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On the re-initialization of fluid interfaces in diffuse interface method

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ABSTRACT

In this paper, a re-initialization method of fluid interfaces is introduced into the Cahn–Hilliard (C–H) model for reducing the continuous numerical and modeling diffusion in the simulation of complex multiphase flows. In this method, the re-initialization process is achieved through three simple steps. Specifically, the order parameter C obtained from the C–H model is first transformed into a roughly estimated distance function d. After that, correction of d is made by using the Hamilton–Jacobian equation. Finally, reconstruction of the fluid interface is then performed to enforce the profile of C to its equilibrium state. The re-initialization of the fluid interface is only required to be implemented occasionally so that the overall computational efficiency is comparable with the original C–H model. In addition to the phase field, the flow field is solved by using the recently-proposed multiphase lattice Boltzmann flux solver. Numerical validations of the proposed method have been carried out by simulating a shearing droplet, Rayleigh–Taylor instability of binary-layered fluids and droplet splashing on a thin film. Good agreements have been achieved with the data published in the literature. The obtained results also show that the present method not only reduces numerical and modeling diffusion substantially but also is able to accurately capture small yet important interfacial structures, such as entrapped air bubbles for the droplet splashing on a thin film.

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1. Introduction

The diffuse interface (DI) method, also known as the phase-field method, has been developed into an effective and powerful numerical tool for simulating a variety of multiphase flows [1–6], such as microfluidics in channels, moving contact lines, breakup and coalescence phenomenon associated with droplets and bubbles and phase change procedures. The wide application of the DI method may be attributed to its simplicity and effectiveness in representing and dealing with complex interfacial structures between different phases. In the DI method, the fluid interface is represented as a thin diffuse layer spreading on several computational grids, where flow properties such as density and viscosity are assumed to change smoothly. Mathematically, the diffuse layer is indicated by the so-called order parameter, for which physical models and governing equations are derived from an energy variation/minimization approach. Based on the physical models proposed, various numerical algorithms for the DI method have been developed and continuously refined for different multiphase problems [6–14].

In earlier numerical studies, the well-known H-Model [7] attracted considerable attentions due to its good performance in the simulation of density-matched fluid flows. In this incompressible model, the volume-averaged velocity is introduced and assumed to satisfy the divergence-free condition in the whole flow field including the interfacial zone, and the Cahn–Hilliard equation is solved for the order parameter. Later, this model was extended for the simulation of more challenging two-phase incompressible flows with large density ratios [8,9]. For instance, Boyer proposed a generalized model for incompressible mixture flows [8], which is well validated by simulating the benchmark of Rayleigh–Taylor instabilities and droplet splashing on a thin film. Ding et al. [9] also derived the Cahn–Hilliard model from the mass conservation law for simulating flows of binary fluids with large density ratios and viscosity ratios. Effective and high-resolution numerical method is introduced for their proposed model, which successfully simulated several challenging two-phase fluid flows, such as bubble rising, head-on collisions of binary droplet and the on-set of droplet entrainment. As compared to the incompressible model, the quasi-incompressible model [10], which allows slightly compressible mixture inside fluid interfaces, has been also proposed by introducing the mass-averaged velocity and enforcing mass conservation law for the flow field. Well-known examples in this cate-

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gories include those of Refs [11,12], which have also been widely applied.

Both incompressible and quasi-incompressible DI models have been widely applied in many complex interfacial flow problems [1,15–17]. They share the same feature that the order parameter is applied to indicate the fluid interface and track its evolutions. One of the most important parameters in the DI simulations is the interface width. It not only affects the numerical accuracy of the phase-filed models [18,19] but also is of direct relevant to mass conservation properties of the method [3,18,20]. In the DI model, the interface width is passively controlled by an artificial parameter proportional to grid spacing and usually involves several computational grids, on which the profile of the interface is resolved numerically. It is quite common that the fluid interface obtained by numerical simulations may be overly diffused or sharpened due to numerical diffusions or convections. However, it is usually preferable to keep the interface profile as close as the equilibrium state in numerical simulations so that the DI method can be accurately implemented [18]. Although it is very challenging to achieve this, many efforts [19] have been recently made in this aspect. Two main strategies are applied. One way is to increase grid resolutions locally or globally for the phase field. Essential examples in this category include the DI method on the adaptive grid [21] and the dual-resolution grid [19]. These methods are able to keep the phase interface sharp but do not guarantee the interface profile in the equilibrium state. The other way is to develop improved DI models by introducing correction terms into the CH equation [18]. Li et al. [18] proposed a modified C–H model with an interfacial correction term and their results showed good accuracy as compared with the original C–H model. It is also noticed that the introduced additional term does not conserve mass exactly in theory.

Up to now, the DI method still can not guarantee its solution being equal or close to the equilibrium profile in the normal direction of the fluid interface, which is a necessity for accurate computation of positions of fluid interfaces and surface tension forces [18]. If one looks into the details of solution obtained by the DI method, the interface can be diffused and flattened too much in some regions, while in some other regions it may be overly compressed and sharpened, leading to numerical instability. As a consequence, the surface tension force may not be accurately computed and the mass of the system cannot be conserved theoretically or numerically. In many multiphase flow problems, the relaxation time of the fluid interface to its equilibrium state is usually smaller than the marching time used in numerical simulation by the C–H model. More importantly, the surface tension force model used by the DI method is not accurate when the profile of the fluid interface is far away from its equilibrium state. It is therefore desirable to re-initialize the fluid interfaces to their equilibrium state in numerical simulations so that the accuracy of the DI method can be improved. In this work, a re-initialization method for the phase field is proposed and examined for simulating incompressible multiphase flows with complex topological changes. In the method, the equilibrium interface profile for the order parameter is used for re-initialization, which will be conducted by introducing a distance function. The flow field is predicted by using the recently proposed multiphase lattice Boltzmann flux solver [22,23] and the interface is obtained by solving the C–H equation directly. Since the re-initialization process is only performed occasionally, the overall computational efficiency of the present method can be retained but the accuracy can be improved. Several numerical examples, including the shearing droplet, Rayleigh–Taylor instability and droplet splashing on a thin film, have been successfully simulated to verify the improvements of the proposed solver.

2. Methodology

2.1. Diffuse interface method with re-initialization of phase interface

2.1.1. Cahn–Hilliard model for interface capturing

For effective simulation of multiphase flows with complex interfacial changes, the DI method usually applies the Cahn–Hilliard model, whose governing equations can be written as:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u}C) = \Gamma \nabla^2 \mu_C, \tag{1}$$

where $C \in [0, 1]$ is the order parameter used to indicate interfacial positions; Γ is the mobility, μ_C represents the chemical potential for fluid-fluid or fluid-wall interfaces, which is a non-linear function of the order parameter C:

$$\mu_C = 2\beta C(C-1)(2C-1) - \kappa \nabla^2 C. \tag{2}$$

Here the constants β and κ are determined by the surface tension coefficient σ and the interface thickness parameter ξ:

$$\kappa = \frac{12\sigma}{\xi}; \quad \beta = \frac{3}{2}\sigma\xi. \tag{3}$$

The local density ρ for each phase of the fluid can be obtained through a linear combination of the heavier and lighter fluids (ρ_H and ρ_L) via the order parameter C:

$$\rho = \rho_L + \Delta\rho \cdot C; \quad \Delta\rho = \rho_H - \rho_L \tag{4}$$

2.1.2. Re-initialization of phase interface for the Cahn–Hilliard model

With the C–H model, the fluid interface can be captured by numerically solving Eq. (1), for which different schemes have been proposed [7,9]. Since the fluid interface in multiphase flows is both temporally and spatially dependent, numerical discretization in space and time is equally important. To maintain spatial stability, upwind schemes are usually applied to discretize the convective term $\nabla \cdot (\boldsymbol{u}C)$ and central schemes are used for the diffusive term $\Gamma \nabla^2 \mu_C$. To accurately track the temporal evolution of interfaces, implicit schemes or explicit schemes, such as the third order TVD (Total Variation Diminishing) Runge–Kutta scheme, for $\partial C/\partial t$ can be adopted. Following our previous work [23], the fifth-order weighted essentially non-oscillatory scheme (WENO) is applied to discretize the convection term $\nabla \cdot (\boldsymbol{u}C)$ and the second-order finite difference scheme is applied to discretize $\Gamma \nabla^2 \mu_C$.

Another important issue is that, when the C–H model is used, it is preferable to maintain the fluid interface as its equilibrium state (a hyperbolic tangent profile) so that mass conservation can be achieved at least in theory and surface tension force can be accurately computed [18]. The mathematical expression for a phase interface, which is derived from the equilibrium state of a one-dimensional interface, can be given by:

$$C(d) = \frac{1}{2}\left[1 + \tanh\left(\frac{2d}{\xi}\right)\right] \tag{5}$$

where d is a signed distance function. It may be noted that, even if high order schemes are applied for Eq. (1), numerical results of fluid interfaces can be expanded or compressed too much due to successive numerical errors in long time computations. This means that the profile of the interface may deviate largely from its equilibrium state indicated in Eq. (5). As a consequence, mass diffusion can be severe and the computation of surface tension may lead to inaccurate results. To remove this drawback, re-initialization of the fluid interface to its equilibrium state can be an effective method, which will be presented below.

The basic idea of the re-initialization method introduced in this work can be described as follows: 1) at the time step $t = t^n$, the order parameter C used to represent the fluid interface is first transformed into a signed distance function d, which is accurate at the

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