Accuracy of the lattice Boltzmann method for low-speed noncontinuum flows

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Simulation of noncontinuum gas flows presents tremendous challenges, especially for nanoscale devices that usually exhibit low speeds and isothermal conditions. Such simulations are often achieved through use of the Boltzmann Bhatnagar-Gross-Krook equation, which forms the foundation for the lattice Boltzmann (LB) method. Accuracy of the LB method in noncontinuum flows is widely assumed to depend on the order of quadrature used. Here, we study noncontinuum Couette flow and discover that interaction of the lattice with the solid boundaries is the dominant mechanism controlling accuracy—quadrature order plays a comparatively minor role. This suggests the applicability of low-order quadrature in LB simulation of wall bounded isothermal noncontinuum flows, and leads to a framework and rationale for accurate implementation of LB models in noncontinuum flows.

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Computational simulation of noncontinuum flows has attracted broad interest over the past century due to its importance in space exploration, motion of hypersonic projectiles, and upper atmospheric science and technology. In recent years, an accurate description of such flows has been the focus of a considerable research effort, motivated by tremendous advances in micro- and nanoscale fabrication. These include ultrasensitive cantilever sensors that are integral to the operation of an atomic force microscope, carbon nanotube resonators capable of atomically resolved mass measurements, and most recently, nanomechanical devices that function in their quantum mechanical ground state [1]. Importantly, the operation of such devices in an ambient environment can yield gas flows not encountered at the macroscopic scale [2]. Gas behavior in these systems is dominated by noncontinuum effects, which arise because the mean free path of gas molecules is significant in comparison to the device dimensions. Critically, such effects cannot be predicted using classical continuum theories, e.g., the Navier-Stokes equation. This poses significant challenges to device modeling, technological development, and application.

Modern numerical techniques for noncontinuum gas flows are commonly based on the Boltzmann equation, e.g., the direct simulation Monte Carlo (DSMC) method. For flows generated by micro- and nanoscale devices, however, DSMC simulations can impose prohibitive computational demands due to the low Mach numbers involved [3]. Consequently, these limitations have promoted significant interest in developing alternate numerical techniques for accurate simulation of low-speed noncontinuum flows.

The lattice Boltzmann (LB) method is a numerical scheme for solving the Bhatnagar-Gross-Krook (BGK) equation [4,5]. Due to its foundation in the BGK equation, recent effort has also examined its validity in simulating noncontinuum flows where the gas mean free path \( \lambda \) is no longer small in comparison to the device dimension, \( L \), i.e., finite Knudsen number \( Kn = \lambda / L \) [6–10]. Significantly, it has been suggested that the accuracy of LB models is controlled by the order of Gaussian-Hermite (G-H) quadrature used for discretization of particle velocity space [6–8]. This motivation has driven a plethora of reports aimed at exploring and applying the LB method to noncontinuum flows (see, e.g., Refs. [9,10]).

Contrary to this accepted convention, Kim et al. [9] recently examined the accuracy of the LB method as a function of algebraic precision (AP) of its G-H quadrature, and surprisingly, found a nonmonotonic dependence. They studied low-speed (low Mach number) Couette and Poiseuille flows ranging from continuum (\( Kn \rightarrow 0 \)), slip (\( Kn \ll 1 \)), through to transition flows [\( Kn \sim O(1) \)]. Strikingly, their results demonstrated that increasing AP in some LB models yields lower accuracy, with this trend becoming particularly pronounced in the transition flow regime. These findings remain unexplained, contradict the above quadrature order convention, and prompt an open and fundamental question: What controls the accuracy of the LB method in noncontinuum flows?

In this Rapid Communication, we address this question using an analytical approach based on a Chapman-Enskog expansion and commensurate numerical results using higher-order LB models developed from G-H quadrature [9,11]. In so doing, we discover that the accuracy of higher-order LB models for wall bounded noncontinuum flows is controlled primarily by the interaction of their lattice with the solid boundaries. This is contrary to previous reports that suggest AP of G-H quadrature is the primary mechanism [6–8]. This discovery leads to a reordering of the LB hierarchy, which precisely predicts and explains the apparent random behavior in the results of Kim et al. [9]. The derived theoretical framework provides (i) a rationale for implementation of higher-order LB models in the accurate simulation of noncontinuum flows and (ii) a means of estimating the degree of accuracy in simulating such flows using LB models.

In its usual finite difference (FD) implementation, the evolution equation of the LB method is

\[
f_i(r + c_i \Delta t, t + \Delta t) - f_i(r, t) = -\omega (f_i - f_i^{eq}),
\]

where \( f_i \) is the distribution function that depends on the discrete particle velocities \( c_i \), whereas \( r, \Delta t, \) and \( \omega \) are position, time, time step, and dimensionless relaxation frequency.

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respectively. The equilibrium distribution \( f_i^\text{eq} \) expanded to second order is sufficient for low-speed noncontinuum simulations [9],

\[
f_i^\text{eq} = w_i \rho \left( 1 + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2} \right),
\]

where \( w_i \) are weights corresponding to discrete velocities \( \mathbf{c}_i \), \( c_s \) is the sound speed, fluid density \( \rho = \sum_i f_i \), and velocity \( \mathbf{u} = \sum_i f_i \mathbf{c}_i / \rho \). In the continuum limit, discretization of particle velocity space is afforded by use of the well-accepted 9-bit (D2Q9) and 27-bit (D3Q27) models for two- and three-dimensional flows, respectively [4]. However, such continuum-based discrete velocity spaces do not account for higher-order nonequilibrium effects, and thus are not expected to exactly capture moments of the distribution function for noncontinuum flows. This casts doubt on the applicability of such conventional discretizations in noncontinuum flows, e.g., transition flows [6,7].

The most direct approach to a more accurate evaluation of nonequilibrium effects in noncontinuum flows is to discretize the particle velocity space using G-H quadrature of higher AP. This motivation has led to the formulation and use of the D2Q16, D2Q25, and D2Q36 models corresponding to four-, five-, and six-point G-H quadrature with AP = 7, 9, and 11, respectively (see Refs. [9,11]). Recently, Kim et al. [9] simulated both Couette and Poiseuille flows ranging from the continuum to transition flow regimes. They found a nonmonotonic and apparently random variation in accuracy with increasing AP. This observation remains unexplained and at odds with the above well-accepted reasoning.

To examine the origin of this behavior, we reinvestigated the findings of Ref. [9] using our own LB simulations of Couette flow and extended their simulations to include a wider range of the Knudsen number, 0.005 \( \leq \text{Kn} \leq 5 \) (see Fig. 1). The D2Q49 and D2Q64 models, developed from seven- and eight-point G-H quadrature with AP = 13 and 15 [11], are also included. The conventional on-lattice algorithm was used for the D2Q9 model while the FD algorithm in Ref. [12] was applied to all other off-lattice LB models. Independence of numerical results on specifics of the FD algorithm was verified by comparison to the alternate formulation of Ref. [9], for which identical results were obtained. We use the definition for Kn in Ref. [9] and also set the Mach number as \( \text{Ma} = 0.16 \). In the FD algorithm, forward Euler and second-order upwind schemes were used for temporal and spatial gradients, respectively. The parameter controlling the explicitness of collisions was set to \( \theta = 0.5 \) [12] and the Courant-Friedricks-Lewey number varied between 0.03 and 0.1. Diffuse boundary conditions [7,9,13], were implemented at the solid walls and periodic boundary conditions utilized at opposite ends of the channel.

Figure 2 shows the computed velocity field for \( \text{Kn} = 1 \), obtained by different LB models; this Knudsen number corresponds to flow in the transition flow regime, where nonequilibrium effects are strong. Such nonequilibrium effects are evident from the data in Fig. 2, which display a slip velocity approximately half that of the wall velocity. Direct numerical solution to the linearized BGK equation (yielding isothermal and constant-density conditions) is also presented [14]—since all LB models are based on the BGK equation, these "exact" results are used as a benchmark.

From Fig. 2(a), we observe that increasing AP from 5 to 7, corresponding to the D2Q9 and D2Q16 models, respectively, dramatically improves accuracy; results from the D2Q16 model are very close to the exact solution. This behavior was previously reported by Ansumali et al. [8]. However, as pointed out by Kim et al. [9], increasing AP to 9, corresponding to D2Q25, recovers results similar to the original (continuum based) D2Q9 model, for which poor accuracy is again observed [see Fig. 2(b)]. Moreover, a further increase to an AP of 11 (D2Q36) gives similar results to D2Q16 albeit with a slight improvement in accuracy near the wall, but less accuracy away from the wall.

Figure 3 gives the relative root mean square error in the velocity field as a function of Knudsen number and quadrature order, highlighting (i) the nonmonotonic behavior in LB accuracy with increasing quadrature order and (ii) that accuracy decreases with increasing Knudsen number, in general. Some results exhibit a small nonmonotonic variation in accuracy with respect to Knudsen number—this may be due to the choice of measure used in assessing accuracy. These results validate the unintuitive findings of Kim et al. [9], and draw into question the primary motivation underpinning the use of higher-order LB models for accurate computation of noncontinuum flows.

Importantly, this motivation focuses purely on the accuracy to which nonequilibrium effects in the flow are evaluated, i.e., away from the boundaries. No consideration is given to
the complete problem, which involves both the flow and its interaction with the solid boundaries. We now examine the influence of this interaction, and in this initial report, focus on the case of pure diffuse reflection at the solid boundaries. This interaction with the solid boundaries. We now examine the complete problem, which involves both the flow and its interaction with the solid boundaries.

To investigate the effect of this discretization in the flow and on the boundaries, LB models are derived specifically for moments over the entire velocity space, i.e., (c – 𝑢₀) · n > 0:

\[
f(\mathbf{r}_b, c) = \frac{\int_{(c \cdot \mathbf{n})_{n=0}}^{(c \cdot \mathbf{n})_{\infty}} \left|(c' - \mathbf{u}_b)\right| \cdot \mathbf{n} \left| f(\mathbf{r}_b, c') \right| d\mathbf{c'}}{\int_{(c \cdot \mathbf{n})_{n=0}}^{(c \cdot \mathbf{n})_{\infty}} \left|(c' - \mathbf{u}_b)\right| \cdot \mathbf{n} \left| f_{eq}(\mathbf{r}_b, c', \rho_b, \mathbf{u}_b, T_b) \right| d\mathbf{c'}} \times f_{eq}(\mathbf{r}_b, c | \rho_b, \mathbf{u}_b, T_b), \tag{3}
\]

where \(n\) is the inward unit vector normal to the boundaries and \(\rho_b, \mathbf{u}_b,\) and \(T_b\) are gas density, velocity, and temperature at the solid boundary position \(\mathbf{r} = \mathbf{r}_b\). The discrete version of Eq. (3) in Ref. [13] is used, where integrals are evaluated based on the discrete particle velocity space of the LB model; an alternate version is in Ref. [15].

To investigate the effect of this discretization in the asymptotic limit of a small Knudsen number, we perform a Chapman-Enskog expansion of the distribution function, \(f = f^{eq} + Kn f^{(1)} + Kn^2 f^{(2)} + Kn^3 f^{(3)} + \cdots\), where \(f^{eq}\) is the local equilibrium distribution and \(f^{(i)}\), \(i = 1, 2, 3, \ldots\), are the nonequilibrium terms. Since we consider low Mach number flows, \(f^{eq}\) is expanded to second order [9]. Chapman-Enskog theory dictates that all nonequilibrium terms \(f^{(i)}\) and their derivatives with respect to time, spatial space, and particle velocity be evaluated using \(f^{eq}\) [16]. Consequently, by substituting the above asymptotic expansion for \(f\) into Eq. (3), the original boundary condition can be expressed formally as an asymptotic series in \(Kn\), involving moments of \(f^{eq}\) (for 2D flows):

\[
I_{mn} = \frac{1}{2\pi RT} \int_0^\infty \int_{-\infty}^\infty c_x'^n c_y'^m \exp \left[-\frac{(c_x'^2 + c_y'^2)}{2RT}\right] dc_x' dc_y', \tag{4}
\]

where \(c_x'\) and \(c_y'\) are the particle velocity components in the Cartesian \(x\) and \(y\) directions (see Fig. 1). The first and second indices in \(I_{mn}\) correspond to the \(x\) direction (streamwise) and \(y\) direction (wall normal), respectively. Note that \(m\) covers all non-negative even integers, whereas \(n\) covers all natural numbers, ensuring that each moment in Eq. (4) is unique. The sum \(m + n\) is the moment order.

In Table I, we assess the accuracy to which the moments in Eq. (4) are captured by each quadrature scheme (D2Q9–D2Q64). Moments ranging in order from \(m + n = 1\) to \(5\) are calculated. For simplicity and without losing generality, Table I presents a few representative odd order moments. Even order moments are not given because they are captured exactly by quadratures of the LB models for \(m + n < 5\).

<table>
<thead>
<tr>
<th>(n)</th>
<th>D2Q9</th>
<th>D2Q16</th>
<th>D2Q25</th>
<th>D2Q36</th>
<th>D2Q49</th>
<th>D2Q64</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-27.6</td>
<td>11.3</td>
<td>-16.5</td>
<td>7.3</td>
<td>-11.8</td>
<td>5.3</td>
</tr>
<tr>
<td>3</td>
<td>8.5</td>
<td>-3.6</td>
<td>2.3</td>
<td>-1.4</td>
<td>1</td>
<td>-0.7</td>
</tr>
<tr>
<td>5</td>
<td>-18.6</td>
<td>2.8</td>
<td>-1</td>
<td>0.5</td>
<td>-0.3</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Note that AP of the LB models increases monotonically from left to right in Table I, following the sequence D2Q9, D2Q16, D2Q25, D2Q36, D2Q49, D2Q64. Table I clearly reveals that accuracy of the quadrature approximations of moments in each LB model does not follow this order. The \(n = 1\) moments are expected to dictate the leading order behavior of the Chapman-Enskog expansion of the boundary condition, since the lattice-wall interaction is controlled by \(c_y\); see Eq. (3). This finding immediately indicates that the naive use of G-H quadrature with higher AP in noncontinuum flows may not necessarily lead to enhanced accuracy, which may indeed be reduced. Such an effect is clearly evident in Figs. 2 and 3 which show that increasing AP leads to a nonmonotonic variation in accuracy of the computed velocity field.

Strikingly, we observe that accuracy of the LB models in Fig. 3 precisely follows the sequence in accuracy of moments \((n = 1)\) in Table I. To be specific, from Table I we find that the accuracy of these moments \((n = 1)\) increases in the following order: D2Q9, D2Q25, D2Q49, D2Q16, D2Q36, D2Q64. This coincides exactly with the ordering in accuracy of the various LB models in Figs. 2 and 3. This agreement indicates a direct link between discretization of the boundary conditions and numerical accuracy of the LB simulations.

To explore the origin of this behavior, we now compare Chapman-Enskog expansions of the diffuse boundary condition and the BGK equation. From Eq. (4), it is clear that the resulting moments in the boundary condition involve integrals over a half velocity space, \(c_y \in [0, \infty)\). This contrasts to moments related to the BGK equation, which are defined over the entire velocity space, \(c_y, c_x \in (-\infty, \infty)\) [16]. Importantly, abscissas of the G-H quadrature schemes of all LB models are derived specifically for moments over the entire velocity space [4,5]. Consequently, their application to half-space integrals can lead to inconsistent accuracy in discretization of moments in the flow and on the boundaries, as we now discuss.
If the discrete velocity space of any LB model includes directions parallel to the boundaries, these discrete particle velocities \((\pm c_i, 0)\) and their corresponding weights \(w_i\) will not contribute to half-space moments. Since these velocity spaces are derived from G-H quadrature, their weights \(w_i\) must satisfy the normalization condition over the entire velocity space: \(\sum_i w_i = 1\). For correct evaluation of half-space moments, the weights of contributing (nonparallel) discrete velocities must sum to \(1/2\) by symmetry. This condition is violated for any LB model that contains discrete velocities parallel to the solid boundaries. Such LB models will thus yield significant error in the half-space moments in Eq. (4).

To assess the practical consequences of this finding, we classify the LB models in Table I into two groups corresponding to discrete particle spaces that have boundary-parallel velocities: G1 (D2Q9, D2Q25, D2Q49), and those without velocities parallel to the boundary: G2 (D2Q16, D2Q36, D2Q64). In agreement with the above discussion, we find that all models in G2 give superior accuracy to those in G1. We also observe that increasing quadrature order has a comparatively small effect on accuracy relative to this boundary discretization phenomenon. This finding shows that careful choice of an LB model is necessary to ensure commensurate discretization of the fluid region and boundary conditions. Discrete particle velocities parallel to the boundaries must be avoided to ensure consistent accuracy of the bulk flow and boundary conditions.

We have examined the accuracy of LB models in simulations of wall bounded low-speed noncontinuum flows and discovered that interaction of the lattice with the solid boundaries primarily controls accuracy. This contrasts strongly to previous reports suggesting quadrature order as the mechanism. Our discovery explains previous observations of a nonmonotonic variation in accuracy with increasing quadrature order, and establishes a theoretical framework to guide accurate implementation of the LB method in wall bounded noncontinuum flows. Generalization to more complex flow configurations, including inclined and curved boundaries, provides interesting avenues for future investigation.

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[9] S. H. Kim, H. Pitsch, and I. D. Boyd, J. Comput. Phys. 227, 8655 (2008); The D2Q12 and D2Q21 models were also studied—these do not originate from 1D G-H quadrature (see Ref. [11]).
[11] Using the production formulas in Ref. [6], all 2D higher-order LB models discussed here are developed from 1D G-H quadrature given by Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).