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Robust preconditioning methods for algebraic problems, arising in multi-phase flow models

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Abstract

The aim of the project is to construct, analyse and implement fast and reliable numerical solution methods to simulate multi-phase flow, modeled by a coupled system consisting of the time-dependent Cahn-Hilliard and incompressible Navier-Stokes equations with variable viscosity and variable density. This thesis mainly discusses the efficient solution methods for the latter equations aiming at constructing preconditioners, which are numerically and computationally efficient, and robust with respect to various problem, discretization and method parameters.

In this work we start by considering the stationary Navier-Stokes problem with constant viscosity. The system matrix arising from the finite element discretization of the linearized Navier-Stokes problem is nonsymmetric of saddle point form, and solving systems with it is the inner kernel of the simulations of numerous physical processes, modeled by the Navier-Stokes equations. Aiming at reducing the simulation time, in this thesis we consider iterative solution methods with efficient preconditioners. When discretized with the finite element method, both the Cahn-Hilliard equations and the stationary Navier-Stokes equations with constant viscosity give raise to linear algebraic systems with nonsymmetric matrices of two-by-two block form. In Paper I we study both problems and apply a common general framework to construct a preconditioner, based on the matrix structure. As a part of the general framework, we use the so-called element-by-element Schur complement approximation. The implementation of this approximation is rather cheap. However, the numerical experiments, provided in the paper, show that the preconditioner is not fully robust with respect to the problem and discretization parameters, in this case the viscosity and the mesh size. On the other hand, for not very convection-dominated flows, i.e., when the viscosity is not very small, this approximation does not depend on the mesh size and works efficiently. Considering the stationary Navier-Stokes equations with constant viscosity, aiming at finding a preconditioner which is fully robust to the problem and discretization parameters, in Paper II we turn to the so-called augmented Lagrangian (AL) approach, where the linear system is transformed into an equivalent one and then the transformed system is iteratively solved with the AL type preconditioner. The analysis in Paper II focuses on two issues, (1) the influence of a scalar method pa-

rameter (a stabilization constant in the AL method) on the convergence rate of the preconditioned method and (2) the choice of a matrix parameter for the AL method, which involves an approximation of the inverse of the finite element mass matrix. In Paper III we consider the stationary Navier-Stokes problem with variable viscosity. We show that the known efficient preconditioning techniques in particular, those for the AL method, derived for constant viscosity, can be straightforwardly applicable also in this case.

One often used technique to solve the incompressible Navier-Stokes problem with variable density is via operator splitting, i.e., decoupling of the solutions for density, velocity and pressure. The operator splitting technique introduces an additional error, namely the splitting error, which should be also considered, together with discretization errors in space and time. Insuring the accuracy of the splitting scheme usually induces additional constrains on the size of the time-step. Aiming at fast numerical simulations and using large time-steps may require to use higher order time-discretization methods. The latter issue and its impact on the preconditioned iterative solution methods for the arising linear systems are envisioned as possible directions for future research.

When modeling multi-phase flows, the Navier-Stokes equations should be considered in their full complexity, namely, the time-dependence, variable viscosity and variable density formulation. Up to the knowledge of the author, there are not many studies considering all aspects simultaneously. Issues on this topic, in particular on the construction of efficient preconditioners of the arising matrices need to be further studied.

List of papers

This thesis is based on the following three papers, which are referred to as Paper I, Paper II and Paper III.

I. M. Neytcheva, M. Do-Quang and X. He, Element-by-element Schur complement approximations for general nonsymmetric matrices of two-by-two block form. *Springer Lecture Notes in Computer Science (LNCS)*, 5910/2010, 2010.

II. X. He, M. Neytcheva and S. Serra Capizzano, On an augmented Lagrangian-based preconditioning of Oseen type problems. *Submitted to BIT Journal, and under revision now, 2010.*

III. X. He and M. Neytcheva, Preconditioning the incompressible Navier-Stokes equations with variable viscosity. Technical Report, 2011, Department of Information Technology, Uppsala University, Sweden.

Contents

Chapter 1

Introduction

Computational fluid dynamics (CFD) is an important branch of fluid mechanics and computational mathematics. Numerical simulations become more and more irreplaceable and indispensable in modern research, not only because the traditional laboratory experiments are costly, but also because the numerical simulations enable us to model the processes, which cannot be experimentally tested, and extend our capability to reproduce physical phenomena in order to obtain a deeper insight of the underlying processes and their interactions.

Simulation of multi-phase flow is an active research area in CFD and has high impact on numerous applications. For example, the phenomenon of solid-liquid interaction when dropping a solid sphere into a liquid and in particular, the splashing phenomenon, observed when the solid sphere penetrates the liquid's surface, are very complicated and have been numerically and experimentally studied during the past. Deeper insights and knowledge about this type of multi-phase flow can be obtained through numerical simulations and used in the context of various applications. The author believes that in future we may use the obtained knowledge to help the athletes to control the splash in the diving competition of the Olympic games.

Numerical simulations of multi-phase flow are based on certain systems of partial differential equations (PDEs), which are, in general, coupled, time-dependent and nonlinear. Those PDEs are then discretized, and since we usually aim at obtaining some stationary solutions or at performing fast numerical simulations, implicit time discretization methods are to be recommended. The nonlinearities are handled via some nonlinear methods, such as Newton's or Picard's iterations. The computational kernel of these complex numerical simulations is the solution of some linear systems of equations. Since the linear solve is in the most inner loop of long time integration, or a nonlinear solution iteration, or both, it is of importance to use reliable, efficient and fast solution methods for those.

The linear systems, arising in such simulations may have huge dimen-

sions, which often outrules direct solution methods due to their high demands for computer resources, enforcing the usage of iterative methods. Further, the matrices of the linear systems, which are in general nonsymmetric, might be very ill-conditioned, which puts extra demands on the possible preconditioning techniques, which are aimed to be not only numerically and computationally efficient but also robust with respect to various parameters, which arise from the PDEs, the discretization and the solution methods.

In this thesis the multi-phase flow is modeled by a coupled system consisting of the time-dependent Cahn-Hilliard and incompressible Navier-Stokes equations. How to construct efficient preconditioners for the nonsymmetric matrices arising from the finite element discretization of the time-dependent and incompressible Navier-Stokes equations with variable viscosity and density is in the focus of this thesis. As to the coupled system, how to construct efficient solution schemes, which permit large time-steps while keeping the accuracy of the obtained solutions, is another main concern in this thesis and the work to follow.

The outline of the thesis is as follows. The coupled model for multi-phase flow is introduced in Chapter 2. The time-dependent Cahn-Hilliard equations and incompressible Navier-Stokes equations are discussed in Chapters 3 and 4. Computational challenges for solving the coupled system are discussed in Chapter 5. A summary of the papers, included in this thesis, is given in Chapter 6 and possible directions of future work are outlined in Chapter 7.

Chapter 2

Coupled model for multi-phase flow

The phase-field model is used to model two immiscible and incompressible fluids. The interface between the fluids is modeled as a narrow interfacial region. The idea that fluid-fluid interface diffuses with finite thickness goes back to Poisson (1831) and Gibbs. Van der Waals (1893) [57] introduced the first diffusive-interface model based on the so-called free energy density and he also suggested that the equilibrium interface profiles are those which minimize the total free energy within the whole domain. Hilliard (1958) [18] and Cahn (1961) [17] extended Van der Waals's idea to the time-dependent case and derived the so-called Cahn-Hilliard equation, which models the creation, movement and dissolution of diffusion-controlled phase interfaces. This diffusive-interface model, where the convective effect of the fluid's motion is not considered, is extensively used in various studies in fluid mechanics, i.e., the study of the dynamics of a near-critical fluid in a shear flow (e.g. [47]); the study of capillary waves (e.g. [54]); the study of contact-line problems (e.g. [53]) and so on. In the above diffusive-interface model, the interface is measured by the so-called *concentration*, which is also referred to as the *phase field*. The *concentration* takes two distinct values (for instance $+1$ and -1) in each of the phases, with a smooth and rapid change between both values in the interface zone. This approach permits to solve the problem by integrating a set of partial differential equations in the whole domain, without explicit treatment of the boundary conditions at the interface.

By taking into account the convective effect of the fluid's motion, a convective form of the time-dependent Cahn-Hilliard equation is derived (see e.g. [19]). More details about the convective Cahn-Hilliard equation are discussed in Chapter 3. The fluids motion is governed by the Navier-Stokes equations, therefore the numerical model for resolving the multi-phase flow involving incompressible fluids is a coupled system consisting of

the time-dependent Cahn-Hilliard (C-H) and incompressible Navier-Stokes (N-S) equation (see e.g. [23]). More details about the C-H and N-S equations involved in the coupled system are discussed in Chapters 3 and 4.

For the coupled system, we are in many cases interested in obtaining the stable solutions. Thus, we have to perform time marching in a large time interval. Since we also aim at fast numerical simulations, we would like to use as large time-steps as possible, meanwhile keeping the accuracy of the solution within some prescribed bounds. One possible approach to match the above requirements is to rewrite the linear systems of PDEs arising from the coupled models for the multi-phase flow as differential-algebraic systems. In this way, the known numerical solution methods for solving the differential algebraic equations DAEs (cf, e.g., [48]) can be utilized. The DAEs formulation permits us to use high-order time integration methods (of order 4 or higher), and allows large time-steps.

Chapter 3

The Cahn-Hilliard equations

3.1 Formulation

The formulation of the phase-field model is derived via the so-called free energy functional, $F(C)$, which depends on a variable C, referred to as the *concentration* (the *phase field*). Van der Waals (1893) [57] suggested that the equilibrium interface profiles are the minimizers of the free energy functional, defined as

$$F(C) = \int_\Omega f(C(\mathbf{x}, t))d\Omega,$$

where the function $f(C)$ denotes the free energy density per volume. Here $\Omega \times (0, T] \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded, connected domain with boundary $\partial\Omega$. Van der Waals derived an explicit expression for the free energy density as $f = \beta\Psi(C) + \frac{1}{2}\alpha \mid \nabla C \mid^2$, where α and β are some constants, proportional to the surface tension coefficient σ and the interface width ϵ, $\alpha \sim \sigma\epsilon$ and $\beta \sim \sigma/\epsilon$ (see e.g. [39]). The interaction between the bulk energy, or molar Gibbs energy, $\beta\Psi(C)$, and the interfacial energy $\frac{1}{2}\alpha \mid \nabla C \mid^2$ determines the position of the interface (see e.g. [19]). The function $\Psi(C)$ is a double well potential with the minimal value at $+1$ and -1 (under the assumption that the *concentration* varies between $+1$ and -1). For instance, $\Psi(C) = \frac{1}{4}(C^2 - 1)^2$.

The equilibrium interface profiles can be obtained, based on the derivative of the free energy functional F with respect to the *concentration* C (cf, e.g., [13]), i.e., $\frac{\partial F}{\partial C} = \int_\Omega (\beta\Psi'(C) - \alpha\Delta C)d\Omega$ where the term $\eta \equiv \beta\Psi'(C) - \alpha\Delta C$ is referred to as the *chemical potential*. By minimizing the integral of the *chemical potential* within the whole domain we obtain the equilibrium profiles of the interface. In other words, the equilibrium profiles are the solutions of $\eta = \beta\Psi'(C) - \alpha\Delta C = const$. In one dimension, for example, the non-unique solution is $C_{1d}(x) = tanh(\frac{x}{\sqrt{2}\epsilon})$ where the coefficient $\epsilon = \sqrt{\frac{\alpha}{\beta}}$ is referred to as the equilibrium interface thickness and the equilibrium surface

tension σ is $\sigma = \alpha \int_{-\infty}^{+\infty} (\frac{dC_{1d}}{dx})^2 dx = \frac{2\sqrt{2}}{3}\sqrt{\alpha\beta}$.

The motion of the fluids in a multi-phase system is, in general, due to diffusion and convection. Thus, the Cahn-Hilliard equation is amended to incorporate the convective process as follows

$$\frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla)C = \nabla \cdot [\kappa(C)\nabla(\beta\Psi'(C) - \alpha\Delta C)], \quad \text{in } \Omega \times (0, T] \tag{3.1}$$

where the coefficient $\kappa(C)$ denotes the so-called mobility, assumed to depend on the *concentration* C and $\mathbf{u}$ is the velocity. Suitable boundary conditions at the solid wall need to be added. The first boundary condition is based on the requirement that there is no flux of the *chemical potential* through solid wall surfaces. Therefore, we set Neumann boundary condition for the *chemical potential* at wall surfaces, i.e., $\mathbf{n} \cdot \nabla\eta = 0$, where the vector $\mathbf{n}$ denotes the unit normal vector outward the wall surface. The second boundary condition at wall surfaces corresponds to physical wetting properties (cf, e.g., [39]).

One can solve Equation (3.1) directly, which means one needs to handle forth order derivatives of the *concentration* C. To avoid this, by introducing the *chemical potential* $\eta = \beta\Psi'(C) - \alpha\Delta C$ as another variable, one can rewrite the time-dependent Cahn-Hilliard equation as a coupled system of two PDEs, as follows,

$$\nabla \cdot (\kappa(C)\nabla\eta) = \frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla)C, \qquad \text{in } \Omega \times (0, T] \tag{3.2}$$

$$\eta = \beta\Psi'(C) - \alpha\Delta C, \qquad \text{in } \Omega \times (0, T] \tag{3.3}$$

with suitable boundary and initial conditions for the *concentration* C and the *chemical potential* η.

Available results regarding the existence and uniqueness of the solution of the C-H equations can be found in [45, 46, 25].

In Equation (3.2), the vector $\mathbf{u}$ denotes the velocity. The term $\mathbf{u} \cdot \nabla$ presents the convective effect of the fluid's motion and constitutes the coupling of the Cahn-Hilliard equation and the time-dependent incompressible Navier-Stokes (N-S) equations, which are discussed in Chapter 4.

3.2 Discretization using the finite element method (FEM)

A standard technique to discretize the Cahn-Hilliard equations (3.2)-(3.3) is to use FEM with the same finite element space for both variables, η and C. The discrete form of the weak formulation reads as follows.
Find $\eta_h, C_h \in X^h \subset H^1(\Omega)$ satisfying

$$\begin{aligned} (\eta_h, v_h) - \beta(\Psi'(C_h), v_h) - \alpha(\nabla C_h, \nabla v_h) &= 0, \\ \kappa(\nabla\eta_h, \nabla v_h) + (\frac{dC_h}{d\mathrm{t}}, v_h) + ((\mathbf{u}_h \cdot \nabla)C_h, v_h) &= 0. \end{aligned} \tag{3.4}$$

for any test function $v_h \in X^h$. Let $\{\phi_i\}_{1\le i\le N}$ be the nodal basis of X^h, then the discrete solutions are of the form $C_h = \sum_{i=1}^N C_i\phi_i$ and $\eta_h = \sum_{i=1}^N \eta_i\phi_i$. The semi-discrete form of the weak formulation of the Cahn-Hilliard equation (3.4) can be presented in matrix form as follows:
Find the solution vectors $\mathbf{C}(t) = \{C_i(t)\}_{i=1}^N$ and $\eta(t) = \{\eta_i(t)\}_{i=1}^N$ to satisfy

$$\begin{aligned} M\eta(t) - \beta f(\mathbf{C}(t)) - \alpha K\mathbf{C}(t) = 0, \\ \kappa K\eta(t) + M\frac{d\mathbf{C}(t)}{dt} + W\mathbf{C}(t) = 0 \end{aligned} \tag{3.5}$$

where the vector $f(\mathbf{C}(t)) = \{f_i(\mathbf{C}(t))\}_{i=1}^N$ and its entries are defined as $f_i(\mathbf{C}(t)) = (\Psi'(\mathbf{C}(t)), \phi_i)$. In Equation (3.5), the involved matrices are M, K and W, which are correspondingly the symmetric and positive definite mass matrix, the symmetric and semi-positive definite stiffness matrix and the matrix, arising from the discretization of the convection term, which is nonsymmetric, and are denoted by

$$\begin{aligned} M &= \{M_{ij}\}_{i,j=1}^N &&= \{(\phi_i, \phi_j)\}_{i,j=1}^N, \\ K &= \{K_{ij}\}_{i,j=1}^N &&= \{(\nabla\phi_i, \nabla\phi_j)\}_{i,j=1}^N, \\ W &= \{W_{ij}\}_{i,j=1}^N &&= \{(\mathbf{u}_h\cdot\nabla\phi_i, \phi_j)\}_{i,j=1}^N. \end{aligned}$$

A method to discretize in time, often used in many numerical simulations, is the θ-method, $\theta \in [0,1]$ (cf, e.g., [2]). Consider a sequence of time-steps, $\{t_k\}$, $k = 0, 1, ...$, where $t_0 = 0$, $t_{k+1} = t_k + \Delta t_k$, and let $\mathbf{X}^{(k)} = \begin{bmatrix} \eta^{(k)} \\ \mathbf{C}^{(k)} \end{bmatrix}$ denote the vector of total unknowns. The fully discretized Cahn-Hilliard equations, which need to be solved at the kth time-step ($k = 0, 1, ...$) is
Find $\mathbf{X}^{(k)} \in \mathbb{R}^{2N}$ satisfying

$$F^{(k)}(\mathbf{X}^{(k)}) \equiv \begin{bmatrix} M\eta^{(k)} - \beta f(\mathbf{C}^{(k)}) - \alpha K\mathbf{C}^{(k)} \\ \theta\Delta t_k\kappa K\eta^{(k)} + M\mathbf{C}^{(k)} + \theta\Delta t_k W\mathbf{C}^{(k)} + (1-\theta)(\Delta t_k\kappa K\eta^{(k-1)} + \Delta t_k W\mathbf{C}^{(k-1)}) - M\mathbf{C}^{(k-1)} \end{bmatrix} = \mathbf{0}. \tag{3.6}$$

For instance, for $\theta = 1$ the scheme corresponds to the backward Euler method (which is first order accurate in time) and for $\theta = 1/2$ the scheme corresponds to the Crank-Nicolson method (with second order accuracy in time).

Due to the presence of the nonlinear term $f(\mathbf{C}^{(k)})$, some linearization technique has to be used. For this purpose, Newton's method is most often used. It is implemented via an iterative procedure as follows. At the kth time-step, we start with an initial guess $\mathbf{X}^{(k,0)}$. An update $\Delta\mathbf{X}^{(k,s)}$ of $\mathbf{X}^{(k,s)}$ at sth Newton step ($s = 0, 1, ...$) is computed by solving the system

$F^{(k)\prime}(\mathbf{X}^{(k,s)})\Delta\mathbf{X}^{(k,s)} = -F^{(k)}(\mathbf{X}^{(k,s)})$, where $\mathbf{X}^{(k,s)}$ is the approximate solution on the sth Newton step and the approximate solution on the next Newton step is formed as $\mathbf{X}^{(k,s+1)} = \mathbf{X}^{(k,s)} + \Delta\mathbf{X}^{(k,s)}$. The above iteration is repeated until the stopping criterion is met.

Here $F^{(k)\prime}(\mathbf{X}^{(k,s)})$ is the Jacobian matrix of $F^{(k)}(\mathbf{X}^{(k,s)})$, which is of the form

$$F^{(k)\prime}(\mathbf{X}^{(k,s)}) = \begin{bmatrix} \theta M & -\theta\beta J(\mathbf{C}^{(k,s)}) - \theta\alpha K \\ \theta\Delta t_k \kappa K & M + \theta\Delta t_k W \end{bmatrix}, \tag{3.7}$$

where $J(\mathbf{C}^{(k,s)})$ is the Jacobian of the nonlinear term $f(\mathbf{C}^{(k,s)})$. For the chosen function $\Psi'(C) = C^3 - C$, the explicit expression of the matrix $J(\mathbf{C}^{(k,s)})$ can be found in [13].

In summary, at the kth time-step, the Newton iterations comprise a sequence of approximate solutions by solving the linear systems with the nonsymmetric Jacobian matrices $F^{(k)\prime}(\mathbf{X})$, which are of two-by-two block form. We note, that, due to the block $-\theta\beta J - \theta\alpha K$ in (3.7), the matrix $F^{(k)\prime}(\mathbf{X})$ is indefinite and even may become singular. Therefore, in general, inexact Newton's method (with an approximate Jacobian matrix) should be used. This issue, however, falls out of the scope of the present work.

3.3 Preconditioning technique

As an illustration of an efficient preconditioner for the C-H equations, we summarize here the results from [13], see also the references therein. Without loss of generality we choose $\theta = 1$ (the implicit Euler Scheme) and the Jacobin matrix in (3.7) reads as follows:

$$\mathcal{A}_{CH} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} M & -J - \epsilon^2 K \\ \delta K & M + \Delta t_k W \end{bmatrix}, \tag{3.8}$$

where the coefficient $\delta = \Delta t_k \kappa$ and $\epsilon^2 = \alpha/\beta$ (for simplicity we choose $\beta = 1$).

The matrix $\mathcal{A}_{CH}$ is first simplified. It has been discussed in [13] that for small enough Δt_k relative to h, the influence of the blocks J and W diminishes and the idea to neglect those arises. The simplified matrix is of the form

$$\mathcal{A}_{CH0} = \begin{bmatrix} M & -\epsilon^2 K \\ \delta K & M \end{bmatrix}. \tag{3.9}$$

Further, it turns out that the matrix

$$\widehat{\mathcal{A}}_{CH0} = \begin{bmatrix} M & -\epsilon^2 K \\ \delta K & M + 2\epsilon\sqrt{\delta} K \end{bmatrix} \tag{3.10}$$

is an optimal preconditioner for $\mathcal{A}_{CH0}$ and all the eigenvalues of the preconditioned matrix $\widehat{\mathcal{A}}_{CH0}^{-1}\mathcal{A}_{CH0}$ belong to the interval [0.5, 1]. This idea

originates from [3] when solving symmetric complex systems, rewritten as twice larger real systems. We point out that even though the system matrix (3.9) is of two-by-two block form, the standard block-factorization methods are not that efficient since they require an approximation of the Schur complement, which is not an easy task. Here, there is no need to approximate the Schur complement. In [13] the systems with the matrix (3.8) are solved using the iterative solution method with the preconditioner $\widehat{\mathcal{A}}_{CH0}$ in (3.10). Theoretical analysis and numerical results about the preconditioner $\widehat{\mathcal{A}}_{CH0}$ can be found there.

Chapter 4

The incompressible Navier-Stokes equations

We now turn to the solution of the incompressible Navier-Stokes (N-S) equations using preconditioned iterative solution methods which, as already mentioned, is the main focus of this thesis. Since the solution of the N-S equations is considered as a part and in the context of the coupling with the Cahn-Hilliard equations, in general, the incompressible N-S equations have to be considered in their full complexity, including time-dependence, variable viscosity and variable density. The formulation reads as follows.

$$\rho(\frac{\partial \mathbf{u}}{\partial \mathrm{t}} + \mathbf{u} \cdot \nabla \mathbf{u}) - \nabla \cdot (2\mu \mathbf{D}\mathbf{u}) + \nabla p = \mathbf{f} - \eta \nabla C, \quad \text{in } \Omega \times (0, T] \tag{4.1}$$

$$\frac{\partial \rho}{\partial \mathrm{t}} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \text{in } \Omega \times (0, T] \tag{4.2}$$

$$\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T] \tag{4.3}$$

with some given boundary and initial conditions for $\mathbf{u}$. The operator $\mathbf{D}\mathbf{u} = (\nabla \mathbf{u} + \nabla^T \mathbf{u})/2$ denotes the rate-of-strain tensor for Newtonian fluids. The coefficient μ denotes the dynamic viscosity and ρ denotes the density. The term $\eta \nabla C$ denotes the surface tension force presented in its potential form (see e.g., [39]) and constitutes the coupling with the Cahn-Hilliard equations (3.2)-(3.3). Equation (4.1) represents the conservation of momentum and Equation (4.2) represents the conservation of mass. Equation (4.3) is the incompressibility condition.

The reason we need to treat density and viscosity as variable is that even though these remain constant within each phase, however they vary in the interfacial region, which evolves with time and in space (cf, e.g., [23]). Therefore, density and viscosity can be seen as smooth functions of the space position and time in the whole computational domain.

In this study, we approach the solution of the N-S equations, starting from the stationary Navier-Stokes problem with constant viscosity and

density, where the expertise in constructing preconditioners to the corresponding discrete equations is most complete and developed, and gradually increase the complexity by next considering the variable viscosity and finally address variable density. Another reason to consider the stationary incompressible Navier-Stokes problem with constant and variable viscosity in more detail is that due to the presence of a mass matrix, the linear system arising from the time-dependent Navier-Stokes problem is relatively better conditioned than that arising from the stationary Navier-Stokes problem.

4.1 Stationary incompressible N-S equations with constant viscosity

We start by considering the stationary incompressible N-S equations with constant viscosity, which read as following:

$$\begin{aligned} -\nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{f}, \quad \text{in } \Omega \\ \nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega \end{aligned} \tag{4.4}$$

with some appropriate boundary conditions. Here the coefficient ν denotes the so-called kinematic viscosity defined as $\nu = \mu/\rho$ and we assume that the density is constant ($\rho = 1$ for simplicity). Due to the presence of the nonlinear convection term, i.e., $\mathbf{u}\cdot\nabla\mathbf{u}$, some linearization technique need to be used, e.g., the Newton or Picard method (see [26]). Here we choose the Picard method, which consists of a sequence of approximate solutions of the linear Oseen's problem with constant viscosity, and reads as follows:
At each Picard iteration, find $\mathbf{u} : \Omega \times (0,T] \to \mathbb{R}^d$ and $p : \Omega \times (0,T] \to \mathbb{R}$ satisfying

$$\begin{aligned} -\nu\Delta\mathbf{u} + (\mathbf{w}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{f}, \quad \text{in } \Omega \\ \nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega \end{aligned} \tag{4.5}$$

subject to suitable boundary conditions for $\mathbf{u}$ on $\partial\Omega$. Here $\mathbf{w} = \mathbf{u}^{(k-1)}$ is the velocity, which has been computed in the previous Picard iteration, and is updated at every Picard iteration.

Let $\mathbf{H}^1_E = \{\mathbf{u} \in \mathcal{H}^1(\Omega)^d |\ \mathbf{u} = \mathbf{w} \text{ on } \partial\Omega_D\}$ and $\mathbf{H}^1_{E_0} = \{\mathbf{v} \in \mathcal{H}^1(\Omega)^d |\ \mathbf{v} = \mathbf{0} \text{ on } \partial\Omega_D\}$ and $\mathbf{X}^h_E$ and P^h are the finite dimensional subspaces of $\mathbf{H}^1_E$ and $L_2(\Omega)$. The discrete form of the weak formulation of (4.5), defined for finite-dimensional spaces, reads (cf, e.g., [26]):
Find $\mathbf{u}_h \in \mathbf{X}^h_E \subset \mathbf{H}^1_E$ and $\mathbf{p}_h \in P^h \subset L_2(\Omega)$ such that

$$\begin{aligned} \nu(\nabla\mathbf{u}_h, \nabla\mathbf{v}_h) + ((\mathbf{w}\cdot\nabla)\mathbf{u}_h, \mathbf{v}_h) - (\nabla\cdot\mathbf{v}_h, \mathbf{p}_h) &= (\mathbf{f}_h, \mathbf{v}_h), \\ (\nabla\cdot\mathbf{u}_h, \mathbf{q}_h) &= 0. \end{aligned} \tag{4.6}$$

for all $\mathbf{v}_h \in \mathbf{X}_{E_0}^h \subset \mathbf{H}_{E_0}^1$ and all $\mathbf{q}_h \in P^h$. Let $\{\varphi_i\}_{1\le i\le n_u}$ be the nodal basis of $\mathbf{X}_E^h$ and $\{\phi_i\}_{1\le i\le n_p}$ be the nodal basis of P^h such that,

$$\mathbf{u}_h = \sum_{i=1}^{n_u} \mathbf{u}_i \vec{\varphi}_i, \quad \mathbf{p}_h = \sum_{i=1}^{n_p} p_i \phi_i,$$

where n_u and n_p are the total number of unknowns for the velocity and pressure. The linear systems, arising from the discrete weak formulation (4.6) with LBB stable FEM (cf, e.g., [26]), are of the form

$$\begin{bmatrix} A & B^T \\ B & O \end{bmatrix} \begin{bmatrix} \mathbf{u}_h \\ \mathbf{p}_h \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \quad \text{or} \quad \mathcal{A}_{CV}\mathbf{x} = \mathbf{b}, \tag{4.7}$$

where the pivot matrix $A \in \mathbb{R}^{n_u \times n_u}$ corresponds to the discrete convection-diffusion operator, i.e., $A = \nu L + N$. The matrix L denotes the discrete Laplacian matrix, which is symmetric and positive definite (after Dirichlet boundary conditions applied), and the matrix N denotes the discrete convection matrix, which is nonsymmetric. The matrix $B \in \mathbb{R}^{n_p \times n_u}$ corresponds to the discrete (negative) divergence operator and the matrix B^T corresponds to the discrete gradient operator. For more details on the properties of the above matrices one can see [26].

The system matrix $\mathcal{A}_{CV}$ is nonsymmetric of saddle point form. Preconditioned iterative solution methods for saddle point problems have been studied intensively during the last 30 years (see e.g. [8, 26] and references therein). Efficient preconditioners are usually constructed based on some approximation of the factorization of the original matrix. In general, the exact factorization of a matrix of two-by-two block form is

$$\mathcal{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & 0 \\ A_{21} & S \end{bmatrix} \begin{bmatrix} I_1 & A_{11}^{-1}A_{12} \\ 0 & I_2 \end{bmatrix}, \tag{4.8}$$

where I_1 and I_2 are identity matrices of proper dimensions. The pivot block A_{11} is assumed to be nonsingular and $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$ is the exact Schur complement matrix. In our case, $A_{11} = A$, $A_{12} = B^T$, $A_{21} = B$ and $A_{22} = O$. So, $S_{\mathcal{A}_{CV}} \equiv S = -BA^{-1}B^T$. The preconditioners for such matrices of two-by-two block form are either of full block-factorized form, such as (4.9) or of block lower- or upper-triangular form, as in (4.10).

$$\mathcal{M}_F = \begin{bmatrix} \widetilde{A}_{11} & O \\ A_{21} & \widetilde{S} \end{bmatrix} \begin{bmatrix} I_1 & \widetilde{A}_{11}^{-1}A_{12} \\ O & I_2 \end{bmatrix}, \tag{4.9}$$

$$\mathcal{M}_L = \begin{bmatrix} \widetilde{A}_{11} & O \\ A_{21} & \widetilde{S} \end{bmatrix}, \qquad \mathcal{M}_U = \begin{bmatrix} \widetilde{A}_{11} & A_{12} \\ 0 & \widetilde{S} \end{bmatrix}. \tag{4.10}$$

where the matrix $\widetilde{A}_{11}^{-1}$ denotes some approximation of A_{11}^{-1}, given on explicit form or implicitly defined via inner iterative solution methods. The matrix $\widetilde{S}$ is some approximation of the exact Schur complement S.

When solving systems with the preconditioner $\mathcal{M}_F$, we need the action of $\widetilde{A}_{11}^{-1}$ twice. This is, clearly, computationally heavier task, compared to $\mathcal{M}_L$ and $\mathcal{M}_U$, where the action of $\widetilde{A}_{11}^{-1}$ is needed once. It is shown in [37] that $\mathcal{M}_L$ and $\mathcal{M}_U$ are equally efficient. In [7] it is pointed out that for indefinite systems, the block-triangular preconditioner, $\mathcal{M}_L$ or $\mathcal{M}_U$, is more efficient than the full block-factorized preconditioner $\mathcal{M}_F$. So, for the Oseen's problem with constant viscosity, the block-triangular preconditioner $\mathcal{M}_L$ or $\mathcal{M}_U$ is the one to choose.

For $\widetilde{A}_{11} = A_{11}$ and $\widetilde{S} = S$ in the preconditioner $\mathcal{M}_L$ (4.10), the preconditioned matrix $\mathcal{M}_L^{-1}\mathcal{A}$ ($\mathcal{A}$ is defined as 4.8) is of the form

$$\mathcal{M}_L^{-1}\mathcal{A} = \begin{bmatrix} A_{11}^{-1} & O \\ -S^{-1}A_{21}A_{11}^{-1} & S^{-1} \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} I_1 & A_{11}^{-1}A_{12} \\ 0 & I_2 \end{bmatrix}$$

where the matrices I_1 and I_2 are the identity matrices with proper dimensions, and the matrices A_{11} and S are nonsingular. The results in [7] show that (i) in this case the minimal polynomial of $\mathcal{M}_L^{-1}\mathcal{A}$, i.e., the polynomial $P(\cdot)$ of the smallest degree for $P(\mathcal{M}_L^{-1}\mathcal{A}) = 0$ takes the form $P = (1-t)^2$ and there will be at most two iterations when solving systems with the matrix $\mathcal{A}$ using iterative solution methods with the preconditioner $\mathcal{M}_L$; (ii) in the general case, where $\widetilde{A}_{11}^{-1} \approx A_{11}^{-1}$ and $\widetilde{S} \approx S$, the eigenvalues of $\mathcal{M}_L^{-1}\mathcal{A}$ are located in disks and the radii of the disks is controlled by making a sufficient number of inner iterations when solving systems with the pivot block matrix A_{11} and by choosing a sufficiently accurate approximation $\widetilde{S}$ of S. Thus, we can see that the quality of the preconditioner $\mathcal{M}_L$ of the matrix $\mathcal{A}$ depends on the accurate solutions of the pivot block matrix and how well the Schur complement matrix is approximated. Compared with the accurate solutions of A_{11}, the most challenging task, however, is how to construct numerically and computationally efficient approximations of the Schur complement matrix, which is in general dense and it is not practical to form it explicitly.

The research on Schur complement approximations for the Stokes and Oseen's problem with constant viscosity is quite active during the past decades (see [49] and [26] and references therein). In Paper II we do a short survey of the known approximations of the Schur complement. The included (problem-dependent) Schur complement approximations may be costly to apply, e.g., the BFBt approximation [27] or may need the construction of an artificial convection-diffusion operator on the finite element space for the pressure, e.g., the pressure convection-diffusion approximation [40]. These approximations are fairly robust with respect to the discretization and problem parameters, i.e., the mesh size h and the viscosity ν. In

Paper I we contribute to the search for efficient Schur complement approximations by trying and analyzing the element-by-element Schur complement approximation. This preconditioner is implemented based on the local features of the finite element discretization, and is of the form

$$S_{EBE} = \sum_{k=1}^{n_E} R_k^T S_e R_k \tag{4.11}$$

where R_k are the Boolean matrices which prescribe the local-to-global correspondence of the degrees of freedom and S_e is the local Schur complement on each macro element. The total number of macro elements is denoted by n_E. From the formula (4.11) we see that the construction of this approximation is relatively cheap. For a uniform mesh, we only need to compute the local Schur complement on one macro element and assemble it for all the macro elements. In several works (see e.g. [41, 6]) it has been shown that, in the case of symmetric and positive definite matrices, split into a two-by-two block form, based on consecutive regular mesh refinements, S_{EBE} is a high quality approximation of the exact Schur complement S, i.e., $(1-\zeta^2)S \leq S_{EBE} \leq S$, where ζ is a positive constant, strictly less that 1, independent on the mesh size and easily computable. (Here the notation $K \leq Z$ means that the matrix $Z - K$ is positive semi-definite.) In Paper I this method is used to approximate the Schur complements of the system matrices arising from the Cahn-Hilliard and Oseen's problem, where the system matrices are non-symmetric and the two-by-two form of the element matrices is due not to the mesh refinement but to the fact that we deal with a system of two equations. Although this approximation is not robust with respect to the mesh size and the viscosity, it is still attractive in some cases because of its low computational cost.

Aiming at finding some preconditioner which is fully independent of the mesh size and the viscosity, we turn to the so-called augmented Lagrangian (AL) approach (see e.g. [29]). Following this approach we first transform the linear system (4.7) into an equivalent one with the same solution, which is of the form

$$\begin{bmatrix} A + \gamma B^T W^{-1} B & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_h \\ \mathbf{p}_h \end{bmatrix} = \begin{bmatrix} \widehat{\mathbf{f}} \\ \mathbf{g} \end{bmatrix} \quad \text{or} \quad \widetilde{\mathcal{A}}_{CV}\mathbf{x} = \widehat{\mathbf{b}}, \tag{4.12}$$

where $\gamma > 0$ and W are suitable scalar and matrix parameters. The modified right hand vector is $\widehat{\mathbf{f}} = \mathbf{f} + \gamma B^T W^{-1} B\ \mathbf{g}$. It is clear that the transformation (4.12) holds for any value of γ, including $\gamma = 1$ or $\gamma \ll 1$, and any nonsingular matrix W. In paper [9] and [10] the AL type preconditioners are proposed for the transformed system (4.12), which are of block lower- or upper-triangular form

$$\widetilde{\mathcal{M}}_{Lcv} = \begin{bmatrix} A+\gamma B^T W^{-1} B & 0 \\ B & -\frac{1}{\gamma} W \end{bmatrix} \quad \text{or} \quad \widetilde{\mathcal{M}}_{Ucv} = \begin{bmatrix} A+\gamma B^T W^{-1} B & B^T \\ 0 & -\frac{1}{\gamma} W \end{bmatrix} \tag{4.13}$$

Now we can explain the purpose of doing the transformation (4.12). Comparing the matrix $\widetilde{\mathcal{A}}_{CV}$ (4.12) with its AL type preconditioner (4.13) and the general two-by-two block matrix $\mathcal{A}$ (4.8) with its block triangular preconditioner (4.10), we can see that the Schur complement $S_{\widetilde{\mathcal{A}}_{CV}} = -B(A+\gamma B^T W^{-1} B)^{-1} B^T$ of the transformed matrix $\widetilde{\mathcal{A}}_{CV}$ (4.12) is approximated by $-\frac{1}{\gamma} W$, where the matrix W can be the pressure mass matrix as shown in [9] or even be the identity matrix as shown in [5].

The AL type preconditioner (4.13) works efficiently for the transformed matrix (4.12) with the requirement that the value of γ should be large (see e.g. [9] and Paper II). However, the modified pivot block matrix of $\widetilde{\mathcal{A}}_{CV}$ (4.12), i.e., $\widetilde{A} = A + \gamma B^T W^{-1} B$, becomes increasingly ill-conditioned with $\gamma \to \infty$, which contradicts to the requirement that γ needs to be large. Numerical experiments in paper II and [9] illustrate that for moderate values of γ, such as $\gamma = 1$, the AL type preconditioners with $W = M_p$ (the pressure mass matrix) work efficiently and do not depend on the mesh size and the viscosity. This observation is very important because it eases the implementation of the AL type preconditioners.

On the other side, although we circumvent the difficulties to approximate the Schur complement of the original system (4.7), we move the challenge to how to efficiently solve systems with the modified pivot matrix $\widetilde{A} = A + \gamma B^T W^{-1} B$, which is much denser than A and is also a Schur complement matrix. Direct methods are used in many research papers, which means that the pivot block has to be explicitly computed first, and then can be factorized. This becomes increasing unacceptable with the size of problems turning bigger and bigger. In other studies, for instance, in [9] and [10], a problem-dependent multigrid method has been derived. In [10], preconditioners for $\widetilde{A} = A + \gamma B^T W^{-1} B$ are derived, which work efficiently, however, requiring that the values of γ have to be relatively small, empirically determined as 0.01 even 0.001. The latter contradicts to the requirement that γ needs to be large so that the AL type preconditioners (4.13) work well for the transformed system (4.12). Our main contribution regarding the AL type preconditioners is that in Paper II we explain the above behavior through a more general framework. The analysis reveals that if we attempt to balance the inner solution (preconditioners to the modified pivot block matrix $\widetilde{A}$) and the outer solution (preconditioners to the transformed system matrix $\widetilde{\mathcal{A}}_{CV}$), then finding a good preconditioner for the Schur complement, i.e., $-BA^{-1}B^T$, of the original system matrix $\mathcal{A}_{CV}$ in (4.7) is unavoidable.

4.2 Stationary incompressible N-S equations with variable viscosity

Consider next the stationary incompressible Navier-Stokes equations with variable viscosity, which read as follows

$$\begin{aligned} -\nabla \cdot (2\nu(\mathbf{x})\mathbf{D}\mathbf{u}) + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p &= \mathbf{f}, \quad \text{in } \Omega \\ \nabla \cdot \mathbf{u} &= 0. \quad \text{in } \Omega \end{aligned} \tag{4.14}$$

with suitable boundary conditions and the assumption that density is constant ($\rho = 1$ for simplicity). This type problems are also studied for non-Newtonian flows, where the variable viscosity may depend on the pressure and the rate-of-strain tensor (cf, e.g., [12, 51]) or the pressure and the shear (cf, e.g., [38, 43, 50]). In Paper III we assume that the kinematic viscosity coefficient is a smooth function, such that

$$0 \leq \nu_{\min} \leq \nu(\mathbf{x}) \leq \nu_{\max},$$

where $\nu_{\min}$ and $\nu_{\max}$ denote its minimal and maximal value. As mentioned already, the motivation of considering the variable viscosity of this form is that in the simulation of the multi-phase flow the density and viscosity remain constant in each phase and vary rapidly and smoothly in the interfacial region.

There are several ways to treat the nonlinear convection term $(\mathbf{u} \cdot \nabla)\mathbf{u}$ in (4.14). (i) One option is to treat it explicitly and move it into the right hand side. This leads to a Stokes-type problem with variable viscosity and the resulting algebraic system matrix is the same on each iteration. For this formulation, block preconditioner involving a mass type matrix for the pressure is proposed and analyzed in [32]. However, the above treatment of the nonlinear term may not be efficient for convection-dominated problems. (ii) Another option is to linearize and discretize the convection term, and incorporate the arising matrix into the system matrix. Thus, Oseen-type problem with variable viscosity arises. In Paper III, we focus on the construction of efficient preconditioners for the matrices arising from Oseen-type problem with variable viscosity.

Here we also choose the Picard method to linearize (4.14) and Oseen-type problem with variable viscosity reads as follows.
At each Picard iteration, find $\mathbf{u} : \Omega \times (0, T] \to \mathbb{R}^d$ and $p : \Omega \times (0, T] \to \mathbb{R}$ satisfying

$$\begin{aligned} -\nabla \cdot (2\nu(\mathbf{x})\mathbf{D}\mathbf{u}) + (\mathbf{w} \cdot \nabla)\mathbf{u} + \nabla p &= \mathbf{f}, \quad \text{in } \Omega \\ \nabla \cdot \mathbf{u} &= 0, \quad \text{in } \Omega \end{aligned} \tag{4.15}$$

subject to suitable boundary conditions for $\mathbf{u}$ on $\partial\Omega$. Here $\mathbf{w} = \mathbf{u}^{(k-1)}$ is the velocity which has been computed in the previous Picard iteration, and is updated at every Picard iteration.

The discrete form of the weak formulation of (4.15) defined using finite-dimensional spaces reads:
Find $\mathbf{u}_h \in \mathbf{X}_E^h \subset \mathbf{H}_E^1$ and $\mathbf{p}_h \in P^h \subset L_2(\Omega)$ such that

$$\begin{aligned}(2\nu(\mathbf{x})\mathbf{D}\mathbf{u}_h, \mathbf{D}\mathbf{v}_h) + ((\mathbf{w}\cdot\nabla)\mathbf{u}_h, \mathbf{v}_h) - (\nabla\cdot\mathbf{v}_h, \mathbf{p}_h) &= (\mathbf{f}_h, \mathbf{v}_h),\\ (\nabla\cdot\mathbf{u}_h, \mathbf{q}_h) &= 0.\end{aligned} \tag{4.16}$$

for all $\mathbf{v}_h \in \mathbf{X}_{E_0}^h \subset \mathbf{H}_{E_0}^1$ and all $\mathbf{q}_h \in P^h$. The definitions of the spaces of $\mathbf{H}_{E_0}^1$ and $\mathbf{H}_E^1$ can be found in Chapter 4.1.

Here we again let $\{\varphi_i\}_{1\le i\le n_u}$ be the nodal basis of $\mathbf{X}_E^h$ and $\{\phi_i\}_{1\le i\le n_p}$ be the nodal basis of P^h such that $\mathbf{u}_h = \sum_{i=1}^{n_u} \mathbf{u}_i\vec{\varphi}_i$ and $\mathbf{p}_h = \sum_{i=1}^{n_p} p_i\phi_i$, where n_u and n_p are the total number of unknowns for the velocity and pressure. The linear systems arising from the discrete weak formulation (4.16) with LBB stable FEM (cf, e.g., [26]) are of the form

$$\begin{bmatrix} F & B^T \\ B & O \end{bmatrix}\begin{bmatrix}\mathbf{u}_h \\ \mathbf{p}_h\end{bmatrix} = \begin{bmatrix}\mathbf{f}\\ \mathbf{g}\end{bmatrix} \quad \text{or} \quad \mathcal{A}_{VV}\mathbf{x} = \mathbf{b}, \tag{4.17}$$

where the system matrix $\mathcal{A}_{VV} = \begin{bmatrix} F & B^T \\ B & O \end{bmatrix}$ is again nonsymmetric of saddle point form. The unknown vector $\mathbf{u}_h$ is the discrete velocity vector and $\mathbf{p}_h$ is the discrete pressure vector. Combining them together we have $\mathbf{x}^T = [\mathbf{u}_h^T \quad \mathbf{p}_h^T]$. The definitions of the matrices B and B^T have been given in Chapter 4.1. Clearly, when considering variable viscosity, the only difference in the arising matrices with FEM, compared to the Oseen's problem with constant viscosity, is observed in the pivot block matrix $F \in \mathbb{R}^{n_u\times n_u}$, which, in the case of variable viscosity has the form $F = A_\nu + N$. The discrete convection matric N has been defined in Chapter 4.1 and the matrix A_ν, which arises from the discretization of the term $(2\nu(\mathbf{x})\mathbf{D}\mathbf{u}, \mathbf{D}\mathbf{v})$, is of the form $[A_\nu]_{i,j} = (2\nu(\mathbf{x})\mathbf{D}\vec{\varphi}_i, \mathbf{D}\vec{\varphi}_j)$. The matrix A_ν is symmetric and positive definite (see more details in Paper III).

In order to construct efficient preconditioners for the system matrix $\mathcal{A}_{VV}$ in (4.17), we consider once again the augmented Lagrangian approach. Namely, we transform the system (4.17) into an equivalent one, which is

$$\begin{bmatrix} F+\gamma B^TW^{-1}B & B^T \\ B & 0 \end{bmatrix}\begin{bmatrix}\mathbf{u}_h \\ \mathbf{p}_h\end{bmatrix} = \begin{bmatrix}\widehat{\mathbf{f}}\\ \mathbf{g}\end{bmatrix} \quad \text{or} \quad \widetilde{\mathcal{A}}_{VV}\mathbf{x} = \widehat{\mathbf{b}}, \tag{4.18}$$

and then propose the AL type preconditioners (4.19) to the transformed matrix $\widetilde{\mathcal{A}}_{VV}$.

$$\widetilde{\mathcal{M}}_{Lvv} = \begin{bmatrix} F+\gamma B^TW^{-1}B & 0 \\ B & -\frac{1}{\gamma}W \end{bmatrix} \quad \text{or} \quad \widetilde{\mathcal{M}}_{Uvv} = \begin{bmatrix} F+\gamma B^TW^{-1}B & B^T \\ 0 & -\frac{1}{\gamma}W \end{bmatrix}. \tag{4.19}$$

Our contributions to constructing the efficient preconditioners of Oseen-type problems with variable viscosity are that (i) in Paper III we theoretically prove that the bounds of the eigenvalues of the preconditioned matrix,

i.e., $\widetilde{\mathcal{M}}_{Lvv}^{-1}\widetilde{\mathcal{A}}_{VV}$ with $W = M_p$ (M_p is the pressure mass matrix) are independent of the mesh size, but dependent of the values of $\nu_{\min}$ and $\nu_{\max}$. The derived bounds are generalizations of those, derived for constant viscosity, as shown in [27] and Paper II. (ii) Numerical experiments in Paper III illustrate that the AL type preconditioner $\widetilde{\mathcal{M}}_{Lvv}$ with $W = M_p$ and $\gamma = 1$ still works efficiently for the transformed system matrix $\widetilde{\mathcal{A}}_{VV}$ for a large range of the values of $\nu_{\min}$ and $\nu_{\max}$.

However, how to efficiently solve systems with the modified pivot block matrix $\widetilde{F} = F + \gamma B^T W^{-1} B$ of the transformed matrix $\widetilde{\mathcal{A}}_{VV}$ in (4.18) is the most difficult part in the application of the AL type preconditioner. This open question is discussed in Chapter 5.

4.3 Incompressible N-S equations with variable density

One often used technique to solve the time-dependent incompressible Navier Stokes equations with variable density is via some operator splitting method. Most of the known splitting methods decouple the diffusion operator and the incompressibility constrain. These are originally developed from the *simple* projection method, which is originally proposed by Chorin [22] and Temam [55] and also referred to as the *non-incremental pressure-correction* algorithm. To understand the splitting technique, we describe the original simple projection algorithm in some detail and for simplicity let the time-step Δt be constant, i.e., $\Delta t = T/N$. Then, the points in time are $t^k = k\Delta t$ for $k = 0, 1, ..., N$. Neglecting the nonlinear convection term in the N-S equations for simplicity and using the implicit Euler time stepping scheme, the non-incremental pressure-correction algorithm applied to solve the time-dependent Stokes problem with constant density reads as follows:
Set $\mathbf{u}^0 = \mathbf{u}_0$, then for all time-steps t^{k+1}, $k \geq 0$, compute $(\tilde{\mathbf{u}}^{k+1}, \mathbf{u}^{k+1}, p^{k+1})$ by solving

$$\begin{aligned} \frac{\rho}{\Delta t}(\tilde{\mathbf{u}}^{k+1} - \mathbf{u}^k) - \mu\Delta\tilde{\mathbf{u}}^{k+1} &= \mathbf{f}(t^{k+1}), \\ \tilde{\mathbf{u}}^{k+1} &= 0 \text{ on } \partial\Omega, \end{aligned} \tag{4.20}$$

and then

$$\begin{aligned} \frac{1}{\Delta t}(\mathbf{u}^{k+1} - \tilde{\mathbf{u}}^{k+1}) + \frac{1}{\rho}\nabla p^{k+1} &= 0, \\ \nabla \cdot \mathbf{u}^{k+1} &= 0 \text{ in } \Omega, \\ \mathbf{u}^{k+1} \cdot \mathbf{n} &= 0 \text{ on } \partial\Omega, \end{aligned} \tag{4.21}$$

where $\mathbf{n}$ denotes the unit outward normal vector. Clearly, at each time-step this algorithm consist of two sub-steps. In the first sub-step, one computes

$\tilde{\mathbf{u}}^{k+1}$ by solving the equation (4.20). Once $\tilde{\mathbf{u}}^{k+1}$ is obtained, the pressure p^{k+1} is computed by solving the following Poisson problem:

$$\Delta p^{k+1} = \frac{\rho}{\Delta t}\nabla \cdot \tilde{\mathbf{u}}^{k+1}, \quad \frac{\partial p^{k+1}}{\partial n} = 0 \text{ on } \partial\Omega. \tag{4.22}$$

Indeed, the second sub-step can be represented as follows:
Using $\tilde{\mathbf{u}}^{k+1}$ and p^{k+1} to compute $\mathbf{u}^{k+1}$ by

$$\begin{aligned} \mathbf{u}^{k+1} + \frac{\Delta t}{\rho}\nabla p^{k+1} &= \tilde{\mathbf{u}}^{k+1}, \\ \nabla \cdot \mathbf{u}^{k+1} &= 0 \text{ in } \Omega, \\ \mathbf{u}^{k+1} \cdot \mathbf{n} &= 0 \text{ on } \partial\Omega. \end{aligned} \tag{4.23}$$

By introducing the Hilbert space

$$\mathbf{H} = \{\mathbf{u} \in L_2(\Omega) \mid \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega; \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega\},$$

the second sub-step can be equivalently rewritten as the projection step $\mathbf{u}^{k+1} = P_{\mathbf{H}}\tilde{\mathbf{u}}^{k+1}$, where $P_{\mathbf{H}}$ is the L_2-projection onto $\mathbf{H}$. This is the reason to refer this method and its other variants as projection methods.

The above algorithm is of first order accuracy in time for the velocity and pressure. The above operator splitting scheme introduces a splitting error of order $O(\Delta t)$ (cf, e.g., [34]), and therefore, there is no improvement of the overall accuracy if one uses higher order time discretization schemes. There are many variants derived from the non-incremental pressure-correction algorithm, e.g., the standard incremental pressure-correction algorithm, the rotational incremental pressure-correction algorithm and so on. Higher order scheme, e.g., the backward difference formula of second order (BDF2) can be used to approximate the time derivative in the standard/rotational incremental pressure-correction algorithms. which are of second order accuracy in time for the velocity. For a comprehensive view of the projection methods for the incompressible flows, we refer to [34].

For the variable density, most of the already known splitting algorithms are similar to the non-incremental pressure-correction algorithm introduced above. They also consist of two sub-steps at each time-step. In the first step, one need to solve problems similar to (4.20), where the pressure is treated explicitly or ignored. In the second step one need to solve problems similar to (4.21). Taking the divergence of the two sides of equations similar to (4.21), one need to solve a variable coefficient Poisson-type problem as follows:

$$-\nabla \cdot (\frac{1}{\rho^{k+1}}\nabla\Phi) = \Psi, \quad \frac{\partial \Phi^{k+1}}{\partial n} = 0 \text{ on } \partial\Omega, \tag{4.24}$$

where ρ^{k+1} is the approximation of the variable density at discrete time t^{k+1} and Ψ is some right hand side with varies at every time-step. The variable

Φ may be the pressure or some other related scalar. Stable algorithms proposed for solving the incompressible N-S equations with variable density can be found in [35, 52].

Due to the variable density one need to assemble and solve a system with the variable coefficient stiffness matrix like (4.24) in the second sub-step. Clearly, it is time consuming. In [36] efficient algorithms are proposed for solving the incompressible flows with variable density, which involve the assemble of the stiffness matrix only once and solving the Poisson problem instead of the Poisson-type problem like (4.24) in the second sub-step. In future study, one research area is the construction of efficient preconditioners of the systems arising from the problems similar to (4.20) in the first sub-step of the algorithms introduced in [36].

Splitting the incompressibility constrain and the diffusion operator reduces the computational complexity to solving problems as in (4.24) and as in (4.20). However, the splitting error and accuracy deficiency are the main limitations of the known splitting techniques. The existing algorithms, which have been proved to be stable, are of up to second order in time for the velocity, which means that we have to use relatively small time-steps to keep the accuracy of the solutions. Another research area in the future is finding some efficient solution methods, which have higher accuracy for the solutions in time and one possible method is very briefly introduced in Chapter 7.

Chapter 5

Computational challenges

In Chapters 4.1 and 4.2 we consider iterative solution methods for the Navier-Stokes problems with constant and variable viscosity. We choose the AL type preconditioner and there are two computational issues which need to be considered.

(1) When constructing and solving systems with the AL type preconditioners, we need an efficient and cheap approximate inverse of the pressure mass matrix. In Paper II, based on local features of the Finite Element discretization (see e.g. [30, 31, 58]), we derive and analyse the so-called element-by-element sparse approximate inverse of the pressure mass matrix. Numerical experiments in Paper II and Paper III show that this approximate inverse of the pressure mass matrix, involved in the AL type preconditioners, works well for both the constant and variable viscosity cases on a low computational cost. For the related topics on the sparse approximate inverse we refer to [11], [16], [33] and [42].

(2) How to efficiently solve systems with the block matrices $\widetilde{A} = A + \gamma B^T W^{-1} B$ (in the constant viscosity case) in (4.13) and $\widetilde{F} = F + \gamma B^T W^{-1} B$ (in the variable viscosity case) in (4.19) is still an open question. We propose an algorithm to compute the exact or approximate inverse of $\widetilde{A}$ and $\widetilde{F}$, based on the inverse Sherman-Morrison's (ISM) formula (e.g. [14] and [15]). The algorithm and its discussion can be seen in paper II. In [21], multiplicative preconditioners are constructed based on the block ISM algorithm and numerical experiments there show that the block ISM algorithm is efficient both in terms of the number of preconditioned iterations and the constructing time. Approximate inverse of $\widetilde{A}$ and $\widetilde{F}$ based on the block ISM algorithm is one possible approach to resolve this challenging open question. In an unpublished work, we have implemented and tested the performance of the ISM method in parallel, using a block-version of it and the standard BLAS operations.

When solving the coupled system comprising the incompressible Navier-Stokes (N-S) and Cahn-Hilliard (C-H) equations, there are two challenging issues to be considered.

(3) In order to decrease the number of the degrees of freedom, the adaptively refined and de-refined meshes are needed. How to determine the domains where the mesh needed to be refined or de-refined and how to choose the stopping tolerances for the refinement and de-refinement are the main challenges. These issues are discussed in [59] and [24].

(5) The smaller time-steps result in better conditioned system matrices arising from the time-dependent N-S and C-H equations and it is easier to solve systems with these matrices. However, smaller time-steps require more computation, especially when the simulation time interval is large. Thus, finding suitable time-steps balancing the aspects mentioned above is also quite important and challenging.

Chapter 6

Summary of Papers

6.1 Paper I

In this paper we consider preconditioned iterative solution methods for the numerical simulation of multi-phase flow, which is governed by the time-dependent Cahn-Hilliard (C-H) and incompressible Navier-Stokes (N-S) equations. The test problems considered in this paper consist of the linearized stationary N-S problem, i.e., Oseen's problem with constant viscosity in 2D and a moving interface with constant speed governed by the C-H equations also in 2D. The matrices arising from the finite element discretization of the above two problems are nonsymmetric of two-by-two block form. The Schur complements of the so-arising matrices are approximated via the element-by-element Schur complement approximation method, which is shown in several works (e.g. [41, 6]) to be a cheap technique resulting in high quality Schur complement approximations for the symmetric and positive definite matrices. In this paper, a framework is suggested to study the quality of the element-by-element Schur complement approximation for general nonsymmetric matrices. The numerical experiments show that due to its low computational cost, the element-by-element Schur complement approximation is still an attractive technique to precondition the exact Schur complement for the considered test problems, in particular for the N-S problems, which are not strongly convection-dominated.

6.2 Paper II

In this paper we mainly focus on constructing efficient preconditioners for the nonsymmetric matrices of saddle point form arising from the finite element discretization of the Oseen's problem with constant viscosity. Aiming at finding some efficient preconditioners, which are fully robust with respect to the mesh size and the viscosity, we choose the augmented Lagrangian (AL) method, where the original system is transformed into an equivalent

one and a block triangular preconditioner is used for the transformed system matrix. The AL type approach involves a scalar parameter γ and an approximate inverse of the pressure mass matrix. The main challenge is how to efficiently solve systems with the modified pivot block matrix of the transformed system matrix, which is much denser than the original one. There exist some preconditioners for the modified pivot block matrix, which work well for relatively small values of γ, such as 0.01 and 0.001 (see e.g. [10]). However, the value of γ needs to be large to make the AL type preconditioner work efficiently for the whole system matrix. The main contribution in this paper is that via a more general framework we analyse the influence of the value of γ on both the convergence rates of the outer (for the whole system matrix) and the inner (for the pivot block matrix) solution methods. Another contribution is that we propose an algorithm to compute the exact (or an approximation of the) inverse of the modified pivot matrix, based on the inverse Sherman-Morrison (ISM) formula. The multiplicative preconditioner, constructed via the block ISM algorithm, is shown to be efficient in terms of the construction time and preconditioning time (see e.g. [21]).

6.3 Paper III

In this paper we consider the construction of efficient preconditioners for the matrices arising from the finite element discretization of Oseen-type problem with variable viscosity. We apply the augmented Lagrangian approach. In Paper III we prove that the AL type preconditioner involving the pressure mass matrix is independent of the mesh size, but depends on the maximal and minimal values of the viscosity, i.e., $\nu_{\max}$ and $\nu_{\min}$. For $\nu_{\max} = \nu_{\min} = \nu$, the theoretical results derived in this paper coincide with those when using the augmented Lagrangian approach and the AL type preconditioner for the Oseen's problem the constant viscosity (see e.g. [28]). Numerical experiments in Paper III show that the AL type preconditioner works efficiently for a large rang of the values of $\nu_{\max}$ and $\nu_{\min}$. However, the efficient solution methods for the modified pivot block matrix of the transformed system matrix is more challenging compared to the case of constant viscosity.

Chapter 7

Summary and future work

A future research direction is the fast solution method for the time-dependent incompressible Navier-Stokes equations with variable density and viscosity. There are two approaches for this problem. The first one is to use the so-called splitting method to decouple the solution for density, velocity and the pressure. This method is also referred to as the projection method, which consists of three sub-steps. In the first two sub-steps one compute the solution for density and velocity. In the third sub-step one need to solve a Poisson problem to compute the solution for pressure. More details about the splitting method can be found in [36]. Efficient solution methods for the Poisson problem have been studied intensively, and the parallel algebraic multi-grid (AMG) (see e.g. [56]) is an efficient method to solve the Poisson problem. We consider iterative solution methods to solve the systems with the matrices arising from the first two sub-steps. Efficient preconditioners for these so-arising matrices need a further study. The known splitting methods, which have been proved to be stable, are up to the second order accuracy in time, therefore, relatively small time-steps are needed to keep the accuracy of the solution.

Aiming at using large time-steps to reduce the simulation time while keeping the accuracy of the solutions within certain bounds, we may consider another approach, namely, to represent the system governing the incompressible and time-dependent Navier-Stokes problem as a system of differential algebraic equations (DAEs) (see e.g. [48]). In this way high-order time integration methods and large time-steps can be used. The solution methods for DAEs and their applications to the Navier-Stokes problems need to be considered in future.

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