Mesh Sensitivity for Numerical Solutions of Phase-Field Equations Using r-Adaptive Finite Element Methods

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Abstract. There have been several recent papers on developing moving mesh methods for solving phase-field equations. However, it is observed that some of these moving mesh solutions are essentially different from the solutions on very fine fixed meshes. One of the purposes of this paper is to understand the reason for the differences. We carried out numerical sensitivity studies systematically in this paper and it can be concluded that for the phase-field equations, the numerical solutions are very sensitive to the starting mesh and the monitor function. As a separate issue, an efficient alternating Crank-Nicolson time discretization scheme is developed for solving the nonlinear system resulting from a finite element approximation to the phase-field equations.

AMS subject classifications: 65M20, 65M50, 65M60, 80A22

Key words: Phase-field equations, moving mesh method, Crank-Nicolson scheme, numerical sensitivity.

1 Introduction

Numerical methods have been proposed to resolve phase change interface between the solid and liquid regions. To avoid the calculation of the position and curvature of the interface, an alternative is to use a so-called diffuse interface model that implicitly defines the position of the interface, see, e.g., [3]. In this model, a phase indicator parameter p is assumed to be smooth on the whole solution domain, which has distinctive values in solid and liquid. With this idea and using the Ginzburg-Landau theory, the phase-field

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equations can be deduced by requiring that the temperature and phase-field evolve such that the free energy decreases [11].

Most numerical methods to solve the phase-field equations have used stationary uniform meshes, see, e.g., [4, 5, 10, 26]. However, it is important that the diffused interface is well resolved if the correct dynamics are to be reproduced. As the phase interface moves in time it is clear that an efficient numerical approach must involve some form of mesh adaptivity. There have been two approaches in doing this. One is to use the local mesh refinement method, i.e. *h*-method, see, e.g., [2, 21–23]. The other is to use moving mesh method which is simpler in implementation and able to resolve the structures as the phase interface with highly anisotropic mesh grids [1, 16, 17, 24].

Recently, Beckett et al. [1] developed a moving mesh strategy for two-dimensional phase-field equations. Their computational mesh was obtained by equidistributing a monitor function tailored for the functional variation of the phase-field in the interfacial region. The same problems were also computed by Tan et al. [24] using the moving mesh finite volume methods. For the solidification of a single solid sphere which is surrounded by uncooled liquid, although the moving mesh results of [1,24] on the radial positions are in quite good agreement with each other, it is found that they are qualitatively different from the (very fine) uniform mesh results given by Elliott and Gardiner [9]. In the Elliott and Gardiner's model, the parameter of the diffuse interface thickness ϵ is taken as 1/80= 0.0125, while in [1,24], ϵ is taken as $1/(160\sqrt{2}) \approx 0.0044$. The smaller value of ϵ has the impact that very fine meshes have to be used in order to resolve the very small transition interfaces. Nevertheless, it is found that the radial position is in fact quite insensitive to the choice of the parameter ϵ . Therefore the differences between the solutions from different authors should be due to some other reasons, such as the numerical methods adopted.

In this work, we try to understand the reason why the results of [1,24] have unreasonable differences from the results obtained on uniform meshes. From the references, one can find that the possible factors leading to the differences among the numerical results therein are relevant to the starting mesh, the monitor function and the time integrating scheme. We first make a numerical convergence study to reveal the fact that the radial position is fairly insensitive to the choice of the parameter ε by computing for both parameters on a sequence of refined uniform meshes. Then we keep the same parameters ε and p_{\pm} as [1,24] and carry out a sequence of computations using different starting meshes, monitor functions and time integrating schemes. The numerical evidences demonstrated that among these three possible factors, the variation in time integrating scheme contributes only slight differences to the numerical solutions, while the other two are on the very contrary. It can be imagined that an inappropriate monitor function will introduce additional error to the numerical solutions, but it is such a surprising fact that the starting mesh can have a similar effect for this problem. Ideally, the moving mesh solutions should not be dependent on the choice of the starting mesh, since the starting mesh will be adapted immediately based on the initial values after the computations begin. However, the numerical results showed that the starting mesh may affect the phase-field