Efficient kinetic method for fluid simulation beyond the Navier-Stokes equation

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We present a further theoretical extension to the kinetic theory based formulation of the lattice Boltzmann method of Shan et al (2006). In addition to the higher order projection of the equilibrium distribution function and a sufficiently accurate Gauss-Hermite quadrature in the original formulation, a new regularization procedure is introduced in this paper. This procedure ensures a consistent order of accuracy control over the non-equilibrium contributions in the Galerkin sense. Using this formulation, we construct a specific lattice Boltzmann model that accurately incorporates up to the third order hydrodynamic moments. Numerical evidences demonstrate that the extended model overcomes some major defects existed in the conventionally known lattice Boltzmann models, so that fluid flows at finite Knudsen number (Kn) can be more quantitatively simulated. Results from force-driven Poiseuille flow simulations predict the Knudsen’s minimum and the asymptotic behavior of flow flux at large Kn.

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I. INTRODUCTION

Understanding and simulating fluid flows possessing substantial non-equilibrium effects pose a long standing challenge to fundamental statistical physics as well as to many other science and engineering disciplines [1, 2]. Due to either rarefaction effects or small geometric scales, such flows are characterized by a finite Knudsen number, defined as the ratio between the particle mean free path, l, and the characteristic length, L. Kn = l/L. At sufficiently large Knudsen numbers, many of the continuum assumptions breakdown [3]. In particular, the Navier-Stokes equation and the no-slip boundary condition become inadequate.

Since the Boltzmann equation is valid for describing fluid flows at any Kn [3], the conventional approach for constructing extended hydrodynamic equations for higher Kn regimes has been through employing higher order Chapman-Enskog approximations resulting in, e.g., the Burnett and super Burnett equations. However, this approach encounters both theoretical and practical difficulties [4, 5]. Alternatively, attempts have been made to extend the Grad’s 13 moment system [6] by including contributions of higher kinetic moments [5]. One major difficulty has been the determination of the boundary condition for these moments because only the lowest few have clear physical meanings. In addition, due to the complexity in the resulting equations, application of this approach is so far limited to simple one-dimensional situations. Nevertheless, the moment based formulation offers an valuable insight into the basic fluid physics for high Kn flows.

Over the past two decades, the lattice Boltzmann method (LBM) has developed into an efficient computational fluid dynamic (CFD) tool [5]. Due to its kinetic nature, LBM intrinsically possesses some essential microscopic physics ingredients and is well suited for handling more general boundary conditions. Certain characteristic phenomena in micro-channel flows were predicted in LBM simulations at least qualitatively [10, 11, 12, 13, 14, 15, 16, 17, 18]. In addition, by introducing a “stochastic virtual wall collision” process mimicking effects of free particle streaming in a long straight channel [14], analytically known asymptotic behavior at very large Kn were also produced. Nevertheless, being historically developed only to recover fluid physics at the Navier-Stokes level, the existing LBM schemes used in these studies possess some well known inaccuracies and numerical artifacts. Therefore, strictly speaking the schemes are not applicable to high Kn flows other than for some rather limited situations. It is important to develop an LBM method capable of performing accurate and quantitative simulations of high Kn flows in general.

Recently, based on the moment expansion formulation [19], a systematic theoretical procedure for extending LBM beyond the Navier-Stokes hydrodynamics was developed [20]. In this work, we present a specific extended LBM model from this procedure containing the next order kinetic moments beyond the Navier-Stokes. A three-dimensional (3D) realization of this LBM model employs a 39-point Gauss-Hermite quadrature with a sixth order isotropy. In addition, a previously reported regularization procedure [21, 22], that is fully consistent with the moment expansion formulation, is incorporated and extended to the corresponding order. Simulations performed with the extended LBM have shown to capture certain characteristic features pertaining to finite Kn flows. There is no empirical models used in the new LBM.

II. BASIC THEORETICAL DESCRIPTION

It is theoretically convenient to describe a lattice Boltzmann equation according to the Hermite expansion representation [20]. The single-particle distribution functions at a set of particular discrete velocity values, \( \{ \xi_a : a = 1, \cdots, d \} \), are used as the state variables to describe a fluid system. The velocity-space discretization is shown to be equivalent to projecting the distribution function onto a sub-space spanned by
the leading \( N \) Hermite orthonormal basis, denoted by \( \mathbb{E}^N \)
hereafter, provided that \( \{ \xi_a \} \) are the abscissas of a sufficiently
accurate Gauss-Hermite quadrature \[19, 20\]. Adopting the
BGK collision model \[23\], the discrete distribution values, \( f_a \),
satisfy the following equation:

\[
\frac{\partial f_a}{\partial t} + \xi_a \cdot \nabla f_a = \Omega_a \tag{1a}
\]

\[
\Omega_a = -\frac{1}{\tau} \left[ f_a - f_a^{(0)} \right] + F_a, \quad a = 1, \cdots, d, \tag{1b}
\]

where \( \tau \) is a relaxation time, \( f_a^{(0)} \) is the truncated Hermite ex-
pansion of the Maxwell-Boltzmann distribution evaluated at
\( \xi_a \), and \( F_a \) is the contribution of the body force term. The
truncation level determines the closeness of the above equation to
approximate the original continuum BGK equation. A Chapman-Enskog
analysis reveals that the Navier-Stokes truncation level determines
the closeness of the above equation to approximate the original
continuum BGK equation. Explicitly speaking, recovering a Chapman-Enskog
analysis to approximate the original continuum BGK equation.

\[
\delta_{ijkl}^{(4)} = \delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} + \delta_{ik}\delta_{jl} \tag{2a}
\]

\[
\delta_{ijklmn}^{(6)} = \delta_{ij}\delta_{kl}\delta_{mn} + \delta_{im}\delta_{jn}\delta_{lk} + \delta_{im}\delta_{jn}\delta_{kl} \tag{2b}
\]

Indeed, direct verification shows that these are satisfied by
the 3D 39-speed model \( (E^{39}_{3,7}) \) and its 2D projection \( (E^{21}_{2,7}) \).

\[
f_a(x + \xi_a, t + 1) = f_a(x, t) - \frac{1}{\tau} \left[ f_a(x, t) - f_a^{(0)} \right] + F_a \tag{5}
\]

As usual, the “lattice convention” with unity time increment is
used here.

### III. THE REGULARIZATION PROCEDURE

An LBM computation is generally carried out in two steps: the
streaming step in which \( f_a \) at \( x \) is moved to \( x + \xi_a \), and the
collision step in which \( f_a(x) \) is replaced with the right-hand-side of
Eq. (5). When viewed as a projection of the continuum BGK equation into \( \mathbb{H}^N \),
this dynamic process introduces an error due to the fact that \( f_a \) does not automatically
lie entirely within \( \mathbb{H}^N \). Borrowing the language from spectral
analysis, this is analogous to the aliasing effect. When the
system is not far from equilibrium, such an error is small and
ignorable. On the other hand, this error can be resolved via
an extension of the “regularization procedure” previously
designed for improvement in stability and isotropy \[21, 22\]. In

\[
\sum_{a=1}^{d} w_a = 1 \tag{3a}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} = \delta_{ij} \tag{3b}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} \xi_{a,k} \xi_{a,l} = \delta_{ijkl}^{(4)} \tag{3c}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} \xi_{a,k} \xi_{a,l} \xi_{a,m} \xi_{a,n} = \delta_{ijklmn}^{(6)} \tag{3d}
\]

where the roman subscripts \( i, j, \ldots \) denote Cartesian com-
ponents. In the above, \( \delta_{ij} \) is the Kronecker delta function,
while \( \delta_{ijkl}^{(4)} \) and \( \delta_{ijklmn}^{(6)} \) represent, respectively, the forth order
and the sixth order generalizations:

\[
\delta_{ijkl}^{(4)} = \delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} + \delta_{ik}\delta_{jl} \tag{4a}
\]

\[
\delta_{ijklmn}^{(6)} = \delta_{ij}\delta_{kl}\delta_{mn} + \delta_{im}\delta_{jn}\delta_{lk} + \delta_{im}\delta_{jn}\delta_{kl} \tag{4b}
\]

According to the previous analysis \[21\], the Gauss-Hermite
quadrature employed for solving a third-order truncated sys-

\[
f_a(x + \xi_a, t + 1) = f_a(x, t) - \frac{1}{\tau} \left[ f_a(x, t) - f_a^{(0)} \right] + F_a \tag{5}
\]

In this work we use a specific model of Eq. (1a) that consists
of moments up to the third order, one order higher than the
Navier-Stokes hydrodynamics in the conventional LBM mod-
els \[9\]. For our present investigation of flows at high
Mach numbers \( (Ma) \), we set the temperature, \( T \), to
a constant for simplicity. Denoting the local fluid density and
velocity by \( \rho \) and \( u \), and defining \( w_a = \xi_a \cdot u \) for brevity, in
the dimensionless units in which all velocities are normalized
by the sound speed \( (i.e., \sqrt{T} = 1) \), \( f_a^{(0)} \) takes the following compact form:

\[
f_a^{(0)} = w_a \rho \left[ 1 + u_a + \frac{u_a^2 - u^2}{2} + \frac{u_a(2u_a^2 - 3u^2)}{6} \right], \tag{2}
\]

where \( u^2 = u \cdot u \), and \( w_a \) is the quadrature weight corre-
ponding to the abscissa \( \xi_a \). The last term inside the brackets
represents the contribution from the third-order kinetic mo-
ments \[24\] which was shown to be related to the velocity-
dependent viscosity \[25\] but generally neglected in the
conventional lattice Boltzmann models.

According to the previous analysis \[20\], the Gaussian-Hermite
quadrature employed for solving a third-order truncated sys-

\[
f_a(x + \xi_a, t + 1) = f_a(x, t) - \frac{1}{\tau} \left[ f_a(x, t) - f_a^{(0)} \right] + F_a \tag{5}
\]

Both LBM models can be verified to admit isotropy for tensors of
the form \( \sum \sum w_a \xi_a \cdots \xi_a \) up to the sixth order instead of fourth
in the conventional LBM models. Explicitly speaking, recovery
of correct hydrodynamic physics up to the third order re-
quires up to six-order isotropy conditions as follows \[24\]:

\[
\sum_{a=1}^{d} w_a = 1 \tag{3a}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} = \delta_{ij} \tag{3b}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} \xi_{a,k} \xi_{a,l} = \delta_{ijkl}^{(4)} \tag{3c}
\]

\[
\sum_{a=1}^{d} w_a \xi_{a,i} \xi_{a,j} \xi_{a,k} \xi_{a,l} \xi_{a,m} \xi_{a,n} = \delta_{ijklmn}^{(6)} \tag{3d}
\]

Indeed, direct verification shows that these are satisfied by
the 3D 39-speed model \( (E^{39}_{3,7}) \) and its 2D projection \( (E^{21}_{2,7}) \).

\[
f_a(x + \xi_a, t + 1) = f_a(x, t) - \frac{1}{\tau} \left[ f_a(x, t) - f_a^{(0)} \right] + F_a \tag{5}
\]

As usual, the “lattice convention” with unity time increment is
used here.
TABLE I: Degree-7 Gauss-Hermite quadratures on Cartesian grid. Listed are the number of points in the symmetry group, \( p \), abscissas, \( \xi_a \), and the weights \( w_a \). Quadratures are named by the convention \( E_{D,n}^m \) where the superscript \( D \) and subscripts \( D \) and \( n \) are respectively the number of abscissas, dimension, and degree of algebraic precision. The subscript \( F S \) denotes permutations with full symmetry. Note that since all velocities are normalized with sound speed, the Cartesian grid spacing has a unit velocity of \( r = \sqrt{3/2} \).

| Quadrature | \( p \) | \( \xi_a \) | \( w_a \) |
|------------|--------|------------|--------|
| \( E_{3,7}^{39} \) | 1 | (0, 0, 0) | 1/12 |
| | 6 | \((r, 0, 0)_{FS}\) | 1/12 |
| | 8 | \((\pm r, \pm r, \pm r)\) | 1/27 |
| | 6 | \((2r, 0, 0)_{FS}\) | 2/135 |
| | 12 | \((2r, 2r, 0)_{FS}\) | 1/432 |
| | 6 | \((3r, 0, 0)_{FS}\) | 1/1620 |
| \( E_{2,7}^{21} \) | 1 | (0, 0) | 91/324 |
| | 4 | \((r, 0)_{FS}\) | 1/12 |
| | 4 | \((\pm r, \pm r)\) | 2/27 |
| | 4 | \((2r, 0)_{FS}\) | 7/360 |
| | 4 | \((\pm 2r, \pm 2r)\) | 1/432 |
| | 6 | \((3r, 0)_{FS}\) | 1/1620 |

terms of the Hermite expansion interpretation, the regularization procedure is more concisely described as the following. We split the post-streaming distribution into two parts:

\[
f_a = f'_a + f_a^{(0)}
\]

(6)

where \( f'_a \) is the deviation from the truncated Maxwellian, or the non-equilibrium part of the distribution. As \( f_a^{(0)} \) already lies entirely in the subspace \( H^N \), the projection is to ensure that the non-equilibrium contribution also lies in the same subspace for all times, and only needs to be applied to \( f'_a \). Effectively, the projection serves as a filtering (or “de-aliasing”) process to ensure the system stay inside the defined subspace in a Galerkin interpretation.

The projection is to convert \( f'_a \) to a new distribution \( \hat{f}_a \) which lies within the subspace spanned by the first three Hermite polynomials. Using the orthogonality relation of the Hermite polynomials and the Gauss-Hermite quadrature, \( \hat{f}_a \) is given by the pair of relations:

\[
\hat{f}_a = w_a \sum_{n=0}^{3} \frac{1}{n!} a^{(n)} H^{(n)}(\xi_a), \quad a = 1, \ldots, d,
\]

(7a)

\[
a^{(n)} = \sum_{a=1}^{d} f'_a H^{(n)}(\xi_a), \quad n = 0, \ldots, 3,
\]

(7b)

where \( H^{(n)} \) is the standard \( n \)-th Hermite polynomial. The differential equation that describes the evolution of the distribution function \( f_a \) is given by:

\[
H^{(0)}(\xi) = 1
\]

\[
H^{(1)}(\xi) = \xi
\]

\[
H^{(2)}(\xi) = \xi_i \delta_{ij} - \delta_{ij}
\]

\[
H^{(3)}(\xi, \xi) = \xi_i \delta_{jk} - \xi_j \delta_{ik} - \xi_k \delta_{ij},
\]

(8a)

(8b)

(8c)

(8d)

and \( a^{(n)} \) the corresponding Hermite expansion coefficient, both rank-\( n \) tensors. The first two Hermite coefficients vanish due to the vanishing contribution from the non-equilibrium distribution to mass and momentum. The second and third Hermite coefficients are:

\[
a^{(2)} = \sum_{a=1}^{d} f'_a \xi_a \xi_a,
\]

\[
a^{(3)} = \sum_{a=1}^{d} f'_a \xi_a \xi_a \xi_a,
\]

(9)

where \( a^{(2)} \) is traceless due to the conservation of energy. Clearly from the above construction or from direct verification, the projected distribution \( \hat{f}_a \) gives the same second order (momentum) and third order fluxes as the original \( f_a \).

\[
\sum_{a=1}^{d} \hat{f}_a \xi_a \xi_a = \sum_{a=1}^{d} f'_a \xi_a \xi_a
\]

\[
\sum_{a=1}^{d} \hat{f}_a \xi_a \xi_a \xi_a = \sum_{a=1}^{d} f'_a \xi_a \xi_a \xi_a,
\]

(10a)

(10b)

This is an essential step to preserve the required non-equilibrium properties affecting macroscopic physics. Furthermore, unlike \( f'_a \) in which all higher order moments are in principle present, the projected distribution \( \hat{f}_a \) can be shown via the orthogonality argument to give zero contributions to fluxes higher than the defined third order above. Consequently, its physical implication is rather apparent: The regularization procedure filters out the higher order non-equilibrium moments that contain strong discrete artifacts due to the insufficient support of the lattice basis.

Overall, given the discrete non-equilibrium distribution, its projection in \( H^N \) is fully specified by:

\[
\hat{f}_a = w_a \left[ \frac{H^{(2)}(\xi_a)}{2} \sum_{b=1}^{d} f'_b \xi_b \xi_b + \frac{H^{(3)}(\xi_a)}{6} \sum_{b=1}^{d} f'_b \xi_b \xi_b \xi_b \right].
\]

(11)

Incorporating the regularization procedure, Eq. 5 is modified to become

\[
f_a(x + \xi_a, t + 1) = f_a^{(0)} + \left(1 - \frac{1}{\tau}\right) \hat{f}_a + F_a.
\]

(12)

It is revealing to realize that the right-hand-side represents a damping operator acting on the “non-equilibrium” part of the distribution function. It is an immediate extension to assign a different relaxation time to each individual Hermite mode. Namely we can recast the collision operator into an equivalent yet slightly more general form:

\[
\Omega_a = \sum_{b=1}^{d} M_{ab} f'_b,
\]

(13)
where the linear matrix operator takes the following generic form

\[ M_{ab} \equiv \delta_{ab} + \left( 1 - \frac{1}{\tau} \right) w_a \left[ \theta_1 \frac{\mathcal{H}^{(2)}(\xi_a)}{2} \xi_b \xi_b + \theta_2 \frac{\mathcal{H}^{(3)}(\xi_a)}{6} \xi_b \xi_b \xi_b \right]. \tag{14} \]

The additional coefficients, \( \theta_1 \) and \( \theta_2 \), can have values between zero and one separately. Indeed, when \( \theta_1 = \theta_2 = 1 \), then we recover the result in Ref. \[21\], the third-order accurate projection operator. On the other hand, comparing Eq. (14) with the similar expression in Ref. \[21\], we find that the latter is a second-order projection operator (i.e., the first term in Eq. (14)), or simply \( \theta_1 = 1 \) and \( \theta_2 = 0 \). It is to be emphasized that the correct application of the third-order projection operator is based on the necessary condition of the third order Hermite quadrature. Hence it cannot be realized via conventional low order LBM such as the popular D3Q19 (or D2Q9).

The explicit form of the body force term comes directly from the Hermite expansion of the continuum BGK equation \[20, 29\]. Up to the third order, it can be expressed as:

\[
F_a = w_a \rho g \cdot (\xi_a + u_a \xi_a - u) \\
+ \frac{1}{2} w_a \left[ a^{(2)}(1) + \rho uu \right] : \left[ g_a \mathcal{H}^{(2)}(\xi_a) - 2g \xi_a \right]. \tag{15}
\]

To be noted here is that, whereas the first term is entirely due to the equilibrium part of the distribution, the term related to \( a^{(2)} \) are contributions from the non-equilibrium part. To our knowledge, the non-equilibrium contribution in the body-force has not been explicitly considered in the existing LBM literature. Nevertheless, although it is expected to play an important role at large \( Kn \), at moderate \( Kn (\lesssim 1) \), no significant effects due to non-equilibrium contribution are observed in the numerical experiments in the present work.

IV. NUMERICAL RESULTS

A. Shear wave decay

The first series of numerical simulations performed are for the benchmark problem of 2D sinusoidal shear wave decay. This set of tests is to evaluate impact from the increased order of accuracy and from the regularization procedure on the resulting isotropy. Obviously, a numerical artifact free wave decay should not depend on its relative orientation with respect to the underlying lattice orientation. The lattice orientation dependent artifact has often plagued discrete fluid models especially at finite Knudsen number when non-equilibrium effects are significant. For this purpose, we have defined two sets of simulations. In the first set, a sinusoidal wave with a wavelength \( L \) of 128 grid spacing is simulated on a \( 128 \times 128 \) periodic domain. The initial velocity field is given by \( u_x = u_0 \sin(y/2\pi L) \) and \( u_y = 0 \). The wave vector is aligned with the lattice. In the second set, the same sinusoidal wave is rotated by 45 degrees from the original orientation and simulated on a matching periodic domain size of \( 181 = 128 \sqrt{2} \times 181 \). The Knudsen number, defined as \( Kn = 2c_s/L \), is chosen to be 0.2, where \( \tau \) is the relaxation time and \( c_s \) the sound speed. These two sets of simulations were conducted using four representative models: the popular 2D 9-state (9s) model (D3Q9), and the present 2D 21-state (21s) model based on \( E_{21s} \), both with and without the regularization process. Note, the 2D 9-state model only admits a second-order regularization projection as discussed in the preceding section. In discussions hereafter we shall refer the models without the regularization as the BGK models, and the ones with regularization the REG models.

In Fig. 1 the dimensionless peak velocity magnitude, normalized by its initial value and measured at the 1/4 width of wavelength, is plotted against the non-dimensional time normalized by the characteristic decay time \( \tau_0 = \lambda^2/\nu \), where \( \nu = c_s^2(\tau - 1/2) \) is kinematic viscosity. As one can easily notice, the decay rate of the shear wave for the 9-s BGK model is substantially different between the lattice oriented setup and the 45 degree one, exhibiting a strong dependence on the orientation of the wave vector with respect to the lattice. This indicates a strong anisotropy of the model at this \( Kn \). This is consistent to our expectation that the 9-s BGK model was originally formulated to only recover the Navier-Stokes hydrodynamics (i.e., at vanishing \( Kn \)). Interestingly this anisotropy is essentially eliminated by the second-order regularization procedure in the resulting 9-s REG model. On the other hand, the amplitude of the shear wave exhibits a strong oscillatory behavior in addition to the exponential decay, implying a greater than physical ballistic effect. These may be explained as the following: The non-equilibrium part of the post-streaming distribution contains contributions from \textit{in principle} all moments, which are highly anisotropic due to inadequate (only up to the second-order moment) symmetry in the underlying discrete model. The regularization procedure filters out all the higher than the second order moment contributions, yielding an isotropic behavior supported by the given lattice. On the other hand, the higher moments
are critical at large \( Kn \). Therefore, though isotropic, the 9-s REG model still should not be expected to show satisfactory physical results at high Knudsen numbers. For the 21-s BGK model, an anisotropic behavior is also very visible, though at a much smaller extent. This may be attributed to the residual anisotropy in the moments higher than the third order. Again, the anisotropy behavior is completely removed once the regularization procedure is applied in the 21-s REG model, as shown from the totally overlapped curves between the lattice oriented and the diagonally oriented simulations. It is also noticeable that the decay history shows a much reduced oscillatory behavior in the 21-s REG model. Because of its correct realization of the third order moment flux, we expect the result is more accurate at this Knudsen number value. It is also curious to observe that the decay of the “lattice aligned” result from 9-s-BGK is surprisingly close to that of 21-s REG model at this \( Kn \). This is likely to be a mere coincidence.

B. Finite Knudsen number channel flows

Using the same four models, we subsequently carried out simulations of the force-driven Poiseuille flow for a range of Knudsen numbers. In order to identify the impact in accuracy in the resulting lattice Boltzmann models as oppose to the effects from various boundary conditions, here a standard half-way bounce-back boundary condition is used in the cross-channel \((y)\) direction. Furthermore, since we are not interested, for the present study, in any physical phenomenon associated with stream-wise variations, a periodic boundary condition is used with only four grid points in the stream-wise \((x)\) direction. In the cross stream \((y)\) direction, two different resolutions, \( L = 40 \) and 80 are both tried to ensure sufficient resolution independence. The Knudsen number is defined as \( Kn = \nu/(c_sL) \). The flow is driven by a constant gravity force, \( g \), pointing in the positive \( x \) direction. The magnitude of the force is set to \( 8\nu U_0/L^2 \), which would give rise to a parabolic velocity profile with a peak velocity of \( U_0 \) in the vanishing \( Kn \) limit. For consistence, a modified definition of fluid velocity, \( u \rightarrow u + g/2 \), is used in \( f_0^{(0)} \). Since the LBM models presently used here are all assuming constant temperature, to enforce an incompressible behavior with negligible thermodynamic effect throughout the simulated \( Kn \) range, we choose a sufficiently small value of \( U_0 \), corresponding to the nominal Mach numbers of \( Ma = U_0/c_s \sim 1.46 \times 10^{-6} \) and \( 2.92 \times 10^{-7} \), and verified that our results are independent of \( Ma \). The actual resulting fluid velocity in these simulations can achieve values much higher than \( U_0 \) at higher \( Kn \).

Plotted in Fig. 2 is the non-dimensionalized mass flux, \( Q \equiv \sum_{y=1}^{L} u_x(y)/Q_0 \), as a function of \( Kn \) in the final steady state of the simulations. Here \( Q_0 = gL^2/c_s \). For comparison we also include two analytical asymptotic solutions \( f_0^{(0)} \) for both small and very large \( Kn \). To be noted first is that at the vanishing \( Kn \) limit, all simulation results agree with each other as well as with the analytical solution. This confirms that all these LBM schemes recover the correct hydrodynamic behavior at vanishing \( Kn \), i.e., the Navier-Stokes limit. Also plotted is the exact Navier-Stokes solution of \( Q = 1/(12Kn) \), a well understood monotonically decreasing line with no minimum. At higher \( Kn \), the 9-s BGK model exhibits a Knudsen’s minimum while over-estimates the flux according to some previously published reports [14]. However, by filtering out moment contributions higher than the second order, such a phenomenon is completely disappeared from the result of 9-s REG, yielding a purely monotonically decreasing behavior. This is a rather interesting but not entirely surprising result. Once again, the regularization process enforces the system to be confined within the second-order Hermite moment space, while all higher order non-equilibrium contributions including both the numerical artifacts and the physical ones, responsible for the finite Knudsen phenomena, are filtered out. Consequently, only the Navier-Stokes order effects are preserved in the 9-s REG model no matter the degree of non-equilibrium at finite \( Kn \). To be further noticed is the impact of the second-order regularization on the near wall properties. In particular, Fig. 3 shows that 9-s REG gives vanishing slip velocity at the wall for a range of \( Kn \) values (\( Kn = 0.1, 0.2, \) and 0.5). This suggests that a bounce-back boundary process is sufficient to realize a no-slip condition once a Navier-Stokes order dynamics in the model equation is enforced. This is yet another confirmation as to why the resulting \( Q \) from 9-s REG model lies very close to the exact Navier-Stokes theoretical curve up to significantly high \( Kn \) values. In comparison, all the other three LBM models show finite slip velocity values, due to the previous discussed reason that they all contain higher than the second-order non-equilibrium contributions. Once again, one must remember that the higher order effects in 9-s BGK (and to a lesser extent the 21-s BGK) have substantial lattice discrete artifacts. To be emphasized is the 21-s REG model: Due to the regularization procedure, only the third-order non-equilibrium moment contribution is preserved. On the other hand, because it has numerically shown to capture the Knudsen minimum phenomenon, correct incorporation of the third-order moment physics is thus essential for accurately simulating some key flow physics beyond the Navier-Stokes. We also wish to emphasize that all these differences are due to the intrinsic natures in these LBM models, and has nothing to do with spatial and temporal resolutions. As a comparison, we plot in Fig. 4 velocity profiles generated from the 21-s REG model.

There are a number of ways that gravity force can be included in LB equations. One can either treat the gravity force outside the collision operator as an external body force term as given by Eq. (15) or by applying a local momentum/velocity shift inside the equilibrium distribution [34]. With regular BGK model, for all \( Kn \), no difference in results are observed when the gravity force is applied in different ways. With the regularization procedure and sufficient isotropy however, some differences are observed at finite (\( > 1 \)) \( Kn \). Generally speaking, applying the body force via Eq. (15) tends to predict higher flux than via momentum/velocity shifting. For the results shown in Fig. 4 the velocity shift applied in \( f_0^{(0)} \) is \( 1/2g \). The other half of the gravity force is applied as an external body force term [15] (Cf., [29]).

The results from both the 21-s BGK and the 21-s REG models predict a Knudsen minimum which resembles that of the
FIG. 3: (Color online) This figure shows the normalized velocity profiles at resolution 40 and $\text{Kn} = 0.1, 0.2,$ and $0.5$. Notice the $9\text{-s BGK}$ model exhibits no visible slip velocity for both small and large $\text{Kn}$.

9-s BGK except with reduced over-estimations at higher $\text{Kn}$. What is interesting, and requires further understanding, is that the flux behavior predicted by the 21-s REG exhibits a reversal of curvature at higher $\text{Kn}$, resembling the analytical asymptotic solution of Cercignani [4].

The qualitative differences seen from these four models suggest that contributions from moments beyond second order are essential for capturing fundamental physical effects at high-$\text{Kn}$. Although the high-order moments are implicitly contained in the second-order BGK model, its dynamics is highly contaminated with numerical lattice artifacts. In contrast, by incorporating the high-order moments explicitly and systematically with the regularization, flows at these $\text{Kn}$ values can indeed be captured by the extended LBM model.

V. CONCLUSION

In summary, the kinetic based representation offers a well-posed approach in formulation of computational models for performing efficient and quantitative numerical simulations of fluid flows at finite $\text{Kn}$. In this work we present a specific extended LBM model that accurately incorporates the physical contributions of kinetic moments up to the third order in Hermite expansion space. The new regularization procedure presented in this paper ensures that both the equilibrium and the non-equilibrium effects are confined in the accurately supported truncated subspace at all times so that the unphysical artifacts are filtered out in the dynamic process. This resulting LBM model is robust and highly efficient. Because of its accurate inclusion of the essential third order contributions, this model is demonstrated to be capable of quantitatively capturing certain fundamental flow physics properties at finite Knudsen numbers. This is accomplished without imposing any empirical models. Furthermore, because of the removal of discrete anisotropy, it is also clear that the new LBM model is not limited to specific uni-directional channel flows, nor it is only applicable for lattice aligned orientations.

Nevertheless, a number of issues are awaiting further studies. For even higher $\text{Kn} \sim 10$, one should expect moment contributions higher than the third order to become physically important. This is straightforward to include via the systematic formulation together with the regularization procedure described here. The issue of boundary condition is also of crucial importance. Even though, as demonstrated in this paper that the realization of the essential slip-velocity effect and the asymptotic behavior is attributed to a significant extent to the third order and higher moment contributions in the intrinsic LBM dynamic model itself. As reported in some previous works, the kinetic boundary condition of Ansumali and Karlin [34] has led to substantial improvements at the Navier-Stokes level micro-channel flow simulations. Boundary condition itself serves as an ef-
factive collision so that it also modifies the degree of the non-equilibrium distribution. Specifically, the well known Maxwell boundary condition (in which the particle distribution function is assumed to be at equilibrium) should be expected give different effect at high Kn compared with that of the bounce-back used in the present study. The latter boundary condition preserves non-equilibrium contributions at all orders. As a consequence, we suspect that the finite slip phenomenon is likely to still be over predicted in our current simulations with the bounce-back boundary condition than what actually would occur in reality. Many more detailed and further investigations particularly pertaining channel flows at finite Knudsen number are certainly extremely important in the future studies.

Thermodynamic effect is also expected to become important at finite Kn when Mach number is not negligibly small. Some distinctive phenomena that is substantial and characteristic only at finite Knudsen numbers with sufficiently large Mach numbers [35]. The work of Xu [35] demonstrates the importance of an accurate formulation of higher than the Navier-Stokes order thermodynamic effect at finite Kn. Theoretically, this additional property is associated with the so called super-Burnett effect in the more conventional language [35], or the fourth-order moment contribution in the Hermite expansion and can be incorporated in a further extended LBM model [20]. The present third-order model is thermodynamically consistent, but only at the Navier-Stokes level [20]. Another interesting point to mention is that both the 21-s BGK or the 21-s REG can allow an expanded equilibrium distribution form including terms up to the fourth power in fluid velocity (as opposed to the square power in 9-s BGK), for that the correct equilibrium energy flux tensor is still preserved. Including the forth power terms immediately results in a desirable positive-definite distribution for the zero-velocity state at all Mach number values.

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