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Fourth-order analysis of force terms in multiphase pseudopotential lattice Boltzmann model

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ABSTRACT

Pseudopotential lattice Boltzmann model (LBM) for multiphase flow has been widely studied due to its conceptual simplicity and computational efficiency. Additional interaction force terms are proposed to adjust mechanical stability condition for thermodynamic consistency in pseudopotential force. However, the additional force terms introduce a new non-physical effect in fourth-order macroscopic equation, which causes a variation of density ratio with different relaxation times in the multiphase-relaxation-time (MRT) LBM. In this work, a fourth-order analysis of force term in MRT LBM is presented to identify the fourth-order terms in recovered Navier–Stokes equations. Through the higher-order analysis, two methods are proposed to eliminate this effect. A series of numerical tests of planar interface and droplet are conducted to validate the analyses.

1. Introduction

The lattice Boltzmann model (LBM) has been developed into an effective approach for computational fluid dynamics (CFD) in recent decades [1,2]. Especially for multiphase flow, LBM has been applied to simulate extensive science and engineering problems, such as phase-change heat transfer, droplet microfluidic, interface deformation and fuel cells [3–7]. In multiphase LBM, there are four major categories of multiphase models [7]: the color-gradient model [8], the pseudopotential model [9,10], the free-energy model [11], and the phase-field model [12,13]. Recently, the pseudopotential LBM and phase-field LBM have been studied extensively in recent researches at large density ratios and relatively high Reynolds numbers [7,14–17]. In addition, the stabilized entropic LBM is developed with enhanced numerical stability [18], and it is used to control the dynamics at liquid–vapor interface in multiphase LBM [19,20].

The pseudopotential LBM introduces an interaction force to mimic the fluid interaction. The inter-particle force not only gives a non-monotonic equation of state (EOS) for phase transition, but also yields a non-zero surface tension [7,21]. Consequently, the phase segregation between different phases can be achieved automatically without interface capturing and tracking methods. If the original SC EOS is used, the pseudopotential LBM can give a Maxwell-construction density ratio at equilibrium state [22], i.e. thermodynamic consistency. However, this SC EOS is not proper to describe a variety of practical fluids in science and engineering applications. Another approach of incorporating arbitrary EOS is the strategy introduced by He and Doolen [23], as well as Yuan and Schaefer [24]. Although this approach is convenient and promising to incorporate general EOSs, subsequent researches found a drawback of thermodynamic inconsistency emerges in this method [25,26]. Some new force schemes were proposed to achieve lower temperatures and approach thermodynamic consistency, such as

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the exact difference method (EDM) [27]. Kupershtokh et al. also proposed a mixed interaction force to adjust the coexistence density of liquid phase and vapor phase to match Maxwell construction [26]. Colosqui et al. used a piecewise linear equation of state to set different sound speeds for gas and liquid phases readily, and the more stable simulations are reached with high density and compressibility ratios [28].

Sbragaglia and Falcucci et al. found the multiphase SC LBM can be implemented better on spurious velocity and stability if multi-range lattice is used [29,30]. Shan and Sbragaglia et al. studied the discrete pressure tensor and gave the mechanical stability condition in pseudopotential model [22,31]. Subsequently, Li et al. [32] pointed out the ϵ in mechanical stability condition has an essential influence on thermodynamic consistency, and presented an improved forcing scheme to adjust density ratio. Later researches [33,34] had analyzed different force schemes up to third-order, such SC, EDM and Guo et al. [35], and found different force schemes have different ϵ in fact. Hu et al. [36] revealed the mixed interaction force of Kupershtokh also adjusts ϵ to achieve thermodynamic consistency in fact. At present, Li et al. and Huang et al. [14,37] proposed a similar method of modifying MRT force scheme to adjust ϵ quantitatively, avoiding other obscure schemes. However, in spite of efficiency in achieving thermodynamic consistency, this kind of adjusting method has a non-physical effect that equilibrium density ratio will vary with different relaxation times at low temperatures in MRT LBM, which has not been stated in previous relevant researches [14,32–34,36,37]. In previous single-relaxation-time LBM [25,38], it is found that coexistence densities given by SC force scheme and EDM scheme vary with the relaxation time τ, but Guo et al.'s force scheme [35] does not change that. In MRT LBM, the Guo et al.'s MRT force scheme [39] recovers the second-order Navier–Stokes equations correctly, and adjustment of relaxation times does not change density ratio. In this work, a force-scheme analysis up to fourth order is conducted to identify the effect introduced by these additional adjustment terms, and gives two methods to eliminate this non-physical effect.

Section 2 gives a brief introduction of MRT pseudopotential LBM. Section 3 presents the Chapman–Enskog analyses from second order to fourth order including the additional force terms. According to the theoretical analysis, Section 4 uses three cases of planar interface, stationary droplet and moving droplet to validate the theoretical results. In addition, two methods are proposed to alleviate this non-physical effect, and the comparison of coexistence densities of different relaxation times are also in good agreement with anticipative results of theoretical analysis. Finally, a conclusion about this work is showed in Section 5.

2. MRT pseudopotential LBM

In this section, a general framework of two-dimensional D2Q9 pseudopotential LBM with the MRT collision operator is presented briefly. This framework has been developed for a dozen years, and MRT LBM gives a better performance than BGK method generally [7,14,40,41]. The MRT LBM can be decomposed into two steps: collision step and streaming step. In velocity space, the density distribution function is written as vector form: $\mathbf{f}(\mathbf{x},t) = [f_0(\mathbf{x},t), f_1(\mathbf{x},t), \ldots, f_8(\mathbf{x},t)]^{\mathrm{T}}$. The collision step is conducted in moment space as follow

$$\mathbf{m}^*(\mathbf{x},t) = \mathbf{m}(\mathbf{x},t) - \mathbf{S}\left[\mathbf{m}(\mathbf{x},t) - \mathbf{m}^{\mathrm{eq}}(\mathbf{x},t)\right] + \delta_t(\mathbf{I} - 0.5\mathbf{S})\mathbf{F}_{\mathrm{m}}(\mathbf{x},t), \tag{1}$$

where $\mathbf{m}(\mathbf{x},t) = \mathbf{M}\mathbf{f}(\mathbf{x},t)$ is the moment converted by transformation matrix $\mathbf{M}$ and density distribution function, $\mathbf{S}$ is a diagonal relaxation matrix, and $s_\rho = s_j = 1$, $\mathbf{m}^{\mathrm{eq}}(\mathbf{x},t)$ is the equilibrium moment, $\mathbf{I}$ is the unit matrix, δ_t is the time step set as 1, and $\mathbf{F}_{\mathrm{m}}(\mathbf{x},t)$ is the discrete force term in moment space. The relevant forms are written as follows:

$$\mathbf{S} = \mathrm{diag}\left(s_\rho, s_e, s_\zeta, s_j, s_q, s_j, s_q, s_\nu, s_\nu\right), \tag{2}$$

$$\mathbf{m}^{\mathrm{eq}} = \rho(1, -2+3|\mathbf{u}|^2, 1-3|\mathbf{u}|^2, u_x, -u_x, u_y, -u_y, u_x^2-u_y^2, u_xu_y)^{\mathrm{T}}, \tag{3}$$

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}, \tag{4}$$

$$\mathbf{F}_{\mathrm{m}} = \left[0, 6(\mathbf{F}\cdot\mathbf{u}), -6(\mathbf{F}\cdot\mathbf{u}), F_x, -F_x, F_y, -F_y, 2(u_xF_x - u_yF_y), (u_xF_y + u_yF_x)\right], \tag{5}$$

where $\mathbf{F} = \left(F_x, F_y\right)$ is the body force, including interaction force, and $\mathbf{u} = \left(u_x, u_y\right)$ is the velocity vector. It should be noted that Eq. (5) is the MRT force scheme proposed by McCracken et al. [42] and Guo et al. [39].

The streaming process is

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha\delta_t, t + \delta_t) = f_\alpha^*(\mathbf{x},t), \tag{6}$$