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On the Fully Implicit Solution of a Phase-Field Model for Binary Alloy Solidification in Three Dimensions

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Abstract. A fully implicit numerical method, based upon a combination of adaptively refined hierarchical meshes and geometric multigrid, is presented for the simulation of binary alloy solidification in three space dimensions. The computational techniques are presented for a particular mathematical model, based upon the phase-field approach, however their applicability is of greater generality than for the specific phase-field model used here. In particular, an implicit second order time discretization is combined with the use of second order spatial differences to yield a large nonlinear system of algebraic equations as each time step. It is demonstrated that these equations may be solved reliably and efficiently through the use of a nonlinear multigrid scheme for locally refined grids. In effect this paper presents an extension of earlier research in two space dimensions (J. Comput. Phys., 225 (2007), pp. 1271–1287) to fully three-dimensional problems. This extension is validated against earlier two-dimensional results and against some of the limited results available in three dimensions, obtained using an explicit scheme. The efficiency of the implicit approach and the multigrid solver are then demonstrated and some sample computational results for the simulation of the growth of dendrite structures are presented.

AMS subject classifications: 65M06, 65M22, 65H10, 65M55

Key words: Phase-field simulations, binary alloys, mesh adaptivity, implicit methods, nonlinear multigrid.

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1 Introduction

The modelling of solidification structures, in particular the growth of dendritic crystals, is a subject of intense and enduring interest within the scientific community, both because dendrites are a prime example of spontaneous pattern formation and due to their pervasive influence on the engineering properties of metals. In all but the most restrictive of cases, analytical solutions to the equations of motion for the solid-liquid interface, using techniques such as boundary integral methods (microscopic solvability theory [1, 4, 26, 40]), cannot be found and recourse must be made to numerical techniques. These include cellular automaton [13, 33], front-tracking [7], one-domain multiphase models [10,32,55] and level set techniques [9,18,27,35]. However, the technique which over the last few years has received the most attention is that of phase-field simulation [8, 28, 29, 39], in which a non-conserved order parameter ϕ is defined over the whole domain, which encodes the phase state of the material. By assuming the interface between the solid and liquid (or different solid phases in multi-phase modelling) to be diffuse, ϕ is rendered continuous, wherein standard techniques for partial differential equations (PDEs) may be used. This allows a regular Eulerian mesh to be used and avoids many of the topological complexities involved with front tracking methods.

However, the application of phase-field modelling leads to a number of issues. The resulting set of coupled PDEs is unsteady, highly non-linear and may moreover suffer from significant multi-scale problems. The latter arises because although the phase-field equations are formulated such that in the asymptotic limit of the diffuse interface width, δ, tending to zero, the corresponding sharp interface equations are recovered exactly, this is not sufficient to ensure that the solutions do not have a dependence upon δ. Such limitations may be overcome by formulating the model in the so-called "thin interface limit" [22–25], whereby asymptotic expansions of the solution on the inner and outer regions of the solid-liquid interface are matched to obtain an equation set in which the solution is independent of the width of the diffuse interface. However, in order to perform the asymptotic matching highly restrictive assumptions need to be made about the thermodynamics governing the phase transformation, which can restrict the applicability of such models. Consequently, in many cases phase-field models are constructed such that δ is much smaller than the other length scales characteristic of the problem. In particular, there is a growing body of opinion that "the sharp interface limit of a phase-field model is not the only meaningful physical limit" [12]. This view draws on the Gibbs [15] interpretation of understanding all interfacial boundaries as being of finite width. In the context of the crystallisation of metals this finite width interface can be understood physically as the number of atom widths over which the long range order characteristic of the crystalline solid is lost, and represents a tendency towards using interface widths in phase-field modelling which may be of the order of the capillary length, typically $2 - 5 \times 10^{-10}$m. This compares with typical microstructural length scales which are of the order $10^{-6} - 10^{-5}$m.

Due to this multi-scale nature phase-field simulations tend to be highly compu-