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Numerical Methods for Two-phase Incompressible Flows

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Dedicated to Agnes and Monique

Preface

Numerical treatment of two-phase incompressible flow problems

In the past few decades there has been tremendous progress in the development and analysis of numerical methods for *one*-phase incompressible Stokes and Navier-Stokes equations. There is an extensive literature on space- and time discretization methods, iterative solvers and other numerical issues, e.g., implementation aspects, related to this problem class. This literature comprises a huge number of papers and many monographs. The research activities resulted in output ranging from new fundamental mathematical insights to software packages that can be used for the simulation of incompressible flow problems. Nowadays open source and commercial software packages are available that perform satisfactory when used as black or gray box solvers for a fairly large class of incompressible one-phase flow problems. Although very big progress has been made, there are still important topics which require further research. For example, in the field of development and analysis of numerical methods for the simulation of turbulent flows, non-Newtonian flows and flows coupled with chemistry the state of the art is not satisfactory, yet.

The work that has been done on numerical methods for one-phase incompressible Navier-Stokes equations forms a solid basis for an extension to the class of *two*-phase incompressible flow problems. In the past decade research on this topic has started. Until now most research results in this field have been published in the engineering literature. There are only few papers that have appeared in the numerical mathematics literature and address rigorous mathematical analysis of methods for two-phase flow problems. This book is meant to give an overview of, and introduction to this field of (analysis of) numerical methods for incompressible two-phase flow problems. We do not know of any other monograph devoted to this topic. In our opinion, time is ripe for substantial progress in the field of numerical analysis of methods for two-phase incompressible flows. There are several important issues relevant for the simulation of two-phase flows that are non-existent in one-phase incompressible flow problems. We briefly address a few of these:

Numerical treatment of the unknown interface. Even in the simplest case of immiscible fluids, i.e. no phase transition or evaporation phenomena, the numerical treatment of the unknown interface is a difficult task. Several numerical techniques are used, ranging from interface tracking, based on an explicit parametrization of the interface, to (VOF or level set) interface capturing methods, which are based on some indicator function. Until now many problems related to e.g. the coupling between the interface evolution and fluid dynamics, mass conservation, accuracy of discretizations and treatment of topological singularities (droplet collision) are largely unsolved. Only very few rigorous mathematical analyses related to these problems are known.
Numerical approximation of surface tension forces. The surface tension force is localized on the interface and in many two-phase systems it determines the flow behavior to a large extent. In case of topological singularities it is not obvious how this force should be modeled. An accurate numerical approximation of this force is often of major importance for a successful simulation, since an insufficient treatment leads to numerical oscillations at the interface (so-called *spurious velocities*). Only few approximation methods are known and analyses of these methods are very scarce.
Simulation of mass and heat transport from one phase into the other. The transport of a dissolved species from one phase into the other is usually modeled by convection-diffusion equations in the two phases that are coupled by a certain condition at the interface. If the species can attach to the interface this gives rise to (open) modeling problems. In general the concentration of the species is *dis*continuous across the interface. In that case one has to determine numerically a solution of a transport problem that is discontinuous across an evolving unknown interface. This topic has hardly been investigated in the literature. In certain systems it may be important to model a dependence of the surface tension on the concentration of the dissolved species or on the fluid temperature at the interface. If this is the case it results in a complicated strongly nonlinear coupling between the two-phase fluid dynamics and the mass or heat transport. The problem of how to handle numerically this coupling has hardly been addressed.
Simulation of surfactants, which are transported on the interface. It may happen that in the two-phase system there is a species (called tenside or surfactant) which adheres to the interface and is transported on the interface due to convection and molecular diffusion. An interesting modeling problem is how adsorption and desorption effects can be described. This surfactant transport results in a convection-diffusion equation on the interface only. As in the case of mass or heat transport discussed above there may be a dependence of the surface tension on the surfactant concentration. First studies of numerical methods for solving such surfactant transport equations, coupled with two-phase fluid dynamics, have appeared only recently.
Further interesting issues, which however will not be treated in this monograph, are the modeling and numerical treatment of evaporation, phase transition, topological singularities and reaction processes at the interface.

In this monograph we address topics, such as the four mentioned above, that are important in the numerical simulation of two-phase incompressible flow problems. We give a fairly complete treatment of such flow problems in the sense that we derive models, discuss appropriate weak formulations, introduce and analyze discretization methods, investigate iterative solvers and finally pay attention to implementation aspects and present results of numerical experiments. On the other hand we restricted ourselves to *in*compressible flows and do not consider important phenomena like phase transition and topological singularities. Also concerning the class of methods we made a severe restriction: we only treat discretizations based on finite elements. Within the problem and method classes considered in this book we tried to give a fairly complete overview. We do not present an overview of work that lies outside this problem class, e.g., flow problems with phase transition or compressible two-phase flows, or outside this method class, e.g., finite difference discretizations of two-phase flows.

Contents of this monograph

We start with an introductory chapter in which the basic models for one- and two-phase incompressible flows, for mass transport between the phases and for surfactant transport are derived. The book consists of five parts. We outline the main topics treated in these parts.

Part I. We first consider the incompressible Stokes and Navier-Stokes equations that model a *one*-phase flow. We treat numerical methods for these one-phase flows that are also used as basic building blocks in the simulation of *two*-phase flows, which is studied in Part II. The space discretizations that we consider are based on finite element methods. Therefore one needs suitable variational (weak) formulations. For this we collect some results on function spaces and variational formulations for (Navier-) Stokes equations known from the standard literature. We explain Hood-Taylor finite element discretization methods on multilevel tetrahedral triangulations and popular time discretization methods for Navier-Stokes equations. The topic of efficient iterative solvers is addressed. We give an introduction to multigrid methods and discuss certain Schur complement preconditioners for saddle point problems. In this part as well as in the other parts, for a specific method (or approach) we often address three aspects: 1. We try to give a clear description of the method. 2. A mathematical analysis of certain important aspects (e.g. discretization error, rate of convergence), often for a simplified model problem, is presented. 3. The method is implemented and results of numerical experiments, which illustrate certain phenomena, are presented.
Part II. We consider the fluid-dynamics in a two-phase incompressible flow problem with surface tension. The issue of interface representation is treated and a weak formulation of a two-phase Navier-Stokes equation with a localized surface tension force is given. Finite element discretization methods are developed and analyzed. In particular a special method for the discretization of

the surface tension force and so-called extended finite element spaces (XFEM) for the pressure approximation are studied. Time discretization schemes are derived and finally iterative solvers are considered.

Part III. We address the numerical simulation of mass transport between the two phases. An appropriate weak formulation is derived. Based on this, finite element space discretization methods and time discretization schemes are discussed. We distinguish between problems with a stationary and with a non-stationary interface. An important issue is the numerical treatment of the discontinuity in the solution across the interface.

Part IV. In this part the convection-diffusion problem which models transport of surfactants is treated. Suitable weak formulations are discussed. Finite element methods based on both interface tracking and interface capturing techniques are presented.

Part V. This is an appendix consisting of two chapters. In the first chapter we collect some elementary results from differential geometry. In the second chapter we give some main results on variational problems in Hilbert spaces (e.g. Lax-Milgram lemma) and on Schur complement preconditioning of saddle point problems in Hilbert spaces.

Among the many numerical approaches treated in this monograph there are some that deserve special attention because these turned out to be particularly useful for the efficient simulation of our two-phase flow problems or we consider them to be promising for future applications. Therefore we emphasize these already in this preface:

- The finite element spaces that we use are based on *a hierarchy of nested tetrahedral triangulations*. The nested hierarchy allows very easy and efficient local refinement and coarsening routines. A (strong) local refinement close to the (evolving) interface in general enhances efficiency significantly. Furthermore, due to the nested hierarchy the use of efficient multigrid solvers is relatively easy.
- In our applications the surface tension is an important driving force. An accurate discretization of this force is essential for reliable simulation results. We use a *Laplace-Beltrami approach* in which the second derivative (curvature) in the surface tension functional can be avoided by partial integration. This technique is based on the representation of the curvature as a Laplace-Beltrami operator applied to the identity. We introduce and analyze an accurate variant of this method. In this method we use a hybrid version of the level set method in the sense that the level set equation is used to describe the evolution of the (implicitly given) interface but for the evaluation of the discrete surface tension functional we need an explicit reconstruction of the interface.
- In the class of two-phase flow problems that we consider there are several quantities which in general are discontinuous across the interface, namely viscosity, density, pressure and, if mass transport is considered, the concentration of a dissolved species. The (approximate) interface is not aligned

with the triangulation and thus we have unknowns (pressure, concentration) that are discontinuous within certain elements. For an accurate approximation of these unknowns we use the *extended finite element method* (XFEM), which has been used in the literature for other applications (e.g. crack propagation in continuum mechanics).

- If mass transport is considered then, due to the so-called Henry interface condition, the ratio of the unknown concentrations on the two sides of the interface has to be equal to a given constant. In general this (Henry) constant is not equal to one, which implies a discontinuity. To satisfy this interface condition we combine the XFEM approach with a *technique due to Nitsche*, in which the bilinear form that represents the partial differential equation is modified such that the jump relation is automatically satisfied in a certain weak sense.
- For one-phase flows and two-phase flows with a stationary interface we use the method of lines ("first space, then time") or the Rothe approach ("first time, then space") to obtain a fully discrete problem. For two-phase flow problems with a non-stationary interface the method of lines approach is not appropriate. The Rothe method is still useful but also *space-time finite element methods* are very suitable. We use the latter method class for the mass transport and for the surfactant transport equation.
- For the spatial discretization of the surfactant transport equation on the interface we introduce and analyze a *new interface finite element method.* The main idea of this method is the use of the trace of a standard outer finite element space (used for discretization of the flow variables) for discretization on the reconstructed approximate interface.
- In the time discretization we use implicit schemes in which the flow variables and the level set function are fully coupled. In each time step a nonlinear problem for these unknowns has to be solved. Due to the surface tension term there is a strongly nonlinear coupling between the flow variables and level set unknowns. We treat efficient *iterative decoupling strategies.*
- After discretization, decoupling and linearization one obtains large sparse linear systems with a saddle point structure. We use block preconditioners for the efficient solution of these linear systems. Special *Schur complement preconditioners* are presented.

Readership

We intended to make a monograph that is of interest for MSc and PhD students with a specialization in Numerical Analysis or Computational Engineering who want to get acquainted with numerical methods for two-phase incompressible flows. Basic knowledge of the numerical treatment of one-phase flow problems is assumed. Some of the topics presented may also be of interest for researchers already working in the field of numerical simulation of two-phase flows.

Further material

Most of the methods treated in this monograph have been implemented in a software package called DROPS, which has been developed at the Chair for Numerical Mathematics at RWTH Aachen. All numerical experiments, the results of which are given in this book, were performed with this package. More background information on DROPS and on publications from our research group is available on the website

www.igpm.rwth-aachen.de/DROPS/

The DROPS package is open source software under the GNU Lesser General Public License.

Acknowledgments

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