Lattice Boltzmann method for linear oscillatory noncontinuum flows

Yong Shi,1,* Ying Wan Yap,2 and John E. Sader2,†

1Department of Mechanical, Materials and Manufacturing Engineering, The University of Nottingham Ningbo China, Ningbo 315100, People’s Republic of China

2Department of Mathematics and Statistics, The University of Melbourne, Victoria 3010, Australia

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Oscillatory gas flows are commonly generated by micro- and nanoelectromechanical systems. Due to their small size and high operating frequencies, these devices often produce noncontinuum gas flows. Theoretical analysis of such flows requires solution of the unsteady Boltzmann equation, which can present a formidable challenge. In this article, we explore the applicability of the lattice Boltzmann (LB) method to such linear oscillatory noncontinuum flows; this method is derived from the linearized Boltzmann Bhatnagar-Gross-Krook (BGK) equation. We formulate four linearized LB models in the frequency domain, based on Gaussian-Hermite quadratures of different algebraic precision (AP). The performance of each model is assessed by comparison to high-accuracy numerical solutions to the linearized Boltzmann-BGK equation for oscillatory Couette flow. The numerical results demonstrate that high even-order LB models provide superior performance over the greatest noncontinuum range. Our results also highlight intrinsic deficiencies in the current LB framework, which is incapable of capturing noncontinuum behavior at high oscillation frequencies, regardless of quadrature AP and the Knudsen number.

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I. INTRODUCTION

Developments in micro- and nanofabrication have spurred tremendous activity in studying flows generated by small-scale devices [1–7]. In contrast to their macroscopic counterparts, flows at micro- and nanometer length scales can deviate significantly from predictions of classical continuum treatments [2,4]. This is particularly the case for gas flows, where noncontinuum effects manifest themselves at both spatial and temporal scales, because (i) the mean free path of the gas is comparable to the device dimensions, and (ii) the characteristic time scale of the flow is not large relative to the molecular relaxation time.

Under steady conditions, noncontinuum effects occur only at the spatial scale and are normally characterized by the Knudsen number, Kn, which is the ratio of mean free path, λ, to the device dimension, L. Conventionally, flows at a very small Kn are considered to be in the continuum limit, and thus obey the Navier-Stokes equation with no slip at solid boundaries. Deviations from this continuum description occur for finite Kn, with flows normally classified in four nominal regimes: continuum flows for Kn < 0.01, slip flows for 0.01 < Kn < 0.1, transition flows for 0.1 < Kn < 10, and free molecular flows for Kn > 10 [8]. Gas flows generated by micro- and nanodevices, under normal atmospheric conditions, usually occur in the slip or transition regimes with the gas mean free path about 70 nm.

While the Knudsen number rigorously quantifies noncontinuum effects for steady flows, its specification alone is insufficient for description of unsteady phenomena. For example, vibrating nanomechanical structures can produce flows whose characteristic time scale is comparable to the molecular relaxation time of the gas [9,10]. In such cases, distinct noncontinuum effects at the temporal scale, in addition to those characterized by the Knudsen number at the spatial scale, can be exhibited. These temporal effects are characterized by a second dimensionless quantity, the frequency ratio, θ = ωτ, where ω and τ are the characteristic oscillatory frequency of the gas flow and the molecular relaxation time, respectively [11,12]. Unsteady noncontinuum flows are thus uniquely described by both Kn and θ; such flows can be profoundly affected by compounding nonequilibrium mechanisms at both the temporal and spatial scales [11–16]. Consequently, the true continuum limit of unsteady gas flows occurs for Kn ≪ 1 and θ ≪ 1—these flows are accurately described by the Navier-Stokes equation [17]. To facilitate discussion, we retain the convention that slip and transitional flows are defined solely in terms of the Knudsen number, as described above. An unsteady slip flow, for which 0.01 < Kn < 0.1, can therefore exhibit strong noncontinuum effects that deviate significantly from the continuum limit when the frequency ratio is large, i.e., θ ≫ 1.

For noncontinuum gas flows at arbitrary Kn and θ, a more fundamental theory is required, one of which is the unsteady Boltzmann Bhatnagar-Gross-Krook (BGK) equation [18]. Importantly, analytical solution of this kinetic equation under general conditions poses a formidable challenge, with exact or high-accuracy numerical solutions known for a few very simple problems [11,12]. Development of efficient numerical schemes for solution of the unsteady Boltzmann-BGK equation is thus highly desirable.

The lattice Boltzmann (LB) method has found widespread use in solving continuum flow problems [19–22]. Since it is based on the Boltzmann-BGK equation [23], the method has also been applied to the solution of noncontinuum gas flows [24–43]. Critically, LB models for noncontinuum flows have thus far mainly focused on steady problems that are only characterized by the Knudsen number, Kn. Most LB models
for steady noncontinuum flows are based on the framework developed for continuum flows. To account for noncontinuum effects, some of these models include ad hoc modifications. Two representative examples are the particle-based kinetic boundary condition [26,27,29], and use of an effective mean free path [31,37]. Such treatments allow the LB method to retain its mathematical simplicity, but limit its applications to weak noncontinuum flows, e.g., the slip flows for 0.01 < Kn < 0.1 and θ ≪ 1.

The accuracy of these modified LB models deteriorates strongly when applied to steady transition and free molecular flows [28]. In an attempt to overcome this problem, several studies [33–36,38,42,43] have proposed the use of high-order LB models—these models include more discrete particle velocities, that are based on Gaussian-Hermite (GH) quadratures of larger algebraic precision (AP) [44]. This enables a more accurate representation of the true (continuous) particle-velocity space by projection onto a finite truncated Hermite basis [23,33]. It has been shown that high-order LB models, in this hierarchy, can well capture steady unbounded flows, in the continuum through to the transition regime [43]. However, this LB hierarchy displays unusual convergence when applied to steady noncontinuum Couette flows, which are bounded by flat walls: Its accuracy does not increase monotonically with GH quadrature order. Significantly, low even-order LB models exhibit higher accuracy than high odd-order LB models [38]. This unexpected phenomenon is due to interaction of the lattice with solid boundaries—this effect dominates the accuracy of solution, with GH quadrature order playing a relatively minor role [42].

In this article, we explore the applicability of even- and odd-order LB models to unsteady bounded noncontinuum flows. This is directly relevant to the simulation of flows generated by modern nanomechanical devices, which are characteristically oscillatory. Interestingly, several studies have applied the LB method to oscillatory gas flows for small frequency ratios, θ, e.g., Refs. [39,41]. The case of arbitrary Knudsen number and frequency ratio remains to be explored—this is the focus of the present study. We develop a hierarchy of LB models based on the linearized Boltzmann-BGK equation using GH quadrature of varying AP, and apply these models to oscillatory Couette flows in the frequency domain. The accuracy of each LB model in this hierarchy, in particular those of high even order, is examined through comparison to high-accuracy numerical solutions to the linearized Boltzmann-BGK equation [12].

The paper is organized as follows: We first develop a GH quadrature-based hierarchy consisting of four linearized LB models in the frequency domain; its derivation is based on the general approach in Ref. [38]. For compatibility with their large discrete particle-velocity space, temporal and spatial derivatives are discretized using finite difference techniques. Linearization and discretization of the diffusive boundary condition is presented in Sec. III. In Sec. IV, we simulate two-dimensional oscillatory Couette flows over a wide range of the Knudsen numbers and frequency ratios. Detailed evaluation of each linearized LB model is then carried out using high-accuracy numerical solutions to the linearized Boltzmann-BGK equation [12] as benchmarks.

II. FINITE DIFFERENCE LINEARIZED LB MODEL IN THE FREQUENCY DOMAIN

In this section, we derive LB models from the linearized Boltzmann-BGK equation in the frequency domain. The merits of the LB model in the frequency domain for oscillatory flows have been discussed previously [40] by comparison to solutions using the conventional time-dependent LB method.

The linearized Boltzmann-BGK equation is [45]

$$\frac{\partial \hat{h}}{\partial t} + c \cdot \frac{\partial \hat{h}}{\partial \mathbf{r}} = -\frac{1}{\tau} (h - h^\text{eq}),$$  

(1)

where $t$, $\mathbf{r}$, $c$, and $\tau$ are the time, position, particle velocity, and relaxation time, respectively. The functions $h$ and $h^\text{eq}$ are perturbations to the distribution function $f$ and its local equilibrium $f^\text{eq}$ from a global equilibrium state, for which the gas has constant density $\rho_0$, constant temperature $T_0$, and zero velocity $\mathbf{u}_0 = 0$. Under isothermal conditions, $h$ and $h^\text{eq}$ are defined [45],

$$h = \hat{f} - \hat{f}^\text{eq} = 1,$$  

(2)

and

$$h^\text{eq} = \frac{\delta \rho}{\rho_0} + \frac{\mathbf{c} \cdot \mathbf{u}}{RT_0},$$  

(3)

where $\hat{f}^\text{eq}$ is the global equilibrium distribution function, $R$ is the gas constant, and $\delta \rho$ and $\mathbf{u}$ are the fluid density and velocity perturbations, respectively. The linearized Boltzmann-BGK equation, i.e., Eq. (1), describes the evolution of $\hat{h}$ in phase space with time $t$ due to gas particle streaming and collisions. It can be rewritten in the frequency domain by a transform $\hat{h}(t,\mathbf{r},c) = h(\omega,\mathbf{r},c) e^{i\omega t}$ [46], with radial frequency $\omega$ and the usual imaginary unit $i$. It follows that

$$\frac{\partial \hat{h}}{\partial t} + c \cdot \frac{\partial \hat{h}}{\partial \mathbf{r}} = -\frac{\hat{h}}{\tau^*} + \frac{\hat{h}^\text{eq}}{\tau},$$  

(4)

where the complex relaxation time $\tau^* = \tau/(1 + i\omega\tau)$ and $h^\text{eq}(\omega,\mathbf{r},c) = \hat{h}^\text{eq}(\omega,\mathbf{r},c) e^{i\omega t}$. Importantly, an explicit time-marching LB algorithm cannot be applied directly to solve Eq. (4). We therefore modify Eq. (4) using the treatment in Ref. [40]—a virtual time $\tau'$ is introduced, which adds the term $\partial \hat{h}/\partial \tau'$ to the left side of Eq. (4). As a consequence, a virtual time-dependent Boltzmann-BGK equation in the frequency domain is obtained:

$$\frac{\partial \hat{\tilde{h}}}{\partial \tau'} + c \cdot \frac{\partial \hat{\tilde{h}}}{\partial \mathbf{r}} = -\frac{\hat{\tilde{h}}}{\tau^*} + \frac{\hat{\tilde{h}}^\text{eq}}{\tau}.$$  

(5)

By definition, the steady-state solution to Eq. (5) gives the required solution to Eq. (4). Equation (5) differs only slightly from the original linearized Boltzmann-BGK equation, Eq. (1), due to the presence of the complex relaxation time $\tau^*$. We thus can numerically solve Eq. (5) using the LB method. To formulate the corresponding algorithm, we first discretize the particle-velocity space in Eq. (5) using GH quadrature, and obtain

$$\frac{\partial \hat{\tilde{h}}}{\partial \tau'} + \mathbf{c}_j \cdot \frac{\partial \hat{\tilde{h}}}{\partial \mathbf{r}} = -\frac{\hat{\tilde{h}}}{\tau^*} + \frac{\hat{\tilde{h}}^\text{eq}}{\tau},$$  

(6)

where $\hat{\tilde{h}}_j$ represents the perturbation in terms of the discrete particle velocity $\mathbf{c}_j$, and the discrete perturbation to the local
equilibrium $\hat{h}_{j}^{eq}$ is

$$
\hat{h}_{j}^{eq} = \frac{\delta \hat{p}}{\rho_0} + \frac{c_j \cdot \mathbf{u}}{c_s^2},
$$

(7)

Here, the sound speed $c_s = \sqrt{RT_0}$, and $\delta \hat{p}$ and $\mathbf{u}$ are the frequency-dependent fluid density and velocity perturbations, respectively. They can be computed from $\hat{h}_j$ and $\hat{h}_j^{eq}$ using

$$
\delta \hat{p} = \rho_0 \sum_j w_j \hat{h}_j = \rho_0 \sum_j w_j \hat{h}_j^{eq},
$$

$$
\mathbf{u} = \sum_j w_j \hat{h}_j \mathbf{e}_j = \sum_j w_j \hat{h}_j^{eq} \mathbf{e}_j,
$$

(8)

where $w_j$ is the moment weight corresponding to $c_j$. The discrete particle-velocity space in Eqs. (6)–(8) is specified through the discrete particle-velocity space in $\hat{h}_j^{eq}$ using

$$
\hat{h}_{j}^{eq} = \frac{\delta \hat{p}}{\rho_0} + \frac{c_j \cdot \mathbf{u}}{c_s^2}.
$$

(7)

The evolution equation reads

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \hat{h}_j(x_0, y_0) - \hat{h}_j(x_0 - \Delta x, y_0)
$$

$$
+ \frac{\hat{h}_j(x_0 + \Delta x, y_0) - 2\hat{h}_j(x_0, y_0) + \hat{h}_j(x_0 - 2\Delta x, y_0)}{2\Delta x},
$$

$$
c_{jx} > 0,
$$

(12a)

while using the hybrid scheme at nodes $(x_1, y_1)$ nearest to the solid boundaries results in [48]

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \frac{\hat{h}_j(x_1, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{\Delta x}
$$

$$
+ (1 - \varepsilon) \frac{\hat{h}_j(x_1 + \Delta x, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{2\Delta x},
$$

$$
c_{jx} > 0,
$$

(13a)

and

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \frac{\hat{h}_j(x_1, y_1) - \hat{h}_j(x_1, y_1)}{\Delta x}
$$

$$
+ (1 - \varepsilon) \frac{\hat{h}_j(x_1 + \Delta x, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{2\Delta x},
$$

$$
c_{jx} < 0,
$$

(13b)

Equation (6) needs to be further discretized in virtual time and physical space. To gain compatibility with the large discrete particle-velocity spaces, namely D2Q16, D2Q25, and D2Q36, we carry out temporal and spatial discretization of Eq. (6) using finite difference techniques. Following the discretization procedure proposed in Ref. [47], we obtain a linearized finite difference LB model in the frequency domain. Its evolution equation reads

$$
\hat{g}_{j+1}^{k+1} = \hat{g}_j + \Delta \tau \cdot \left( \hat{g}_{j+1} - \hat{g}_j \right) + \frac{\delta \hat{h}_j}{\delta x} + \frac{\Omega_g \hat{g}_{j+1}^k}{\Omega_g - \hat{g}_j^k},
$$

(9)

In Eq. (9), we introduce a new function $\hat{g}_j$:

$$
\hat{g}_j = \hat{h}_j \left( \frac{1 + \Omega \theta_1}{2} \right) + \frac{\Omega}{2} \left( \hat{h}_j - \hat{h}_j^{eq} \right).
$$

(10)

This function is used to compute $\delta \hat{p}$ and $\mathbf{u}$:

$$
\delta \hat{p} = \rho_0 \sum_j w_j \hat{g}_j, \quad \mathbf{u} = \sum_j w_j \hat{g}_j \mathbf{e}_j.
$$

(11)

Spatial discretization has been formally represented by a term in brackets on the left side of Eq. (9). In this article, we adopt the second-order upwind scheme to approximate the spatial gradients on bulk nodes, while the hybrid scheme is used for those on the nodes in the vicinity of solid boundaries. To be specific, the second-order upwind scheme computes the derivative $\partial \hat{h}_j/\partial x$ at bulk nodes $(x_0, y_0)$ in Cartesian coordinates as follows [48]:

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \frac{\hat{h}_j(x_0, y_0) - \hat{h}_j(x_0 - \Delta x, y_0)}{\Delta x}
$$

$$
+ \frac{\hat{h}_j(x_0 + \Delta x, y_0) - 2\hat{h}_j(x_0, y_0) + \hat{h}_j(x_0 - 2\Delta x, y_0)}{2\Delta x},
$$

$$
c_{jx} > 0,
$$

(12a)

while using the hybrid scheme at nodes $(x_1, y_1)$ nearest to the solid boundaries results in [48]

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \frac{\hat{h}_j(x_1, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{\Delta x}
$$

$$
+ (1 - \varepsilon) \frac{\hat{h}_j(x_1 + \Delta x, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{2\Delta x},
$$

$$
c_{jx} > 0,
$$

(13a)

and

$$
\frac{\partial \hat{h}_j}{\partial x} \approx \frac{\hat{h}_j(x_1, y_1) - \hat{h}_j(x_1, y_1)}{\Delta x}
$$

$$
+ (1 - \varepsilon) \frac{\hat{h}_j(x_1 + \Delta x, y_1) - \hat{h}_j(x_1 - \Delta x, y_1)}{2\Delta x},
$$

$$
c_{jx} < 0,
$$

(13b)

where $\Delta x$ denotes the grid spacing. The prefactor $\varepsilon$ in Eqs. (13a) and (13b) is determined from numerical tests. In this article, we choose $\varepsilon = 0.05$ to ensure LB simulations are stable while nearly second-order accurate.

In summary, Eqs. (7), (9)–(11), together with the discrete particle-velocity spaces D2Q9, D2Q16, D2Q25, and D2Q36 [38,42]; see Appendix A.

III. BOUNDARY CONDITIONS AT SOLID WALLS

The conventional no-slip boundary condition does not apply to noncontinuum flows. Maxwell proposed a different approximation at the kinetic scale, the so-called diffusive boundary condition. This boundary condition specifies the distribution function $f$ for particles leaving the walls by [49]

$$
f(r_p, c) = \int_{(r_p - u_b, c) \cdot n > 0} f(r_p, c) d\mathbf{c}
$$

$$
\times f^{eq}(r_p, c, \rho_b, u_b, T_b) d\mathbf{c},
$$

(14)

where $n$ is the unit vector normal to the wall and into the gas, and $\rho_b$, $u_b$, and $T_b$ are the fluid density, wall velocity, and wall temperature at the position $r = r_p$, respectively. Equation (14) is specified in terms of the full nonlinear time-dependent distribution function $f$, which is continuous in particle-velocity space. Consequently, it cannot be directly
applied to simulation of the linearized LB models developed in Sec II. We therefore linearize Eq. (14) and discretize its particle-velocity space. For compatibility with the LB models, it is derived in the frequency domain. Importantly, for flat walls such as the solid boundaries in oscillatory Couette flows, Eq. (14) simplifies to

\[
\hat{h}_j = \hat{h}_j^{eq} - \frac{2\pi}{c_j} \left[ \sum_{\epsilon_j, n < 0} w_j (c_j' \cdot n) \hat{h}_j' \right] + \sum_{\epsilon_j, n > 0} w_j (c_j' \cdot n) \hat{h}_j^{eq} , \quad c_j \cdot n > 0 .
\]  

Equation (15) is the frequency-dependent linearized discrete diffusive boundary condition. Its detailed derivation is given in Appendix B. In simulations, we apply it locally to update the perturbation functions with velocities \( c_j \cdot n > 0 \) at a wall node while those with velocities \( c_j \cdot n \leq 0 \) are interpolated from their neighboring nodes inside the fluid zone or on the wall through Eq. (9). With this boundary treatment, we do not require any ghost nodes in the wall to close the computation, even for high-order LB models.

**IV. NUMERICAL SIMULATIONS AND DISCUSSION**

In this section, we will apply the developed linearized LB hierarchy, consisting of a linearized on-lattice D2Q9 LB model and linearized finite difference D2Q16, D2Q25, D2Q36 LB models, to simulate oscillatory Couette flows over a wide range of the Knudsen numbers and frequency ratios. The Couette flow geometry is illustrated in Fig. 1, which includes two parallel plates separated by a distance \( L \). These plates oscillate in opposite directions along their planes with identical velocity amplitudes \( u_0 \) and radial frequency \( \omega \). Throughout this section, all time-dependent variables are expressed in the complex frequency domain. For example, the velocity of the top plate in the \( x \) direction is \( u_{wall} = U_0 e^{i \omega t} \).

We perform LB simulations for Knudsen numbers in the range \( 0.1 \leq Kn \leq 5 \) and frequency ratios \( 0.05 \leq \theta \leq 5 \). The linearized discrete diffusive boundary condition, Eq. (15), is applied to specify \( h_j \) at the solid walls and periodic boundary conditions are used in the \( x \) direction (see Fig. 1).

For simplicity, numerical results are nondimensionalized by setting the plate separation, \( L = 1 \), the reference density \( \rho_0 = 1 \), and the oscillation amplitude \( u_0 = 1 \). Capitalis are used to represent these dimensionless parameters, e.g., \( \bar{Y} = y/L \) and \( \bar{U} = u/u_0 \). We introduce the Courant-Friedricks-Lewey number CFL = \( c_m \Delta t / \Delta x \) in the linearized finite difference LB simulations, where \( c_m \) is the maximum particle speed; CFL is required to range between 0.1 and 0.2 to ensure numerical stability. All simulations are performed on a uniform \( 200 \times 200 \) grid, except for the simulation with \( Kn = 0.1 \) and \( \theta = 5 \), where a dense \( 400 \times 400 \) grid is used to achieve the grid-independent results. The Mach number \( M = 0.16 \), and the two dimensionless relaxation frequencies \( \Omega \) and \( \Omega^* \) are calculated from Kn and \( \theta \). Numerical convergence is tracked by comparing the absolute difference between the results obtained at the \( N \)th and the \( (N + 1500) \)th time steps. The criterion for convergence is defined as \( |U_{\delta t = 15000} - U_N| \leq 10^{-4} \), where \( U_N \) represents the real or imaginary part of the velocity at the \( N \)th time step.

The D2Q9 LB model gives excellent agreement with the known exact analytical solution for continuum flows (\( Kn \ll 1 \) and \( \theta \ll 1 \)) [17]; the interested reader is referred to Ref. [40]. In this article, we focus on noncontinuum flows and begin by examining the slip regime, \( 0.01 \leq Kn < 0.1 \), for various frequency ratios \( \theta \). It is known that under these circumstances, significant slip exists at the solid walls. Figure 2 gives numerical results, including both real and imaginary parts, from the linearized LB hierarchy for flows with \( Kn = 0.1 \) and \( \theta = 0.05, 1, \) and 5. Only the top half of the flow, i.e., \( 0.5 \leq y \leq 1 \), is shown due to the inherent symmetry. In Fig. 2(a) for \( \theta = 0.05 \), we observe that the slip velocity obtained using various LB models differs, as does the nature of the flow in the vicinity of the plate. To assess the relative merits of these LB models, we compare their predictions to high-accuracy numerical solutions of the linearized Boltzmann-BGK equation [12]. This comparison shows that the accuracy of the linearized LB hierarchy for small-\( \theta \) oscillatory Couette flows varies nonmonotonically as the discrete particle-velocity space expands. Significantly, as was previously observed for steady Couette flows [38,42], even-order GH quadrature-based LB models (D2Q16 and D2Q36) possess superior accuracy to odd-order models (D2Q9 and D2Q25). This numerical observation shows that unsteady slip flows, at small \( \theta \), behave in a similar fashion to steady noncontinuum flows, for identical Kn. As such, computational accuracy is controlled primarily by the interaction between the lattice and solid boundaries [42]. It remains to be seen if this finding holds for unsteady flows at higher values of \( \theta \).

Figures 2(b) and 2(c) present the results of unsteady slip flows under the same conditions as Fig. 2(a) but at two larger frequency ratios: \( \theta = 1 \) and 5. In these two cases, we clearly observe a boundary layer in the vicinity of the plate. Its thickness can be coarsely approximated by the continuum result \( \delta \approx \sqrt{2Kn} / \nu = 2 Kn L / (\sqrt{\pi \theta}) \), which depends on both the Knudsen number \( Kn \) and frequency ratio \( \theta \); \( \nu \) is the kinematic viscosity of the gas. The high-accuracy numerical solutions in Figs. 2(a)–2(c) also obey this relation, with the “thickness” of the boundary layer, and hence the length scale of the flow, decreasing with increasing \( \theta \) (at fixed Kn).
FIG. 2. (Color online) Velocity fields for oscillatory Couette flows with Kn = 0.1 for (a) θ = 0.05, (b) θ = 1, (c) θ = 5, using D2Q9, D2Q16, D2Q25, and D2Q36. High-accuracy numerical solutions to the linearized Boltzmann-BGK equation (denoted BGK) in Ref. [12]. D2Q9 is unstable for θ = 5.

In Fig. 2(b), even-order LB models (D2Q16 and D2Q36) for θ = 1 exhibit better accuracy than the odd-order LB models (D2Q9 and D2Q25) in the vicinity of solid walls. However, unusual behavior is observed away from the walls: The velocity fields predicted by even-order LB models exhibit spatial oscillations—this differs considerably from small-θ flows in Fig. 2(a). We also find the amplitudes of these oscillatory velocity profiles depend strongly on the discrete particle-velocity space. Use of a larger discrete velocity space, e.g., the D2Q36 model, attenuates these (artificial) numerical oscillations, leading to better agreement with the high-accuracy numerical solution [12].

These unexpected artificial oscillations increase in intensity for θ = 5 [see Fig. 2(c)], with even-order LB models exhibiting larger amplitudes and shorter spatial wavelengths in the velocity field than those present in Fig. 2(b). Oscillations also
These artificial oscillations are independent of the central finite difference scheme in Eqs. (13a) and (13b)—this was verified by changing $\epsilon$ from 0.05 to 1, for which the observed oscillations were identical. These oscillations are therefore not due to instability in the numerical procedure but point to a significant deficiency in the present LB framework for simulating flows at small Kn, but moderate to high $\theta$. Such anomalous behavior is not entirely unexpected, since it is known that increasing $\theta$ enhances noncontinuum effects on the temporal scale, even at small mean free paths. We are thus led to the conclusion that the accuracy of these LB models decreases with increasing $\theta$, at fixed and small Kn.

In Fig. 3, we present results for the shear stress under identical conditions to Fig. 2. High-accuracy numerical solutions obtained directly from the linearized Boltzmann-BGK equation [12] are also provided as benchmark data. For flows with small to moderate frequency ratios, i.e., Figs. 3(a)

![Graphs showing shear stress distribution for $\theta = 0.05$, $\theta = 1$, and $\theta = 5$, with results from different LB models compared to benchmark data.](image)
and 3(b), we again observe numerical phenomena similar to Fig. 2—even-order LB models exhibit better accuracy than odd-order LB models for small-$\theta$ flows, while they suffer from spatial oscillations when $\theta$ grows to a moderate value, e.g., $\theta = 1$. Even so, the accuracy of both even- and odd-order LB models gradually improves as the discrete particle-velocity space expands; e.g., D2Q25 is more accurate than D2Q9, and D2Q36 is better than D2Q16. For flows at large $\theta$, the current linearized LB hierarchy again fails to provide reasonable predictions; see Fig. 3(c). Similar to the velocity fields, we observe strong artificial spatial oscillations in the shear stress profiles that deviate from the high-accuracy solutions from Ref. [12].

These artificial spatial oscillations in the LB simulations appear to be due to the unsteady nature of the flow. To explore this phenomenon further, we perform LB simulations in the transition flow regime. Figure 4 shows the resulting velocity profiles for oscillatory Couette flows with $Kn = 1$.
and $\theta = 0.05, 1, and 5$, while Fig. 5 presents the corresponding shear stress distributions.

As expected for flows in the transition regime, all four LB models exhibit significant deviations from high-accuracy numerical solutions to the linearized Boltzmann-BGK equation [12]. However, the nature and magnitudes of these deviations in each case are intrinsically different. For the lowest frequency ratio, $K_n = 1$ and $\theta = 0.05$, LB simulations still qualitatively capture the velocity [Fig. 4(a)] and shear stress [Fig. 5(a)] profiles, albeit with larger error than for slip flow. In particular, D2Q36 gives rather close agreement with the high-accuracy numerical solution. This is not surprising since noncontinuum effects at small frequency ratios are mainly characterized by $K_n$, which can be effectively captured by LB models with even-order discrete particle-velocity spaces [38,42]. However, at high frequency ratios, temporal noncontinuum effects are strong, which compound existing spatial noncontinuum effects in the transition regime. None of the four LB models effectively predict flow behavior under such circumstances. In Figs. 4(b) and 5(b), we observe...
significant deviations in LB results for flows with $\text{Kn} = 1$ and $\theta = 1$, while LB results are qualitatively incorrect for $\text{Kn} = 1$ and $\theta = 5$; see Figs. 4(c) and 5(c).

The presented results for unsteady slip and transition flows demonstrate an essential shortcoming in the LB method for unsteady noncontinuum flows. The presence of significant noncontinuum effects, whether it is of a spatial or temporal nature, leads to significant deterioration in accuracy of LB models. Critically, this shows that use of high-order LB models based on GH quadratures with large AP is not an effective approach for simulating strongly unsteady noncontinuum flows, characterized by large frequency ratios.

V. CONCLUSIONS

We have explored the applicability of the linearized frequency-dependent LB method to unsteady Couette flows, at finite Knudsen numbers and frequency ratios; diffusive boundary conditions were applied at the solid walls. As previously suggested, particle-velocity space was discretized using high-order GH quadrature to account for noncontinuum effects. This led to a hierarchy of linearized frequency-dependent LB models, ranging from D2Q9 to D2Q36.

The computational accuracy of each LB model was explored in the unsteady slip and transition regimes. This accuracy was found to decrease with increasing Knudsen number and/or frequency ratio, with their effects compounding. For slip flows ($0.01 \leq \text{Kn} \leq 0.1$), increasing the frequency ratio $\theta$ decreases LB accuracy with unphysical spatial oscillations appearing in both the velocity and shear stress profiles. The situation is exacerbated for transition flows, $\text{Kn} \sim O(1)$. Nonetheless, LB models of high even order allow for application of the LB method over the greatest noncontinuum range, spanned by both the Knudsen number and frequency ratio. The findings of this study show that the present LB models based on GH quadratures of different AP are incapable of capturing strongly unsteady noncontinuum flows, regardless of the Knudsen number.

ACKNOWLEDGMENTS

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FIG. 6. (Color online) Configuration of the two-dimensional discrete particle-velocity spaces developed from a GH hierarchy of AP = 5, 7, 9, and 11, for noncontinuum flows.
The discrete particle velocity $c_j$ and its moment weight $w_j$, for D2Q9, D2Q16, D2Q25, and D2Q36. The coefficients, $a$, $b$, and $c$, specify velocity components in Cartesian coordinates, which are obtained by multiplying the abscissae of the GH quadrature with the sound speed $c_s$. The subscript, $FS$, denotes full symmetry.

**TABLE I**

| D2Q9   | $c_j = \begin{cases} 
(a,0)_{FS}, & j = 1 - 4 \\
(±a, ±a), & j = 5 - 8 \\
(0,0), & j = 9 
\end{cases}$ | $a = \sqrt{3} c_s$ | $w_{1-4} = 1/9$ |
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<td>$w_{5-8} = 1/36$</td>
<td>$w_9 = 4/9$</td>
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| D2Q16  | $c_j = \begin{cases} 
(±a, ±a), & j = 1 - 4 \\
(±b, ±b), & j = 5 - 8 \\
(a,b)_{FS}, & j = 9 - 16 
\end{cases}$ | $a = \sqrt{3 - \sqrt{6}} c_s$ | $w_{1-4} = (5 + 2\sqrt{6})/48$ |
|        | $w_{5-8} = (5 - 2\sqrt{6})/48$ | $w_{9-16} = 1/48$ | |
| D2Q25  | $c_j = \begin{cases} 
(±a, ±a), & j = 1 - 4 \\
(±b, ±b), & j = 5 - 8 \\
(a,b)_{FS}, & j = 9 - 12 \\
(0,0), & j = 13 - 24 
\end{cases}$ | $a = \sqrt{5 - \sqrt{10}} c_s$ | $w_{1-4} = (14 + 4\sqrt{10})/225$ |
|        | $w_{5-8} = (14 - 4\sqrt{10})/225$ | $w_{9-12} = (89 + 28\sqrt{10})/3600$ | |
|        | $w_{13-16} = (89 - 28\sqrt{10})/3600$ | $w_{17-24} = 1/400$ | |
|        | $w_{25} = 64/225$ | $w_{26} = 0.1671$ | |
| D2Q36  | $c_j = \begin{cases} 
(±a, ±a), & j = 1 - 4 \\
(±b, ±b), & j = 5 - 8 \\
(±c, ±c), & j = 9 - 12 \\
(a,b)_{FS}, & j = 13 - 20 \\
(a,c)_{FS}, & j = 21 - 28 \\
(b,c)_{FS}, & j = 29 - 36 
\end{cases}$ | $a = 0.6167 c_s$ | $w_{1-4} = 7.85 \times 10^{-3}$ |
|        | $w_{5-8} = 6.53 \times 10^{-6}$ | $w_{9-12} = 3.62 \times 10^{-2}$ | |
|        | $w_{13-20} = 1.04 \times 10^{-3}$ | $w_{21-28} = 2.26 \times 10^{-4}$ | |

**APPENDIX A: DISCRETE PARTICLE VELOCITY SPACES**

In this Appendix, we present the four discrete particle-velocity spaces used in the LB method. We follow the conventional notation $DmQn$ [50], where $m$ is the dimensionality of physical space and $n$ is the number of discrete particle velocities. Figure 6 schematically illustrates the configurations of these four discrete particle-velocity spaces in two-dimensional Cartesian coordinates (i.e., $m = 2$). Table I summarizes their mathematical specifications.

**APPENDIX B: DERIVATION OF THE LINEARIZED discrete DIFFUSIVE BOUNDARY CONDITION IN THE FREQUENCY DOMAIN**

Here, the linearized discrete diffusive boundary condition in the frequency domain is derived. We start from the Maxwell diffusive boundary condition, Eq. (14), which is rewritten in terms of $h$:

$$
\frac{h(r_b, c) + 1}{h^{eq}(r_b, c) + 1} = \frac{\int_{(c - u_b) \cdot n > 0} |(c' - u_b) \cdot n|^2 f^{eq}(c') h(r_b, c') d c' + \int_{(c - u_b) \cdot n < 0} |(c' - u_b) \cdot n|^2 f^{eq}(c') d c'}{\int_{(c - u_b) \cdot n > 0} |(c' - u_b) \cdot n|^2 f^{eq}(c') h(r_b, c') d c' + \int_{(c - u_b) \cdot n < 0} |(c' - u_b) \cdot n|^2 f^{eq}(c') d c'}. \quad (B1)
$$

The diffusive boundary condition is applied to solid boundaries in oscillatory Couette flows—these boundaries are flat walls that exhibit in-plane oscillations, i.e., $u_b \cdot n = 0$; see Fig. 1. Equation (B1) thus reduces to

$$
\frac{h(r_b, c) + 1}{h^{eq}(r_b, c) + 1} = \frac{\Delta \frac{d h}{d c}}{\Delta \frac{d h^{eq}}{d c} + \int_{n > 0} |(c' - n) f^{eq}(c') h^{eq}(r_b, c') d c'|} \leq 0. \quad (B2)
$$

Next, we discretize the particle-velocity space in Eq. (B2) using the same procedure as that for the LB models. At the wall position, $r = r_b$, we have

$$
h_j = \frac{-\sum_{c_j, n < 0} w_j (c_j' \cdot n) h_j + c_j/\sqrt{2\pi} (h_j^{eq} + 1) - 1, \quad c_j \cdot n > 0. \quad (B3)
$$

As both perturbation functions, $h_j$ and $h_j^{eq}$, are small, we neglect nonlinear terms of the form of $h_j^{eq} \cdot h_j$ in Eq. (B3). After several manipulations, we obtain a simple linearized discrete diffusive boundary condition,

$$
h_j = h_j^{eq} - \frac{\sqrt{2\pi}}{c_s} \left[ \sum_{c_j, n < 0} w_j (c_j' \cdot n) h_j + \sum_{c_j, n > 0} w_j (c_j' \cdot n) h_j^{eq} \right], \quad c_j \cdot n > 0. \quad (B4)
$$
In the frequency domain, this boundary condition becomes
\[ \hat{h}_j \equiv \hat{h}_j^{\text{eq}} - \frac{\sqrt{2\pi}}{c_s} \left[ \sum_{c'_j, n < 0} w_j(c'_j \cdot n)\hat{h}_j + \sum_{c'_j, n > 0} w_j(c'_j \cdot n)\hat{h}_j^{\text{eq}} \right], \quad c'_j \cdot n > 0. \tag{B5} \]

and is used in all linear LB simulations.