as for the Navier–Stokes equations, though. An alternative would be to coarsen the level set mesh in regions away from the interface. This is reasonable since in these remote regions, only the momentum and continuity balances need to be represented accurately, while the level set equation does not contain any additional information. Similarly, the interface region can be resolved by more mesh points than there are used for the Navier–Stokes equations. However, this requires a special implementation for the evaluation of the surface tension force in the finite element algorithms because the variables are related to different meshes.

An alternative hybrid approach that might be taken into account is to not mix the level set formulation with the phase field formulation as has been done in Paper III, but to use the phase field model as a micro-scale input to a macro-scale formulation based on a level set description of two-phase flow. A heterogeneous multiscale approach has been proposed by Ren and E [75] for modeling the interaction of macro-scale fluid flow by micro-scale information from molecular dynamics. The response on molecular level provides information about the expected motion of contact lines during one time step. This coupled model behaves differently than large-scale level set model, which would assume zero velocity. It is conceivable that a similar interaction could be applied for a micro-scale simulation done with the phase field model. The difficulty of such a micro-macro coupling is to find appropriate transfer operations from the micro scales to the macro scales. Suitable boundary conditions for the Cahn–Hilliard sub-problem given the solution of a macro-scale level set model are needed, as well as a shear velocity for the macro-scale Navier–Stokes equations, based on the results from a micro model.

Acknowledgments

I am very grateful to my adviser Gunilla Kreiss for introducing me to this interesting subject and for stimulating discussions on various aspects of multiphase flow. My thanks go to Volker Gravemeier who acquainted me with the subject of variational multiscale large eddy simulation for turbulent flow and stimulated ideas. I acknowledge discussions with Wolfgang Bangerth on implementation aspects of finite element programming. Finally, I would like to thank Katharina Kormann and Eddie Wadbro for countless discussions on computational mathematics as well as proof-reading manuscripts of my articles and this thesis.

This work was supported by the Graduate School in Mathematics and Computing (FMB).

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