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Construction of seamless immersed boundary phase-field method

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ABSTRACT

In this paper, we try to construct the seamless immersed boundary phase-field method for simulating the two-phase flows. The seamless immersed boundary method is one of the Cartesian grid approaches, in which the forcing term is added to the incompressible Navier–Stokes equations in order to satisfy the velocity condition on the boundary. In the seamless immersed boundary method, the forcing term is added not only on the grid points near the boundary but also on the grid points inside the boundary. This method is applied to the phase-field equation, i.e., the Cahn–Hilliard equation for the two-phase flow analysis. By using the Taylor series expansion in multi-variable, the correction term for satisfying the Neumann boundary condition is estimated. The phase separation in a rotated square cavity is considered, in order to validate the present approach. It is found that the rotated solutions obtained on the Cartesian coordinates are the same as the original solution at any time. Then, it is concluded that the present seamless immersed boundary phase-field method is very fruitful for simulating the complicated two-phase flows.

1. Introduction

The many numerical simulations of two-phase flow have been conducted with the development of the computer, in particular, since the 1990s. In order to simulate the incompressible two-phase flow, the volume-of-fluid (VOF) [1] and level set [2] methods are usually applied. In recent years, the phase-field method [3,4] is spotlighted in place of these conventional methods. The phase-field method is based on the Van der Waals' hypothesis as the equilibrium interface is found by minimizing fluid free energy. The phase-field variable (order parameter) which varies smoothly through the diffuse interface is introduced in the computational domain. The behavior of phase-field variable is typically governed by the Cahn–Hilliard equation [5] with the variables of the phase-field and the chemical potential, and as a result, the phase is determined by minimizing a free energy. However, to solve the Cahn–Hilliard equation numerically is difficult, because this equation includes the fourth-order spatial derivatives, so that the severe time step restriction is introduced, e.g., $\Delta t \sim \Delta x^4$ for the explicit methods [6]. In the presence of flow, the Cahn–Hilliard equation has to be solved together with the incompressible Navier–Stokes equations. Then, this severe time step restriction for the Cahn–Hilliard equation provides the low computational efficiency in the system of the incompressible Navier–Stokes and the Cahn–Hilliard equations solver. In order to improve this weak point, we proposed the stabilized phase-field method [7]. As a result, the computation can be executed stably with about 10 timed time step of conventional time integration schemes. In simulating complicated two-phase flows, the Cahn–Hilliard equation has another weak point that the transformation of the Cahn–Hilliard equation to the boundary fitted coordinates (BFC) is very complicated, because of the fourth-order derivatives in this equation. Therefore, in most cases, the coordinate transformation of the Cahn–Hilliard equation was applied to the simple coordinate system [8,9]. In practice, many simulations were performed by the finite element method [10–13], the finite volume method [14], and the lattice Boltzmann method [15–17]. Since the transformed Cahn–Hilliard equation on the computational plane has more terms than the equation on the Cartesian coordinates, so that the computational effort becomes larger, it is desirable to simulate on the Cartesian coordinates. For the complicated geometries, however, simulation on the Cartesian coordinates has not been carried out enough. Then, it is very important to construct the Cahn–Hilliard equation solver on the Cartesian coordinates for effective numerical simulation of complicated two-phase flows.

In the flow simulations with complicated geometry on the Cartesian coordinates, the immersed boundary method [18–21] is very popular today. In this paper, the seamless immersed boundary method [22] which is the smart approach without the unphysical pressure oscillations on the Cartesian coordinates is applied to the Cahn–Hilliard equation. The conventional immersed bound-

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ary method gives the unphysical pressure oscillations near the boundary. On the other hand, in the seamless immersed boundary method for the incompressible Navier–Stokes equations, the external forcing term which satisfies the velocity condition on the boundary is added not only on the grid points near the boundary but also on the grid points inside the boundary. As a result, the unphysical pressure oscillations can be removed [23]. The seamless immersed boundary method was applied to the moving boundary problem [24], flow with heat transfer [22], turbulent flow [25], and lattice Boltzmann equation [26] successfully. Similar to the incompressible Navier–Stokes equations, the correction term which satisfies the boundary condition can be added to the Cahn–Hilliard equation. Conventionally the Neumann boundary condition, i.e., $\partial c/\partial n = 0$ and $\partial \mu/\partial n = 0$, is imposed for the phase-field variable, c, and the chemical potential, μ, on the solid boundary with contact angle of $\pi/2$. Therefore, we try to estimate the correction term which satisfies the Neumann boundary condition for the phase-field method. In order to estimate such a term, the Taylor series expansion in multi-variable is introduced. The boundary value and its derivatives in the Cartesian directions can be determined in this procedure. This approach is applied to the phase separation problem in a rotated square cavity. The effectiveness of the present approach is discussed.

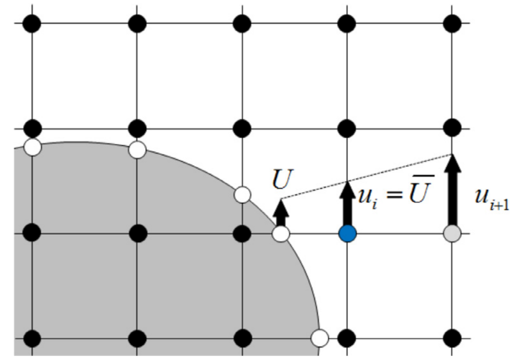

Fig. 1. Direct forcing.

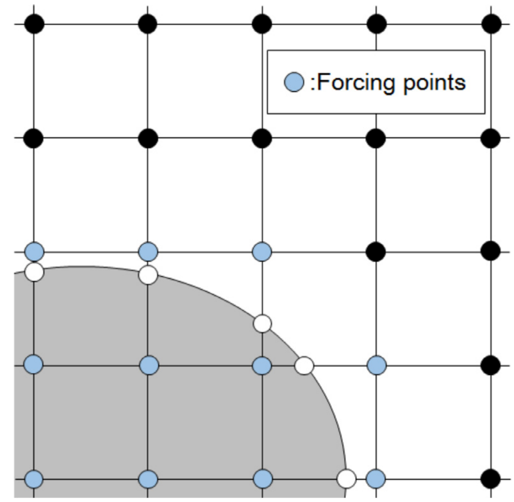

Fig. 2. Grid points added forcing term.

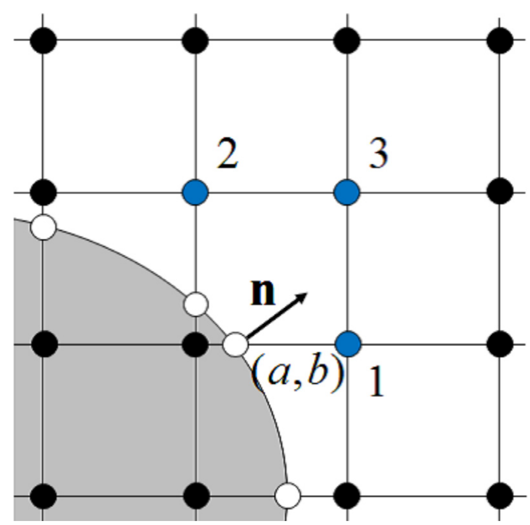

Fig. 3. Grid points used the Taylor series expansion.

2. Phase-field method

2.1. Phase-field equation

In the phase-field method, it is assumed that the interface between two phases at any time can be described by the phase-field variable (order parameter) c which is defined by the function of location $\mathbf{x}$. A free energy J can be written as a functional of $c(\mathbf{x})$,

$$J(c) = \int_\Omega \left[F(c) + \frac{\varepsilon^2}{2} |\nabla c|^2 \right] d\mathbf{x}, \tag{1}$$

where Ω denotes the computational region and the first term, $F(c)$, and the second term are the Helmholtz free energy and the surface energy, respectively. In this paper, the conventional quartic free energy is adopted, which is defined by

$$F(c) = \frac{1}{4} c^2 (1-c)^2. \tag{2}$$

The equilibrium interface profile is determined by minimizing the functional $J(c)$ with respect to variations of the function $c(\mathbf{x})$. Assuming that the fluid is incompressible with equal density and isothermal condition is satisfied, the phase-field variable $c(\mathbf{x})$ is governed by the following non-dimensional Cahn–Hilliard equation,

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = \frac{1}{Pe} \frac{\partial}{\partial x_j} \left(M(c) \frac{\partial \mu}{\partial x_j} \right) + G_c, \tag{3}$$

$$\mu = \frac{dF}{dc} - \varepsilon^2 \frac{\partial^2 c}{\partial x_j \partial x_j} + G_\mu, \tag{4}$$

where u_j denotes the flow velocity, $M(c) > 0$ is the non-dimensional mobility, and μ is the generalized chemical potential. These variables are non-dimensionalized by the reference length $\bar{L}$, the reference velocity $\bar{U}$, the reference chemical potential $\bar{\mu}$, and the reference mobility $\bar{M}$. $Pe(= \bar{L}\bar{U}/(\bar{M}\bar{\mu}))$ is the diffusional Peclet number which means the relative strength of advection and diffusion. $\varepsilon > 0$ is the interface thickness. In this paper, the mobility is set to be constant, i.e., $M(c) = 1$. Also, the last terms, G_c in Eq. (3) and G_μ in Eq. (4), denote the correction terms satisfied the boundary condition for the described immersed boundary method.

2.2. Incompressible flow equations

In the presence of flow, the aforementioned Cahn–Hilliard equation is solved together with the flow equations. For the incompressible flow, the flow is governed by the continuity equation and the momentum equations, i.e., the incompressible Navier–Stokes equations with surface tension term. These governing equa-