Intermediate Lattice Boltzmann-BGK method and its application to micro-flows

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Abstract. A novel discretization approach for the Bhatnager-Gross-Krook (BGK) kinetic equation is proposed. The method inherits properties of the Lattice Boltzmann (LB) method like linear streaming step, conservation of moments. Similar to the finite-difference methods for the BGK model the presented approach describes high-order moments of the distribution function with controllable error. Two test problems are considered: the Poiseuille flow between two parallel plates and plane Couette flow. Significant increase in precision over the conventional LB models is observed.

1. Introduction
The Lattice Boltzmann (LB) method is supposed to be an adequate approach for the modeling of non-equilibrium flows and kinetic effects beyond the Navier-Stokes level [1]. Nevertheless, when the flow is rarefied and the role of high-order moments of the velocity distribution in a rarefied media increases the precision of conventional LB models go down. In the real world, the large values of the rarefaction parameter - the Knudsen number can be observed in the micro, nano-flows, in shale gas flow inside porous media, water transport inside nano-graphene membranes [2].

The Lattice Boltzmann method is based on the idea of the full discretization (in velocity and physical space) of the BGK kinetic equation [3], which reads as

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \frac{1}{\tau} (\Phi - f),$$

where \(f(t, x, \xi)\) is the gas distribution function, \(t, x, \xi\) are the time, spatial coordinate, particle velocity respectively; \(\Phi(t, x, \xi) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|x-u|^2}{2\theta}\right)\) is the local Maxwell state and \(\rho(t, x), u(t, x), \theta(t, x)\) are the macro-parameters (the density, bulk velocity, temperature), \(D\) is the number of spatial dimensions, \(\tau\) is the relaxation time.

In the conventional LB method the discretization is performed in a such way that the LB distribution function (DF) is equivalent to the solution for the BGK equation projected on a finite basis in velocity space spanned by the Hermite polynomials (the Grad expansion). This equivalence is achieved via the Gauss-Hermite quadratures [4, 5, 3]. Since the first moments of the LB local equilibrium are reproduced in the same form as for the local Maxwell state then LB method is conservative by the construction. Moreover, the streaming step is modeled in a
simple linear form, the particles in this step travel from one lattice site to another. The latter guarantees second order accuracy in physical space.

Instead of the exact reproduction of the first moments for the distribution function, the finite-difference methods for the BGK model are aimed to recover the distribution function in overall [6], including high-order moments. The cost to pay is the usage of relatively large discrete velocity sets, moreover conservation of moments requires some additional efforts.

The present research is aimed to develop a new LB based discrete velocity (DV) method which is able to cope with the kinetic high-order moments in the rarefied flow but without drastic increase in number of discrete velocities.

2. Hierarchy LB models
2.1. The construction of LB hierarchy
The simplest LB one-dimensional discretization of the BGK equation (1) \((D = 1)\) which is able to reproduce the Navier-Stokes equations at the limit of low Mach numbers is D1Q3 model \((D\) is the number of dimensions, \(Q\) is the number of the discrete velocities) [1]

\[
f_{-1}(t + \Delta t, x - c\Delta t) - f_{-1}(t, x) = \frac{1}{\tau} \left( f^e_{-1}(t, x) - f_{-1}(t, x) \right),
\]

\[
f_{0}(t + \Delta t, x) - f_{0}(t, x) = \frac{1}{\tau} \left( f^e_{0}(t, x) - f_{0}(t, x) \right),
\]

\[
f_{+1}(t + \Delta t, x + c\Delta t) - f_{+1}(t, x) = \frac{1}{\tau} \left( f^e_{+1}(t, x) - f_{+1}(t, x) \right),
\]

where \(\tau\) is the relaxation time, \(f_{\pm1}, f_0\) are the lattice distribution functions corresponding to the lattice velocities \(\pm c, 0\). The equilibrium states \(f^e_{\pm1}, f^e_0\) are defined as

\[
f^e_{\pm1}(t, x) = \frac{\rho(t, x)}{6} \left( 1 \pm 3 \frac{u(t, x)}{c} + 3 \frac{u(t, x)^2}{c^2} \right),
\]

\[
f^e_0(t, x) = \frac{4\rho(t, x)}{6} \left( 1 - 3 \frac{u(t, x)^2}{2c^2} \right),
\]

where the macroscopic parameters \(\rho, u\) are defined from the expressions

\[
\rho(t, x) = f_{-1}(t, x) + f_0(t, x) + f_{+1}(t, x), \quad \rho(t, x)u(t, x) = -f_{-1}(t, x)c + f_{+1}(t, x)c,
\]

moreover the full energy is calculated as follows

\[
\rho(t, x)(u(t, x)^2 + c_s^2) = (f_{-1}(t, x) + f_{+1}(t, x))c^2,
\]

where the sound velocity \(c_s = \sqrt{\frac{\rho}{\rho}}\), i.e. the model describes only isothermal flows.

Now lets associate with the local equilibrium distribution function for D1Q3 model a random variable \(X(N)\), here \(N = 1\) (the first step in the hierarchy). Assume that this random variable has three outcomes \(-c, 0, +c\). We also assume that this random variable has the distribution function same as the local equilibrium distribution for D1Q3 model. At the present moment this procedure is formal and does not give any additional information. The underlying reason for the introduction of the random variable \(X(1)\) will be clear at the next step.

Next, consider two independent identically distributed (i.i.d.) random variables \(X_1(2), X_2(2)\) (here \(N = 2\), the second step) in a such way that their sum has the same expected value (the bulk velocity \(u\)) and the same variance (the temperature \(c_s^2\)) as for \(N = 1\) case.
Now, generalizing the previous step I consider a sum of $N$ i.i.d. random variables such that their sum has again an expected value $u$ and variance $c^2_s$. The variable $\sum_j^N X_j(N)$ has $2N + 1$ possible outcomes $-Nc, (-N + 1)c \ldots Nc$. Since this sum is composed from the independent identical random variables the corresponding distribution function can be calculated in an exact closed form (see below the expression for $Prob(\sum_j^N X_j = nc)$). The Central Limit Theorem (CLT) for sequences in the form of Lyapunov or Lindeberg-Feller guarantees that the sequence of the distribution functions in the hierarchy converges to the Gaussian distribution (Maxwell state with bulk velocity $u$ and temperature $c^2_s$).

Finally, at $N$-s step the following $2N + 1$ discrete velocity model can be introduced for $-Nc, (-N + 1)c \ldots Nc$ lattice

$$f_n(t+1, x, c_n t) - f_n(t, x) = \frac{1}{\tau} \left( f^eq_{n, N} - f_n \right)(t, x), \quad n = -N \ldots N, \quad c_n = nc$$  \hspace{1cm} (2)

$$f^eq_{n} = \rho \cdot Prob \left( \sum_j^N X_j = nc \right)$$  \hspace{1cm} (3)

$$Prob \left( \sum_j^N X_j = nc \right) = \sum_{m=0}^{n-1} \frac{N!}{(n+m)!m!(N-n-2m)!} P_N(c)^{n+m} P_N(-c)^m P_N(0)^{N-n-2m},$$  \hspace{1cm} (4)

for $n \geq 0$, and where

$$P_N(\pm c) = \frac{1}{2e^2(N)N} \left( c_s^2 \pm cu + \frac{u^2}{N} \right), \quad P_N(0) = 1 - P(c) - P(-c)$$  \hspace{1cm} (5)

and

$$c_s^2 = \frac{Nc^2}{3}.$$  \hspace{1cm} (6)

To keep the temperature constant $c^2_s = \theta_0$ at the all levels of the hierarchy it should be required that

$$c = c(N) = \sqrt{3\theta_0/N},$$

thus the lattice step is decreasing when $N$ grows.

Similar expressions can be obtained for $n < 0$ by taking $|n|$ instead of $n$ and changing $P_N(\pm c)$ by $P_N(\mp c)$.

The model (2)-(6) is the main result of the paper. It can considered as a new LB type discretization for the BGK kinetic equation (for isothermal flows) since the CLT guarantees the convergence of the local equilibrium to the local Maxwell distribution.

### 2.2. Some analytical properties

The equilibrium states in the hierarchy contain $P(\pm c), P(0)$ functions. This states are non-negative if $P(\pm c), P(0)$ are non-negative. This requirement leads to the following inequality

$$u \leq \sqrt{\frac{2}{3}} Nc.$$  

Therefore, the domain of non-negativity is growing when $N$ increases. Potentially this property can result in better stability for the models with $N > 1$ in comparison with the conventional $D1Q3$. 
The straightforward computation of the moment generating function (MGF) defined by $M(s)$ is complicated. One has

$$M(s) \equiv \langle e^{ns} \rangle = \sum_{n=0}^{N} e^{ns} \sum_{m=0}^{[N-n]} \frac{N!}{(n+m)!m!(N-n-2m)!} P_n(c)^{n+m} P_n(-c)^m P_n(0)^{N-n-2m}$$

and the further convolution of the sums seems to be problematic. Nevertheless, the result can be obtained if one takes into account the fact that the local equilibrium is related to a sum $Y = \sum_{j} X_j(N)$ of independent random variables $X_j(N)$. Then the moment generating function for $Y$ is a product of the moment generating functions for $X_j(N)$, they are defined as $M_X(s)$. One has

$$M(s) = M_X(s)^N = (P_N(-c)e^{-cs} + P_N(0) + P_N(c)e^{cs})^N,$$

then any moment $m_k$ of order $k$ can be calculated from Eq. (7) using the formula $m_k = \frac{d^k M(s)}{ds^k}|_{s=0}$. Now taking logarithm from the MGF function (7) and using the expressions (5) for $P_N(\pm c), P_N(0)$ one obtains after some lengthy algebra

$$\log(M(s)) = \frac{\theta s^2}{2} + us + \left\{ (9/6! - 1/16)s^6 + \ldots + (-u^3/2)s^3 \right\} \frac{1}{N^2} + O\left(\frac{1}{N^3}\right)$$

where $\frac{\theta s^2}{2} + us$ is the logarithm of MGF for the Gaussian distribution and $\theta = \frac{Nc^2}{2}$. Therefore, the difference between the logarithms of MGF for the intermediate LB local equilibrium state and the local Maxwell state is of $O(1/N^2)$ order. Then one concludes that the moments for the presented intermediate LB models converge to the local Maxwell ones with the error decreasing as $O(1/N^2)$.

### 2.3. Models in several dimensions

The models in several dimensions can be constructed as a tensor product of 1D models. Since all the models in the discussed above hierarchy have the same order of isotropy ($D1Q3, D1Q5, D1Q7$ and so on) then one can construct 3D models in the form $D1Qn \times D1Qm \times D1Qk$ with $n \times m \times k$ velocities preserving the order of isotropy of 1D models. The local equilibrium takes the product form of equilibrium states in 1D models. This product form approach is based on the ideas from [7]. For instance, one can construct 15 velocity model $D2Q15$ composed by the $D1Q5$ (the formal sum of $D1Q3$ and $D1Q3$) and $D1Q3$ model.

### 2.4. Ballistic streamers removal

As was discussed above, 2D and 3D models can be obtained by taking a tensor product of 1D LB models. This models have velocities parallel to the axis - a streaming directions which do not touch a wall if the wall is placed parallel to the axis (ballistic streamers effect) [8]. The removal of zero lattice velocity mitigates the problem and significantly increases the calculation precision for several problems [8, 9].

Having $(2N+1)$ velocity model in the hierarchy for $[-Nc \ldots 0 \ldots Nc]$ lattice I construct $(2N+2)$ velocity model (zero velocity is removed) in $[-(N+0.5)c, -(N-0.5)c, \ldots (N-0.5)c, (N+0.5)c]$ lattice, the local equilibrium is given by the formulas

$$\tilde{f}_n = \begin{cases} f^{eq}(nc + \frac{1}{2}c) & 0 \leq n < N; \\ f^{eq}(nc + \frac{1}{2}c) & N \leq m \leq 0; \\ \frac{1}{2} f^{eq}(Nc), & N \leq m \leq 0; \end{cases}$$

$$\tilde{f}_m = \begin{cases} f^{eq}(mc - \frac{1}{2}c) & 0 \leq n < N; \\ f^{eq}(mc - \frac{1}{2}c) & N \leq m \leq 0; \end{cases}$$

$$\tilde{f}_n = \begin{cases} f^{eq}(nc - \frac{1}{2}c) & 0 \leq n < N; \\ f^{eq}(nc - \frac{1}{2}c) & N \leq m \leq 0; \end{cases}$$

$$\tilde{f}_m = \begin{cases} f^{eq}(mc + \frac{1}{2}c) & 0 \leq n < N; \\ f^{eq}(mc + \frac{1}{2}c) & N \leq m \leq 0; \end{cases}$$
the temperature $\theta$ is now equals to

$$\theta = c_s^2 + \frac{c^2}{4}$$

and remembering that $c_s^2 = \frac{Nc^2}{3}$ (in the case of $2N+1$ velocity models the temperature is equal to $c_s^2$) one has

$$\theta = \frac{4N + 3}{12} c^2,$$

then the requirement of constant temperature $\theta = \theta_0$ at the all levels of the hierarchy leads to the following formula for the lattice velocities

$$c = \sqrt{\frac{12}{4N + 3} \theta_0}.$$

Finally, it is worth to mention that the error terms in the third moment for $2N+2$ hierarchy in comparison to the Maxwell distribution are the same as for $2N+1$ hierarchy.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Poiseuille flow across flat walls and Knudsen paradox. Volumetric flow vs Knudsen number is presented. The left slide corresponds to the models from $2N+1$ hierarchy, right slide for the models from $2N+2$ hierarchy. The increase of $N$ obviously leads to the convergence of the LB results to the solution for the linearized BGK model. The Knudsen number ($Kn$) is defined as $Kn = \sqrt{\frac{c^2}{8T_0} \frac{\tau}{H}}$, where $T_0$ is unit temperature, $\tau$ is the relaxation time and $H$ the distance between the walls. The volumetric flow rate results for the linearized BGK solution are taken from [10].}
\end{figure}

3. Numerical validation

The first test problem is the Poiseuille flow between two parallel plates. The convergence to the theoretical results can be observed (Fig. 1). For instance, $D1Q7 \times D1Q3 = D2Q21$ model shows approximately 10 percent departure from the linearized BGK solution up to $Kn=0.5$; In ballistic regime runaway effects prevent the correct computation of the flux for $2N+1$ hierarchy.
Figure 2. Plane Couette flow. Slip velocities vs Knudsen number are presented. The application of the model $D1Q5 \times D1Q3$ significantly improves the precision over $D2Q9$ model. The Knudsen number for Couette flow is defined as $Kn = \frac{\sqrt{T_0 H \tau}}{H}$, where $T_0, H, \tau$ are the wall temperature equals to unity, the distance between the walls and the relaxation time respectively. The solutions of the linearized BGK model [11, 12] are adopted as benchmark (black squares).

while for the models from $2N+2$ hierarchy runaway effects are absent but the flow does not have minimum. This result is very typical for LB models with a single relaxation time: the models with velocities parallel to the wall suffer from runaway effects, while the models which are free of such lattice velocities do not reproduce the minimum at $Kn \sim 1$, see [13, 9]. Nevertheless, the accuracy of the models in the present study is very good for slip and transitional regimes which are most important in microfluidics (Fig. 1).

Here it is important to emphasize that for 2D models in the form $D1Q5 \times D1Q3$ and etc, the part $D1Q5, D1Q6, D1Q7$ and etc is responsible for the dynamics transverse to the flow direction while the component $D1Q3$ is responsible to the streamwise direction. The kinetic boundary conditions for high-order lattices are stated at the walls [14, 15]. For the Poiseuille flow the periodic boundary conditions with pressure variations [16] and the addition of pressure as a force term were tested. The both methods give very closed results. For the numerical study 200 spatial cross-stream nodes are taken, the boundary conditions are taken in a such form that the flow is very slow, $Ma \sim 10^{-4}$.

The last test case is the plane Couette flow between parallel walls. Again, the kinetic boundary boundary are adopted [14, 15]. The wall velocity is $Ma^{-4}$. The application of the model $D1Q5 \times D1Q3$ significantly improves the precision over $D2Q9$ model (Fig. 2).

The results regarding the Poiseuille and Couette flows can be compared with the results obtained using high-order and regularized LB models [13, 17, 18, 19], on-lattice and off-lattice models with correct half-fluxes [9, 20].

4. Conclusion

The new discretization approach for the kinetic BGK model is proposed. The method is based on the ideas of the LB method (linear streaming step, conservation of moments) and the discrete velocity method for the BGK model (the description of high moments with controllable error).
Two test case problems are considered (the plane Poiseuille flow, the plane Couette flow), the method shows better results in the description of the Knudsen paradox and the slip velocities than the conventional LB approach.

The presented method is restricted to slow isothermal flows, the further developments towards transonic and supersonic flows are interesting.

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