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Lattice Boltzmann phase-field modelling of binary-alloy solidification

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Abstract

A lattice Boltzmann phase-field method for flows of binary-alloys with liquid–solid phase-transitions is introduced. Applications to two-dimensional flows with solidification fronts are presented and commented on.

Keywords: Lattice Boltzmann equation; Phase-field equation; Binary alloys; Solidification; Cellular structure; Convection

1. Introduction

Fluid flows with phase-transitions play an important role both in natural and industrial solidification processes. Though the dimensions of the entire system are often macroscopic, as e.g., in casting or bulk crystal growth, the pattern formation during the solidification takes place on a mesoscopic scale. On the macroscopic scale the fluid flow and diffusion define the species and heat distribution, whereas on the mesoscopic scale the details of the liquid–solid phase-transition come into play. A state-of-the-art method to describe the phase-transition is the phase-field method, which is based on a Ginzburg–Landau-type theory with a continuous order parameter defining the state of matter at a certain spatial point. Since there is no sharp interface the numerical solution of the resulting phase-field method does not require a front tracking of the interface. A uniform grid can be used for solving the phase-field equation as well as for applying the lattice Boltzmann equation to compute the fluid motion and its coupling with solid.

In this paper we describe a combination of the phase-field method and the lattice Boltzmann equation for the simulation of fluid flows with first-order phase-transitions. This combination appears particularly interesting because the dynamics of the phase-fields describing the interface evolution is most naturally incorporated within the particle-like dynamics underlying the lattice Boltzmann formulation of fluid flow. A similar approach is used also by Medvedev et al. for studying dendritic growth of monocomponent melts [1]. In this paper we combine advanced features of the lattice Boltzmann method, such as grid refinement [2] and moving interfaces [3], to the case of fluid flows with binary-alloy solidification. To the best of our knowledge, this is the first time that binary-alloy solidification is handled by lattice Boltzmann techniques.

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2. Phase-field model of a binary-alloy

Crystallization processes in a binary-alloy can be described by a pair of scalar fields, $\phi(\vec{r},t)$ and $c(\vec{r},t)$. The first one, also known as phase-field, acts as a continuous order parameter which distinguishes between the solid and liquid phase ($0\leqslant\phi\leqslant 1$ with $\phi=0$ completely liquid and $\phi=1$ completely solid). The second scalar field, c, represents the fraction of solute (say A) to solvent (say B), so that $c=1$ corresponds to full A and $c=0$ to full B, respectively. There is a third scalar field, namely the temperature, which for simplicity will be treated in this paper as a static quantity affecting the evolution of the scalar fields only via boundary conditions.

The scalar fields obey the following set of coupled, non-linear, advection-reaction–diffusion equations:

$$\tau_\phi D_t\phi = -Wg'(\phi)+\Theta p'(\phi)+\xi^2\Delta\phi, \tag{1}$$

$$D_t c = \nabla[D(\phi)\nabla c + D(\phi)(c_l-c_s)\nabla p(\phi)], \tag{2}$$

where D_t is the total derivative along the flow and τ_ϕ is a typical relaxation time of the phase-field.

The rate equation for the phase-field is governed by the potential of the phase-field (first term on right-hand side of Eq. (1)), the constitutional undercooling, $\Theta=\Theta(\phi,c)$ and the curvature of the interface (third term). These equations can be derived by minimization of a free-energy functional $\mathscr{F}(\phi,c)=\int[f(\phi,c)+(\xi^2/2)|\nabla\phi|^2]\,\mathrm{d}V$, where f is the free-energy density in the bulk and the second term describes the effects of interfacial energy, i.e., the cost of maintaining an interface of thickness proportional to ξ.

The bulk free-energy density consists of two contributions. The first, $Wg(\phi)=W\phi^2(1-\phi^2)$, is a typical double-well potential, whose height, $W/4$, controls the transition from liquid to solid and viceversa.

The function $p(\phi)$ is a monotonic switch fulfilling the conditions $p(0)=0$, $p(1)=1$, $p'(0)=p'(1)=0$, prime standing for derivative with respect to ϕ. A suitable choice is $p(\phi)=3\phi^2-2\phi^3$.

The terms f_s and f_l are the free energy of solid and liquid phases, respectively. They are taken in the forms: $f_l=CT(\overline{\ln T_m}-\ln T)+(RT/V_m)(c\ln c+(1-c)\ln(1-c))$, $f_s=f_l-f_L$, where $\overline{\ln T_m}\equiv c\ln T_A+(1-c)\ln T_B$.

The quantity f_L corresponds to latent heat production, $f_L=T(cL_A(1/T-1/T_A)+(1-c)L_B(1/T-1/T_B)$. The terms L_A, L_B are the latent heats of the corresponding alloy components and T_A and T_B are the melting temperatures.

Finally, the diffusion coefficient of the solvent is taken in the form $D(\phi)=D_0(1-\phi)$, in order to enforce zero diffusivity in the solid phase.

In terms of the standard classification [4], our model is one with one conserved and one non-conserved order parameters, c and ϕ, respectively.

3. Lattice Boltzmann scheme with moving interfaces

The general form of the lattice Boltzmann equation reads as follows (see e.g., [7–9])

$$f_i(\vec{x}+\vec{c}_i\Delta t,t+\Delta t)-f_i(\vec{x},t)=-\Omega_{ij}\Delta t[f_j-f_j^e](\vec{x},t)+S_i\Delta t, \tag{3}$$

where $f_i(\vec{x},t)\equiv f(\vec{x},\vec{v}=\vec{c}_i,t)$, $i=0,b$, is the discrete one-body distribution function describing particles moving along the lattice direction defined by discrete speed $\vec{c}_i$. All the symbols have the standard meaning [10–12], except for the source term, S_i, which encodes the fluid interaction with the solidification front.

This interaction is dealt with as follows. At each lattice site, only a fraction $1-r(\phi)$ is transmitted to the next link, so that the reflection step reads as:

$$\tilde{f}_{\bar{i}}(\vec{x}+\vec{c}_i\Delta t,t+\Delta t)=(1-r(\vec{x},t))\,f_i(\vec{x},t)+r(\vec{x},t)\,f_{\bar{i}}(\vec{x},t),$$

where bar denotes the mirror conjugate to direction i ($\vec{c}_{\bar{i}}+\vec{c}_i=0$). Consequently, the modified LB update, including reflections, reads as follows:

$$f_i(\vec{x}+\vec{c}_i\Delta t,t+\Delta t)=\tilde{f}_{\bar{i}}-(1-r(\vec{x},t))\Omega_{ij}\Delta t[f_j-f_j^e(\vec{x},t)]+\tilde{S}_i\Delta t. \tag{4}$$