

Simulation of Anisotropic Microstructure Growth in Solidification

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1 Introduction

The aim of the article is to present simulation of non-convex pattern growth for the system of phase-field equations endowed by anisotropy. The equations represent a mathematical model of solidification of pure crystalline substances at micro-scale. The mentioned physical phenomenon is accompanied by presence of an interface between phases which can move in space and is determined intrinsically by the state of the physical system, its boundary and initial data. The paper deals with the anisotropic model has been presented in the following form:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla^2 u + L\chi'(p)\frac{\partial p}{\partial t}, \\ \alpha\xi\frac{\partial p}{\partial t} &= \xi\nabla \cdot T^0(\nabla p) + \frac{1}{\xi}f_0(p) + F(u)\xi\Phi^0(\nabla p), \end{aligned} \quad (1)$$

with initial conditions

$$u|_{t=0} = u_0, \quad p|_{t=0} = p_0,$$

and with boundary conditions of Dirichlet type

$$u|_{\partial\Omega} = 0, \quad p|_{\partial\Omega} = 0.$$

Here, $\xi > 0$ is the "small" parameter (thickness of the interface), and f_0 the derivative of double-well potential. The coupling function $F(u)$ is bounded and continuous, or even Lipschitz-continuous. The anisotropy is included using the monotone operator T^0 operating with the field gradient. We consider $f_0(p) = ap(1-p)(p - \frac{1}{2})$ with $a > 0$. The enthalpy is given by $\mathcal{H}(u) = u - L\chi(p)$, where the coupling function χ is monotone with bounded, Lipschitz-continuous derivative: $\chi(0) = 0$, $\chi(0.5) = 0.5$, $\chi(1) = 1$, $\text{supp}(\chi') \subset \langle 0, 1 \rangle$. For the sake of simplicity, Ω is rectangle. Obviously, the extension to higher dimensions, and to other boundary conditions is possible. The analysis presented in this article has been motivated by numerical studies obtained by the model both for the case of curve dynamics in the plane (see [2]), and for the case of microstructure growth in solidification (see [1]). The model works with an anisotropy rigorously implemented into the equations. Finally, the model gives reasonable results even in case of non-convex anisotropies, when the mentioned theory is not applied. Our aim is to present numerical convergence results for the onset of dendritic growth.

2 Computational results

The model (1) is proved to have a unique weak solution with suitable properties. The numerical scheme based on the method of lines is convergent (see [1]). We have performed a series of computations to show that it yields a good approximation of the original problem and to investigate the solution itself.

Example shows the growing dendrite with imposed weak (convex) anisotropy. The shape of the solution is presented in Figure 1. The computation demonstrates development of primary dendrite branches.

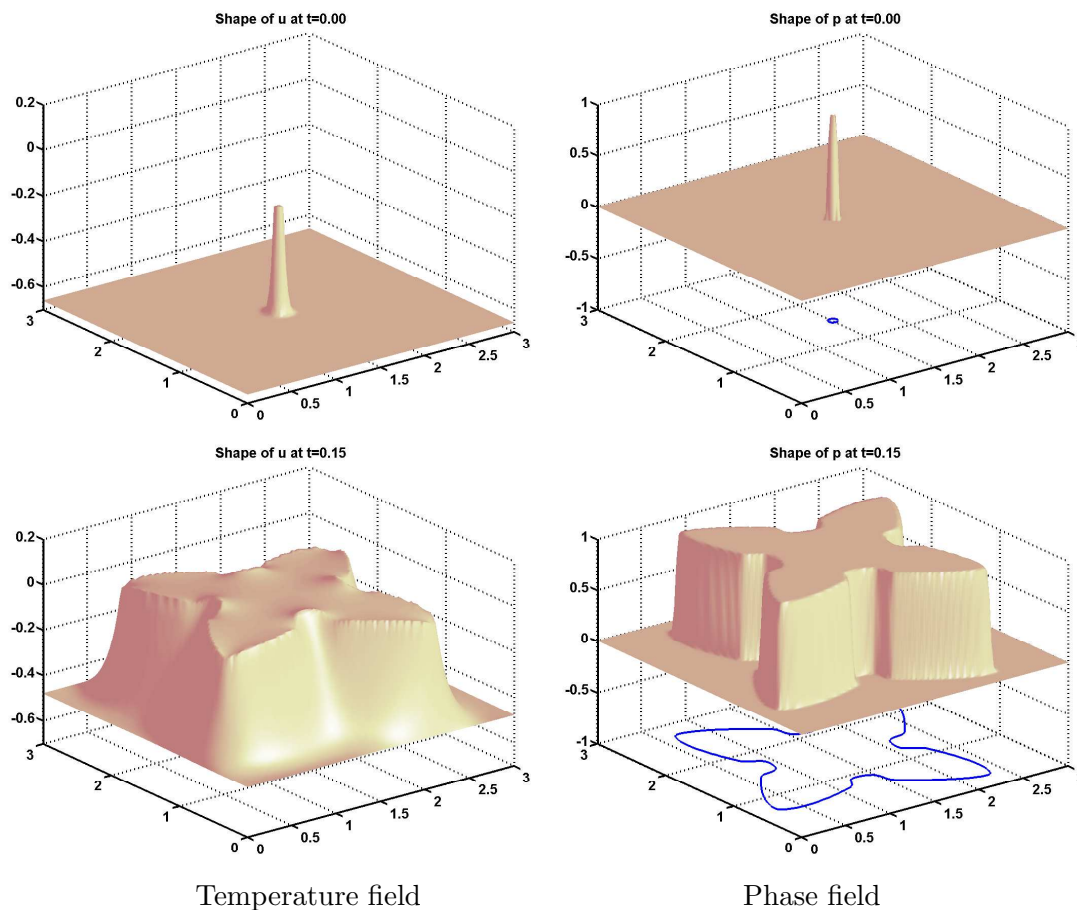


Figure 1: Shape of the solution for Example.

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References

- [1] M. Beneš. Anisotropic phase-field model with focused latent-heat release. In *FREE BOUNDARY PROBLEMS: Theory and Applications II*, pages 18–30, Chiba, Japan, 2000. GAKUTO International Series Mathematical Sciences and Applications, Vol.14.
- [2] M. Beneš. Diffuse-interface treatment of the anisotropic mean-curvature flow. *Applications of Mathematics*, 48, No. 6:437–453, 2003.