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Referee's Report on the PhD thesis
Variational Methods in Phase Transition Modelling
by Aleš Wodecki

Content of the thesis:
The thesis is divided in two main parts. Part I is devoted to several fundamental aspects of phase field modeling applied to pure substance solidification. It is concerned with the phase-field model that governs the solidification of a pure melt. Part II is focused on PDE-constrained optimization problem with respect to the Dirichlet boundary condition for the heat equation. It leads to a particular phase field profile at the final time. Chapter 2 is concerned with the derivation of a phase field model. It governs the solidification of pure substances. In Chapter 3 the novel reaction terms for this problem are proposed. These reaction terms are validated using asymptotic analysis. It also contains several interesting numerical examples and comparison with experimental results. Fundamentals of PDE-constrained optimization iare summarized n Chapter 4. The optimization methods and techniques are investigated in Chapter 5. The existence of a weak solution to the problem is shown. First order optimality conditions are derived using the Fréchet differential of the solution operator. Numerical aspects of solving the infinite dimensional optimization problem are investigated in Chapters 6 and 7. The methods are based on the solution of the adjoint problem. Using the adjoint problem leads to gradient computation. Finally, several numerical examples in one and two spatial dimensions demonstrate the advantages of using the newly proposed reaction term for optimization purposes.

Comments and suggestions:
1. The regularized cost functional $J(p,u,\theta)$ (see (6.5)) depends on the Dirichlet boundary condition control profile θ through the solution (p,u) of the Allen-Cahn system of phase-field equations (6.6)-(6.11). It is not clear wheter the functional J is a convex function of θ. Did the author computed, at least numericaly, the second Frechet derivative of J with respe to θ? Is it positive definite operator? Otherwise, the proposed numerical method may converge to one of local minimizers. A discussion is needed.

2. On arxive.org I found a related paper: Convergence of the Finite Volume Method on Unstructured Meshes for a 3D Phase Field Model of Solidification by A Wodecki, P Strachota, M Beneš - arXiv preprint arXiv:2010.04132, 2020. What is the status of the paper? Is its content contained in parts of the thesis too?

Conclusion:
This is a carefully written and valuable dissertation thesis. I recommend Ing. Aleš Wodecki to be awarded the degree Ph.D. (Doctor of Philosophy) from the Faculty of Nuclear Engineering, Czech Technical University.

Sincerely yours,

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