Journal of Computational Physics 231 (2012) 1781–1796

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

An implicit parallel multigrid computing scheme to solve coupled thermal-solute phase-field equations for dendrite evolution

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ARTICLE INFO

Article history:
Received 27 February 2011
Received in revised form 3 November 2011
Accepted 5 November 2011
Available online 16 November 2011

Keywords:
Parallel computing
Multigrid method
Phase field
Dendrite evolution
Solidification

ABSTRACT

An implicit, second-order space and time discretization scheme together with a parallel multigrid method involving a strip grid domain partitioning has been developed to solve fully coupled, nonlinear phase field equations involving solute and heat transport for multiple solidifying dendrites. The computational algorithm has been shown to be stable and monotonously convergent, and allowed time marching steps that were 3–4 orders of magnitude larger than those employed in similar explicit approaches, resulting in an increase of 3–4 orders of magnitude in computing efficiency. Full solute and thermal coupling was achieved for metallic alloys with a realistic, high Lewis number of $>10^4$. The parallel multigrid computing scheme is shown to provide a scalable methodology that allowed the efficient use of distributed supercomputing resource to simulate the evolution of tens of complex shaped 2D dendrites in a computational domain containing tens or even hundreds of millions of grid points. The simulations have provided insight into the dynamic interplay of many growing dendrites in a more realistic fully coupled thermal-solute condition, capturing for the first time fine scale features such as dendrite splitting.

1. Introduction

Since the successful demonstration of the phase field (PF) approach for the simulation of dendrite shape during solidification by Kobayashi in 1994 [1], the PF method has been developed intensively worldwide for the simulation of pure metal and alloy dendrite microstructural evolution [2–7]. The PF method employs a diffuse interface concept with a continuous PF variable ϕ that varies smoothly but steeply across a diffuse interface that represents the separation between solid and liquid phases and avoids the need for explicit tracking of the physical position of the solid–liquid interface [8]. Generally, the evolution of ϕ is governed by the spatial and temporal distribution of alloy internal energy (specific and latent heat) and the interface gradient energy, and the introduction of ϕ produces a set of partial differential equations (PDEs) governing the phase field, solute and temperature. Because temperature and the composition of both liquid and solid phases in an alloy are linked by thermodynamic considerations, the PDEs are strongly coupled and non-linear, and consequently are difficult to solve efficiently. Hence, in most of the studies concerning PF based simulations of dendrite evolution during solidification reported so far simplified version of the PDEs have been used to decouple the thermal and solute fields e.g. dendrite growth in an isothermal field (without transient heat transfer) [9], at a constant pre-determined cooling rate [10], or under an applied predefined and fixed thermal gradient [11,12]. Finite difference discretization and an explicit time-marching method have generally been used to solve the discretized PDEs. Consequently, in order to make the complex, coupled case of alloy

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doi:10.1016/j.jcp.2011.11.006

dendritic solidification tractable, the resulting simulations either omit some of the underlying physics, or predict unrealistic dendrite morphologies compared with reality. Further serious challenges concern the time-stepping constraint and small discretization distances required for stability in the explicit method so that computing times become enormous and even the most powerful supercomputers can calculate dendrite shape evolution for only a few tens of dendrites, making it very difficult, if not impossible, to simulate microstructures over meaningful volumes of material with a sensible computer burden, and with sufficient underlying physics (linked solute and thermal transport), to be insightful for practical solidification problems.

To take the coupled thermal-solute effect into account, Karma and Rappel [13,14] and Ramirez et al. [15] have recently developed a coupled thermal-solute PF model for dilute binary alloys. By introducing a term named the "anti-trapping" current to the solute conservation equation, non-equilibrium effects such as interface stretching and surface diffusion effects arising when the solid and liquid diffusivities are unequal were eliminated, and very good quantitative agreement between simulation and analytical equations based on the Gibbs–Thomson equation for curvature effects on solid–liquid interfaces were obtained. However, the required coupling of a thermal field into the solidifying system introduces further computing complexity due to the multi-scale character of the very large difference between the thermal and solute diffusion rate characterized by the Lewis number i.e. the ratio between the thermal and solute diffusivities, which is typically $\sim 10^4$ for metallic alloys. As a consequence, for the study of fully coupled thermal-solute dendrite growth in metallic alloys, typically only one quarter or half of a solidifying primary dendrite can be simulated, and even then an artificially low Lewis number of order of magnitude 10^1–10^2 must be assumed [15] in order to reduce computational cost.

In an effort to address more practical Lewis numbers, length and time scales, implicit rather than explicit algorithms have been developed. Rosam et al. [16,17] presented an adaptive mesh, multigrid algorithm and showed that this approach could simulate successfully dendrite shape evolution during solidification at a lower computational cost by refining the discretized grid at the diffuse interface area only. More importantly, due to the inherent high stability of the implicit approach, limits on the Lewis number were removed. In comparison with the other numerical methods that might be applied to phase field equations such as the generalized minimal residual (GMRES) or conjugated gradient (CG) [18], a multigrid approach can provide solutions involving a number of computational operations that are near linearly proportional to the problem scale or dimension [19].

In summary, the many phase field approaches to the simulation of the way in which dendrite shape evolves during solidification usually suffer from one or more of the following restrictions:

(1) artificially low Lewis number,
(2) very small length and time scales associated with the explicit method,
(3) a decoupling of thermal and solute fields (that are strongly coupled in practice), and
(4) only a few dendrites can be considered and therefore microstructure prediction is non-sensible.

In this paper we present a new numerical approach with dramatic increases in computational efficiency for the phase field method in order to simulate the evolution of dendritic microstructures, including multiple dendrite growth, impingement and solute segregation. The approach is a major extension of the multigrid algorithm applied by Rosam et al. [16,17] but implemented here with a new highly parallelized computing scheme. As a consequence of the improved robustness and computational efficiency, we then present results for the first time of multiple dendrite growth for realistic Lewis numbers of $\sim 10^4$ corresponding to metallic alloys in a fully coupled thermal-solute field, including secondary dendrite arm stretching and dendrite impingement.

2. The phase field model

2.1. Governing equations

The coupled thermal-solute PF model for the solidification of dilute binary alloys proposed by Ramirez et al. [15] was adopted in this study. The governing PDEs are:

$$\frac{\partial \phi}{\partial t} = -K_\phi \frac{\delta F}{\delta \phi} \tag{1}$$

$$\frac{\partial c}{\partial t} = \vec{\nabla} \cdot \left(K_c \vec{\nabla} \frac{\delta F}{\delta c} - \vec{j}_{at} \right) \tag{2}$$

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{L}{2c_p} \frac{\partial \phi}{\partial t} \tag{3}$$

where t is time, ϕ, c, T are phase field, solute concentration (molar), and temperature respectively, K_ϕ and K_c are constants, α is thermal diffusivity, L is latent heat, and c_p is alloy specific heat. F is the system free energy and during the solidification of a dilute binary alloy is given by [15]: