Parellelization of Phase-field Model for Phase Transformation Problem

Ying Xu, Tianliang Yang, James M. McDonough* and Kaveh A. Tagavi

Department of Mechanical Engineering
University of Kentucky
151 RGAN Bldg., Lexington, KY 40506-0108, USA

Introduction

The problem of crystal growth into an undercooled melt has attracted much interest for decades because of its importance in industrial applications such as castings, ingots and weldings. Many mathmatical models and numerical applications have been developed in this area. Among those widely-used models in recent years, the phase-field model provides a convenient basis for the numerical solution of complicated solidification problems with many morphologies. In the phase-field model, in addition to the customary thermal energy, an additional variable, phase field ϕ, is introduced to explicitly label the liquid and solid phases. In this approach, the phase-field takes on a constant value in each bulk phase; e.g., $\phi = 0$ in the solid phase, and $\phi = 1$ in the liquid phase. The transformation from solid to liquid occurs over a thin transition region through which ϕ varies smoothly from zero to one. Since significant changes in the phase-field variable only occur over a very small part of the whole domain, the algorithms must allow the interface width to be very small, in order to capture the small-scale features such as liquid trapping and tip splitting. Hence, the mesh sizes must be small enough to resolve these phenomena and obtain accurate solutions. One drawback of phase-field model is its CPU intensity. To solve this problem, it is necessary to apply parallelization to phase-field model algorithms in order to decrease wall-clock time.

We introduce the phase-field model in the first part of this paper. Numerical solutions corresponding to growth of dendrites are also given in this part. Finally we discuss the approach to parallelization and the speedups obtained.

Governing Equations of Phase-Field Model

In this section we present the equations of the phase-field model along with the scalings employed to render them dimensionless. Boundary and initial conditions required to formulate a well-posed mathematics problem are also prescribed.

The coupled thermodynamically consistent dimensionless governing equations for the phase field and temperature (Chen [1]) can be written as:

$$\phi_t = m\Delta\phi + \frac{m}{\epsilon^2}\phi(1-\phi)\left[\phi - \frac{1}{2} + 30\epsilon a S\theta\phi(1-\phi)\right], \tag{1a}$$

$$\theta_t = \Delta\theta - \frac{30\phi^2(1-\phi)^2}{S}\phi_t. \tag{1b}$$

In the above equations, ϕ is the dimensionless phase value. By introducing the length scale w (the geometric size of the domain) and the reference time scale w^2/α (the thermal diffusion time, where $\alpha = k/\rho c_p$ is the thermal diffusivity of the liquid-assumed to be a constant), dimensionless temperature θ, spatial variable $\mathbf{x}$, time t are defined by:

$$\theta = \frac{T - T_m}{T_m - T_0}, \quad x = \frac{\mathbf{X}}{w}, \quad t = \frac{\tau}{w^2/\alpha},$$

*E-mail: jmmcd@uky.edu

where T is temperature; T_m is the equilibrium melting temperature; T_0 is the initial temperature of the domain; $\mathbf{X}$ and τ are the spatial and temporal variables, respectively.

In addition, the four dimensionless parameters of this isotropic phase-field model are defined in the following form:

$$S = \frac{c_p(T_m - T_0)}{L}, \quad \epsilon = \frac{\delta}{w}, \quad m = \frac{\mu\sigma T_m}{\alpha L}, \quad a = \frac{\sqrt{2}w}{12d},$$

where $d = \rho c_p \sigma T_m / L^2$ is capillary length; S is the Stefan number; L is latent heat per unit volume; σ is the surface energy; μ is the interface kinetic coefficient, and δ is a length scale for the interface thickness (see details in [2]).

In the present study, the domain size $X_0 \times Y_0 = 2.25 \times 2.25$ is chosen so that it is sufficient for approximating an unbounded domain. The boundary conditions are:

$$\frac{\partial\theta(0,y,t)}{\partial x} = 0, \quad \frac{\partial\theta(X_0,y,t)}{\partial x} = 0, \quad \forall t > 0, \forall y \in [0, Y_0], \tag{2a}$$

$$\frac{\partial\theta(x,0,t)}{\partial y} = 0, \quad \frac{\partial\theta(x,Y_0,t)}{\partial x} = 0, \quad \forall t > 0, \forall y \in [0, X_0], \tag{2b}$$

$$\frac{\partial\phi(0,y,t)}{\partial x} = 0, \quad \frac{\partial\phi(X_0,y,t)}{\partial x} = 0, \quad \forall t > 0, \forall y \in [0, Y_0], \tag{2c}$$

$$\frac{\partial\phi(x,0,t)}{\partial y} = 0, \quad \frac{\partial\phi(x,Y_0,t)}{\partial y} = 0, \quad \forall t > 0, \forall y \in [0, X_0]. \tag{2d}$$

At the initial time dimensionless temperature is set at the melt temperature on a small rectangle 1/75 the domain size in the center of the domain. Hence prescribed initial data take the form:

$$\theta(x_0, y_0, t) = 0, \quad \phi(x_0, y_0, t) = 0, \quad (x_0, y_0) \in \Omega_0, \tag{3a}$$

$$\theta(x, y, t) = -1, \quad \phi(x, y, t) = 1, \quad (x_0, y_0) \in \Omega \setminus \Omega_0, \tag{3b}$$

where

$$\Omega_0 \equiv \left[\frac{37}{75}X_0, \frac{38}{75}X_0\right] \times \left[\frac{37}{75}Y_0, \frac{38}{75}Y_0\right], \quad \Omega \equiv [0, X_0] \times [0, Y_0].$$

Numerical methods and results

The governing equations (1) are a pair of coupled nonlinear parabolic equations. Note that the heat equation (1b) is linear in the temperature θ but contains a source term depending nonlinearly on ϕ, which depends on θ only in the interfacial region. On the other hand, Eq. (1a) contains a quartic nonlinearity in ϕ.

A δ-form Douglas-Gunn procedure is employed to solve the parabolic phase-field governing equations. Quasilinearization of the nonlinear term $g(\phi,\theta)$ in Eq. (1a) use a Fréchet-Taylor expansion [3, 4] that ignores terms beyond first order. Figure 1 displays the state of dendritic growth at 0.2 units of dimensionless time.

Approach to parallelization and results

Parallelization of the numerical solution procedure is based on the shared-memory programming paradigm using the HP Fortran 90 HP-UX compiler. The program is parallelized using OpenMP running on the HP SuperDome at the University of Kentucky Computing Center. The maximum number of threads available on the HP SuperDome is 64, and in the current study each processor is used to compute one part of the whole domain. The mesh grid is set to be

600×600 corresponding to the domain size 2.25×2.25, and the time step is 1.25×10^{-5}. To study the speed-up of the parallelization, different numbers n of processors (n=1,2,4,8,16) are used to execute the algorithm at t=0.2. Figure 2 shows the speed-up factor versus the number of processors. It shows that, as the numbers of processors increase, the speed-up factor increases sub-linearly. The curve in Fig. 2 also shows that the speed-up factor attains its maximum at a certain number of processors for the present problem.

Fig. 1. Dendritic growth from the center at t=0.2.

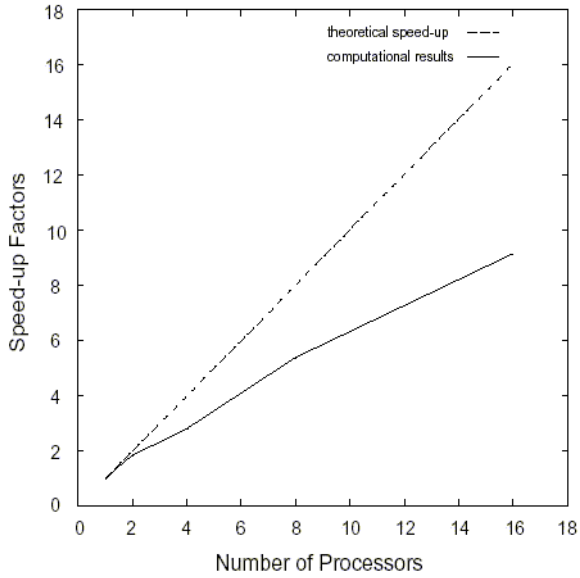

Fig. 2. Speed-up performance of the parallelized phase-field model.

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