GPU phase-field lattice Boltzmann simulations of growth and motion of a binary alloy dendrite

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Abstract. A GPU code has been developed for a phase-field lattice Boltzmann (PFLB) method, which can simulate the dendritic growth with motion of solids in a dilute binary alloy melt. The GPU accelerated PFLB method has been implemented using CUDA C. The equiaxed dendritic growth in a shear flow and settling condition have been simulated by the developed GPU code. It has been confirmed that the PFLB simulations were efficiently accelerated by introducing the GPU computation. The characteristic dendrite morphologies which depend on the melt flow and the motion of the dendrite could also be confirmed by the simulations.

1. Introduction

Melt flow plays a crucial role in the formation process of solidification microstructures. The melt flow transports heat and solute rejected from solid during solidification, and greatly changes the dendritic growth speed and morphology compared to the free dendritic growth, i.e. growth without flow. In addition, the homogeneously nucleated solid seeds and the detached dendrite arms are also transferred by the melt flow, and those form the equiaxed grains. Recently, in situ and real time observations of solidifying metals using synchrotron radiation facility have revealed the mechanical bending and fragmentation of dendrite arms by the melt flow [1-6]. In this way, the melt flow occurring during solidification drastically changes the solidification morphologies.

In order to accurately control and predict the solidification microstructures, it is of key importance to express the dendrite or cellular structures with high accuracy. Phase-field (PF) method has emerged as the most powerful numerical tool to simulate dendrite structures [7-10]. The PF method is also applied to the solidification problem including the melt flow [11-18]. However, almost all the studies are focused on the stationary dendritic growth, i.e. without motion. Very few papers treat the simultaneous growth and motion of dendrites using the PF method. Do-Quang and Amberg [19] simulated a settling dendrite due to gravity. They expressed the rigid body motion of a dendrite using two different meshes to compute the dendritic growth and the fluid flow separately. Although the rigid body motion of a growing dendrite could be well represented, it would be difficult to apply this method to the multiple dendrite growth problem and large scale computation. Medvedev et al. [20] developed a dendritic solidification model with translation and rotation by employing multi-phase-field method and lattice Boltzmann method. Although they simulated dendritic growth in shear and...
duct flows, the accuracy examinations of the model were not performed. Recently, we also developed a phase-field lattice Boltzmann (PFLB) model to simultaneously simulate the dendritic growth and motion of solid due to melt flow [21]. Because of the simplicity in the algorithm of the PFLB, it is relatively straightforward to apply it to large scale parallel computation.

In this study, we develop a graphics processing unit (GPU) code for the PFLB model to make faster computations. Using the developed code, we simulate the dendritic growth in a shear flow and the settling dendritic growth due to gravity. The PF method is very well suited for the GPU single GPU, it can be easily applied to the three-dimensional problem and multi-GPUs computation.

2. Model
In the PFLB model, we employed a quantitative phase-field model for isothermal solidification of a dilute binary alloy [9] and lattice Boltzmann method for the melt flow [25].

2.1. Phase-field method
The phase-field variable \( \phi \) is defined as \( \phi = +1 \) in solid and \( \phi = -1 \) in liquid. The solute concentration \( c \) is considered by introducing a nondimensional supersaturation \( u \) defined by \( u = (c_{L} - c_{S}^e)/c_{L}^p - c_{S}^p \) where \( c_{L} \) is the concentration in liquid and \( c_{L}^p \) and \( c_{S}^p \) are the equilibrium concentrations of the liquid and solid at a constant temperature \( T_0 \). The time evolution equation of \( \phi \) is expressed as

\[
\tau(\theta) \left( \frac{\partial \phi}{\partial t} + U_s \cdot \nabla \phi \right) = \nabla \cdot \left( W(\theta)^\gamma \nabla \phi \right) - \frac{\partial}{\partial x} \left[ W(\theta) \frac{\partial W(\theta)}{\partial \theta} \frac{\partial \phi}{\partial y} \right] + \frac{\partial}{\partial y} \left[ W(\theta) \frac{\partial W(\theta)}{\partial \theta} \frac{\partial \phi}{\partial x} \right] - \frac{df(\phi)}{d\phi} - \chi \frac{dg(\phi)}{d\phi} u
\]

(1)

Here, \( W(\theta) \) is the interface thickness expressed by \( W(\theta) = W_0 a_{1}(\theta) \) where \( W_0 \) is the standard interface thickness, and \( a_{1}(\theta) \) is the anisotropy function expressed by \( a_{1}(\theta) = 1 + \varepsilon_{s} \cos(4\theta) \) which depends on the crystal orientation, \( \theta \). \( \tau(\theta) \) is the relaxation time considering the anisotropy by \( \tau(\theta) = \tau a_{1}(\theta)^2 \). The interpolating functions \( f(\phi) \) and \( g(\phi) \) are chosen as \( df(\phi)/d\phi = -\phi + \phi^3 \) and \( dg(\phi)/d\phi = (1 - \phi^2)^2 \), respectively. \( \lambda^* \) is associated with the thermodynamic driving force and is expressed as \( \lambda^* = a_{1} W_0/\delta_0 \), where \( a_{1} = 0.88388 \) and \( \delta_0 \) is the chemical capillary length. \( U_s \) is the solid velocity. The time evolution equation of \( u \) is expressed as

\[
\frac{1}{2} \left[ 1 + k - (1 - k) \phi \right] \left( \frac{\partial u}{\partial t} + U \cdot \nabla u \right) = \nabla \cdot \left[ D_L q(\phi) \nabla u - J_{AT} \right] + \frac{1}{2} \left[ 1 + (1 - k) \phi \right] \frac{\partial \phi}{\partial t} - \nabla \cdot J,
\]

(2)

where, \( k = c_{S}^p/c_{L}^p = c_{S}/c_{L} \) is the partition coefficient and \( q(\phi) \) is the interpolating function selected as \( q(\phi) = (kD_s + D_L + (kD_s - D_L)\phi)/2D_L \). \( D_L \) and \( D_s \) are the diffusion coefficients in liquid and solid, respectively, \( J_{AT} \) and \( J \) are the antitrapping and the fluctuation currents, respectively, and \( U \) is the fluid velocity.

2.2. Lattice Boltzmann method
The lattice Boltzmann equation is given by

\[
f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau} [f_i(x+t) - f_i^{eq}(x, t)] + G_i(x, t) \Delta t.
\]

(3)

where, \( \tau \) is the single relaxation time, \( f_i \) is the particle distribution function in the \( i \)th direction, \( x \) is the position vector, \( c_i \) is the discrete particle velocity, \( \Delta t \) is the time step, and \( G_i \) is the discrete force. The equilibrium distribution function \( f_i^{eq} \) is expressed as

\[
f_i^{eq} = w_i \rho \left[ 1 + \frac{3[(c_i \cdot U) c_i]}{c_i^2} + \frac{9[(c_i \cdot U)^2]}{2c_i^4} - \frac{3U \cdot U}{2c_i^2} \right].
\]

(4)
where, $w_i$ is the weighting function depending on the employed model and $c$ is the lattice velocity defined by $c = \Delta x/\Delta t$ using lattice size $\Delta x$ and time increment $\Delta t$. The fluid density $\rho$ and velocity $U$ are computed by

$$\rho = \sum_{i=0}^{Q-1} f_i,$$

$$\rho U = \sum_{i=0}^{Q-1} c_i f_i,$$

where, $Q$ is the number of discrete velocities. The discrete force $G_i$ in equation (1) is given with second-order accuracy as [26]

$$G_i = \rho w_i \left[ 3 \frac{c_i - U}{c^2} + 9 \left( \frac{c_i \cdot U}{c^4} \right) \right] G,$$

where, $G$ is the external force on the solid-liquid interface, where the phase-field $\phi$ changes from -1 to +1, to satisfy the non-slip boundary condition. $G$ is modeled as a dissipative drag [11]:

$$G(x,t) = \frac{2 \rho \nu h}{W_0} \left( \frac{1 + \phi}{2} \right)^2 (U_S - U),$$

where, $\nu$ is the kinematic viscosity, $h$ is a constant of $h = 2.757$ and $U_i$ is the solid velocity. In the following simulations, the two-dimensional nine-velocity (D2Q9) model is used.

### 2.3. Solid motion

The motion of solids is determined by solving the following set of equations [27; 28]:

$$M_S \frac{dU_T}{dt} = G_S,$$

$$I_S \frac{d\omega_S}{dt} = T_S,$$

where, $M_S$ is the mass of the solid, $U_T$ is the translational velocity of the solid, $I_S$ the tensor for the moment of inertia, $\omega_S$ is the angular velocity, and $G_S$ and $T_S$ are the total force and torque acting on the solid, respectively. $G_S$ and $T_S$ are calculated by

$$G_S = -\sum_{x \in \Omega} G(x,t) \Delta V + \left( 1 - \frac{\rho_l}{\rho_S} \right) M_S g,$$

$$T_S = -\sum_{x \in \Omega} (x - X_S) \times G(x,t) \Delta V,$$

where, $\Delta V$ is the volume of the computational domain, $\Omega$ is the domain in the vicinity of the interface, $\rho_l$ and $\rho_S$ are the density of the liquid and solid phases, $g$ is the gravity, and $X_S$ is the center of mass of the solid. The solid velocity $U_S$ is given by

$$U_S = U_T + \omega_S \times (x - X_S).$$

### 3. Computations

The dendritic growth in a shear flow and the sedimentation of a growing dendrite due to gravity are simulated using the developed code. In both simulations, the dendrites grow with translation and rotation. An Al-3wt%Cu binary alloy is used in the following simulations and the material parameters are the same as those used in the reference [22].
3.1. Dendritic growth in a shear flow

Figure 1(a) shows the computational domain and the initial condition. The size of the computational domain is set to \( L_x \times L_y = 8,192 \Delta x \times 1,024 \Delta y \) with a lattice size \( \Delta x = \Delta y = 0.5 \mu m \). A solid seed with radius of \( 3 \Delta x \) is placed at the point of \( (200 \Delta x, 512 \Delta y) \). Bottom and top flow velocities are fixed to \( U_0 = 6 \text{ mm/s} \) and \(-U_0/2\), respectively. The initial distribution of flow velocity in \( x \)-direction is set to \( U(y) = U_0(1-3y/2L_y) \) and the initial velocity in \( y \)-direction is set to \( V = 0 \) in all domain. Periodic boundary conditions are set to the melt flows at the left and right sides. For phase-field \( \phi \) and the supersaturation \( u \), zero Neumann conditions are set to all boundaries.

Figure 1 shows the time changes of the dendrite morphology and the concentration distribution. The dendrite shape is expressed by the solid black line which is the counter of \( \phi = 0 \). The color indicates the concentration distribution. It can be observed that the dendrite grows with translation and rotation. The four dendrite arms are designated by a1, a2, a3 and a4. Initially, the arm a1 grows toward \( x \)-axis direction and its location changes with time. We can see that the dendrite rotates about 180º every 25,000 steps.

Figure 2(a) shows the variation of area of the dendrite, \( A_s \), during the computation shown in figure 1. The dashed line indicates the variation in \( A_s \) of a free growth dendrite computed without flow. It can be observed that the melt flow largely enhances the dendritic growth. Figure 2(b) shows the variations of the dendrite migration velocity in the \( x \)-direction, \( U_x \), and the \( y \)-coordinate of the center of mass of the dendrite, \( Y_s \). The dendrite migration velocity \( U_x \) increases almost linearly until about 75,000 steps and then accelerates. These velocity changes can be explained by the change of \( Y_s \).

![Figure 1](image_url)

**Figure 1.** Time slices during dendrite growth in shear flow.
Figure 2. Variations of (a) area of the dendrite, $A_S$, and (b) velocity in $x$-direction, $U_S$, and position in the $y$-direction, $Y_S$, of center of mass of the dendrite.

3.2. Dendritic growth during settling

The settling of growing dendrites, which are caused by the density difference between solid and liquid, is a very important phenomenon in solidification and casting [29-34]. Figures 3-5 show the dendrite morphological changes and the changes of concentration field obtained in the dendrite settling simulations under three different initial supersaturations, i.e. $u_0 = -0.2$, -0.3 and -0.4. The computational domain is set to $L_x \times L_y = 2,048\Delta x \times 4,096\Delta y$ with a lattice size $\Delta x = \Delta y = 0.5$ $\mu$m. A solid seed with radius of $3\Delta x$ is placed at the point of $(1,024\Delta x, 3,896\Delta y)$. The no-slip condition and the zero Neumann condition for $\phi$ and $u$ are set to all boundaries. The density ratio, $\rho_s/\rho_L$, is assumed to be 1.05, and the gravity acts along the $y$-direction.

From figures 3-5, it can be observed that the dendrites settle straightly until about $y = 3,000\Delta y$. The dendrite arm growing downward becomes longer compared to the other three arms, and the growth of the one oriented upward is suppressed by the high concentration field. The dendrite arms with the preferred growth direction along the $x$-axis slightly grow downward. This nonsymmetrical growth of the four dendrite arms is caused by the melt flow initiated in the settling of the dendrite. This behavior is very similar to the experimental observations of a transparent material [32]. Then, as shown in figure 3-5(b), the rotation of the dendrite starts. The rotation is caused due to the non-symmetry in the left and right sides of the dendrite morphology.

Figure 3. Dendrite settling simulation for $u_0 = -0.2$. 
Figure 4. Dendrite settling simulation for $u_0 = -0.3$.

Figure 5. Dendrite settling simulation for $u_0 = -0.4$.

Figure 6. Variations of (a) area of the dendrite, $A_s$, and (b) settling speed, $V_s$, for three different initial supersaturations, $u_0$.

Figure 6 shows the variations of the dendrite area, $A_s$, and the settling velocity, $V_s$. The four solid circles on each curve correspond to the time step in figures 3-5. As can be seen, the growth speed increases as the supersaturation reduces, and that is why the settling speed, $V_s$, is faster for a smaller
supersaturation. Although $A_t$ increases monotonically, $V_s$ fluctuates around the velocity before the solid starts rotating. Therefore, the fluctuations in figure 6(b) are due to the rotations of the dendrite. For $u_0 = -0.3$ and -0.4, large speed reductions are observed at the last stage of the computations. This is due to the interaction with the boundary as shown in figures 4(d) and 5(d).

The computational time of the shear flow and the settling simulations using 8,388,608 meshes was about 140 minutes for 150,000 steps which includes the data output time every 1,000 steps. Here, single GPU of the NVIDIA Tesla K20X was used. The computational efficiency can be improved even further by modifying the developed code. However, the computational time in the present study is thought to be reasonable for larger computations and systematical investigations.

4. Conclusions
In this study, we have developed a GPU code for the PFLB method, which can simulate the dendritic growth with translation and rotation. The GPU accelerated PFLB method has been implemented using CUDA C. The dendritic growth in a shear flow and settling condition has been simulated by the developed GPU code using a single NVIDIA Tesla K20X. As a result, the characteristic dendrite morphologies and the growth speed differences depending on the melt flow could be observed. It has been also confirmed that the GPU accelerated PFLB computations were enabled in reasonable computational times. By parallelizing the developed GPU code using multiple-GPUs, larger computations and three-dimensional computations of dendritic growth with motion will be possible.

Acknowledgements
This work was supported by a Grant-in-Aid for Scientific Research (KAKENHI) (Grant Number 25289006 and 26220002) from the Japan Society for the Promotion of Science (JSPS) and a Research Promotion Grant from the Iron and Steel Institute of Japan (ISIJ).

References
[1] Ruvalcaba D, Mathiesen R H, Eskin D G, Arnberg L and Katgerman L 2007 In situ observations of dendritic fragmentation due to local solute-enrichment during directional solidification of an aluminum alloy Acta Mater. 55 4287
[2] Yasuda H, Yamamoto Y, Nakatsuka N, Yoshiya M, Nagira T, Sugiyama A, Ohnaka I, Uesugi K and Umetani K 2009 In situ observation of solidification phenomena in Al-Cu and Fe-Si-Al alloys Int. J. Cast Met. Res. 22 15
[3] Billia B, Nguyen-Thi H, Mangelinck-Noel N, Bergeon N, Jung H, Reinhart G, Bogno A, Buffet A, Hartwig J, Baruchel J and Schenk T 2010 In Situ synchrotron x-ray characterization of microstructure formation in solidification processing of Al-based metallic alloys ISIJ Int. 50 1929
[4] Mirihanage W U, Arnberg L and Mathiesen R H IOP Conference Series: Materials Science and Engineering,2012, vol. Series 33)
[5] Liotti E, Lui A, Vincent R, Kumar S, Guo Z, Connolley T, Dolbnya I P, Hart M, Arnberg L, Mathiesen R H and Grant P S 2014 A synchrotron X-ray radiography study of dendrite fragmentation induced by a pulsed electromagnetic field in an Al-15Cu alloy Acta Mater. 70 228
[6] Reinhart G, Nguyen-Thi H, Mangelinck-Noël N, Baruchel J and Billia B 2014 In situ investigation of dendrite deformation during upward solidification of Al-7wt.%Si  JOM 66 1408
[7] Kobayashi R 1993 Modeling and numerical simulations of dendritic crystal growth Physica D: Nonlinear Phenomena 63 410
[8] Karma A and Rappel W J 1996 Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics 53 R3017
[9] Ohno M and Matsuura K 2009 Quantitative phase-field modeling for dilute alloy solidification involving diffusion in the solid Physical Review E - Statistical, Nonlinear, and Soft Matter Physics 79
[10] Takaki T 2014 Phase-field modeling and simulations of dendrite growth *ISIJ Int.* **54** 437
[11] Beckermann C, Diepers H J, Steinbach I, Karma A and Tong X 1999 Modeling Melt Convection in Phase-Field Simulations of Solidification *J. Comput. Phys.* **154** 468
[12] Tong X, Beckermann C and Karma A 2000 Velocity and shape selection of dendritic crystals in a forced flow *Physical Review E - Statistical, Plasmas, Fluids, and Related Interdisciplinary Topics* **61** R49
[13] Beckermann C, Li Q and Tong X 2001 Microstructure evolution in equiaxed dendritic growth *Science and Technology of Advanced Materials* **2** 117
[14] Jeong J H, Goldenfeld N and Dantzig J A 2001 Phase field model for three-dimensional dendritic growth with fluid flow *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **64** 416021
[15] Tong X, Beckermann C, Karma A and Li Q 2001 Phase-field simulations of dendritic crystal growth in a forced flow *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **63** 061601/1
[16] Al-Rawahi N and Tryggvason G 2002 Numerical simulation of dendritic solidification with convection: Two-dimensional geometry *J. Comput. Phys.* **180** 471
[17] Al-Rawahi N and Tryggvason G 2004 Numerical simulation of dendritic solidification with convection: Three-dimensional flow *J. Comput. Phys.* **194** 677
[18] Guo Z, Mi J, Xiong S and Grant P S 2013 Phase Field Simulation of Binary Alloy Dendrite Growth Under Thermal- and Forced-Flow Fields: An Implementation of the Parallel–Multigrid Approach *Metallurgical and Materials Transactions B* **44** 924
[19] Do-Quang M and Amberg G 2008 Simulation of free dendritic crystal growth in a gravity environment *J. Comput. Phys.* **227** 1772
[20] Medvedev D, Varnik F and Steinbach I *Procedia Computer Science, 2013*, vol. Series 18) pp 2512
[21] Rojas R, Takaki T and Ohno M 2015 Submitting
[22] Takaki T, Ohno M, Shimokawabe T and Aoki T 2014 Two-dimensional phase-field simulations of dendrite competitive growth during the directional solidification of a binary alloy bccystal *Acta Mater.* **81** 272
[23] Takaki T, Shimokawabe T, Ohno M, Yamanaka A and Aoki T 2013 Unexpected selection of growing dendrites by very-large-scale phase-field simulation *J. Cryst. Growth* **382** 21
[24] Yamanaka A, Aoki T, Ogawa S and Takaki T 2011 GPU-accelerated phase-field simulation of dendritic solidification in a binary alloy *J. Cryst. Growth* **318** 40
[25] Chen S and Doolen G D 1998 Lattice boltzmann method for fluid flows. In: *Annual Review of Fluid Mechanics*, pp 329
[26] Medvedev D, Fischaleck T and Kassner K 2006 Influence of external flows on crystal growth: Numerical investigation *Physical Review E* **74** 031606
[27] Glowinski R, Pan T W, Hesla T I, Joseph D D and Périaux J 2001 A Fictitious Domain Approach to the Direct Numerical Simulation of Incompressible Viscous Flow past Moving Rigid Bodies: Application to Particulate Flow *J. Comput. Phys.* **169** 363
[28] Feng Z G and Michaelides E E 2004 The immersed boundary-lattice Boltzmann method for solving fluid-particles interaction problems *J. Comput. Phys.* **195** 602
[29] Badillo A, Ceynar D and Beckermann C 2007 Growth of equiaxed dendritic crystals settling in an undercooled melt, Part 2: Internal solid fraction *J. Cryst. Growth* **309** 216
[30] Badillo A, Ceynar D and Beckermann C 2007 Growth of equiaxed dendritic crystals settling in an undercooled melt, Part 1: Tip kinetics *J. Cryst. Growth* **309** 197
[31] Lesoult G 2005 Macrosegregation in steel strands and ingots: Characterisation, formation and consequences *Materials Science and Engineering: A* **413–414** 19
[32] Appolaire B, Albert V, Combeau H and Lesoult G 1999 Experimental study of free growth of equiaxed NH4Cl crystals settling in undercooled NH4Cl-H2O melts *ISIJ Int.* **39** 263
[33] Appolaire B, Albert V, Combeau H and Lesoult G 1998 Free growth of equiaxed crystals settling in undercooled NH4Cl-H2O melts *Acta Mater.* **46** 5851
[34] Ramani A and Beckermann C 1997 Dendrite tip growth velocities of settling NH4Cl equiaxed crystals *Scripta Mater.* **36** 633