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A pseudopotential multiphase lattice Boltzmann model based on high-order difference

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ABSTRACT

The hyperbolic tangent function is usually used as a reliable approximation of the equilibrium density distributions of a system with phase transitions. However, analyzing the accuracies of the numerical derivatives, we find that its numerical derivatives computed by central difference method (CDM) may deviate significantly from its analytical solutions, while those computed by high-order difference method (HDM) can agree very well. Therefore, we introduce HDM to evaluate the interparticle interactions instead of popular CDM, and propose a pseudopotential multiphase lattice Boltzmann model based on high-order difference method. The present model not only retains the advantages of the pseudopotential model, such as easy implementation, high efficiency, full parallelism and so on, but also achieves higher accuracies. To verify the performances of this model, several multiphase flow simulations are conducted, including both stationary and dynamic situations. Firstly, full thermodynamic consistencies for the popular equations of state have been achieved in large temperature range and at large density ratio, without any combining interaction and any additional adjustable parameter of interaction. Secondly, with high-order difference, either the interparticle interaction proposed by Shan-Chen or by Zhang-Chen can equally depict the phase transitions of the fluids with all selected equations of the state. These numerical agreements based on HDM are consistent to the theoretical analysis that the two interactions are mathematically identical. Thirdly, the present model is stable and can be easily applied to various practical simulations and expected to obtain some more interesting results.

1. Introduction

Due to its numerous advantages, including clear physical backgrounds, simple algorithm, high efficiency and full parallelization, lattice Boltzmann method (LBM) has been successfully applied in modeling complex fluid systems involving interfacial dynamics and phase transitions [1–3]. In past two decades, a considerable number of efforts have been devoted to developing multiphase lattice Boltzmann models, and three main kinds of models have been proposed, i.e., color model proposed by Gunstensen et al. [4], pseudopotential methods by Shan and Chen [5,6] and free energy model by Swift et al. [7]. Among them, the pseudopotential model has been popularly applied due to its easy implementation and high efficiency in multiphase flow simulations [8,9]. In the original pseudopotential model, the interparticle force is mimicked by a so called "effective mass", $\psi(\boldsymbol{x})$, which is usually set to $\psi(\boldsymbol{x}) = 1 - \exp(-\rho/\rho_0)$ empirically, where ρ_0 is a reference density [10]. Although this model is able to reproduce phase transition phenomena, it is thermodynamic inconsistent, and cannot be applied to those fluids with the usual equations of state or applied to large density ration systems. By incorporating different equations of state (EOS) into the pseudopotential model, Yuan and Schaefer [11] extended its application range, and achieved higher density ratios. However, as the interparticle force form remains unchanged, it is still thermodynamic inconsistent slightly. Furthermore, the applying range of the temperature of the improved model is still small, and thus the density ratio is limited. Falcucci et al. [12,13] and Chibbaro et al. [14] proposed a two-belt pseudopotential model with multi-range interactions and achieved phase separation at liquid-gas density ratios in excess of 500. The model was compared with free energy model and front tracking approach in order to assess its effectiveness [15]. The pseudopotential model was also implemented on higher-order lattices for multiphase flow simulations at high density ratios [16]. To obtain thermodynamic consistency and achieve larger density ratios, Kupershtokh et al. [17,18] proposed a new pseudopotential model by integrating reduced equations of state, in which the interparticle interaction is evaluated by combining the general effective

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mass method [5] and the method based on potential function [19]. Consequently, the simulation stability is greatly improved, the temperature range is extended, and the thermodynamic consistency is also ensured numerically. Subsequently, Gong et al. [20] and Hu et al. [21] also proposed pseudopotential models like Kupershtokh's successively, and good results were again retrieved as expected. In Hu's model, a method of modifying equations of state was proposed in terms of the Maxwell construction theory, and the simulation stability was greatly enhanced with the modified equations of state. Due to their excellent performances, the three hybrid interaction models have been widely used in multiphase flow simulations [22–25]. For constructing the pseudopotential multiphase lattice Boltzmann model, from the usual views, two problems must be addressed: obtaining a correct interaction with clear physical concept and solid theory foundation, and developing an effective method to incorporate the interaction into the basic lattice Boltzmann equation. In recent years, many works have been done to obtain better pseudopotential interactions, and three main forms with good performances have been developed, including "effective mass" interactions [5], interactions with potential forms [19], and the hybrid interactions by combining the former two forms with weight coefficient method [17,20,21]. Among them, the hybrid interactions have been popularly used owing to their high accuracies. As the methods of incorporating the interaction into the lattice Boltzmann equation, so called forcing technologies, many variants of the method have been developed [5,17,26–29]. These forcing technologies can be all used to incorporate the interactions into the basic lattice Boltzmann equations with different degrees of approximation. It is worth to mentioning that the technology proposed by Kupershtokh et al. is simple, accurate and independent of the relaxation time, thus it becomes popular recently. Reviewing the developments of the pseudopotential multiphase lattice Boltzmann models, no matter the interparticle interaction forms or the forcing technologies have been achieved considerable progresses, it seems as if two of the most important problems have already resolved. Deeply analyzing the existing interactions forms shows that, both the effective mass interaction and the interaction with potential form have numerous successful applications, and they really are identical mathematically. From the literatures [17,20,21], neither of these two interaction forms can well describe the phase transitions of the usually used equations of state, however their linear combination with an adjustable coefficient gives better descriptions. This means that the linear combination of two mathematically identical interactions provides new physical results, which is hardly understood. On the other hand, in order to obtain the optimal results, the adjustable parameter in the hybrid interaction must take different values for different equations of state, thus this interaction form may have artificial arbitrariness [17,20]. Furthermore, seeing the literatures [17,20,21], the adjustable parameter needs to be negative or larger than 1 in order to obtain the optimal solutions in these cases; this parameter may lose its meaning of weight. Therefore, we think that there should be a third issue for constructing the pseudopotential multiphase lattice Boltzmann models, which may have not been attracted much attentions before, e.g. for a specific interaction, how can we numerically evaluate the interaction with the required accuracies? As far as we know, this third problem has seldom been investigated in the published literatures. In this paper, we will investigate the numerical methods for calculating the interactions, and reveal the importance of the numerical accuracies of the interactions. Then, we introduce a new numerical scheme to evaluate the interparticle interactions and construct an effective pseudopotential multiphase lattice Boltzmann model. Finally, several testing cases are conducted to demonstrate the performances of the proposed model.

The rest of this paper is organized as follows. Firstly, a brief introduction is given to the pseudopotential multiphase lattice Boltzmann model. Secondly, the central difference and the high-order difference methods are investigated. Thirdly, a pseudopotential multiphase lattice Boltzmann model based on high-order difference is constructed. Fourthly, the performances of the present model are investigated by using the multiphase flows with several usual equations of state, such as van der Waals (VDW) EOS, Peng-Robinson (PR) EOS, Carnahan-Starling (CS) EOS and Redlich-Kwong (RK) EOS. Finally, a brief conclusion is drawn.

2. Pseudopotential models

Originating from the cellular automaton concept and kinetic theory, the intrinsic mesoscopic properties make lattice Boltzmann method (LBM) outstanding in modeling complex fluid systems involving interfacial dynamics [30–32] and phase transitions [8,9]. In basic approach of LBM, a particle distribution function is used to depict the behavior of the multiphase flows, which obeys the following lattice Boltzmann equation

$$f_i(\boldsymbol{x}+\boldsymbol{e}_i\delta t, t+\delta t) - f_i(\boldsymbol{x},t) = -\frac{1}{\tau}[f_i(\boldsymbol{x},t) - f_i^{(eq)}(\boldsymbol{x},t)] + F_i, \tag{1}$$

where $f_i(\boldsymbol{x},t)$ is the particle distribution function at lattice site $\boldsymbol{x}$ and time t, δt is the time step, which is usually taken to be unit, $\boldsymbol{e}_i$ with $i = 0,\ldots,N$ is the discrete speed, τ is the relaxation time, and $f_i^{(eq)}$ is the equilibrium density distribution function, it can be represented as (D2Q9 model)

$$f_i^{(eq)}(\boldsymbol{x},t) = \rho\omega_i\left[1 + 3(\boldsymbol{e}_i\cdot\boldsymbol{u}) + \frac{9}{2}(\boldsymbol{e}_i\cdot\boldsymbol{u})^2 - \frac{3}{2}u^2\right], \tag{2}$$

where ω_i is the weight coefficient, and $\boldsymbol{u}$ is the fluid velocity. The fluid density ρ and the velocity $\boldsymbol{u}$ (in the absence of body fore) can be calculated by

$$\rho = \sum_{i=0}^{N} f_i, \quad \rho\boldsymbol{u} = \sum_{i=0}^{N}\boldsymbol{e}_i f_i, \tag{3}$$

In pseudopotential models, the body force term F_i is the discrete version of the interparticle interaction. A widely used interparticle interaction is proposed by Shan-Chen [5], which is so called "the effective mass based interaction" and can be written as

$$\boldsymbol{F}^{SC}(\boldsymbol{x},t) = -G\psi(\rho(\boldsymbol{x},t))\nabla\psi(\rho(\boldsymbol{x},t)), \tag{4}$$

where $\psi(\rho(\boldsymbol{x},t))$ is the "effective mass", and G is the interaction strength. In the early applications, "effective mass" is usually taken the simple form $\psi(\rho) = 1 - \exp(-\rho/\rho_0)$, and thus the model can't be directly applied to the fluids with usual equations of state. With Eq. (4), the corresponding equation of state is

$$p = c_s^2\rho + \frac{G}{2}\psi^2(\rho), \tag{5}$$

In order to extend the pseudopotential model for including the fluids with the usual equations of state, Yuan and Schaefer [11] incorporated the equations of state into LBM by introducing the following relation between the "effective mass" and the equation of state

$$\psi(\rho) = \sqrt{\frac{2(p-\rho c_s^2)}{G}}, \tag{6}$$

where c_s is the "sound speed", and takes the value $c_s^2 = \frac{1}{3}$ in D2Q9 model.

Another popular interparticle interaction is presented by Zhang-Chen [19], which is so called "the interaction based on potential function" and can be written as