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Finite-difference lattice Boltzmann model for liquid–vapor systems

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Abstract

A two-dimensional finite-difference lattice Boltzmann model for liquid–vapor systems is introduced and analyzed. Two different numerical schemes are used and compared in recovering equilibrium density and velocity profiles for a planar interface. We show that flux limiter techniques can be conveniently adopted to minimize spurious numerical effects and improve the numerical accuracy of the model.

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1. Introduction

Lattice Boltzmann (LB) models are based on the physics at the mesoscopic scale (collisions are accounted for by local interactions) [1]. Due to their ability to incorporate particle interactions at the mesoscopic level, LB models fit for simulating the behavior of multi-phase/component fluid systems [1].

In this paper, we will consider a finite-difference lattice Boltzmann (FDLB) model [2] for liquid–vapor systems [9]. In the finite-difference formulation of LB models the Boltzmann equation is discretized in the phase space and time and solved by using one of the several available finite-difference numerical schemes. This gives more freedom to choose the discrete velocity set in the phase space, since space step δx and time step δt are no more related via the lattice speed as in the standard ("collide and stream") formulations of LB models [1]. This finite-difference based approach revealed very useful in developing a thermal FDLB model for a simple fluid [11] where the possibility of having different sets of velocities allows to release the constraint of constant temperature. This is a possible route if one aims to extending the proposed model for non-ideal fluids to the situation where the full set of thermo-hydrodynamic equations [5] has to be taken into account so that the temperature is free to evolve fulfilling the heat equation. The main

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problem in following this strategy comes from the fact that all the LB models are known to introduce spurious terms in the continuum conservation equations, which depend on δx and δt [2].

As a preliminary study before addressing more complex problems, we investigate the effects of different finite difference schemes and restrict our attention in the present paper to the case of isothermal liquid–vapor systems to reduce the number of independent degrees of freedom that can affect numerical results. We mainly consider how the chosen numerical scheme influences the numerical accuracy in recovering the coexistence curve and a planar interface between the liquid and vapor phases. This problem still lacks necessary clarification and should be always considered in order to recover the correct physical interpretation of simulation results.

2. The model

The starting point of any FDLB model is the Boltzmann equation. If we use the forward finite difference scheme for the time derivative, linearize the collision term using the Bhatnagar–Gross–Krook approximation [1] after introducing the relaxation time τ, and discretize phase space, then the distribution functions $f_i(\mathbf{r}, t)$ are defined only in the nodes $\mathbf{r}$ of a discrete lattice $\mathcal{L}$ while the velocities are reduced to a discrete set $\{\mathbf{e}_i\}$ $(i = 0, 1, \ldots, \mathcal{N})$. We get the following set of LB evolution equations in nondimensional form:

$$f_i(\mathbf{r}, t + \delta t) = f_i(\mathbf{r}, t) - \frac{\delta t}{\tau}[f_i(\mathbf{r}, t) - f_i^{\mathrm{eq}}(\mathbf{r}, t)] - \delta t\, \mathbf{e}_i \cdot \nabla f_i(\mathbf{r}, t) + \frac{\delta t}{\chi c^2}\mathbf{F}(\mathbf{r}, t) \cdot [\mathbf{e}_i - \mathbf{u}(\mathbf{r}, t)] f_i \mathrm{eq}(\mathbf{r}, t);$$
$$i = 0, 1, \ldots, \mathcal{N} \tag{1}$$

where $\mathbf{F}(\mathbf{r}, t)$ is the acting force. Macroscopic variables, e.g., the density n and the local velocity $\mathbf{u}$ are computed from the distribution functions as $n = \sum_{i=0}^{i=\mathcal{N}} f_i$ and $\mathbf{u} = \frac{1}{n}\sum_{i=0}^{i=\mathcal{N}} \mathbf{e}_i f_i$. In the two-dimensional (2D) case here considered, $\mathcal{N} = 8$ and the velocities $\mathbf{e}_i$ are given by $\mathbf{e}_i/c = (\pm 1, 0)$, $(0, \pm 1)$, $(\pm 1, \pm 1)$, $(0, 0)$, where $c = \sqrt{\theta/\chi}$ is the thermal speed with θ the dimensionless temperature and $\chi = 1/3$ is a characteristic constant of the 2D lattice. The equilibrium distribution functions are expressed as a series expansion in the velocity $\mathbf{u}$ [6].

The force term in Eq. (1) is given by $\mathbf{F} = (1/n)\nabla(p^i - p^w) + \kappa\nabla(\nabla^2 n)$ [3], where $p^i = \theta n$ and $p^w = 3\theta n/(3 - n) - 9n^2/8$ are the non-dimensionalized ideal and van der Waals equations of state, respectively. With the equation of state in this form, the critical point is located at $\theta = 1$ and $n = 1$. The parameter κ controls the surface tension. The mass and momentum equations for a van der Waals fluid are recovered from Eq. (1) after using the standard Chapman–Enskog procedure up to second-order with respect to Knudsen number [7]. In this way, it is possible to take correctly into account hydrodynamic effects as in model H of a liquid–vapor fluid [4]. The particular numerical scheme used to solve Eq. (1) may introduce spurious terms that appear in the conservation equations.

3. Flux limiters techniques for finite-difference LB models

When using FDLB models the value of δx is no more related to the time step δt via the relation $\delta x = c\delta t$ as in the "collide and stream" LB models. To compute the term $\mathbf{e}_i \cdot \nabla f_i$ in hyperbolic equation systems like (1) we may use one of the characteristics based finite-difference schemes, such as first-order upwind (in the following denoted as UP), second-order space centered, and Lax–Wendroff [8]. Although, only first-order in space, the UP scheme is preferred since this one is more stable than the space centered scheme when dealing with large density gradients, as is the case for two component systems. However, the UP scheme exhibits numerical diffusion and viscosity [8], which may affect the simulation results. Even if the second-order Lax–Wendroff scheme is more accurate, the wiggle phenomenon introduces unphysical oscillations of the fluid density [10]. Flux limiter schemes introduced below provide a possibility to overcome these well known problems of FDLB models.

If we refer to a node j on the lattice and to its neighbors $j - 1$ and $j + 1$ on the characteristics line along to the vector $\{\mathbf{e}_i\}$, the Lax–Wendroff scheme [10] for updating the value of the distribution function in node j at time step $n + 1$ in accordance to the partial differential equation $\partial_t f_i + \mathbf{e}_i \cdot \nabla f_i = 0$ is

$$f_{i,j}^{n+1} = f_{i,j}^n - \frac{c\delta t}{\delta x}[f_{i,j+1}^n - f_{i,j-1}^n] + \frac{1}{2}\left(\frac{c\delta t}{\delta x}\right)^2 [f_{i,j+1}^n - 2f_{i,j}^n + f_{i,j-1}^n]. \tag{2}$$

According to the general approach for constructing high order Total Variation Diminishing (TVD) schemes using *flux limiters* [10], we rewrite the updating rule (2) in a conservative form using two fluxes

$$f_{i,j}^{n+1} = f_{i,j}^{n} - \mathrm{CFL}[F_{i,j+1/2}^{n} - F_{i,j-1/2}^{n}] \tag{3}$$

where

$$F_{i,j+1/2}^{n} = f_{i,j}^{n} + \tfrac{1}{2}(1 - \mathrm{CFL})[f_{i,j+1}^{n} - f_{i,j}^{n}]\psi(\theta_{i,j}^{n}) \tag{4}$$

and

$$F_{i,j-1/2}^{n} = F_{i,(j-1)+1/2}^{n} = f_{i,j-1}^{n} + \tfrac{1}{2}(1 - \mathrm{CFL})[f_{i,j}^{n} - f_{i,j-1}^{n}]\psi(\theta_{i,j-1}^{n}). \tag{5}$$

$\mathrm{CFL} = c\delta t/\delta x$ is the Courant–Friedrichs–Levy number which in FDLB models can be done smaller than 1 to increase stability.

The flux limiter $\psi(\theta_{i,j}^{n})$ introduced in (4) is expressed as a function of the *smoothness* $\theta_{i,j}^{n} = \frac{f_{i,j}^{n} - f_{i,j-1}^{n}}{f_{i,j+1}^{n} - f_{i,j}^{n}}$. In particular, the Lax–Wendroff scheme is recovered for the flux limiter $\psi(\theta_{i,j}^{n}) = 1$. The first-order UP scheme is recovered as another particular case, when $\psi(\theta_{i,j}^{n}) = 0$. A wide choice of other flux limiters is at our disposal in the literature [10]. Here, we will consider the Monitorized Central Difference (MCD) scheme

$$\psi(\theta_{i,j}^{n}) = \begin{cases} 0, & \theta_{i,j}^{n} \le 0 \\ 2\theta_{i,j}^{n}, & 0 \le \theta_{i,j}^{n} \le \frac{1}{3} \\ \frac{1}{2}(1 + \theta_{i,j}^{n}), & \frac{1}{3} \le \theta_{i,j}^{n} \le 3 \\ 2, & 3 \le \theta_{i,j}^{n} \end{cases} \tag{6}$$

Finite-difference schemes are known to introduce spurious numerical terms in the conservation equations [8]. When using the first-order UP scheme, these terms are linearly dependent on the lattice spacing δx. Since, flux limiter schemes are adapting themselves to the local smoothness of the distribution functions, it is rather cumbersome to derive analytical expressions of the spurious numerical terms in these cases. However, the numerical diffusivity introduced by flux limiter schemes was found to closely follow a second-order dependence on δx [8]. Since, the lattice spacing is a small quantity, the use of flux limiter schemes is expected to improve the accuracy of FDLB simulations.

4. Numerical results and discussion

Simulation results reported here were obtained on a 128×5 lattice using the UP and the MCD schemes with $\delta x = 1/128$, $\delta t = 10^{-5}$, $\tau = 10^{-4}$, and $\kappa = 10^{-5}$. First, densities of the coexisting phases at different temperatures are verified. The theoretical densities computed by Maxwell construction are compared with numerical results in

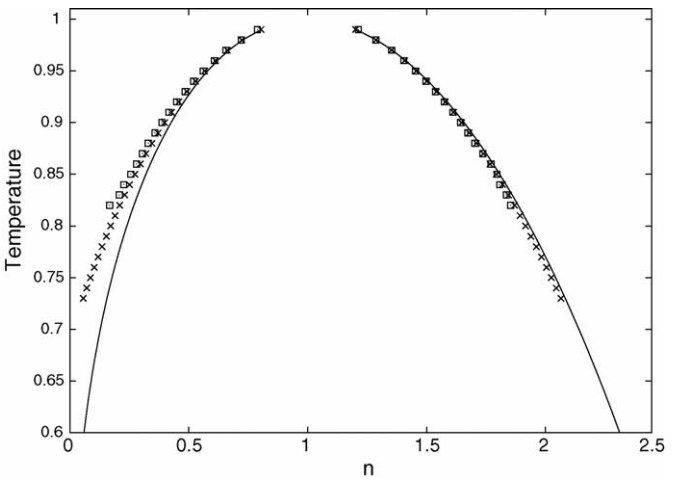

Fig. 1. Coexistence curve recovered with the Maxwell construction (—), the UP (×), and the MCD (□) schemes.

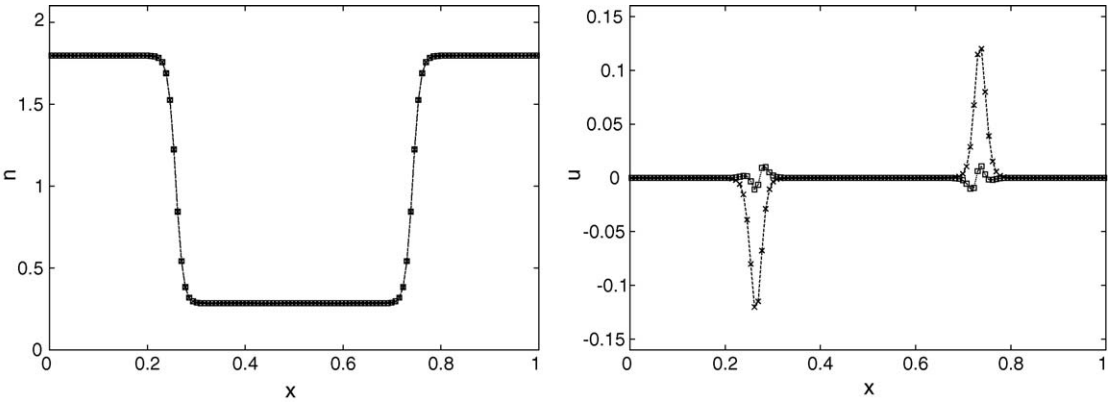

Fig. 2. Left panel: equilibrium density profiles recovered with the UP (×) and the MCD (□) schemes. Right panel: equilibrium velocity profiles recovered with the UP (×) and the MCD (□) schemes. In both the cases, it is $\theta = 0.85$.

Fig. 1. For values of the temperature $\theta \geq 0.85$, UP and MCD data points do almost overlap and a good agreement with the theoretical curve is found (larger discrepancies are found in the vapor branch). An evident difference in using UP and MCD comes out when considering effects at interfaces of coexisting phases. Equilibrium density and velocity profiles are shown in Fig. 2, starting from an initial sharp interface. Density profiles are not affected by the particular numerical scheme and interfaces are smooth. Their width can be controlled by the surface tension tuned by κ. It is more interesting what happens with velocity profiles. At equilibrium, we should expect zero velocities but spurious numerical terms produce non-zero velocities. An effective damping of spurious velocity at interfaces can be observed when using the MCD scheme. The reason is related to the fact that spurious numerical schemes are second-order in δx compared to UP where they are first-order in δx. As shown in Ref. [8], the velocity profile with UP is proportional to the first derivative of the density profile. When using MCD, we expect the velocity profile to be proportional to the second derivative of the density profile. This expectation seems to be confirmed by the fact the we see a double peak in the velocity at interfaces where the density goes from one phase to the other. These results suggest that numerical schemes have to be carefully chosen when dealing with multiphase systems and that the MCD scheme can be conveniently used in the proposed model of liquid–vapor system to reduce spurious numerical contributions.

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