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Application of mixed quadrature lattice Boltzmann models for the simulation of Poiseuille flow at non-negligible values of the Knudsen number

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ABSTRACT

We consider the 2D force-driven Poiseuille flow between parallel plates, on which diffuse reflection boundary conditions apply. We present a systematic procedure for the construction of the force term in lattice Boltzmann models based on mixed Cartesian quadratures, where the quadrature on each axis is selected independently. We find that, at non-negligible value of the Knudsen number, half-range quadratures outperform the full-range Gauss–Hermite quadratures for the direction perpendicular to the diffuse-reflecting plates, while the quadrature on the periodic direction along the flow is the full-range Gauss–Hermite quadrature. Our results are validated against numerical results available in the literature.

1. Introduction

At non-negligible values of the Knudsen number *Kn* (defined as the ratio λ/L between the mean free path λ of the fluid particles and the characteristic length scale of the channel *L*), microfluidics effects beyond the reach of the Navier–Stokes continuum formulation become important. The boundary conditions imposed on the channel walls must account for the microscopic nature of the fluid constituents. According to the diffuse reflection concept [1,2], the particles incident on the wall are fully thermalised due to particle–wall interactions before being re-emitted back into the fluid. For a planar boundary, having outwards-directed normal $\boldsymbol{\chi}$, mass conservation is ensured by imposing zero flux at the wall:

$$\int_{\boldsymbol{p}\cdot\boldsymbol{\chi}<0} d^D p f^{(\text{eq})}(n_w, \boldsymbol{u}_w, T_w; \boldsymbol{p})(\boldsymbol{p}\cdot\boldsymbol{\chi}) = -\int_{\boldsymbol{p}\cdot\boldsymbol{\chi}>0} d^D p f(\boldsymbol{p})(\boldsymbol{p}\cdot\boldsymbol{\chi}), \tag{1}$$

where n_w, $\boldsymbol{u}_w$ and T_w are the particle number density, macroscopic velocity and temperature of the bounding wall. For prescribed wall velocity $\boldsymbol{u}_w$ and wall temperature T_w, the above equation can be used to find the number density n_w in the wall nodes. Non-planar walls can be approximated by successions of walls which are perpendicular to the coordinate axes [3,4], provided that the lattice is sufficiently fine.

In this paper, we focus on the study of the 2*D* force-driven Poiseuille flow between parallel plates using lattice Boltzmann (LB) models. Many excellent studies of the Poiseuille flow have been performed using the lattice Boltzmann method, mostly in isothermal conditions and at low Mach numbers [5–12]. Non-isothermal flows were considered in [13–18] and it was found, by comparison with analytic works [19–22] and with Direct Simulation Monte Carlo (DSMC) results [6,11,12,16–18] or experimental data [15], that high-order LB models (i.e. with large velocity sets) must be employed to access the physics beyond the Navier–Stokes level, which gives rise to microfluidis specific effects (e.g. slip velocity, temperature dip, Knudsen paradox, etc). A similar conclusion was reached through the analysis of the Couette flow [23].

As suggested in Refs. [6,16] for the Poiseuille flow, and also in Refs. [24–27], the implementation of diffuse reflection in LB models cannot be performed exactly when full-space quadratures are employed. Based on the analytic analysis of flows between diffuse reflective boundaries [28–37], a solution to correctly account for half-range integrals of the form in Eq. (1) is to consider half-range polynomial expansions of the distribution function. This idea can be implemented in LB models by employing quadratures based on half-range polynomials, such as the Laguerre [38–40] and the

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half-range Hermite [41–43] polynomials, as well as by explicitly constructing velocity sets and quadrature weights that recover half-range moments [12].

The novelty of this paper lies in extending the mixed quadrature LB models introduced in Ref. [43] by introducing a force term on the direction where the full-range Gauss–Hermite quadrature is employed. Our approach to the simulation of Poiseuille flow follows closely the one employed in Ref. [43] for the Couette flow, which we summarise here. Noting that $f^{(\rm eq)}$ can be factorised with respect to the Cartesian components of the momentum and in order to reduce computational effort, we follow Refs. [36,37] and consider thermal LB models based on mixed Cartesian quadratures. On the direction parallel to the walls (the y axis), we always employ a full-range Gauss–Hermite quadrature, since the boundary conditions on this direction are periodic. On the direction perpendicular to the walls (the x axis), we compare the full-range Gauss–Hermite, Laguerre and half-range Gauss–Hermite quadratures in terms of convergence. We work with the BGK collision term, expanding $f^{(\rm eq)}$ with respect to each axis independently, as described in Refs. [39,40,43]. Thus, when half-range quadratures are considered, the expansion of $f^{(\rm eq)}$ can be performed such that its half-range moments are exactly recovered, thereby extending the work in Refs. [12,41,42], where the expansion of $f^{(\rm eq)}$ does not allow the exact recovery of its half-range moments. Since the force for this flow is applied only on the axis parallel to the walls, the method introduced in Ref. [44] is used to derive an expression for the force term when the full-range Gauss–Hermite quadrature is employed.

In general, the quadrature points corresponding to Gauss quadratures are irrational numbers, giving rise to velocity vectors having irrational components on the coordinate axes. In order to implement arbitrary quadrature orders, we employ a finite difference flux-limiter scheme [16,45,27].

This paper is organised as follows. In Section 2, the Boltzmann–BGK equation is discussed in the context of the 2D force-driven Poiseuille flow. Mixed quadrature thermal lattice Boltzmann models are introduced in Section 3 and the general formula for the force term when full-range Gauss–Hermite quadratures are considered is given in Section 3.3. The numerical method employed for the Poiseuille flow is described in Section 4 and the numerical results are presented in Section 5. Appendix A lists some basic ingredients required for the construction of LB models based on half-range Hermite quadratures.

In this paper, all physical quantities are non-dimensionalised as presented in Refs. [46–49].

2. Boltzmann–BGK equation for the 2D Poiseuille flow

The Boltzmann equation in the presence of an external force $\boldsymbol{F}$ can be written as:

$$\partial_t f + \frac{1}{m}\boldsymbol{p}\cdot\nabla f + \boldsymbol{F}\cdot\nabla_{\boldsymbol{p}} f = J[f], \tag{2}$$

where m is the particle mass and $f \equiv f(\boldsymbol{x}, \boldsymbol{p}, t)$ is the Boltzmann distribution function, giving the number of particles per unit phase space volume centred at position $\boldsymbol{x}$ and momentum $\boldsymbol{p}$ at time t. In this paper, we consider the Bhatnagar–Gross–Krook (BGK) approximation [50] for the collision term $J[f]$. Specialising to the case of the 2D Poiseuille flow between parallel plates driven by a constant force $\boldsymbol{F} = (0, ma)$ (where a is the acceleration along the y direction) reduces Eq. (2) to:

$$\partial_t f + \frac{1}{m} p_x \partial_x f + ma\partial_{p_y} f = -\frac{1}{\tau}(f - f^{(\rm eq)}), \tag{3}$$

where the flow is considered to be homogeneous along the periodic direction y, while diffuse reflection boundary conditions apply on the x direction. The plates are placed at $x = \pm L/2$ and are kept at rest at the temperature T_w. The relaxation time τ is related to the (constant) Knudsen number Kn through [51]

$$\tau = \frac{Kn}{n}. \tag{4}$$

In this paper, we focus on obtaining the profiles of the macroscopic density n, fluid velocity $\boldsymbol{u}$, stress tensor $T_{\alpha\beta}$ and heat flux $\boldsymbol{q}$, defined as:

$$n = \int d^2p f = \int d^2p f^{(\rm eq)}, \tag{5a}$$

$$\rho u_\alpha = \int d^2p\, p_\alpha f = \int d^2p\, p_\alpha f^{(\rm eq)}, \tag{5b}$$

$$T_{\alpha\beta} = \int d^2p \frac{p_\alpha p_\beta}{m} f, \tag{5c}$$

$$q_\alpha = \int d^2p \frac{\boldsymbol{\xi}^2}{2m}\frac{\xi_\alpha}{m} f, \tag{5d}$$

where $\rho = mn$ is the mass density and $\xi_\alpha \equiv p_\alpha - mu_\alpha$ is the peculiar momentum.

The temperature is defined in terms of the trace of the stress tensor:

$$nT + \frac{1}{2}\rho\boldsymbol{u}^2 = \frac{1}{2}\left(T_{xx} + T_{yy}\right) = \int d^2p \frac{\boldsymbol{p}^2}{2m} f^{(\rm eq)}. \tag{6}$$

The equality between the moments of f and $f^{(\rm eq)}$ in Eqs. (5a), (5b) and (6) is a statement of the fact that 1, p_α and $\boldsymbol{p}^2/2m$ are collision invariants of the Boltzmann collision term $J[f]$ (in particular, also of the BGK collision term).

In order to study the macroscopic evolution equations contained in the Boltzmann equation, it is convenient to introduce the following notations:

$$M_{s_x,s_y} = \int d^2p p_x^{s_x} p_y^{s_y} f, \qquad M^{\rm eq}_{s_x,s_y} = \int d^2p\, p_x^{s_x} p_y^{s_y} f^{(\rm eq)}. \tag{7}$$

Thus, the evolution equation for M_{s_x,s_y} can be written as:

$$\partial_t M_{s_x,s_y} + \frac{1}{m}\partial_x M_{s_x+1,s_y} = mas_y M_{s_x,s_y-1} - \frac{1}{\tau}(M_{s_x,s_y} - M^{\rm eq}_{s_x,s_y}), \tag{8}$$

where integration by parts was used to obtain the coefficient of a. For the Poiseuille flow considered here, the evolution of a moment of order s_x on the x axis requires information about the moment of order $s_x + 1$ on the x axis, while the evolution of moments of order s_y on the y axis can be written completely in terms of moments of order less than or equal to s_y on the y axis. This implies that the evolution of moments of order up to N_y on the y axis can be recovered with a quadrature that exactly recovers moments of order up to N_y on the y axis. Thus, when investigating the moments in Eqs. (5), the results of simulations employing quadratures that recover moments of order up to $N_y \geq 4$ yield identical results when N_x is kept fixed.

3. Lattice Boltzmann models based on mixed Cartesian quadratures

As discussed in Refs. [28,36,37,43], half-range quadratures are only appropriate on the directions perpendicular to the bounding walls. While in Ref. [40], the half-range Gauss–Laguerre quadrature was employed on all axes to study the 3D Poiseuille flow, here we employ full-range Gauss–Hermite quadratures on the y axis (the axis parallel to the walls). For the x direction, we consider the cases of full-range Gauss–Hermite, Gauss–Laguerre and half-range Gauss–Hermite quadratures, which we discuss separately in what follows. We refer to such models for which the quadrature