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Force method in a pseudo-potential lattice Boltzmann model

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ABSTRACT

Single component pseudo-potential lattice Boltzmann models have been widely studied due to their simplicity and stability in multiphase simulations. While numerous models have been proposed, comparative analysis and advantages and disadvantages of different force schemes are often lacking. A pseudo-potential model to simulate large density ratios proposed by Kupershtokh et al. [1] is analyzed in detail in this work. Several common used force schemes are utilized and results compared. Based on the numerical results, the relatively most accurate force scheme proposed by Guo et al. [2] is selected and applied to improve the accuracy of Kupershtokh et al.'s model. Results obtained using the modified Kupershtokh et al.'s model [1] for different value of τ are compared with those obtained using Li et al.'s model [3]. Effect of relaxation time τ on the accuracy of the results is reported. Moreover, it is noted that the error in the density ratio predicted by the model is directly correlated with the magnitude of the spurious velocities on (curved) interfaces. Simulation results show that, the accuracy of Kupershtokh et al.'s model can be improved with Guo et al.'s force scheme [2]. However, the errors and τ's effects are still noticeable when density ratios are large. To improve the accuracy of the pseudo-potential model and to reduce the effects of τ, two possible methods were discussed in the present work. Both, a rescaling of the equation of state and multi-relaxation time, are applied and are shown to improve the prediction of the density ratios.

1. Introduction

Lattice Boltzmann Equation (LBE) method [4], also known as Lattice Boltzmann Method (LBM), has attracted a significant attention due to its potential to solve problems at the mesoscopic scale. From its origin in lattice gas automation method, it has been developed into a numerical method to simulate fluid flows and other nonlinear problems. One promising application of LBE method is multiphase flow simulation. Due to its kinetic nature, a well-developed theoretical basis, and the ability of self-capturing the interface, LBE method has many advantages when simulating multiphase problems. Several LBE multiphase models have thus been developed. These models can be summarized into four categories: color models [5], pseudo-potential methods [6], free energy models [7,8] and kinetic models [9–11]. Gunstensen et al. [5] proposed the first color LBE model by labeling components and particles by colors in the LBE model. Several extensions were developed based on Gunstensen et al.'s model and have been successfully applied to complex interfacial flows [12,13]. However, these models suffer from several limitations, such as the anisotropy of surface tension and spurious currents [14]. Due to their simplicity

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and stability at a high density ratio, pseudo-potential models first proposed by Shan and Chen [6] are widely used, but they also have drawbacks such as spurious currents [14]. The first free energy type LBE model was proposed by Swift et al. [7]. However, it is restricted to low density ratios, and the early free energy LBE models often suffered from Galilean invariance [8]. Kinetic LBE models, as the name suggests, are based on kinetic methods. A typical kinetic LBE model is by He, Shan and Doolen [9], which is based on a modified Boltzmann equation. With a special discrete method, Lee and Lin [15] successfully extended the He–Shan–Doolen model for large density ratios. However, in addition to the sensitivity of the discrete approach, it has been shown that the mass conservation of these models is weak for large density ratios [16].

These LBE multiphase models have been widely used in simulations. However, most of the above models are limited to multiphase flows with small density ratios. To solve this problem, several additional LBE multiphase models for large density ratios were proposed [15,17–19]. Among these models, single component pseudo-potential models show promise to solve large density ratio flows since they are stable for large density ratios without fancy numerical methods. However, Yuan and Schaefer [19] found that the stabilities of these models vary with equations of state introduced in the pseudo-potential models. To address this issue, they developed the large density ratio pseudo-potential model by choosing an appropriate Equation Of State (EOS). However, it has been shown that the pseudo-potential models are consistent with thermodynamic theories only when the EOS takes a special exponent form [20]. The stability of the pseudo-potential is related to the pressure tensor which varies with the inter-particle interaction force models and the LBE force schemes adopted in the model [3,21].

To address these problems, several approaches have been proposed to reduce the thermodynamic error and to increase the stability of the pseudo-potential method. The most common approach is the multi-range pseudo-potential model, developed by Sbragaglia et al. [22], which combines the nearest-neighbor interactions and the next-nearest-neighbor interactions. Though much improved, the introduction of the next-nearest-neighbor interactions leads to difficulties in programming especially for the boundary conditions. Li et al. [3] recently put forward a method to reduce the thermodynamic error by introducing an additional term in the force scheme. It successfully improved the stability without adding much numerical cost. However, the special treatment of the inter-particle interaction force is developed specifically for the force scheme proposed by Guo et al. [2].

In a parallel effort to reduce the thermodynamic error, Kupershtokh et al. [1,23,24] pointed out that the scale of the EOS is the main reason for the stability of the pseudo-potential model. They also developed an interparticle-force model by combining two nearest-neighbor interactions models and adjusting the scale of the reduced EOS. Later, Hu et al. [25] extended this method to general EOS.

The development of Kupershtokh et al.'s model is however somewhat ad hoc. Thus the choice of the parameters introduced in the model lacks theoretical foundation. Moreover, some studies have shown that the Exact Difference Method (EDM) force scheme [26] applied in Kupershtokh et al.'s work leads to error terms in the corresponding macroscopic equation, and thus the numerical problem being solved is different from the original macroscopic problem [3,21]. Huang et al. did attempt to integrate different LBE approaches, and provided some theoretical foundation for the Kupershtokh et al. model. However in Huang et al.'s work [21], the density distributions of the EDM force scheme vary with the relaxation time, which is not the case in Kupershtokh et al.'s work.

We here report a numerical error analysis of the Kupershtokh et al.'s model for EDM force scheme. We then extend and improve the model by applying the force scheme proposed by Guo et al. [2], instead of using the EDM forcing scheme, thus eliminating the error in the corresponding macroscopic equation. Finally, numerical results obtained using the improved method developed here and those obtained using Li et al.'s method [3], which adopted a different approach to approximately satisfy the thermodynamic constraints, are compared.

Rest of the paper is organized as follows. The pseudo-potential LB model is briefly introduced in Section 2. In Section 3, interparticle interaction force calculation methods and the forcing schemes are theoretically analyzed. Numerical investigations and comparisons are presented in Section 4. Finally, conclusion are drawn in Section 5.

2. Pseudo-potential model

In the LBE method, the motion of the fluid is described by evolution of the density distribution function. The evolution equation can be written in the form of the BGK operator [27] as

$$f_\alpha(\boldsymbol{x}+\boldsymbol{e}_\alpha\Delta t, t+\Delta t) - f_\alpha(\boldsymbol{x},t) = -(f_\alpha(\boldsymbol{x},t) - f_\alpha^{\mathrm{eq}}(\boldsymbol{x},t))/\tau + \boldsymbol{F}_\alpha, \tag{1}$$

where τ is the reduced relaxation time, $f_\alpha(\boldsymbol{x},t)$ is the density distribution function of particles at node $\boldsymbol{x}$ and time t, and $\boldsymbol{e}_\alpha$ is the velocity where $\alpha = 0, 1, 2, \cdots, N$. The right side of the equation is a collision operator, $\boldsymbol{F}_\alpha$ is the force term, $f_\alpha^{\mathrm{eq}}(\boldsymbol{x},t)$ is the equilibrium distribution function which can be represented in the following form for the two-dimensional nine-velocity (D2Q9) lattice:

$$f_\alpha^{\mathrm{eq}}(\boldsymbol{x},t) = w_\alpha\rho(\boldsymbol{x},t)[1 + (e_\alpha\cdot\boldsymbol{u}^{\mathrm{eq}})/c_s^2 + (e_\alpha\cdot\boldsymbol{u}^{\mathrm{eq}})^2/(2c_s^4) - (\boldsymbol{u}^{\mathrm{eq}})^2/(2c_s^2)], \tag{2}$$