ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
FAKULTA JADERNÁ A FYZIKÁLNĚ INŽENÝRSKÁ
KATEDRA MATEMATIKY

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Supervisor's report of doctoral thesis

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Thesis: Variational Methods in Phase Transition Modelling

The submitted doctoral thesis deals with modeling of phase transitions by the means of the phase-field model. The thesis is divided into two main parts:

I. phase field modeling of pure substance solidification (Chapters 2 and 3),

II. optimization on normed linear spaces (Chapter 4, 5 and 6).

In Part I, the candidate describes a statistical model for phase transition. This leads to a general expression for free energy which is difficult to use for numerical simulations. Based on the general form of the free energy, the author suggests a new reaction term for the phase-field model. The new reaction term is designed to exhibit better physical properties. Specifically, it does not suffer from spontaneous nucleation when significant under-cooling occurs. The author also employs the new reaction term in the anisotropic phase-field model based on the Finsler dual metric. A detailed computational study is presented in the third chapter where the new reaction term is compared with several other reaction terms [1, 2, 3]. Among other things, the author compares the dendrite tip velocity with experimental data, where a good agreement is found. These results are the subject of a scientific paper [4].

In Part II, optimization on normed linear spaces is studied. This part of the thesis is motivated by an optimal control problem in which the phase-field model is the state equation and a Dirichlet boundary condition is optimized. This optimization problem allows to control the growth of the crystals to reach the prescribed shape. This problem is formulated as an optimization problem with constraints given by partial differential equations. Such problems can be solved by the gradient descent method, where the gradient can be efficiently computed by the adjoint equation. For this purpose, the author first describes the theory of optimization on Banach spaces in the fourth chapter. In the fifth chapter, the problem of the Dirichlet control of the phase-field model together with its weak formulation is defined and the existence of the solution is proven. Next, the proof of Fréchet differentiability of the solution operator is also given which leads to derivation of the optimality conditions. The sixth chapter deals with the numerical solution of the optimal control problem for the phase-field model. Only isotropic models are considered in the computational study and therefore the finite difference method is used for the numerical approximation of the problem. First, the candidate discusses details of 1D simulations. 1D simulations are valuable for basic understanding of the behavior of the studied problems. In this case, the author deals with the solution of the adjoint equations which do not have any physical meaning and so understanding their behavior is not trivial. Next, the author presents results of numerical simulations in 2D which are closer to real applications. The problem of optimal control is very demanding when it comes to computational resources like system memory and computational power and so 3D simulations were not performed. Without use of the adjoint equation even computations in 2D would not be possible. The results show that the model is really capable of driving the crystal growth towards prescribed shape just based on the proper choice of the time dependent Dirichlet boundary condition. Possibly, the numerical solver of this optimal control problem could be useful in some applications in material sciences. The results presented in the second part are the subject of the papers [5, 6] which are under review in scientific journals.

The work on the thesis was conducted as part of the OP RDE project no. CZ.02.1.01-0.0-0.0-16-019-0000765: *Research Center for Informatics* of Ministry of Education, Youth and Sports of the Czech Republic, AZV project No. NV19-08-00071: *Analysis of flow character and prediction of evolution in endovascular treated arteries by magnetic resonance imaging coupled with mathematical modeling* of Ministry of Health of the Czech Republic and OP RDE project no. CZ.02.1.01-0.0-0.0-16-019-0000778: *Centre for Advanced Applied Sciences*, group MATE, Operational Programme of Research, Development and Education of the Ministry of Education, Youth and Sports of the Czech Republic. During his study, the candidate visited Technical University in Delft for a short-term stay (five weeks). He has also actively attended six international conferences and he is co-author of two impacted papers listed Web of Science. The candidate also assisted in the education of students by guiding exercises in mathematical analysis and by supervising one bachelor student.

The candidate proved his ability to deal with complex mathematical problems. He is able to write advanced code in C++ on one hand but also study advanced theoretical works in mathematics on the other hand. Especially deep understanding of the mathematical background of various real problems is one of his most significant strengths. His excellent knowledge of different parts of mathematical analysis and applied mathematics is very valuable in our research group. The submitted thesis is of very high quality and it presents a valuable contribution to numerical methods of phase transition modeling.

The thesis fulfills all requirements for Ph.D. theses. Hence, I recommend the candidate to the committee for the doctoral theses to bestow him the title of Doctor of Philosophy.

Prague, December 9, 2022

doc. Ing. Tomáš Oberhuber, Ph.D.

References

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