Journal of Computational Science xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Studies of accurate multi-component lattice Boltzmann models on benchmark cases required for engineering applications

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ARTICLE INFO

Article history:
Received 24 December 2015
Received in revised form 2 May 2016
Accepted 4 May 2016
Available online xxx

MSC:
00-01
99-00

Keywords:
Multi-component flow
Lattice Boltzmann

ABSTRACT

We present recent developments in lattice Boltzmann modeling for multi-component flows, implemented on the platform of a general purpose, arbitrary geometry solver PowerFLOW. Presented benchmark cases demonstrate the method's accuracy and robustness necessary for handling real world engineering applications at practical resolution and computational cost. The key requirements for such approach are that the relevant physical properties and flow characteristics do not strongly depend on numerics. In particular, the strength of surface tension obtained using our new approach is independent of viscosity and resolution, while the spurious currents are significantly suppressed. Using a much improved surface wetting model, undesirable numerical artifacts including thin film and artificial droplet movement on inclined wall are significantly reduced.

1. Introduction

Recently, there has been increased interest in engineering applications of multi-component flow simulation with the lattice Boltzmann (LB) method, because of its advantages for complex geometry and turnaround time efficiency. The lattice Boltzmann method (LBM) is based on the kinetic theory which allows to construct physical models from microscopic as well as from macroscopic viewpoints.

While multi-component LBM's have shown promising results on a large number of academic cases, numerical accuracy and stability still represent challenges under extreme conditions such as coarse resolution and low viscosity. Actually, these conditions are likely to be encountered in many engineering applications. In this paper, issues with currently existing schemes and models are pointed out, and an improved LB scheme is tested.

The paper is organized as follows. In Section 2, the standard LBM for multi-component flow is briefly reviewed. In Section 3, issues related to the basic functionality are specified, and an improved scheme is proposed and tested via the simulation of a two-dimensional droplet. In Section 4, cases with wall boundaries are discussed and typical issues associated with boundary models are pointed out. A new boundary model is tested on some benchmark cases. We discuss results in Section 6. In this paper, all physical quantities are written in lattice units, and the discrete lattice time and space increments are $\Delta x = \Delta t = 1$.

2. Multi-component lattice Bolzmann method

The commonly used LB equation for multi-component flow can be written as:

$$f_i^\alpha(\boldsymbol{x} + \boldsymbol{c}_i\Delta t, t + \Delta t) - f_i^\alpha(\boldsymbol{x}, t) = \mathcal{C}_i^\alpha + \mathcal{F}_i^\alpha, \tag{1}$$

where α stands for different components (species), $\boldsymbol{c}_i$ is the discrete velocity and $\mathcal{F}_i^\alpha$ is inter-component interaction force [1]. The D3Q19 lattice model [2] is used so that i ranges from 1 to 19, and $\mathcal{C}_i^\alpha$ is the particle collision operator. The simplest and commonly used one is the BGK collision operator [2–5] with a single relaxation time τ_α for the α-species:

$$\mathcal{C}_i^\alpha = -\frac{1}{\tau_\alpha}(f_i^\alpha - f_i^{eq,\alpha}). \tag{2}$$

The equilibrium state $f_i^{eq,\alpha}$ with the third order expansion is defined as:

$$f_i^{eq,\alpha}(\rho^\alpha, \boldsymbol{u}) = \rho^\alpha w_i \left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{T_0} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2T_0^2} - \frac{\boldsymbol{u}^2}{2T_0} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^3}{6T_0^3} - \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{2T_0^2}\boldsymbol{u}^2\right]. \tag{3}$$

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http://dx.doi.org/10.1016/j.jocs.2016.05.001
1877-7503/

Here $T_0 = 1/3$ is the lattice temperature, w_i is the isotropic weight in D3Q19, ρ^α is the density of the component α, and $\boldsymbol{u}$ is the mixture flow velocity:

$$\rho^\alpha = \sum_i f_i^\alpha \tag{4}$$

$$\rho = \sum_\alpha \rho^\alpha = \sum_\alpha \sum_i f_i^\alpha \tag{5}$$

$$\boldsymbol{u} = \frac{\sum_\alpha \sum_i \boldsymbol{c}_i \cdot f_i^\alpha}{\rho}. \tag{6}$$

There exist several models that introduce local interactions between components that are responsible for separation between the components [1,6]. One of the most commonly used ones is the Shan-Chen potential force:

$$\boldsymbol{F}^{\alpha,\beta}(\boldsymbol{x}) = G^{\alpha,\beta}\rho^\alpha(\boldsymbol{x}) \sum_i w_i \boldsymbol{c}_i \rho^\beta(\boldsymbol{x} + \boldsymbol{c}_i \Delta t). \tag{7}$$

Here, the matrix $G^{\alpha,\beta}$ defines parameters which determine the strength of interaction between components. If $G^{\alpha,\alpha} = 0$ and $G^{\alpha,\beta} \neq 0$ where $\alpha \neq \beta$, the interaction forces only exist between different components. The equation of state for each component is that of ideal gas. If $G^{\alpha,\alpha}$ is nonzero, in addition to the interaction forces between different components, there is also a body force within the α-component. As a result, the α-component acquires the equation of state of a non-ideal gas and phase transition within that component becomes possible. In this paper, phase transitions of single components are neglected and $G^{\alpha,\alpha} = 0$.

There are several ways to apply the forcing term $\mathcal{F}_i^\alpha$. The existing approaches have the same body force representation at the first order in space/time resolution, but different at the second and higher orders. The high order difference does have significant influence on simulation quality. In this work we use the forcing term described in [7].

The resulting fluid velocity $\boldsymbol{u}_F$ is the velocity averaged over pre- and post-collision steps,

$$\boldsymbol{u}_F = \boldsymbol{u} + \frac{\boldsymbol{g}\Delta t}{2} \tag{8}$$

$$\boldsymbol{g} = \frac{\sum_\alpha \boldsymbol{g}^\alpha \rho^\alpha}{\rho}. \tag{9}$$

where $\boldsymbol{g}^\alpha$ is the acceleration of the component α derived from the intercomponent force $\boldsymbol{F}^{\alpha,\beta}$: $\boldsymbol{g}^\alpha = \sum_\beta \boldsymbol{F}^{\alpha,\beta}/\rho^\alpha$. This quantity $\boldsymbol{u}_F$ is henceforth called simply *velocity*.

3. High accuracy bulk solver

Engineering applications usually require simulations involving various material properties and flow scenarios. Due to the jump of physical characteristics at the interface between components, accurate representation and simulation of these interfaces represents a significant difficulty. There is a consensus that numerical stability and accuracy remain two major challenges in development of multi-phase/multi-component LB flow solvers. To ensure numerical stability, the viscosities cannot be too small, and also the viscosity ratio between different components cannot be too large. Numerical artifacts including spurious current could often contaminate flow physics near the interface region. It becomes even more challenging when the solid-fluid interaction, i.e. surface wetting, is also considered. A new LB algorithm for the multi-component flow used in this work improves these numerical issues.

Even when the interface is static, numerical artifacts could provide a source of artificial velocity, which is called spurious velocity (cf. [8]). The proper treatment of these phenomena is recognized as one of the key requirements for accuracy and stability of the multi-component flow modeling. In previous studies [9,10], it is pointed out that the spurious current is associated with the insufficient isotropy of the numerical system caused by the discretization.

Instead of BGK, we use here a regularized filter collision operator [11]:

$$f_i^\alpha(\boldsymbol{x} + \boldsymbol{c}_i\Delta t, t + \Delta t) = f_i^{eq,\alpha}(\rho^\alpha, \boldsymbol{u}) + \left(1 - \frac{1}{\tau_\alpha}\right) f_i^{neq,\alpha} + \mathcal{F}_i^\alpha. \tag{10}$$

Here τ_α is the relaxation time of the fluid component α that is related to the kinematic viscosity of that component ν_α [12]. $f_i^{neq,\alpha}$ is the regularized non-equilibrium distribution function,

$$f_i^{neq,\alpha} = \Phi^\alpha : \Pi^\alpha, \tag{11}$$

where Φ is a regularized filter collision operator based on Hermite polynomials [11,13,14] and Π^α is the non-equilibrium momentum flux tensor for the component α. $\mathcal{F}_i^\alpha$ is the interaction body force. The general idea and relevant algorithm details of the regularization can be found in [11,13–16]. Here we would like to emphasize that this filter collision operator keeps the nonequilibrium information of moments up to the desired order, for example the 2nd order for the momentum flux and the 3rd order for the energy flux, and removes other higher order nonequilibrium moments in the Hermite space. Such a filtering procedure could substantially reduce unphysical noise and numerical artifacts and improve numerical stability and accuracy.

As a first test of this approach, a two-dimensional static droplet is simulated with the variable initial droplet radius, $R = \{8, 12, 16, 24\}$, and relaxation time, $\tau^\alpha = \{0.525, 0.55, 1.0, 1.5, 3.0\}$ for each component. The simulation domain size is five times the droplet radius and the initial density for each component is 0.22. After a steady state is reached, the droplet radius is measured by fitting the hyperbolic tangent curve to the density profile so that the interface position is accurately estimated.

In Fig. 1, the pressure differences across the droplet interface, dP, are plotted with respect to the inverse droplet radius $1/R$, using four sets of τ^α combinations with the maximum viscosity ratio of 100. The subscripts 1 and 2 for τ denote quantities inside and outside the droplet, respectively. Results for all τ options are fitted by a line. According to the Young-Laplace law,

$$dP = \frac{\sigma}{R}, \tag{12}$$

the slope of the fitted line numerically achieves the surface tension σ, which is independent of the viscosity and droplet size. Achieving such independence is an important first step toward simulating complex practical problems.

As mentioned above the spurious current problem is believed to be caused by insufficient isotropy of discrete schemes [9,10]. In Fig. 2, maximum spurious currents are plotted in terms of τ_2 and R. In the left figure, τ_2 is varied while τ_1 is fixed corresponding to the initial $R = 8$. It is seen that the spurious current of the modified scheme is lower than the original one for all cases. Furthermore, with the modified version the spurious current dependence upon τ and R is much reduced. As a result, one can estimate the spurious velocity quantitatively even before simulation, evaluate its effect on the main flow, and reduce numerical artifacts.

In Fig. 3, the distributions of the velocity field and the second component density are presented. Here the initial R is 24 and the relaxation times are $\tau_1 = 0.525$ and $\tau_2 = 3.0$. The results demonstrate that the new scheme significantly reduces the spurious current while preserving the density profile and the interface thickness.

Please cite this article in press as: H. Otomo, et al., Studies of accurate multi-component lattice Boltzmann models on benchmark cases required for engineering applications, J. Comput. Sci. (2016), http://dx.doi.org/10.1016/j.jocs.2016.05.001