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Improved stability strategies for pseudo-potential models of lattice Boltzmann simulation of multiphase flow

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ABSTRACT

Since the pseudo-potential lattice-Boltzmann (LB) model was proposed, it has been suffering from low density ratio, small Reynolds number and flow instabilities, which hamper its application in many science and engineering problems. In this work, we analyze the reasons of flow instabilities in the pseudo-potential LB models, and propose some methods to improve the simulation stability. It is shown that the inter-particle interaction force term and the equations of state (EOS) can result in numerical instability in the particle distribution functions and density. Some straightforward and universal techniques are proposed here in order to achieve larger density ratio, higher Reynolds number and lower temperature as well as suppressing spurious velocity in multiphase flow in the pseudo-potential LB models without additional influences on the equilibrium properties in most cases. These methods contribute to extending the pseudo-potential LB models to realistic multiphase flow further. Finally, we demonstrate the method application for droplet splashing with $Re = 15000$, $We = 120$ and density ratio = 4792 at $0.45T_c$ successfully.

1. Introduction

The lattice Boltzmann (LB) method has been developed as an efficient numerical method for a large number of applications in science and engineering. Different from the conventional macroscopic Navier-Stokes (NS) methods, LB method is a mesoscopic approach based on the kinetic theory derived from the Boltzmann equation [1,2]. Particularly, this characteristic provides a platform to simulate complex fluid flows where macroscopic behavior of the flow is originated from the microscopic physics [3]. LB method is also useful for modeling multiphase flows. The interface dynamics description is usually associated with some free energy functions, pressure tensor and chemical potentials [4]. The phase segregation in multiphase flows can proceed automatically without tracking or capturing the interface between different phases through other equations, which are often used in conventional methods with many simplified assumptions and empirical correlations [5].

In the last 25 years, lots of efforts have been made to extend the LB method to practical multiphase flows. Most multiphase LB models can be classified as the following categories: the color-gradient LB method [6], the pseudo-potential LB method [7,8], the free-energy LB method [9], and the kinetic-theory-based LB method [10–12]. In these models, the pseudo-potential LB method proposed by Shan and Chen (SC) [7,8] has been applied extensively due to its simple inter-particle interaction model and computational efficiency. In addition, the pseudo-potential LB method is regarded as more robust than others, and has been widely employed to simulate lots of multiphase cases with larger density ratios and higher Reynolds numbers [1]. In the pseudo-potential LB method, the inter-particle interaction is imposed through an artificial potential linked with density and temperature, which causes the phase separation by a short-range attraction within the varying density interface. Note that this potential goes to zero in the limit $\rho \rightarrow 0$ and reaches a maximum value at a large density, leading to a stable phase separation without mass collapse [13].

Another advantage of the pseudo-potential LB method is that any equation of state can be incorporated readily through the strategy introduced by He and Doolen [12] and Yuan & Schaefer [14], which is a very crucial and promising characteristic to describe the practical fluid. In 2003, Zhang and Chen [15] also proposed a new and straightforward scheme of force term that can incorporate an arbitrary equation of state, which is regarded as a similar method to the pseudo-potential model. In 2006, Yuan and Schaefer [14] found that the largest density ratio of pseudo-potential

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simulation can be improved by choosing an appropriate equation of state. Subsequently, some works pointed out some drawbacks of this method, including large spurious currents, thermodynamic inconsistency and numerical instability at low temperatures [16,17]. Sbragaglia and Falcucci et al. found the multiphase SC model will give better performance on spurious velocity and stability if the multi-range lattice is used [18,19]. Moreover, exact difference method (EDM) was proposed by Kupershtokh and Medvedev [20] to incorporate the force term into the particle distribution function. Unlike SC force scheme (velocity shifting method), it was found [17,21] that the coexistence of liquid-vapor densities given by EDM and Guo et al.'s [22] scheme hardly vary with relaxation time τ. These two methods are more stable than others. Nevertheless, density ratios derived by EDM still change with τ to some extent at large density ratios [21]. Kupershtokh et al. [16] had proposed a mixed interaction force to adjust the coexistence density of liquid and vapor phases to match the Maxwell construction. With this interaction force, the lower reduced temperature can be reached, and stationary droplet simulation is more stable [16,17]. Recently, Hu et al. [23] had analyzed this interaction force scheme, which shows that an additional force term emerging in this interaction force can adjust the parameters ε in the mechanical stability condition [24]. A more precise method to adjust the interaction force has been proposed by Li et al. [25,26], and Huang and Wu [27]. This method produces a steerable force in LBGK or MRT schemes to adjust ε and achieve large density ratios and thermodynamic consistency stably. Considering their analyses, it shows that different forcing schemes will lead to different values of ε, which mainly affects the vapor phase density. Furthermore, Huang and Wu [27] have analyzed the third order Chapman-Enskog expansion and found that the third order terms of force will affect the isotropic property of LB method and the equilibrium density. They proposed an additional term at third order to adjust the ε in mechanical stability condition. Besides, the dynamic multiphase flow, droplet splashing, at large density ratio has been investigated in Li et al.'s work to illustrate the performance of this kind of method [25,28].

In addition, Wagner and Pooley [29] found that multiplying a pre-factor p_0 in the pressure tensor, which gives $p_{EOS}^{new} = p_0 p_{EOS}$, can enhance the achievable largest density ratio and stability with widening the interface thickness. Similar strategies have also been proposed by Kupershtokh et al. [16] and Hu et al. [30]. Moreover, Huang et al. [21] found that the parameters a and b in the equations of state affect the interface thickness and stability. Li et al. [25] also found that the interface thickness is approximately proportional to $1/\sqrt{a}$, and a smaller parameter a can stably achieve larger density ratio and lower reduced temperature. Later, Liu and Cheng [31] pointed out that these two tuning methods of Li et al. and Hu et al. are equivalent in math. Although this kind of method can yield to better results compared to previous methods, in fact, it will reduce the sound speed in both phases [29] since a different parameter a means a different fluid. In addition, it is stated that using the pre-factor or the parameter a will not change the liquid-coexistence densities given by the Maxwell construction equation [25,30]. However, the coexistence densities will be changed in the pseudo-potential LB methods due to the term ψ'/ψ determined by mechanical stability condition [1,24]. Recently, Khajepor et al. [32,33] proposed another multi-pseudo-potential interaction based on the previous analyses [13,24] to achieve intrinsic thermodynamic consistency. However, this method can only incorporate the cubic equations of state through equation decomposing and parameter matching. Moreover, the numerical stability of this method should be investigated further since the parameters in the equations of state in their paper are obviously smaller than that in other literatures.

To the best of our knowledge, in current pseudo-potential LB method, the main methods to obtain large density ratio and low temperature stably are to either use a small parameter a or adjust ε. However, some other reasons for numerical instability of the pseudo-potential LB method haven't been illustrated in previous literatures. Consequently, there appears to be a need for relevant methods that can prevent some numerical instability at low reduced temperature in some cases, especially in the dynamic multiphase processes.

It should be noted that there are some instabilities existing in LBMs, including LBGK and MRT. The discretization gives rise to some high order deviations from correct NS equations. Brownlee et al. [34,35] studied LBM by free flight and proposed the dissipative method and non-dissipative method for stabilization. Furthermore, the later paper [35] achieved the regularization of LBMs, where the entropic LB-BGK method as well as entropic limiters was conceived based on the maximization of entropy in entropic LBM. A stabilization solution is based on the use of multiple relaxation times tuned to equilibrate the "ghost modes" when non equilibrium entropy passes a certain threshold [35]. In addition, given that the larger density variation between phase interface will cause a larger error in the cubic velocity term, elimination or reducing these aspects of instability in LBMs itself can contribute to improving simulation further. An approach to modify the collision operator to eliminate the cubic velocity related terms has been suggested by Dellar [36]. These works are outstanding due to realizing the intrinsic instability mechanisms of LBM itself. As for this paper, we focus on studying several numerical instabilities caused by pseudo-potential force, spurious velocity and equations of state, which are based on the pseudo-potential multiphase MRT-LBM.

In this paper, we present four numerical instabilities caused by the preceding pseudo-potential LB methods, and propose four optimization techniques in Sections 3.1-3.4, aiming to extend the existing pseudo-potential LB methods to stably simulate multiphase flow at larger density ratio and higher Reynolds number in the both of static and dynamic processes. First, the negative probability density distribution function f_α, which is caused by large interaction force and low vapor density at lower temperature, will result in negative density and make simulation unstable. Therefore, the average interpolation method and tuning relaxation times around adjacent vapor points are proposed in Section 3.1 to prevent density from converting into negative number. Second, numerical instabilities due to the singularity in EOSs and the sign reversal in the square root have been analyzed. Both of the instabilities occur since the liquid density goes larger, which gives rise to the singularity in EOSs and the sign reversal in the square root. The corresponding limiter functions and a new pseudo-potential interaction are proposed in Sections 3.2 and 3.3 respectively to prevent from these situations. Finally, based on the cognition of compressibility in pseudo-potential multiphase flow calculation as well as Cramer's research [37], we find the larger bulk viscosity that is tens or hundreds of times of dynamic viscosity will suppress spurious velocity well.

In Section 4, due to various simulations and method parameters in different papers and considering the rigorous contrast in this paper, we compare the cases' results with Li et al.'s result [25] under the completely same MRT framework as well as simulation argument setting. In the stationary droplet cases with the same parameters of CS EOS ($a = 0.5$), we employ these limiter functions to obtain a stable result with density ratio = 4039.6 and spurious velocity = 0.02229 at $0.4T_c$, and the lowest achievable temperature of $0.35T_c$. Using these limiter functions and strategies, a case of droplet splashing on a thin film is implemented with $Re = 15000$, $We = 120$ and density ratio = 4792 at 0.45 T_c ($a = 0.25$ in CS-EOS).