Multi-Scale Scheme Implemented on Phase-Field Model to Simulate Freezing in Turbulent Flow

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1. INTRODUCTION

Phase-field models have been applied to phase transformation problems for decades. Numerous studies have been conducted using phase-field methods on solidification problems, including phase transitions in pure materials and binary alloys, and solidification in an induced flow field. A detailed literature survey can be found in Xu et al. [1] [2].

We notice that all of the previous research on solidification in a flow field involves length and time scales in microns and nanoseconds, respectively, which is not appropriate for studying freezing in a flow field. Therefore, the concepts of multiscale methods should be introduced to phase-field models with convection. Even such formulations still have the drawback of being very CPU intensive. Hence, it is necessary to apply parallelization to phase-field model algorithms in order to decrease wall-clock time. The task of this research is to simulate dendrite growth in a turbulent flow (in this case lid-driven-cavity flow). We have noticed that previous solidification with convection problems have been solved under small Reynolds number. We will implement a two-level scale method, i.e., a macroscale for flow field and a microscale for dendrite growth, which enables us to solve phase-change problems in a turbulent flow.

We introduce the phase-field model with convection in the first part of this paper, followed by a brief description of the implementation of multi-scale scheme. Finally we present the numerical solutions and discuss the approach to parallelization and the speedups obtained.

2. GOVERNING EQUATIONS OF PHASE-FIELD MODEL WITH CONVECTION

In this section we introduce the equations of the phase-field model. The difference of length scales between dendrites and flow field make it unreasonable to implement the dimensionless form. Therefore, dimensional governing equations are introduced. Boundary and initial conditions required to formulate a well-posed mathematical problem are also prescribed. The coupled 2-D Navier–Stokes equations and phase-field model are

$$u_x + v_y = 0\,, \tag{1a}$$

$$u_t + (u^2)_x + (uv)_y = -\frac{1}{\rho_0}p_x + \frac{\mu(\phi)}{\rho_0}\Delta u + X_1(\phi)\,, \tag{1b}$$

$$v_t + (uv)_x + (v^2)_y = -\frac{1}{\rho_0}p_y + \frac{\mu(\phi)}{\rho_0}\Delta v + X_2(\phi) - \frac{\rho(\phi,T)}{\rho_0}g\,, \tag{1c}$$

$$\phi_t + (u\phi)_x + (v\phi)_y = \frac{\epsilon^2}{M}\nabla\cdot((\boldsymbol{\xi}\cdot\nabla\phi)\boldsymbol{\xi}) - \frac{30\rho_0 L_0}{T_m M}\psi(\phi)(T_m - T) - \frac{\rho_0}{aM}\psi'(\phi)T + Y(\phi,T)\,, \tag{1d}$$

$$T_t + (uT)_x + (vT)_y = \frac{k}{\rho_0 c_p(\phi)}\Delta T + \left[\frac{\epsilon^2}{2}\nabla\cdot((\boldsymbol{\xi}\cdot\nabla\phi)\boldsymbol{\xi}) - \frac{30L_0\psi(\phi)}{c_p(\phi)}\right]\frac{D\phi}{Dt} + W(u,v,\phi)\,. \tag{1e}$$

where

$$X_1(\phi) = -\frac{\epsilon^2}{\rho_0}\phi_x\left(\xi_1^2\phi_{xx} + 2\xi_1\xi_2\phi_{xy} + +\xi_2^2\phi_{yy}\right), \tag{2a}$$

$$X_2(\phi) = -\frac{\epsilon^2}{\rho_0}\phi_y\left(\xi_1^2\phi_{xx} + 2\xi_1\xi_2\phi_{xy} + +\xi_2^2\phi_{yy}\right), \tag{2b}$$

$$Y(\phi,T) = \frac{30(p-p_0)}{\rho_0 M}\psi(\phi)[\rho_L - \rho_S + \beta\rho_L(T-T_m)], \tag{2c}$$

$$W(u,v,\phi) = \frac{\mu(\phi)}{\rho_0 c_p(\phi)}\left[2u_x^2 + v_y^2 + (u_y+v_x)^2\right] + \frac{\epsilon^2}{4\rho_0 c_p(\phi)}\left(\xi_1^2\phi_x^2 - \xi_2^2\phi_y^2\right)(v_y - u_x) \tag{2d}$$

$$- \frac{\epsilon^2}{2\rho_0 c_p(\phi)}\left[v_x\left(\xi_1\xi_2\phi_x^2 + \xi_2^2\phi_x\phi_y\right) + u_y\left(\xi_1^2\phi_x\phi_y + \xi_1\xi_2\phi_y^2\right)\right] \tag{2e}$$

For the sake of brevity we introduce only a few of the key notations for the phase-field model; a full description has been given in [1]. Most variables in Eqs. (1) have their usual meanings, and ϕ is the phase-field variable. The variable ϵ is related to freezing-front thickness; T_m is the melting temperature, and L_0 is latent heat.

3. MULTI-SCALE SCHEME

We implement the multi-scale scheme as shown in Fig. 1. In Figure 1, we denote a large domain by Ω and a small domain inside one grid cell of Ω by Ω_s. We first solve the equations of motion Eqs. (1a–1c) on a macroscopic level in Ω to obtain u, v and pressure p. We then interpolate the large-scale solutions to every grid point of Ω_s to prepare for the computation on the small scale. Small-scale computation is conducted to simulate ice growth in the flow field during one time step of large-scale calculation. We assume that the small-scale computation does not affect the velocity field and pressure on large scale. Phase field ϕ and temperature T on the small scale are computed by Eqs. (1d) and (1e) with Neumann boundary conditions to approximate an infinite domain. Moreover, velocity and pressure on the small scale are obtained using Eqs. (1a–1b) with Dirichlet boundary conditions which are calculated from the interpolation of large-scale solutions.

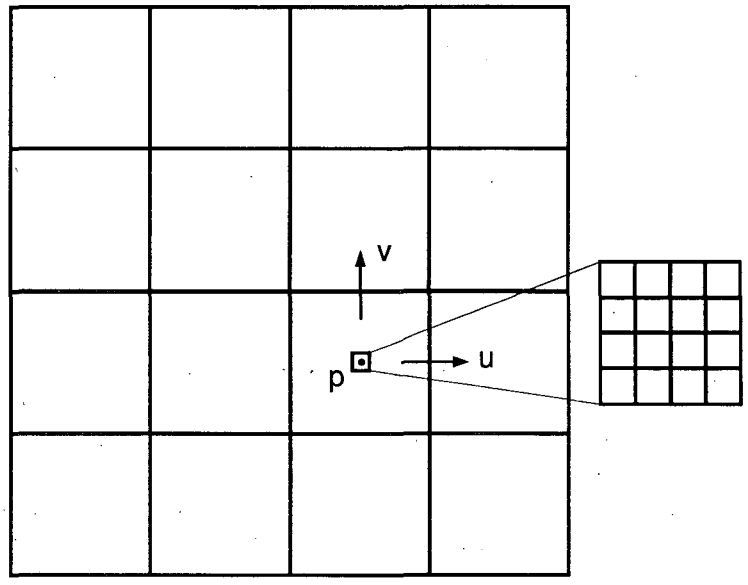


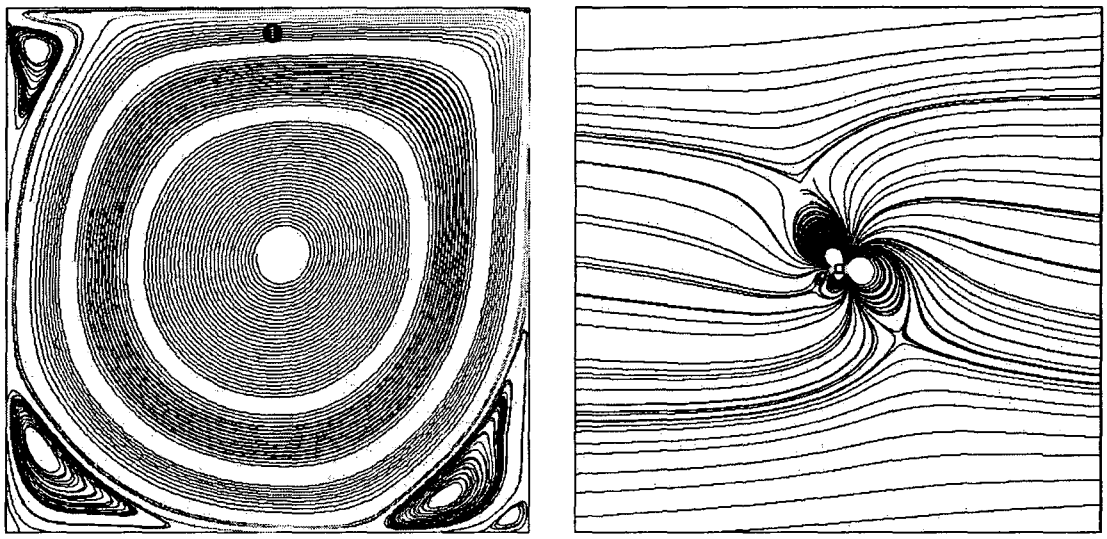
Figure 1: Sketch of Multi-Scale Scheme.

4. NUMERICAL METHODS AND RESULTS

The governing equations (1b–e) are four coupled nonlinear parabolic equations in conserved form. We apply Leray projection to the momentum equations and use a Shuman filter [3] to mollify the solutions. Since time-

splitting methods are efficient for solving multi-dimensional problems by decomposing them into sequences of 1-D problems, a δ-form Douglas & Gunn [4] procedure is applied to the current model. Quasilinearization of ϕ is constructed by Fréchet–Taylor expansion in "δ-form" [5].

On the domain $\Omega = [0, L] \times [0, L] \equiv (0, 0.1m) \times (0, 0.1m)$, prescribed boundary conditions for velocity are no slip boundary condition on $\partial\Omega$ with $u = U$ on $y = L$, and $u \equiv 0$ on $\partial\Omega\backslash\{y = L\}$. Here U determines the Reynolds number, i.e., $Re = UL/\nu_L$. The boundary condition for pressure is the Neumann condition $\partial p/\partial n = 0$. For small-scale computations on $\Omega_s = l \times l \equiv 40\mu m \times 40\mu m$, the boundary conditions for velocity and pressure are obtained from interpolation of the large-scale solution. The boundary conditions for ice growth on the small scale are the Neumann conditions $\partial\phi/\partial n = \partial T/\partial n = 0$. Initial conditions are $\phi_0 = 0$, $T_0 = 233K < T_m$ in Ω_0, where Ω_0 is a square-shaped seed with side length $l_c = 0.6\mu m$ in the center of the domain, and $u_0 = v_0 = 0$. The spatial and time step sizes for large-scale computation are $\Delta x = \Delta y = 10^{-3}m$, $\Delta t = 10^{-3}s$, respectively, and those for small-scale are $\Delta x = \Delta y = 10^{-7}m$, $\Delta t = 2 \times 10^{-12}s$. Figure 2 displays streamlines for large-scale velocity and those for the small-scale near point 1, where the small-scale computation is introduced at $t = 100s$ and centered at the point $(0.05m, 0.09m)$. As would be expected, flow is quite complicated in the neighborhood of the growing dendrite, even at early times.



(a) (b)

Figure 2: (a) Streamlines of Lid-Driven-Cavity Flow at $t = 100s$ with $Re = 10,000$; (b) Streamlines around Ice Crystal for Small-Scale Computation at Point 1 in (a).

5. APPROACH TO PARALLELIZATION AND RESULTS

Parallelization of the numerical solution procedure is based on the MPI algorithm using the HP Fortran 90 HP-UX compiler. The program is parallelized using MPI running on the HP SuperDome at the University of Kentucky Computing Center. We parallelize the loops in the Douglas & Gunn time splitting and line SOR, which is equivalent to distributing the computations on a 2-D domain line by line to each processor. 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. To study speed-up of parallelization, different numbers n of processors ($n = 2, 4, 8, 16, 32$) are used to execute the algorithm. Figure 3 shows the speed-up factor versus the number of processors. It shows that, as the number of processors increases, the speed-up factor increases sub-linearly, suggesting that the demonstrated speedups are not extremely good for $n \geq 32$.

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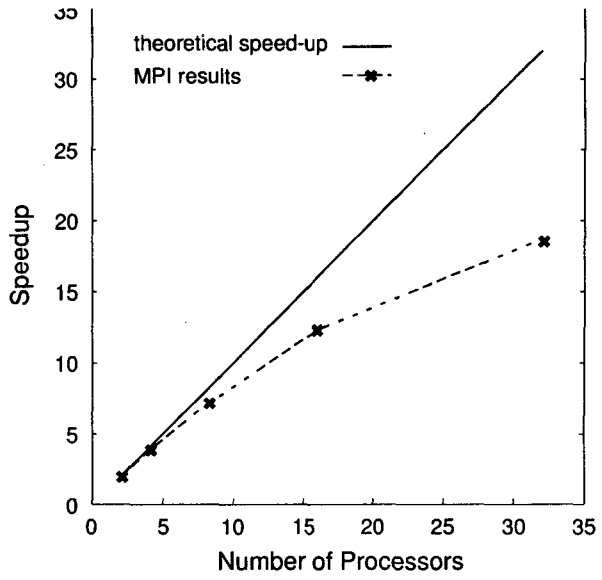

Figure 3: Speed-up performance of the parallelized phase-field model with convection

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