MESOSCOPIC SIMULATION OF SOLIDIFICATION PROCESS WITH MELT CONVECTION

Medvedev D.A.[1,2,3,a], *Varnik F.*[3], *Steinbach I.*[3]

[1]Lavrentyev Institute of Hydrodynamicsics, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia
[3]ICAMS, Ruhr University, Bochum, Germany
[a]dmedv@hydro.nsc.ru

Dendritic solidification is a phenomenon with immense technical and theoretical importance. Its technical importance clearly stems from the fact that the overwhelming majority of all metallic workpieces have once in their lifetime undergone solidification with a dendritic structure. The grain size, shape and the solute distribution affects significantly the mechanical properties of the materials produced.

Under normal growth conditions, i.e., if we do not have a microgravity setup, the inhomogenous distribution of temperature and solute concentration in the solidification sample will inevitably lead to thermal convection. Convective flows can substantially influence the growth process and the features of the resulting pattern.

The phase-field method is widely used in simulations of dendritic solidification (e.g. Refs. [1-2]). Its main advantage is the absence of the necessity of tracking the interface, together with the possibility of keeping good accuracy at moderate computational cost. The lattice Boltzmann (LB) method is presently a well-established tool to simulate fluid flows, especially flows in complex geometries [3].

We describe the combined mesoscopic scheme for the simulation of solidification with presence of melt flow. We consider the case of the solute-driven process, but the thermal-driven case can be considered as well [4]. The scheme is based on the multiphase-field method [1] for calculating the solidification. The interphase boundary is considered as a thin transition layer in which all the material parameters change gradually. The dynamics of the phase-field variable which represents the local concentration of the solid phase is governed by the minimization of the free-energy functional. The concentration of solute is obtained from the diffusion equation, with the local redistribution of solute between solid and liquid phases according to the linear phase diagram.

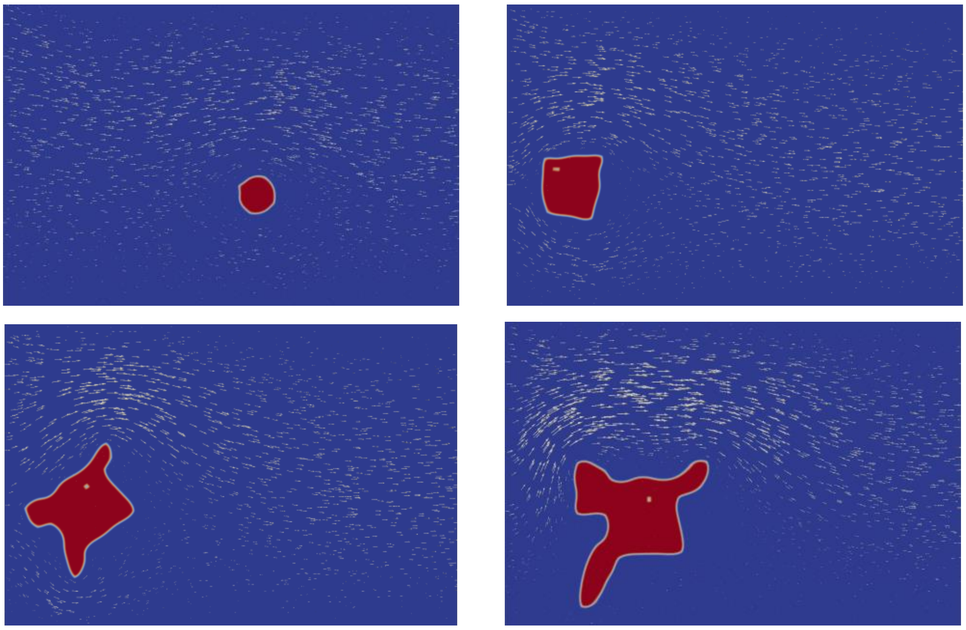
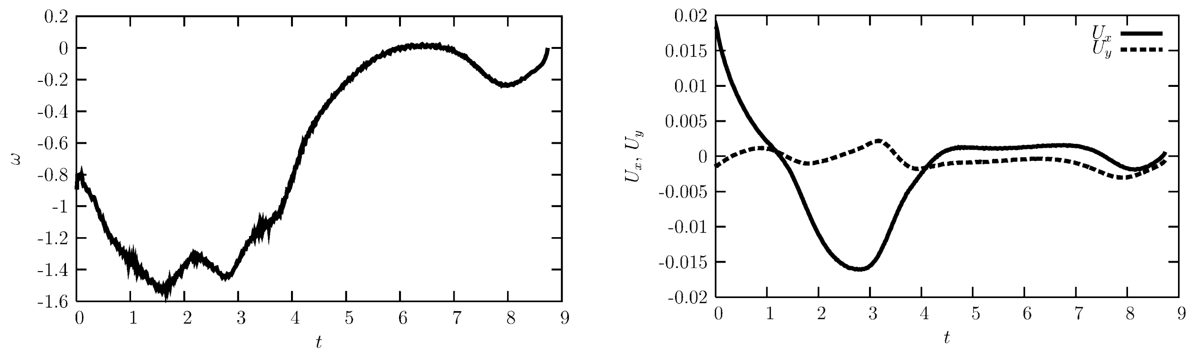


Figure 1. Moving grain in a channel flow. Time is (left to right, top to bottom) t = 0:5 s, 1 s, 1.5 s.

The lattice Boltzmann method [3] is used to simulate the fluid flows. The fluid is presented as a set of pseudoparticles which stream to neighbor lattice nodes and undergo local collisions. Friction forces due to the relative velocity of solid and liquid phases are taken into account by the Exact Difference Method [4]. Buoyancy force due to the thermal expansion and the inhomogeneous distribution of the solute concentration can also be included. Motion and rotation of growing solid grains is described by the equation of motion of a rigid body.



a b

Figure 2. Moving grain in a channel flow
a) time dependence of the grain velocity and b) angular velocity

We simulated the growth and the rotation of a dendrite in a parabolic flow, the grain growth and rotation in a shear flow, and the grain evolution and motion in a parabolic flow under the action of gravity. In first two cases, the growing dendrite rotates due to the interaction with the flow. Results for the moving grain are shown in Fig. 1. The direction of low is from left to right, the gravitational force is directed to the left. Time dependence of the center of mass velocity and the angular velocity is shown in Fig. 2. When the size of the grain increases, the drag force also increases, and the grain stops and then starts to move with the flow. The angular velocity also first increases, then decreases and changes sign. In all the cases, the upwind branches grow faster since the flow brings fresh material into its vicinity.

In conclusion, the mesoscopic approach based on the combination of the phase-field and lattice Boltzmann methods can be successfully applied to simulation of solidification processes with melt convection in a wide range of problems.

References

1. Steinbach I. Phase-field models in materials science. *Modelling Simul. Mater. Sci. Eng.* 17. P. 073001 (2009).
2. Karma A., Rappel W.-J. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Rev. E* 57 P. 4323 (1998).
3. Chen S., Doolen G. Lattice Boltzmann method for fluid flows. *Annual Review of Fluid Mechanics.* 30. P. 329–364 (1998).
4. Medvedev D., Kassner K. Lattice-Boltzmann scheme for crystal growth in external flows. *Phys. Rev. E* 72. P. 056703 (2005).
5. Kupershtokh A.L. Incorporating a body force term into the lattice Boltzmann equation // *Vestnik NGU (Quarterly Journal of Novosibirsk State Univ.) Series: Math., Mech. and Informatics*. 4(2). P. 75–96. (2004).

© Medvedev D.A., Varnik F., Steinbach I., 2017