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GAUSS QUADRATURES – THE KEYSTONE OF LATTICE BOLTZMANN MODELS

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In this paper we compare two families of Lattice-Boltzmann models derived by means of Gauss quadratures in the momentum space. The first one is the $\mathrm{HLB}(\mathrm{N}; \mathrm{Q_x}, \mathrm{Q_y}, \mathrm{Q_z})$ family, derived by using the Cartesian coordinate system and the Gauss-Hermite quadrature. The second one is the $\mathrm{SLB}(\mathrm{N}; \mathrm{K}, \mathrm{L}, \mathrm{M})$ family, derived by using the spherical coordinate system and the Gauss-Laguerre, as well as the Gauss-Legendre quadratures. These models order themselves according to the maximum order N of the moments of the equilibrium distribution function that are exactly recovered. Microfluidics effects (slip velocity, temperature jump, as well as the longitudinal heat flux that is not driven by a temperature gradient) are accurately captured during the simulation of Couette flow for Knudsen number up to 0.25.

Keywords: Lattice Boltzmann; Gauss quadrature; microfluidics; Couette flow

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1. Introduction

In their early days, the Lattice Boltzmann (LB) models were designed to retrieve the Navier-Stokes equation in the incompressible limit by using a discrete set of vectors in the two- (2D) or three-dimensional (3D) momentum space.[1,2,3,4,5] More convenient LB models (isothermal or with variable temperature) were derived later using

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the Gauss-Hermite quadrature.[6,7,8,9] Such models form a hierarchy and higher order moments of the equilibrium distribution functions are successively achieved when increasing the position of an LB model in the hierarchy.[10,11,12] This is particularly important when approaching microfluidics problems.[13,14,15,16,17,18]

In this paper, we briefly outline the basics of the derivation of three-dimensional ($3D$) LB models based on Gauss quadratures. There are two families of such models, which differ by the coordinate system (Cartesian of spherical) used in the momentum space and we consider the thermal Couette flow problem to compare the results obtained by using both models.

2. Lattice Boltzmann models derived by Gauss quadratures

Let us consider the equilibrium distribution function $f^{eq} \equiv f^{eq}(\mathbf{p}; n, \mathbf{u}, T) = n(\beta/\pi)^{D/2} e^{-\beta(\mathbf{p}-m\mathbf{u})^2}$, where $\mathbf{p}$ is the momentum vector (whose Cartesian components in the D-dimensional space are p_α, $1 \leq \alpha \leq D$), m is the mass of the fluid particles, n is the local particle number density, $\mathbf{u}$ is the local fluid velocity, T is the local fluid temperature and $\beta = 1/2mT$. According to the Chapman-Enskog method, the derivation of the conservation equations from the Boltzmann equation involves the calculation of the moments of the distribution functions up to a certain order S ($0 \leq s \leq S$):

$$\mathcal{M}^{(s)}_{\{\alpha_l\}} \equiv \mathcal{M}^{(s)}_{\alpha_1\alpha_2\ldots\alpha_s} = \int d^D p f^{eq} \prod_{l=1}^{s} p_{\alpha_l} \qquad (1 \leq \alpha_l \leq D) \tag{1}$$

In the LB models, the integral in the equation above is replaced by summation over a discrete set of momentum vectors $\{\mathbf{p}_{i\in\mathcal{I}}\}$, where $\mathcal{I}$ is an index set. Accordingly, the equilibrium distribution function $f^{(eq)}$ is replaced by the set of distribution functions $f_i^{eq} \equiv w_i n E_N(\mathbf{p}_i; u, T)$, $i \in \mathcal{I}$, where $E_N(\mathbf{p}; u, T)$ is a polynomial of order N with respect to $\mathbf{p}$. After these replacements, Eq. (1) becomes:

$$\widetilde{\mathcal{M}}^{(s)}_{\{\alpha_l\}} \equiv \widetilde{\mathcal{M}}^{(s)}_{\alpha_1\alpha_2\ldots\alpha_s} = \sum_{i\in\mathcal{I}} f_i^{eq} \prod_{l=1}^{s} p_{i\alpha_l} \tag{2}$$

In practice, $E_N(\mathbf{p}; u, T)$ might be expanded with respect to some orthogonal polynomials set, e.g., Hermite polynomials.[6,7,8,9,19,20,21] This allows one to determine the momentum vectors $\mathbf{p}_i$, as well as their associated weights w_i ($i \in \mathcal{I}$) by using appropriate Gauss quadratures[21] that ensure $\mathcal{M}^{(s)}_{\{\alpha_l\}} = \widetilde{\mathcal{M}}^{(s)}_{\{\alpha_l\}}$ for $0 \leq s \leq S$.[7,8,18,20] As stated in Refs. 19 and 20, the condition $N \geq S$ needs to be satisfied in other to retain all relevant moments up to order S.

The integration over the whole momentum space, which appears in Eq. (1), may be performed in using the separation of variables along the axes of the coordinate system. When $D = 3$, both the Cartesian and the spherical coordinate systems may be used for this purpose. In the first case, the equilibrium distribution function is expanded with respect to the Hermite polynomials,[19,20] while a more elaborated expansion involving the generalized Laguerre polynomials, as well as the Legendre polynomials, is used in the second case.[18,22]

In principle, the Gauss quadrature method allows one to build LB models of order N as large as needed by using appropriate momentum vector sets. The number of the vectors is determined by the quadrature order(s) and the projections of these vectors on the axes of the coordinate system are related to the roots of orthogonal polynomials.[7,8,9,10,18,19,20] This feature greatly facilitates the assembling of LB models of any order and LB models with momentum sets up to 8,000 elements, which run successfully on high performance computing systems, were already reported.[17,18,23] Although the number of momentum vectors in the set becomes very large when increasing N, it can be reduced by pruning techniques at the cost of sacrificing the accuracy of some higher-order moments of the distribution function or by taking advantage of the symmetry group of the lattice.[11,15,24] However, such techniques are very elaborated and need to be carefully designed for each N.

In the sequel, we will denote by $HLB(N; Q_x, Q_y, Q_z)$ the 3D LB model of order N based on Gauss-Hermite quadratures, where Q_l is the order of the quadrature used along the l axis ($1 \leq l \leq 3$). The spherical LB models are denoted by $SLB(N; K, L, M)$, where K, L, M are the orders of the quadratures with respect to the spherical coordinates r, θ and ϕ, respectively.[18,22] Since both models are off-lattice, a flux limiter numerical scheme[17,18,25] involving the projection of the discrete momenta on the Cartesian axes was used to compute the evolution of the distribution functions after each time step. The Shakhov collision term[18,26,27,28] was used in these models to achieve the right value (2/3) of the Prandtl number.

3. Computer results

To compare the characteristics of the two families of quadrature-based LB models (HLB and SLB), we considered the problem of thermal Couette flow between two parallel plates perpendicular to the z axis. The plates are located at $z_b = -0.5$ and $z_t = 0.5$, respectively and move in opposite directions along the y axis with speed $u_w = 0.63$. Their temperatures is $T = 1.0$ (nondimensionalized units[18] are used). The computer simulations were done on a cubic lattice with 128 nodes in the z direction and 2 nodes in the x and y direction. Periodic boundary conditions were applied along the x and y axes and the diffuse reflection boundary conditions[17,18,29] were applied on the plates. The results reported in this paper were obtained with the lattice spacing $\delta s = 1/128$ and the time step $\delta t = 10^{-4}$.

Figure 1 shows the transversal profiles of the longitudinal velocity u_y, the temperature T, the transversal heat flux q_z, as well as the longitudinal heat flux q_y. These profiles were obtained in the stationary state with the Shakhov collision term by using the models HLB(6;20,20,20) and SLB(6;20,20,20), for three values of the Knudsen number. The profiles are compared to the Direct Simulation Monte Carlo (DSMC) results for hard sphere molecules reported in Refs. 30 and 31. We used the Shakhov collision term[18] to ensure the right value of the Prandtl number (Pr $= 2/3$).

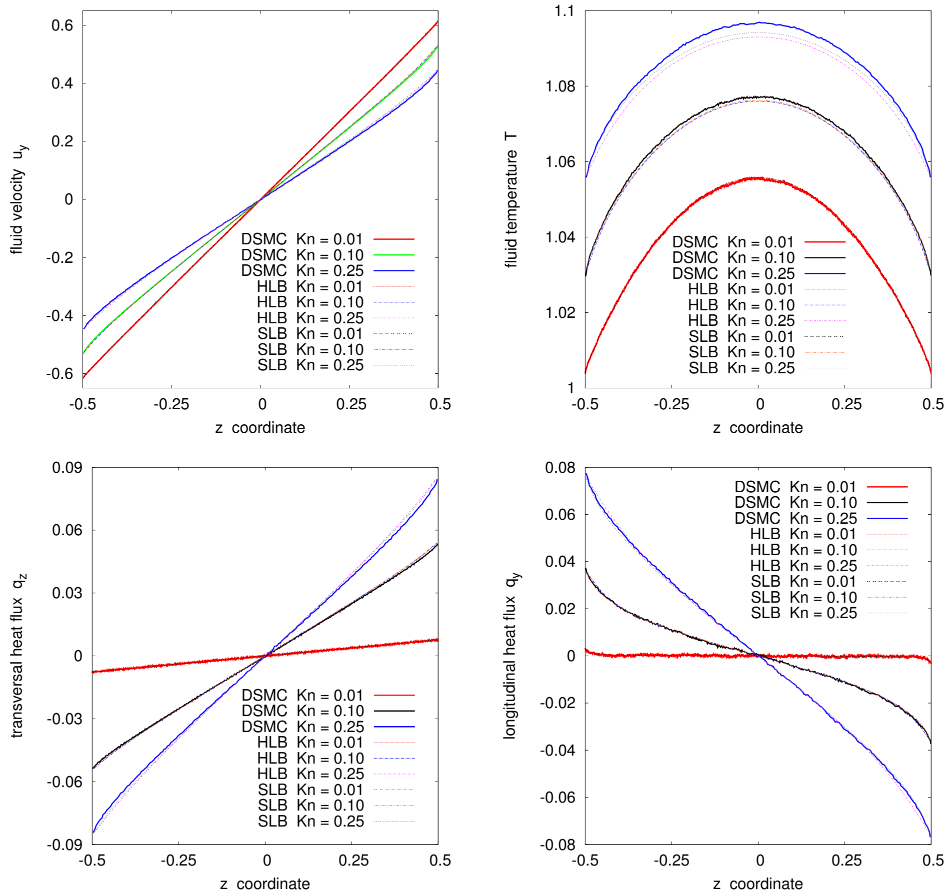

Fig. 1. Velocity, temperature and heat flux profiles in Couette flow obtained with models HLB(6;20,20,20) and SLB(6;20,20,20 at three values of the Knudsen number Kn.

Good agreement between the LB and DSMC results is observed for all quantities, excepting the temperature results at $Kn = 0.25$.[18] The specific microfluidics effects (slip velocity, temperature jump, as well as the longitudinal heat flux that is not driven by a temperature gradient) are accurately captured.

According to Figure 2, the HLB(N;20,20,20) and SLB(N;20,20,20) results get well superposed for $N \geq 4$ and $N \geq 3$, respectively. As seen in Figure 3, both the HLB and the SLB models are found to be very sensible with respect to the quadrature orders when the Knudsen number is large enough. This behavior originates from the half-space integrals involved in the implementation of the diffuse reflection boundary conditions. As mentioned in the literature, the errors are reduced and the simulation results converge when the quadrature orders (i.e., the number of momentum vectors) in the LB model) are large enough.[13,17,18,29,32,33]

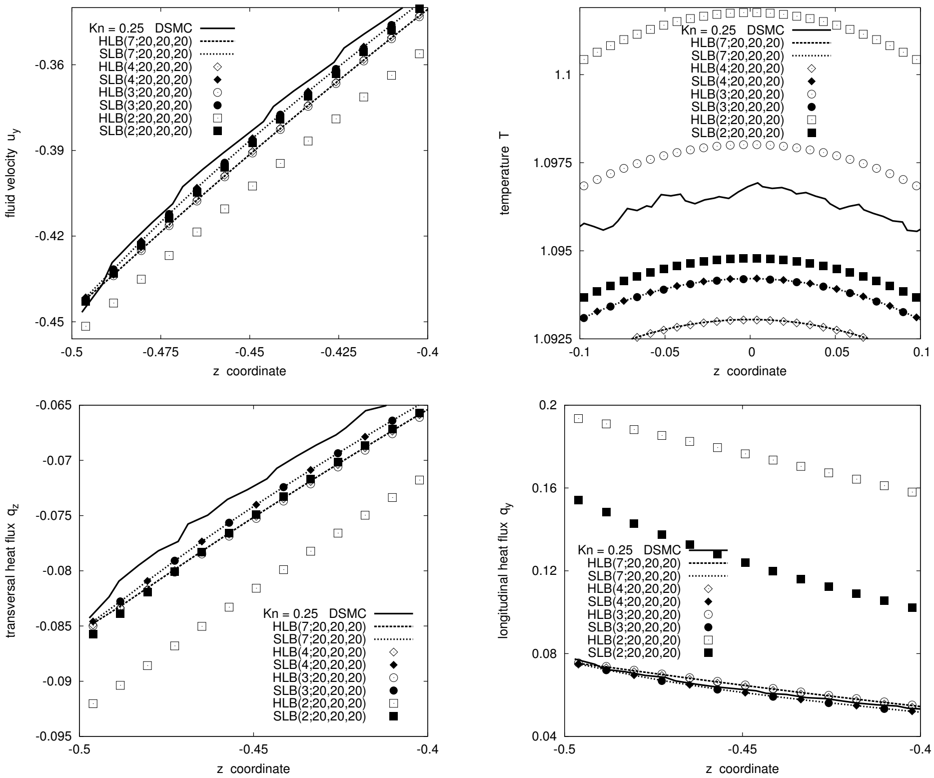

Fig. 2. Velocity and heat flux profiles near the left wall, as well as temperature profiles in the central region of Couette flow at Kn = 0.25, for various values of N.

4. Conclusion

In this paper we compared the simulation results obtained by using two families of LB models based on Gauss quadratures. When using the Shakhov collision term, both families of LB models allows one to accurately capture microfluidics effects (slip velocity, temperature jump, as well as the longitudinal heat flux that is not driven by a temperature gradient) in Couette flow when $Kn < 0.25$. The main advantage of these models is that the momentum vector sets can be easily constructed, regardless of the order N of the model. This feature is particularly helpful for the accurate implementation of the diffuse reflection boundary conditions, which needs large momentum sets as Kn increases.

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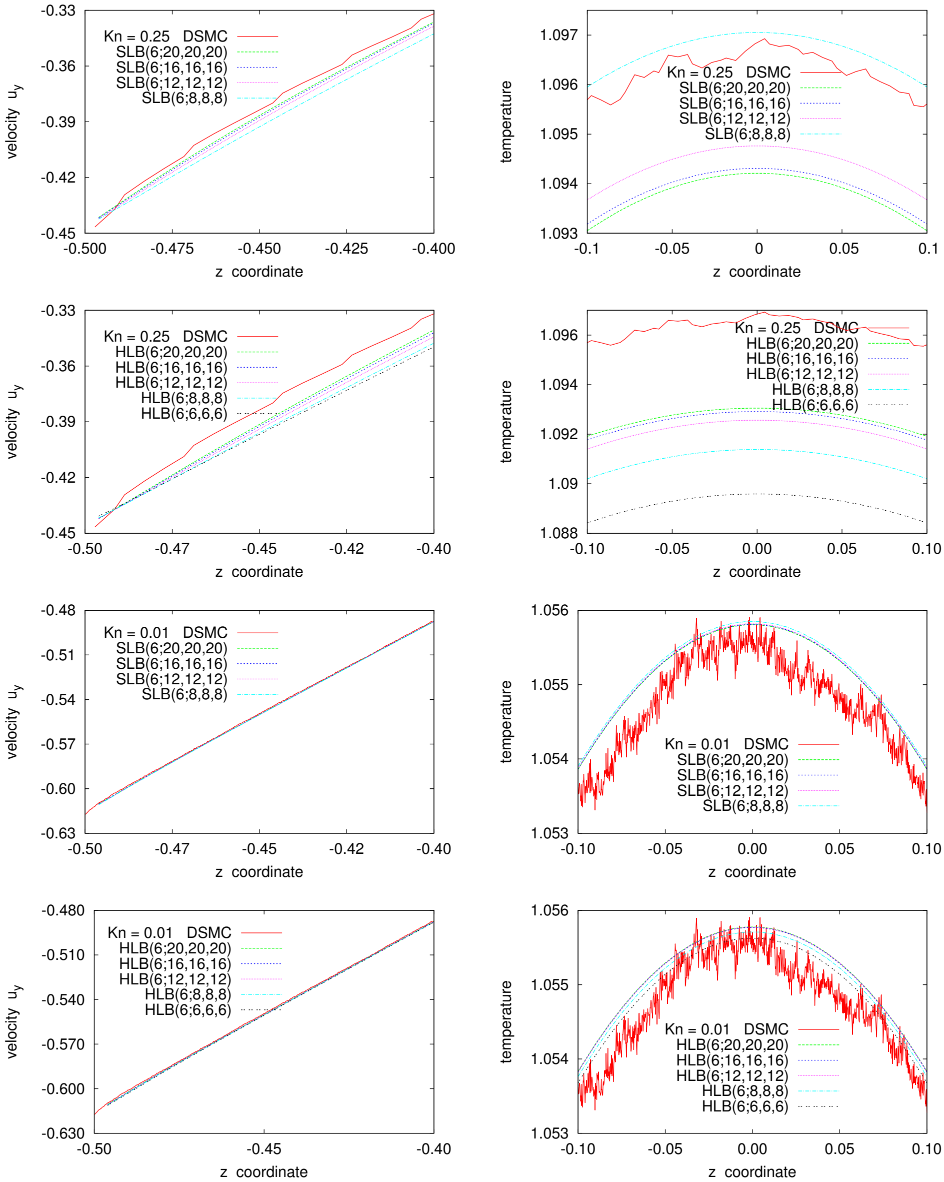

Fig. 3. Velocity profile parallel to the velocity of the walls (left) and temperature profile (right) at Kn = 0.25 (rows 1 and 2) and Kn = 0.01 (rows 3 and 4) in the SLB (rows 1 and 3) and HLB (rows 2 and 4) models, compared with DSMC results.

thors are grateful to Professor Henning Struchtrup (Department of Mechanical Engineering, University of Victoria, Canada) for the DSMC simulation results[30,31] used in this work. The computer simulations were done on the IBM Blue Gene / P

system at the West University of Timişoara (Romania) using the Portable Extensible Toolkit for Scientific Computation (PETSc) developed at Argonne National Laboratory, Argonne, Illinois.[34]

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