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A kinetic theory-based lattice Boltzmann model for multicomponent systems with non-unitary molecular mass ratios

Maria R. A. F. Lisboa[1], Ricardo L. M. Bazarin[2], Paulo C. Philippi[1]

[1]*Mechanical Engineering Graduate Program, Pontifical Catholic University of Paraná*
R. Imac. Conceição, 1155 - Prado Velho, Curitiba - PR, 80215-901
lisboa.maria@pucpr.edu.br, paulo.philippi@pucpr.br
[2]*Federeal University of Santa Catarina*
Estr. Dona Francisca, 8300 - Bloco U - Zona Industrial Norte, Joinville - SC, 89219-600
ricardo.bazarin@posgrad.ufsc.br

Abstract. In a kinetic model, the mean velocity of a particle is a function of the temperature and molecular mass. For a kinetic-based model, the introduction of a non-unitary mass ratio for multicomponent systems is relevant to LBM discretization, presenting a challenge for physically consistent model formulation. The purpose of this work is to explore the use of non-unitary molecular mass ratios on the lattice Boltzmann method starting from the continuous Boltzmann equation. Keeping the kinetic theory-based LB model with prescribed abcissas quadrature of the Maxwell-Boltzmann equilibrium distribution, the authors reached mass ratios of 10^6 for the layered Poiseuille flow.

Keywords: Lattice Boltzmann Method, Multicomponent flow, non-unitary mass-ratio

1 Introduction

In a multicomponent flow, portraying fluids with different masses is essential for accurately representing fluid behavior, where variations in density and composition significantly affect flow dynamics. However, this presents a major challenge in numerical simulation, as it requires solving sharp density gradients, often demanding sophisticated algorithms and significant computational resources. The lattice Boltzmann method, already known for its efficiency and accuracy, has been improving in representing fluids with different densities over the last decades.

Describing a non-unity density ratio requires either varying the molecular mass or adjusting the molar volume for each component. From a simulation perspective, these are achieved by modifying the scale factor c_s or introducing a non-ideal equation of state (EOS), respectively. This work focuses on the mass ratio approach. Introducing a non-unitary mass ratio usually alters the model discretization [1]. The sound speed c_s, commonly used as a scale factor in LBM, is directly related to the mass m, as $c_s = \sqrt{kT/m}$, where k is the Boltzmann constant and T is the temperature. Consequently, for an isothermal multicomponent system, the mass ratio between components implies an effective sound speed ratio.

In the literature, many authors use *ad hoc* procedures, adding tunable free parameters and solving linear systems to achieve an equilibrium distribution function representative for the macroscopic moments of fluids with different masses [2–6]. Nevertheless, the final effect of these procedures is the modification of the sound speed, as it can be shown algebraically. These procedures modify almost arbitrarily the equilibrium, distancing it from the Maxwellian distribution.

It has already been established that the Maxwell-Boltzmann equilibrium distribution (MBD) aligns with thermodynamic equilibrium, corresponding to the maximum entropy state, as described by the H-theorem [7]. The present work proposes an approach without *ad hoc* impositions in the discretization of the equilibrium distribution function, keeping the usual kinetic-based Hermite polynomial quadrature [1]. This work uses the color gradient model[8] with the segregation operator proposed by Latva-Kokko and Rothman [9], achieving density ratios of 10^6 in the layered Poiseuille flow.

2 Multicomponent equations for the Continuum

From the continuum space of mesoscopic binary collisions, the balance equations governing the interactions among different fluid components can be represented by the Boltzmann equation. Considering a multi-component system with N immiscible fluid components, the Boltzmann equation is represented by:

$$\partial_t f^{(k)} + \xi_\alpha \partial_\alpha f^{(k)} + g_\alpha^{(e)} \partial_{\xi_\alpha} f^{(k)} = \sum_s \Omega^{(ks)}, \tag{1}$$

where t is the time, $f^{(k)}$ is the distribution function for component k, ξ_α is the molecular velocity vector, $g_\alpha^{(e)}$ is the acceleration resulting from a external body force, and $\Omega^{(ks)}$ is a collision operator usually modeled using the Bhatnagar-Gross-Krook (BGK) collision operator [10]. To account for the immiscibility of fluids, collisions between particles of different components can be disregarded, which implies that $\Omega^{(ks)} = 0$ for $k \neq s$. The BGK collision operator represents the relaxation of the populations around an equilibrium state $f^{(k),eq}\left(n^{(k)}, u_\alpha, T, m^{(k)}\right)$, that depends on particle density $n^{(k)}$, macroscopic velocity u_α, temperature T and molecular mass $m^{(k)}$. The equilibrium distribution function is frequently modeled by the Maxwell–Boltzmann distribution:

$$f^{(k),eq}\left(n^{(k)}, u_\alpha, T, m^{(k)}\right) = \frac{n^{(k)}}{\left(2\pi \dfrac{kT}{m^{(k)}}\right)^{\frac{D}{2}}} exp\left[-\frac{\left(\xi_\alpha - u_\alpha\right)^2}{2\dfrac{kT}{m^{(k)}}}\right], \tag{2}$$

where D denotes the number of spatial dimensions under consideration.

3 Proposed equilibrium discretization

Aiming to keep the thermodynamic representation of the MBD, we develop our modeling keeping the usual Gauss-Hermitian quadrature. Equation (2), can be written as:

$$f_{i,(N)}^{(k),eq} = n^{(k)} W_i \sum_{\eta=0}^{N} \frac{1}{\eta!} a_{eq}^{(k),(\eta)}\left(u_\alpha, \Theta^{(k)}\right) H_i^{(\eta)}\left(e_{i,\alpha}\right), \tag{3}$$

where $a_{eq}^{(k),(\eta)}\left(u_\alpha, \Theta^{(k)}\right)$ are the macroscopic moments, $H^{(\eta)}\left(e_{i,\alpha}\right)$ are the Hermitian polynomial and N is the order of truncation. In this representation the sound speed is given as $c_s^2 = kT_0/m_0$, where T_0 and m_0 are the temperature and mass of reference, respectively. The macroscopic moments are a function of u_α and $\Theta^{(k)}$, an energy deviation term given by: $\Theta^{(k)} = \frac{\theta}{r^{(k)}} - 1$, where $r^{(k)} = m^{(k)}/m_0$ and $\theta = T/T_0$ are related to the mass and temperature of reference. The mass deviation term contributes to the energy representation of each component. For a system at isothermal conditions, heavier particles move more slowly compared to lighter ones, reflecting the inverse relationship between the particle mass and the mean peculiar kinetic energy. Consequently, the modified sound speed of the component is defined by $c_{s,(k)}^2 = \frac{c_s^2}{r^{(k)}}$.

In the discrete domain, the conservation moments are recovered by:

$$\sum_k r^{(k)} \sum_i f_i^{(k)} = \sum_k r^{(k)} \sum_i f_{i,(N)}^{(k),eq} = \sum_k r^{(k)} n^{(k)} = \rho, \tag{4}$$

$$\sum_k r^{(k)} \sum_i f_i^{(k)} e_{i,\alpha} = \sum_k r^{(k)} \sum_i f_{i,(N)}^{(k),eq} e_{i,\alpha} = \rho u_\alpha, \tag{5}$$

$$\sum_k r^{(k)} \sum_i f_i^{(k)} e_i^2 = \sum_k r^{(k)} \sum_i f_{i,(N)}^{(k),eq} e_i^2 = \rho u^2 + Dnc_s^2\left(\Theta + 1\right). \tag{6}$$

It has been demonstrated in the literature that at least third-order Hermite moments are required to correctly recover the hydrodynamic moments when varying the speed of sound [1, 11, 12]. Using a second-order velocity set, Huang et al. [11] and Leclaire et al. [13] proposed correction terms to mitigate this discretization error. A third-order representation of the D2Q9 helps to reduce these errors, once it can retrieve non-diagonal third-order moments[14]. Nevertheless, these moments are incomplete and still require correction for representing complex flow, once it may add error terms that may be relevant depending on the mass ratio. However, this discretization allows for an effortless extension to higher-order lattices, which can naturally recover third-order moments and directly eliminate the source of this error.

The mass range reached by this model is intrinsically associated with the velocity space discretizaton, once the truncation of Eq. (3) may result in negative populations arising from $\Theta^{(k)}$, when $r^{(k)}$ exceeds a given $r^{(k)}_{max}$ or falls below a certain $r^{(k)}_{min}$. Considering an isothermal fluid in a static condition ($u_\alpha = 0$), an equilibrium distribution where $N = 2$ or 3 will only be non-negative when $a^{(k),(2)}_{eq} H^{(2)}_i > -2a^{(k),(0)}_{eq} H^{(0)}_i$. Consequently, for specific lattice directions, when $r^{(k)} > r^{(k)}_{max}$ or $r^{(k)} < r^{(k)}_{min}$, the equilibrium leads to negative populations and possible numerical instabilities. For the D2Q9 lattice, the mass range is $(0.5, 2)$, while for the D2V17 this interval is approximately $(0.5, 1.1)$. On the other hand, a fourth-order representation of the D2Q9 velocity set holds, in theory, non-negative populations for $r^{(k)} \in (0.5, +\infty)$.

4 Results

The layered Poiseuille flow became an important benchmark for models with a non-unitary mass ratio. A fully developed two-dimensional layered Poiseuille flow describes the steady, laminar flow of immiscible fluids confined between two parallel, static walls. In here, the velocity field is considered along the y-axis, with a wetting fluid adhering to both walls and a non-wetting fluid occupying the central region. The flow is driven by a constant pressure, resulting in a parabolic velocity profile within each fluid layer.

According to the Navier-Stokes equations for steady flow, the velocity profile for a non-unitary density ratio is given by[15]:

$$u_{ana}\left(x\right) = \begin{cases} A_1 x^2 + C_1 & \text{for } 0 \leq |x| \leq a, \\ A_2 x^2 + B_2 x + C_2 & \text{for } a \leq |x| \leq b, \end{cases} \tag{7}$$

where the coefficients are given by: $A_1 = -\frac{P}{2\rho_1 \nu}$, $A_2 = -\frac{P}{2\rho_2 \nu}$, $B_2 = 2\left(A_1\gamma - A_2\right)a$, $C_1 = \left(A_2 - A_1\right)a^2 - B_2\left(b - a\right) - A_2 b^2$, $C_2 = -A_2 b^2 - B_2 b$, in which $\gamma = \frac{\rho_1}{\rho_2}$ is the density ratio and P is the pressure.

The simulations were made using the color gradient segregation model, considering half-way bounce-back on the static walls and periodic boundaries on the remaining ones. For the simulation parameters, it was used $2b = 4a = L$, where L is the length of the simulation domain, $G = 1.5 \times 10^{-8}$ and Latva-Kokko and Rothman [9] segregation parameter $\beta = 0.7$. The results are illustrated in Fig. 1, for a D2Q9 velocity set, using a 4^{th}-order equilibrium distribution, for $\gamma = 10^{-6}, 10^{-3}, 10^{-1}, 10^{1}, 10^{3}$, along with the errors obtained comparing the analytical and numerical solutions, $Error(\%) = \frac{\sum_x u_{ana}(x) - u_{num}(x)}{\sum_x u_{ana}(x)} \times 100\%$. The present work was able to simulate mass ratios up to 10^{-6}, while most color gradient models in literature are restricted to mass ratios up to 10^{-4} [16]. A good fit was obtained even for smaller meshes of $2b = 50$.

5 Conclusions

The Gauss-Hermitian quadrature is able to represent mass variation correctly in LBM. Nevertheless, choosing a velocity space that represents well the relevant moments to the intended problem and which can reach the mass ratio of interest is key. In future work, results for more complex flows will be presented as, for example, for the Rayleigh-Taylor instability.

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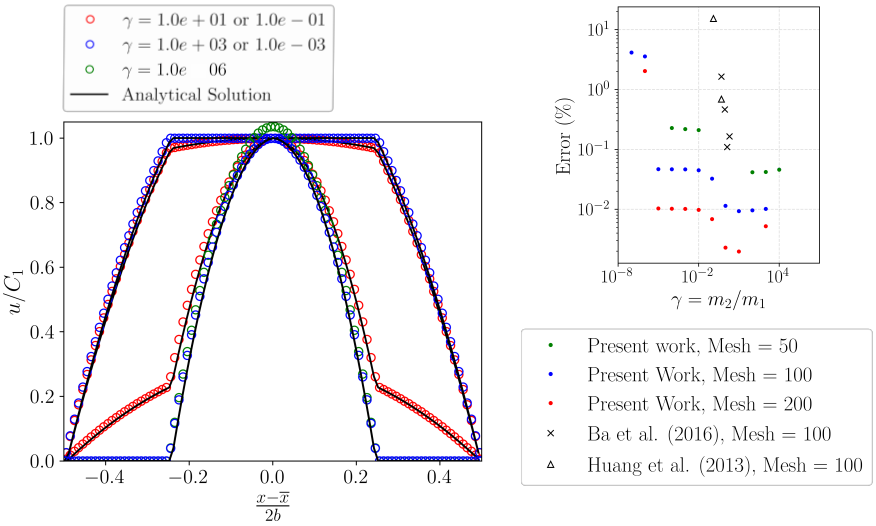


Figure 1. Steady velocity profile for a layered Poiseuille flow for $\gamma = 10^{-6}, 10^{-3}, 10^{-1}, 10^{1}, 10^{3}$, comparing the present work, for $2b = 100$ with the analytical solution given by Eq. (7) in the solid black line. The error between the analytical and numeric solutions are given on the right side for different meshes.

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