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Numerical Investigation to the Effect of Initial Guess for Phase-Field Models

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Abstract. The construction of relevant initial conditions in the phase-field models for interfacial problems is discussed. If the model is supposed to have a local equilibrium at the interface, it must be based on a local distance function. However, since for the Cartesian coordinates non-uniform boundaries occur, the initial conditions have to be corrected in order to match the actual phenomena. We discuss the volume correction method, image initialisation, non-overlapping multi component concentration, etc. The methods presented can be used in the initial guess constructions for various phase-field models.

AMS subject classifications: 65M06, 68U10

Key words: Allen-Cahn equation, Cahn-Hilliard equation, phase-field model, level set function.

1. Introduction

The phase-field model, a mathematical model for solving interfacial problems, was introduced in [24, 39]. Examples of such problems include dendritic growth [34, 58], spinodal decomposition [45], micro-phase pattern formation [11, 61], image inpainting [5], image segmentation [55], vesicle dynamics [47, 53], tumor growth [13, 44], two-phase flow [1, 38], and multi-phase fluid flow [3, 23, 59]. In the phase-field model, the boundary conditions at the interface are replaced by the phase-field equation. The phase-field function takes distinct values at each phase and has a smooth interfacial transition layer between distinct values. We define the interface as a contour in the two-dimensional space or an isosurface in the three-dimensional space. In the limit of an infinitesimal interfacial parameter, we can have the correct interfacial dynamics. Therefore, instead of direct treatment of the corresponding boundary conditions at the interface, the interfacial related problems can be reduced to the solution of equations over the whole domain.

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The first example of the phase-field equations is the Allen-Cahn (AC) equation [2] which governs the motion of anti-phase boundaries in crystalline solids

$$\frac{\partial \phi}{\partial t}(\mathbf{x},t) = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta\phi(\mathbf{x},t), \quad \mathbf{x}\in\Omega, \quad t>0, \tag{1.1}$$

where Ω is a domain, ϕ the difference of concentrations, $F(\phi) = 0.25(\phi^2-1)^2$, and ϵ a positive parameter related to the interfacial thickness. Fig. 1 shows the temporal evolution of the contour and the isosurface of the numerical solutions of the AC equation (1.1) with the initial conditions described in [42].

Next example is the dendritic growth equations with a four-fold symmetry in the two-dimensional space [34, 58]

$$\begin{aligned}
\epsilon^2(\phi)\frac{\partial \phi}{\partial t} &= \nabla\cdot\left(\epsilon^2(\phi)\nabla\phi\right) + \left[\phi - \lambda U\left(1-\phi^2\right)\right]\left(1-\phi^2\right) \\
&\quad + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_x}\right)_x + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_y}\right)_y, \\
\frac{\partial U}{\partial t} &= D\Delta U + \frac{1}{2}\frac{\partial\phi}{\partial t}, \quad \text{for} \quad \mathbf{x}\in\Omega, \quad t>0, \\
\epsilon(\phi) &= W_0\left(1-3\delta_4+4\delta_4\frac{\phi_x^4+\phi_y^4}{|\nabla\phi|^4}\right),
\end{aligned} \tag{1.2}$$

where Ω is a domain, $\phi(\mathbf{x},t)$ the order parameter taking values between -1 (liquid phase) and 1 (solid phase), W_0 the measure of the interface width, $\epsilon(\phi)$ the anisotropic function, δ_4 the anisotropic strength, λ the dimensionless coupling parameter, D the diffusion rate

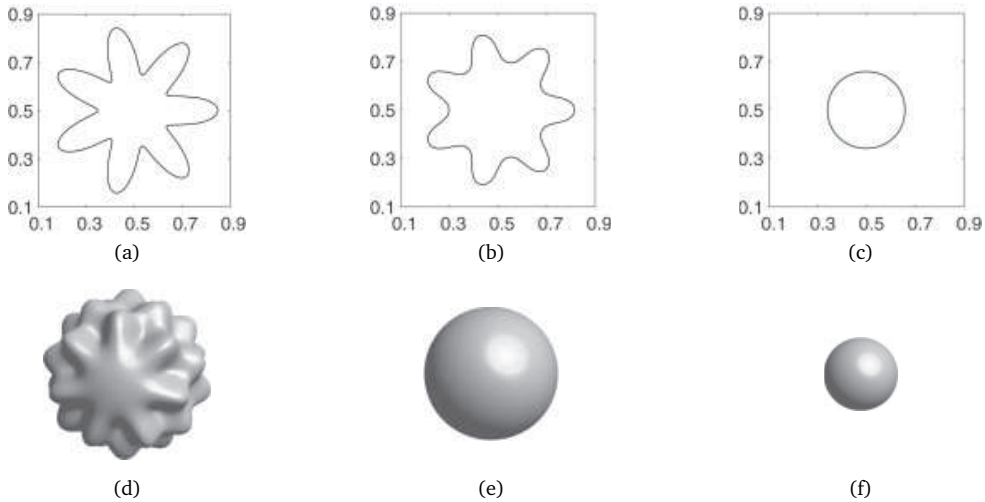

Figure 1: Motion by mean curvature. (a)-(c) and (d)-(f) show the results in two- and three-dimensional spaces, respectively. Reprinted from Li *et al.* [42] with permission of Elsevier Science.