Thermal Lattice Boltzmann models derived by Gauss quadrature using the spherical coordinate system

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Abstract. A hierarchy of thermal Lattice Boltzmann models is derived by separation of variables using the spherical coordinate system in the momentum space. The moments of the equilibrium distribution function are computed by means of Gauss-Legendre and Gauss-Laguerre quadratures. This procedure allows us to find the discrete momentum vectors for each model in the hierarchy. The Shakov collision term is used to get the right value of the Prandtl number. Computer simulation of Couette flow is used to illustrate the capability of these models to capture specific effects in microfluidics.

1. Introduction
Lattice Boltzmann (LB) models are derived from the Boltzmann equation using a simplified version of the collision operator. These models provide an alternative to the simulation techniques of Computational Fluid Dynamics (CFD) or Direct Simulation Monte Carlo (DSMC) and have been recognized as efficient tools for the investigation of single- or multi-component complex fluids with or without structure formation, as well as for the investigation of microfluidics problems [1, 2, 3].

At their beginning (more than two decades ago), the LB models were designed to retrieve the Navier-Stokes equation in the incompressible limit [1] by using a discrete set of velocities in the two- (2D) or three-dimensional (3D) space. Later, the LB models were rigorously derived by using the Chapman-Enskog method, as well as the Gauss-Hermite quadrature after separation of variables in the Cartesian coordinate system [4]. This way, the LB models approach the discrete velocity method (DVM) well known in kinetic theory of rarefied gases [5, 6].

As the Knudsen number increases and the fluid system goes farther away from equilibrium, higher order moments of the equilibrium distribution function need to be considered in order to account for the complexity of flow phenomena when using the Chapman-Enskog method. As pointed in the literature [4, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17], higher order moments of the equilibrium distribution function can be achieved in LB models by increasing the number of velocity vectors in the discrete set. Since the number of vectors in the discrete set increases monotonically with the order of the Gauss-Hermite quadrature, the corresponding LB models...
form a hierarchy. Higher order moments of the equilibrium distribution function are successively satisfied when increasing the position of a LB model in this hierarchy.

The LB models currently reported in the literature are mainly isothermal or of low order. High order LB models with variable temperature are computationally expensive and were not considered until recently [17, 18, 19, 20]. Application of the Gauss-Hermite LB models to investigate gas flow phenomena at non-negligible values of the Knudsen number is very encouraging [17, 20]. In these models, the Cartesian coordinate system is used in the momentum space. The purpose of this contribution is to introduce a new class of LB models in 3D, which are derived using the spherical coordinate system in the momentum space, as well as the Gauss-Laguerre and Gauss-Legendre quadratures.

All quantities of interest in the LB models introduced in this paper are made dimensionless by using three basic reference quantities [21]: a characteristic length \( l_R \), a reference mass \( m_R \) and a reference energy \( e_R = k_B T_R \), where \( k_B \) is Boltzmann’s constant and \( T_R \) is a reference temperature. Other references are derived from the basic quantities: particle number density \( n_R = 1/l_R^3 \), speed \( c_R = \sqrt{k_B T_R/m_R} \), time \( l_R/c_R \), and so on.

2. Description of the model

We take advantage of the spherical shell models introduced by Watari and Tsutahara [22, 23, 24, 25, 26] and build a hierarchy of three-dimensional thermal Lattice Boltzmann models by using the spherical coordinate system in the momentum space. According to the discretization procedure [8], the continuum momentum space is now replaced by a discrete set \( \{ \alpha \} \) having \( N \) elements. The corresponding density functions and equilibrium density functions are denoted \( f_\kappa \) and \( f_\kappa^{(eq)} \), respectively.

The highest natural number \( N \) for which all tensors of order \( s \) \( (0 \leq s \leq N) \)

\[
\tilde{M}^{(s)}_{\{\alpha\}} \equiv \tilde{M}^{(s)}_{\alpha_1 \alpha_2 \ldots \alpha_s} = \sum_\kappa f_\kappa^{(eq)} \prod_{l=1}^s p_{\alpha_\lambda} 
\]

(1)

equal the corresponding ones in the continuum space [8]

\[
M^{(s)}_{\{\alpha\}} \equiv M^{(s)}_{\alpha_1 \alpha_2 \ldots \alpha_s} = \int d^D p f^{(eq)} \prod_{l=1}^s p_{\alpha_\lambda} 
\]

(2)

defines the order of the LB model in the hierarchy \( (p_{\alpha_\lambda} \text{ and } p_{\alpha_\lambda}, \alpha_\lambda \in \{1, 2, 3\} \text{ are the Cartesian components of the vectors } \p_\kappa \text{ and } \p, \text{ respectively}) \). For given \( N \), the momenta \( \p_\kappa \), as well as the expression of the equilibrium density functions \( f_\kappa^{(eq)} \) can be established by means of series expansion and Gauss quadrature.

The equilibrium distribution function in the continuum space, i.e., the Maxwell - Boltzmann distribution function, is given by [1, 27, 28]

\[
f^{(eq)} = f^{(eq)}(\p; n, u, T) = n(\beta/\pi)^{D/2} e^{-\beta(p - mu)^2}
\]

(3)

where \( n = M^{(0)} \) is the particle number density, \( u_\alpha = M^{(1)}_{\alpha} / mn \) is the fluid velocity and \( T = \delta_{\alpha_1 \alpha_2} M^{(2)}_{\alpha_1 \alpha_2}/Dmn - mu^2/D \) is the fluid temperature, respectively \( (\beta = 1/2mT, D = 3, m \text{ is the mass of fluid particles and } \delta_{\alpha_1 \alpha_2} \text{ is Kronecker’s symbol; the sum rule over repeated } \alpha_\lambda \text{ indices is understood}) \). Since mass, momentum and energy are conserved during fluid particle collisions, the local quantities \( n, u_\alpha \) and \( T \) are also recovered by computing the corresponding moments of \( f_\kappa \) and \( f \) [1, 8, 13, 27, 28]. Splitting Eq.(3) yields \( (p = \sqrt{\p^2}) \)

\[
f^{(eq)} = f^{(eq)}(\p; n, u, T) = nF(p^2; T)E(\p; u, T)
\]

(4)
When replacing is a polynomial of order $s$

This means that the $s^{th}$ order moment

$$
N^{(s)} = \left\lfloor \frac{N}{2} \right\rfloor \frac{1}{j!} \left( -\frac{m u^2}{2T} \right)^j \sum_{r=0}^{N-2j} \frac{1}{r!} \left( \frac{p u}{T} \right)^r
$$

is a polynomial of order $s$ in the fluid velocity $\mathbf{u}$. Hence Eq. (2) is preserved for $0 \leq s \leq N$ when replacing $E$ in (4) with its series expansion with respect to $\mathbf{u}/\sqrt{T/m}$ up to order $N$:

$$
E^{(N)} = \sum_{j=0}^{[N/2]} \frac{1}{j!} \left( -\frac{m u^2}{2T} \right)^j \sum_{r=0}^{N-2j} \frac{1}{r!} \left( \frac{p u}{T} \right)^r
$$

($[x]$ is the largest integer less than or equal to $x$).

When using the spherical coordinate system $(p, \theta, \varphi)$ in the momentum space, such that

$p_{\alpha} = p e_{\alpha}(\theta, \varphi), e_1(\theta, \varphi) = \sin \theta \cos \varphi, e_2(\theta, \varphi) = \sin \theta \sin \varphi, e_3(\theta, \varphi) = \cos \theta$, we get $E^{(N)} \equiv E^{(N)}(p, \theta, \varphi; \mathbf{u}, T)$ and

$$
N^{(s)} = n \int_0^\infty dp d\theta d\varphi \left( \frac{p^2}{p} \right)^{N+1} w_{\alpha_1, \alpha_2, \ldots, \alpha_s} = \sum_{\lambda=0}^{M} A_{\lambda, \mu, \nu}(p, \mathbf{u}) \times (\sin \theta)^{\mu+\nu}(\cos \theta)^{\lambda}(\sin \varphi)^{\mu}(\cos \varphi)^{\nu}
$$

According to [30, 31], the following quadrature formula

$$
Q^{(s)}(\alpha_1) = \int_0^{2\pi} d\varphi S^{(s)}(\alpha_1)(\theta, \varphi) = \frac{2\pi}{M} \sum_{i=1}^{M} S^{(s)}(\alpha_1)(\theta, \varphi_i)
$$

with $\varphi_i = \varphi + 2\pi(i-1)/M$ and $\phi$ an arbitrary angle, is exact for any integer $M \geq 2N+1$. Terms with odd $(\mu + \nu)$ in $S^{(s)}(\alpha_1)$ do not contribute to the integral with respect to $\varphi$. The even powers of $\sin \theta$ are easily changed in powers of $\cos \theta$ and $Q^{(s)}(\alpha_1)$ is eventually expressed as a polynomial of order at most $2N$ in $z = \cos \theta$ [29]. The *Gauss-Legendre* quadrature [31, 32] gives

$$
E^{(s)}(\alpha_1) = \int_{-1}^{+1} dz Q^{(s)}(\alpha_1) = \sum_{j=1}^{L} w_{j}(P) E^{(s)}(\alpha_1)(z_j)
$$

$$
w_{j}(P) = \frac{2(1-z_j^2)}{(L+1)^2[P_{L+1}(z_j)]^2}
$$

where $z_j, 1 \leq j \leq L$ are the roots of the Legendre polynomial $P_L(z)$ of order $L \geq N + 1$. Because of the symmetry of the integration domain, odd powers of $z = \cos \theta$ do not contribute
Figure 1. First two members of the SLB family: SLB\((1; 2, 2, 3)\) and \(SLB(2; 3, 3, 5)\).

to \(\mathcal{E}_{\{\alpha\}}^{(s)}\). Thus, the appropriate use of quadrature formulae during integration over the angular coordinates \((\theta, \varphi)\) gives us the polynomial \(\mathcal{E}_{\{\alpha\}}^{(s)} \equiv \mathcal{E}_{\{\alpha\}}^{(s)}(p^2; \mathbf{u}, T)\) containing only even powers of \(p\) [29]

\[
\mathcal{E}_{\{\alpha\}}^{(s)} = \frac{2\pi}{M} \sum_{j=1}^{L} \sum_{i=1}^{M} w_j^{(p)} p^s \mathcal{E}^{(N)}(p, \theta_j, \varphi_i; \mathbf{u}, T) \prod_{l=1}^{s} e_{j|i\alpha_l} \tag{15}
\]

where \(e_{j|i\alpha_l} \equiv e_{\alpha_l}(\theta_j, \varphi_i), \theta_j \equiv \arccos(z_j)\) and \(\varphi_i = \phi + 2\pi(i - 1)/M\). This allows us to use the Gauss-Laguerre quadrature [31, 32] after changing the integration variable from \(p\) to \(x \equiv p^2\) in Eq. (10). Since

\[
\mathcal{M}_{\{\alpha\}}^{(s)} = \frac{n}{2} \int_{0}^{\infty} dx \, x^{1/2} e^{-x} \mathcal{F}(x; T) \mathcal{E}_{\{\alpha\}}^{(s)}(x; \mathbf{u}, T) \tag{16}
\]

contains the term \(x^{1/2}\), we expand \(\mathcal{F}(x; T) \equiv e^x \mathcal{F}(x; T)\) with respect to the generalized Laguerre polynomials \(L_{\ell}^{(1/2)}(x)\):

\[
\mathcal{F}(x; T) = \pi^{-3/2} \sum_{\ell=0}^{K-1} (1 - 2mT)\ell L_{\ell}^{(1/2)}(x) \tag{17}
\]

The order \(K - 1\) of this expansion must be greater than or equal to \(N\) because \(\mathcal{E}_{\{\alpha\}}^{(s)}(x; \mathbf{u}, T)\) is a polynomial of order at most \(N\) in \(x\) and hence is orthogonal to all \(L_{\ell}^{(1/2)}(x)\) of order \(\ell > N\). Application of the Gauss-Laguerre quadrature rule gives [29]

\[
\mathcal{M}_{\{\alpha\}}^{(s)} = \frac{n}{2} \sum_{k=1}^{K} w_k^{(L)} \mathcal{F}(x_k; T) \mathcal{E}_{\{\alpha\}}^{(s)}(x_k; \mathbf{u}, T) \tag{18} \\
w_k^{(L)} = \frac{x_k \Gamma(K + 3/2)}{K!(K + 1)^2[L_{K+1}^{(1/2)}(x)]^2} \tag{19}
\]

where \(x_k, 1 \leq k \leq K, K \geq N + 1\) are the roots of the generalized Laguerre polynomial \(L_K^{(1/2)}(x)\), \(w_k^{(L)}\) are the quadrature weights and \(\Gamma(x)\) is the factorial function [32].

Comparison of Eqs. (1) and (18) gives the expression of the equilibrium distribution functions \(f_k^{(eq)} \equiv f_{kji}^{(eq)}\) in the LB model of order \(N\) with Gauss quadrature in spherical coordinates [29],

\[4\]
as well as the Cartesian components \( p_{\alpha} = p_{kji\alpha} \) (\( \alpha = 1, 2, 3 \)) of the corresponding momentum vectors \( p_{kji} \) (\( 1 \leq k \leq N + 1, 1 \leq j \leq K, 1 \leq i \leq M \)):

\[
\begin{align*}
    f_{kji}^{(eq)} &= n F_k E_{kji} \\
    F_k &= \frac{w_k^{(L)}}{M \sqrt{\pi}} \sum_{\ell=0}^{K-1} (1 - 2mT)^{\ell} L_{\ell}^{(1/2)} (p_k^2) \\
    E_{kji} &= w_j^{(P)} E^{(N)} (p_k, \theta_j, \varphi_i; u, T) \\
    p_{kji\alpha} &= p_k e_{ji\alpha}, \quad p_k = \sqrt{E_k}
\end{align*}
\]

The members of this family (hierarchy) of spherical shell LB models will be denoted \( SLB(N; K, L, M) \). More details on the derivation of these models can be found in [29]. The first two members of the SLB family are shown in Figure 1.

### 3. Preliminary results

To illustrate the capability of the SLB models introduced in this paper to capture the physics of flow phenomena at various values of Knudsen number, we consider the problem of Couette flow between parallel plates perpendicular to the \( z \) axis and located at \( z_b = -0.5 \) and \( z_t = 0.5 \), respectively. The plates have equal temperatures \( T(x, y, z_b) = T(x, y, z_t) = T_w = 1.0 \) and move in opposite directions along the \( x \) axis with speed \( u_w = 0.63 \) (as stated in Section 2, all quantities of interest are non-dimensionalized). To ensure the right value of Prandtl number for the ideal gas (\( \text{Pr} = 2/3 \)), we use the Shakov collision term [33, 34, 35, 36] in the evolution equation of the distribution functions, instead of the BGK collision term [1]:

\[
\partial_t f_{kji} + \frac{p_{kji\alpha}}{m} \partial_\alpha f_{kji} = -\frac{1}{\tau} \left[ f_{kji} - f_{kji}^{(eq)} (1 + S_{kji}) \right]
\]

where \( \tau = \text{Kn}/n \) [27] and

\[
S_{kji} = \frac{1 - \text{Pr}}{nT^2} q_\alpha (p_{kji\alpha} - mu_\alpha) \left[ \frac{(p_{kji} - mu)^2}{(D + 2mT)} - 1 \right]
\]

\[
q_\alpha = \frac{1}{2m^2} \sum_{k,j,i} f_{kji} (p_{kji\alpha} - mu_\alpha) (p_{kji} - mu)^2
\]

The evolution equations (21) are numerically solved by projecting the discrete moments \( p_{kji} \) on the Cartesian axes and using the MCD flux limiter scheme [17, 29, 37, 38, 39]. Diffuse reflection boundary conditions were implemented on the walls [3, 17, 21, 29, 39]. We used a cubic lattice with 100 nodes in the \( z \) direction and 2 nodes in the \( x \) and \( y \) directions where periodic conditions apply. The lattice spacing had the value \( \delta s = 1/100 \) and the time step was set to \( \delta t = 10^{-4} \).

Simulation results recovered with SLB(6; 8, 8, 13) for two values of Kn (0.01 and 0.10) are compared to DSMC results for hard sphere molecules [40, 41, 42, 43] in Figures 2 and 3. The Knudsen layer, where the velocity profile is nonlinear and a longitudinal heat flux is generated, is well captured by the SLB models up to Kn=0.10, despite the large value of \( u_w \). Differences between the SLB temperature profiles and the corresponding DSMC results were observed for larger values of Kn [29].

### 4. Conclusion

The spherical coordinate system may be used in the momentum space in order to derive a hierarchy of Lattice Boltzmann models \( SLB(N; K, L, M) \) based on Gauss-Laguerre and Gauss-Legendre quadratures. These models ensure the recovery of all moments of the equilibrium
distribution function up to order \( N \). Couette flow simulation was used to validate these models and the preliminary computer results fit well to DSMC simulations up to \( Kn = 0.1 \). Further investigations need to be performed in the future in order to explore the capabilities of the \( SLB \) models, as well as to compare them with the existing LB models in the literature.

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Figure 2. Stationary profiles (velocity, temperature and heat fluxes) across the channel in Couette flow at \( Kn = 0.01 \) \((T_w = 1.0; u_w = 0.63)\).
Figure 3. Stationary profiles (velocity, temperature and heat fluxes) across the channel in Couette flow at Kn=0.10 ($T_w = 1.0; u_w = 0.63$).
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