Universität Regensburg

FAKULTÄT FÜR MATHEMATIK
Lehrstuhl für Mathematik

Universität Regensburg Mathematik D-93040 Regensburg

Prof. Dr. Harald Garcke
Telefon +49 941 943-2992
Telefax +49 941 943-3263
Sekretariat:
Telefon +49 941 943-2773
Telefax +49 941 943-3263
Universitätsstraße 31
D-93053 Regensburg

harald.garcke@ur.de
www.mathematik.uni-regensburg.de/Mat8/lst

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Referee report

on the doctoral thesis

Diffuse interface models in theory of interacting continua

by RNDr. Martin Řehoř

Diffuse or phase field models for two- and multiphase systems have been in the focus of modeling, analysis and scientific computing in the last two decades. Early modelling goes back to the work of Hohenberg and Halperin in the seventies who studied two-phase flow of two fluids with matched densities. Matched or better nearly equal densities severely restricts the applicability of the early works. After the pioneering work of Hohenberg and Halperin several authors generalised diffuse interface models to situations with non-matched densities. A by now classic work of Lowengrub and Truskinovsky uses the assumption of quasi-incompressibility to obtain a mathematical model for non-matched densities. However, in this model the velocity is not divergence-free although the two fluids are assumed to be incompressible. Later Boyer; Ding, Spelt, Shu and Abels, Garcke, Grün developed models for non-matched densities for which the velocity field is solenoidal (divergence-free). These last models made the analysis and computations simpler when compared to the model of Lowengrub and Truskinovksy.

The non-isothermal case was not studied intensively so far. For matched densities Eleuteri, Rocca and Schimperna introduced a non-isothermal diffuse interface model for two-phase flows of incompressible fluids. They also showed existence of solutions. Incompressible models for the general case of non-matched densities in an isothermal situation are missing so far. In his thesis Martin Řehoř gives a systematic derivation of non-isothermal diffuse interface models for multiphase fluids with non-matched densities, i.e. in particular he also studies more than two phases. He studies the fully-compressible, the quasi-incompressible and the fully-incompressible situations. He hence fills a gap in the literature and this systematic derivation is one of the main new achievements of the thesis. A second main topic of the thesis is the numerical solution of the Cahn–Hilliard–Navier–Stokes model in the isothermal case. Let me now discuss the parts of the thesis in more detail.

In an introduction Martin Řehoř motivates the use of diffuse interface models with the help of applications in the glass forming process. Here three immiscible fluids (glass/tin/nitrogen) simultaneously appear and interfaces between the three fluids have to be tracked. It was demonstrated in an already appeared publication by Řehoř, Blechta and Souček that a diffuse interface approach successfully can describe the float glass forming process. In the introduction also different modeling approaches (sharp interface versus diffuse interface models) are discussed and a systematic presentation of results in the literature are given.

Chapter 2 gives a systematic introduction to rational thermodynamics and of the theory of mixtures in particular. The general approach follows the classic works of Truesdell; Noll; Gurtin; Hutter; de Groot, Mazur and others. In particular, a dependence of the entropy on gradients of an order parameter is allowed as necessary for diffuse interface models. Chapter 3 contains the main new results of the thesis. First generalisations of Helmholtz free energies of Ginzburg-Landau type for multi-phase situations are discussed. Then new fully compressible multi-phase models are introduced. These models generalise earlier models introduced by Heida, Málek and Rajagopal. In a second part quasi-incompressible models in a non-isothermal, multi-phase situation are derived. These models generalise the model of Lowengrub and Truskinovsky to the non-isothermal multi-phase case. In the fully-incompressible case also new models are derived in Section 3.4. Here the model of Abels, Garcke and Grün is generalised to the non-isothermal case and the model of Eleuteri, Rocca and Schimperna for the non-isothermal case with matched densities is generalised to the non-matched and multi-phase case.

The general models are very complex and neither a mathematical analysis nor a numerical implementation of these models is given in the thesis. However, for an isothermal model which is introduced in Chapter 4 a numerical approach based on finite elements is given in Chapter 5. The isothermal model is a variant of models of Boyer et al. and generalises the model of Abels et al. to the multi-phase case. With respect to the mobility the model is a little to simplifying as the same mobility is used for all order parameters.

Based on a time discretization of Minjeaud and Guillen-Gonzales, Tierra a decoupling between the Cahn-Hilliard equation and the Navier–Stokes system is achieved. However this splitting might cause some accuracy and stability issues and should be compared with fully coupled discretizations like the one in Garcke, H., Hinze, M., Kahle, C., *A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow*, Applied Numerical Mathematics 99, 151–171 (2016). Using ideas of Minjeaud and Guillen-Gonzales, Tierra a discrete stability result is shown for the multi-phase case.

The discrete Cahn-Hilliard part is solved using a Newton method and the large discrete linear systems stemming from the Navier-Stokes part need some preconditioning to be solved in an efficient way. Here a preconditioner based on the pressure convection diffusion strategy is used. It is also discussed how to solve the resulting discrete systems with sparse direct solvers and how to solve the resulting equations on parallel architectures. Overall efficient solution strategies have been developed and implemented. This is demonstrated in Section 6 by several numerical experiments. In particular, convergence tests for simple shear flow problems and computations for a standard benchmark problem introduced by Hysing et al. (2009) validate the algorithms and the code. In particular, the developed code allows for the computations of general multi-phase systems in the isothermal case. The non-isothermal case studied in the first part of the thesis is highly non-linear and efficient solvers for these general systems would be quite difficult to achieve.

In conclusion, the thesis contains new scientific results. First of all the generalisation of Cahn-Hilliard/Navier-Stokes models to the non-isothermal, multi-phase case with non-matched densities is new. Although some parts of the modeling has been done previously by other authors for some specific situations (I name for example the model introduced by Eleuteri, Rocca, Schimperna for the non-isothermal two phase case with matched densities) a general model was missing so far. This definitely demonstrates the ability of the author for creative scientific work. Another part with new ideas are the chapters with the derivation of discretization methods for general Cahn-Hilliard systems with non-matched densities in the isothermal case. This part is restricted to the isothermal, fully incompressible case. However, the computational challenges are already very high and it is also a major achievement developing stable discretizations and efficient numerical solvers.

Multi-phase flows appear in many situations in nature and modeling and computation for these flows have many applications. In the thesis the float glass forming process is mentioned and discussed in detail as one such application. Overall the thesis has new interesting contributions to mathematics and to the natural and engineering sciences. In addition, the thesis is very well written and very careful in the details. I hence recommend to accept the thesis.

Prof. Dr. Harald Garcke