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Renormalization of the lattice Boltzmann hierarchy

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Is it possible to solve Boltzmann-type kinetic equations using only a small number of particle velocities? We introduce a technique of solving kinetic equations with a (arbitrarily) large number of particle velocities using only a lattice Boltzmann method on standard, low-symmetry lattices. The renormalized kinetic equation is validated with an exact solution of the planar Couette flow at moderate Knudsen numbers.

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The lattice Boltzmann (LB) method has met with considerable success in a wide range of fluid dynamics problems ranging from turbulent to multiphase flows [1]. Recently, much of the attention was focused on the use of the LB models for simulation of microflows at moderate Knudsen numbers (Kn), the ratio of the mean free path to a characteristic flow scale [2–8]. It is understood by now that LB models form a well-defined hierarchy [9–12]. Each level $N \geq 3$ of the LB hierarchy is characterized by a set of discrete velocities chosen as roots of Hermite polynomials of the order N [9,11] or rational-number approximations thereof [12]. The number of discrete velocities scales as N^D, where D is the spatial dimension. With increasing the level N, the LB hierarchy constitutes a novel approximation of the classical kinetic theory and has to be considered as an alternative to more traditional approaches such as higher-order hydrodynamics (Burnett or super-Burnett [13]) or Grad's moment systems [14]. One salient feature of the LB hierarchy, which is crucial for any realistic application and which distinguishes it from traditional approaches, is that it is equipped with relevant boundary conditions derived directly from Maxwell-Boltzmann theory [2]. However, proceeding to the higher levels N (a must in microflow applications) constitutes an increasingly difficult computational problem.

In this Rapid Communication, we solve the problem of simulating the LB models with large velocity sets on small lattices, without sacrificing any physics or accuracy. The first step in this direction is to realize that the lower-order models are nothing but closures within the higher-order models. This simple yet important observation enables us to formulate the renormalized LB models on the lower levels in such a way that the additional physics of the higher-order models is correctly incorporated. In particular, we show with an example of exact solution in the stationary Couette flow that the accuracy of the most commonly used planar $D2Q9$ LB model can be enhanced drastically, without introducing additional velocities. Thus, we introduce a way of increasing the accuracy of the LB models without significantly increasing the computational cost. The methodology developed herein can be used to renormalize other computational kinetic theories.

We consider the isothermal LB hierarchy of kinetic equations,

$$\partial_t f_i + c_{i\alpha}\partial_\alpha f_i = Q_i(f), \tag{1}$$

where f_i are populations of discrete velocities c_i, $i=1,\ldots,N^D$, summation convention is assumed, and Q is the collision integral satisfying local conservation of density and momentum and vanishing at the equilibrium $f^{\rm eq}$, where

$$f_i^{\rm eq} = w_i\left(\rho + \frac{j_\alpha c_{i\alpha}}{c_{\rm s}^2} + \frac{j_\alpha j_\beta}{2\rho c_{\rm s}^4}(c_{i\alpha}c_{i\beta} - c_{\rm s}^2\delta_{\alpha\beta})\right). \tag{2}$$

Here $\rho=\Sigma_{i=1}^{N^D} f_i$ is the density, $j_\alpha=\Sigma_{i=1}^{N^D} c_{i\alpha} f_i$ is the momentum density, $c_{\rm s}$ is the speed of sound, and we shall use units in which $c_{\rm s}=1$. The weights w_i and the velocities c_i are so chosen that, at each level N, the hydrodynamic limit of the kinetic equation (1) at low Mach numbers is the Navier-Stokes equation. While the hydrodynamic limit of all models (1) is the same at each level N, their behavior is markedly different when exploring the microflow domain. Our goal is to modify the lowest-level kinetic equation (1) in such a way that the nonhydrodynamic features of the higher-level models are correctly captured by the lower-order models.

In order to introduce the main ideas, we first consider the one-dimensional case. For $D=1$, the lowest-order ($N=3$) model with three velocities $\{-\sqrt{3},0,\sqrt{3}\}$ ($D1Q3$) and collision integral in the Bhatnagar-Gross-Krook (BGK) form, $Q_i=(f_i^{\rm eq}-f_i)/\tau$, with a relaxation time τ, can be written as a moment system for ρ, j and pressure $P=\Sigma_{i=1}^3 c_i^2 f_i$:

$$\partial_t\rho = -\partial_x j,$$

$$\partial_t j = -\partial_x P,$$

$$\partial_t P = -3\partial_x j - \frac{1}{\tau}(P - P^{\rm eq}), \tag{3}$$

where $P^{\rm eq}=\rho+(j^2/\rho)$ is the equilibrium value of the pressure. Note that when writing the equation for the pressure we have used identity for the energy flux, $q=\Sigma_{i=1}^3 c_i^3 f_i = 3j$, which appears as a consequence of a lattice constraint, $c_i^3=3c_i$. The next ($N=4$) member of the LB hierarchy is an off-lattice four-velocity model based on the roots of the fourth-order

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Hermite polynomial $\{\pm a, \pm b\}$, where $a=\sqrt{3-\sqrt{6}}$ and $b=\sqrt{3+\sqrt{6}}$ ($D1Q4$) [see, e.g., Refs. [11,12] where the equilibrium (2) is given explicitly for this model]. The starting point is the moment system corresponding to the kinetic equation (1),

$$\partial_t \rho = -\partial_x j,$$

$$\partial_t j = -\partial_x P,$$

$$\partial_t P = -\partial_x q - \frac{1}{\tau}(P - P^{\mathrm{eq}}),$$

$$\partial_t q = -\partial_x(\alpha P + \beta \rho) - \frac{1}{\theta}(q - q^{\mathrm{eq}}), \tag{4}$$

where $\alpha=\frac{b^4-a^4}{b^2-a^2}=6$ and $\beta=\frac{a^4b^2-b^4a^2}{b^2-a^2}=-3$ are constants of the four-velocity set and $q^{\mathrm{eq}}=3j$ is the equilibrium value of the energy flux. We have introduced two relaxation times τ and θ in order to distinguish the relaxation of P and q. System (4) can be realized, for example, as the moment system of an appropriately chosen quasiequilibrium kinetic model [15,16] with two relaxation times. We remark that it is not required to write explicitly a kinetic equation leading to the system (4), so that (4) is the sole and convenient starting point for the analysis. Note that the subset of equations for $\{\rho, j, P\}$ is not closed within the system (4).

Now it is easy to see that the $D1Q3$ model (3) is a closure of the $D1Q4$ moment system (4). Indeed, assuming $\theta \ll \tau$ and substituting $q \approx q^{(0)}=q^{\mathrm{eq}}$ into the equation for pressure, one arrives at a closed subsystem for $\{\rho, j, P\}$ which is identical to (3). Note that, from this new angle of view, the aforementioned identity for the energy flux, $q=3j$ in (3), appears as an implication of the closure rather than the lattice constraint.

Upon realizing this relation between the higher- and lower-level "bare" kinetic equations (1), it is tempting to seek improvements for the closure. The simplest way to do this is to rescale the time with τ, to introduce a bookkeeping parameter $\eta=\theta/\tau$, and to compute the first correction $q=q^{(0)}+q^{(1)}$, where $q^{(1)}$ is found from the equation

$$q^{(1)} = -\eta\tau[\partial_t^{(0)} q^{(0)} + \partial_x(\alpha P + \beta\rho)], \tag{5}$$

while the zeroth-order derivative $\partial_t^{(0)} q^{(0)}$ is evaluated by the chain rule: $\partial_t^{(0)} q^{(0)}=(\partial q^{(0)}/\partial j)\partial_t j$ and $\partial_t j=-\partial_x P$. Using $q^{(0)}=3j$, we immediately find, from (5),

$$q^{(1)} = \tau\eta[(3-\alpha)\partial_x P - \beta\partial_x \rho]. \tag{6}$$

This is certainly in the spirit of the Chapman-Enskog method although note that a closed system does not consist solely of local conservation laws but also includes relaxation.

The resulting corrected moment system [first three equations in (4) supplemented with the closure relation $q=q^{(0)}+q^{(1)}$] is equivalent to a renormalized kinetic equation

$$\partial_t f_i + c_i \partial_x f_i - \lambda_i \tau\eta \partial_x^2[(\alpha-3)P + \beta\rho] = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}}), \tag{7}$$

with $\lambda_{\mp}=1/6$ and $\lambda_0=-1/3$. Thus, we can realize the one-step renormalization (OSR) (6) as a (source term supplemented) kinetic equation for populations on the same three-velocity lattice.

The renormalized kinetic equation (7) is a convenient starting point for a space-time discretization. The corresponding technique is standard [17] and has been already used for other kinetic equations with a source term containing second-order derivatives (in particular, for the thermal lattice Boltzmann models—e.g., in Ref. [18]). Details of the numerical implementation will be reported in a separate publication.

Now we shall apply the one-step renormalization to the particularly important two-dimensional 16-velocity model ($D2Q16, N=4$). The $D2Q16$ model is a tensor product of the two copies of the $D1Q4$ model considered above, and it (or its analogs) has attracted attention recently [7,19,20] as the first LB model which is capable of describing correctly the transient Knudsen regime, unlike the standard nine-velocity $D2Q9$ ($N=3$) LB model.

The set of 16 moments describing the $D2Q16$ model is split into the locally conserved (C), slow relaxing (S_τ), and fast relaxing (F_θ) subsystems

$$C = \{\rho, j_x, j_y\}, \tag{8}$$

$$S_\tau = \{P_{xx}, P_{yy}, P_{xy}, Q_{xyy}, Q_{yxx}, \psi\}, \tag{9}$$

$$F_\theta = \{Q_{xxx}, Q_{yyy}, \psi_x, \psi_y, L_x, L_y, \phi\}, \tag{10}$$

where $(\langle \mathrm{s}\rangle=\Sigma_{i=1}^{16} \mathrm{s}_i f_i)$

$$P_{\alpha\beta} = \langle c_\alpha c_\beta\rangle, \quad Q_{\alpha\beta\gamma} = \langle c_\alpha c_\beta c_\gamma\rangle,$$

$$\psi = \langle (c_x^2-1)(c_y^2-1)\rangle, \quad \psi_\alpha = \langle (c_\alpha^2-3)c_x c_y\rangle,$$

$$L_\alpha = \langle c_\alpha(c_x^2-3)(c_y^2-3)\rangle, \quad \phi = \langle c_x c_y(c_x^2-3)(c_y^2-3)\rangle.$$

The closure of the fast subsystem (10), $F_\theta^{(0)}=F^{\mathrm{eq}}$, where

$$F_\theta^{(0)} = \{3j_x, 3j_y, 0, 0, 0, 0, 0\}, \tag{11}$$

renders the moment subsystem for the nine moments C and S_τ equivalent to the moment system of the $D2Q9$ model [1]. Thus, again, the standard LBGK model on the nine-velocity lattice appears as a closure of the higher-level theory. The one-step renormalization $F_\theta^{(1)}$ is found to be [cf. (6)]

$$Q_{\alpha\alpha\alpha}^{(1)} = 3\tau\eta(\partial_\alpha \rho - \partial_\alpha P_{\alpha\alpha}),$$

$$\psi_x^{(1)} = -3\tau\eta\partial_x(Q_{yxx} - j_y),$$

$$\psi_y^{(1)} = -3\tau\eta\partial_y(Q_{xyy} - j_x),$$

$$L_\alpha^{(1)} = -3\tau\eta\partial_\alpha \psi,$$

$$\phi^{(1)} = 0. \tag{12}$$

With (12), it is straightforward to write down the renormalized $D2Q9$ kinetic equation [cf. (7)] and to implement the space-time discretization. We do not address this here. Instead, in order to clearly see the implication of the one-step renormalization (12), we consider the exact solution of the renormalized $D2Q9$ system in stationary Couette flow, where a fluid is enclosed between two parallel plates separated by a distance L. The bottom plate at $y=-L/2$ moves with velocity U_1 and the top plate at $y=L/2$ moves with velocity U_2. The solution of the renormalized model proceeds essentially along the lines of [7]: First, the steady-state OSR $D2Q9$ moment system is integrated under the assumption of unidirectional flow and no mass flux through the walls. Second, the boundary conditions are applied to compute the integration constants of the solution. This step is particularly important: The boundary conditions for the OSR $D2Q9$ model are *induced* by the boundary conditions of the $D2Q16$ model. Namely, when the diffusive wall boundary conditions [2] are applied to the $D2Q16$ model, the result is presented in terms of all the moments C, S_τ, and F_θ. Indeed, the diffusive boundary condition for $D2Q16$ model in the present setup can be written as

$$f_i|_{c_i\cdot e>0} = \left[\frac{P_{yy}}{\rho c_s^2} + \frac{\sqrt{6}(b-a)}{2(a+b)}\left(1-\frac{P_{yy}}{\rho c_s^2}\right)\right] f_i^{\mathrm{eq}}(\rho, U_{\mathrm{wall}}), \tag{13}$$

where e is the wall normal. Now, based on a one-to-one relation between moments and populations, we can generate the boundary condition for $D2Q16$ model in terms of C, S_τ, and F_θ moments. Finally, we use the latter relationship by replacing $F_\theta \to F_\theta^{(0)} + F_\theta^{(1)}$. This step provides the boundary conditions for the OSR $D2Q9$ moment system in terms of the C and S_τ moments only.

Let us introduce the mean free path $l=\sqrt{3}\tau c_s$ and the Knudsen number $\mathrm{Kn}=l/L$. The x component of the velocity as predicted by the OSR $D2Q9$ model for any $\eta=\theta/\tau$ is

$$u_x(y) = A \sinh\left(\frac{y}{\mathrm{Kn}\sqrt{\eta}L}\right)\Delta U + B\left(\frac{y}{L}\right)\Delta U + U, \tag{14}$$

where $\Delta U = U_2 - U_1$ is the relative velocity of the plates, $U=(U_1+U_2)/2$ is the centerline velocity, and A and B are constants which depend only on Kn and η:

$$B = \frac{\mu\sqrt{\eta} + 2\sqrt{3}\tanh\left(\frac{1}{2\sqrt{\eta}\mathrm{Kn}}\right)}{(4\mathrm{Kn}+\mu)\sqrt{\eta} + 2(\mu\mathrm{Kn}+\sqrt{3})\tanh\left(\frac{1}{2\sqrt{\eta}\mathrm{Kn}}\right)},$$

$$A = \frac{4\mathrm{Kn}}{\mu^2\sqrt{\eta}\cosh\left(\frac{1}{2\sqrt{\eta}\mathrm{Kn}}\right) + 2\sqrt{3}\mu\sinh\left(\frac{1}{2\sqrt{\eta}\mathrm{Kn}}\right)} B, \tag{15}$$

and $\mu=a+b\approx 3.076$.

It is striking that for $\eta=1$ ($\theta=\tau$), the result (14) and (15) becomes *identical* to the one obtained in [7] for the BGK $D2Q16$ model. We recall (see [5,7]) that the bare $D2Q9$ model predicts only a linear velocity profile in this problem,

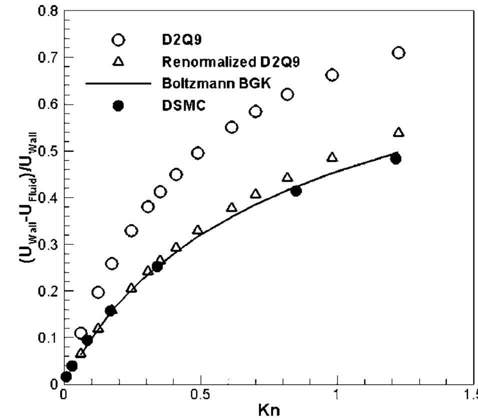

FIG. 1. Slip velocity at the wall as a function of Knudsen number. Line: linearized Boltzmann-BGK model [22]. Solid circles: DSMC simulation. Open circles: standard (bare) $D2Q9$ model [5,7]. Open triangles: one-step renormalized $D2Q9$ model (14), $\eta=1$.

$u_x=(1+2\mathrm{Kn})^{-1}(y/L)\Delta U+U$, stripped of the nonlinear Knudsen layer at the walls. Quite on the contrary, the renormalized $D2Q9$ model shows clearly the Knudsen layer [first term in (14)], which is exactly the same as in the $D2Q16$ model itself. The reason for this can be traced to the fact that the renormalization removes the lattice constraint pertinent to the bare $D2Q9$ model—namely, $Q_{\alpha\alpha\alpha}=3j_\alpha$. In the present approach, this constraint is recognized as a closure relation $F_\theta^{(0)}$ which is then corrected by the first term in (12). Thus, the sense of the renormalization is to dress the bare kinetic equations with nonhydrodynamic modes so that they reveal the correct behavior at nonvanishing Kn. This is indeed much in spirit of the renormalization group method [21] for spin-lattice models where renormalization improves on the mean-field approximation to dress it with correlations.

In Fig. 1, the value of the velocity slip at the wall resulting from (14) is compared at various Kn with the classical data of Willis [22] for the linearized Boltzmann-BGK equation, and with results obtained with the direct-simulation Monte Carlo (DSMC) method [23]. The result for the bare $D2Q9$ model is also plotted for comparison. It is clear that the agreement for the renormalized $D2Q9$ model remains excellent for large values of Kn and the renormalization leads to a drastic improvement of the bare $D2Q9$ model. We conclude this Rapid Communication with a number of comments using again the simple $D1Q4$ model for the sake of argument.

(i) The physical meaning of the renormalization in the present context is to establish an intermediate level between kinetics and hydrodynamics. This intermediate level happens when the dynamics of q becomes slaved by the dynamics of $\{\rho, j, P\}$ but the dynamics of P is not yet slaved by the dynamics of $\{\rho, j\}$. The hydrodynamic limit of model (4) assumes two smallness parameters $\epsilon=\tau/T$ and $\mu=\theta/T$ where T is a flow time scale. Instead, we rearrange it in terms of two other parameters ϵ and $\eta=\theta/\tau=\mu/\epsilon$. Note that η need not be small.

(ii) Although the simple one-step renormalization is quite reliable, a rigorous approach to the nonperturbative renormalization can be based on the invariance equation [24]

$$\Delta(q) = \partial_t q - \left(\frac{\partial q}{\partial \rho} \partial_t \rho + \frac{\partial q}{\partial j} \partial_t j + \frac{\partial q}{\partial P} \partial_t P \right) = 0. \qquad (16)$$

A stable fixed point of (16) is a fully renormalized q. Owing to a specific feature of the LB hierarchy (linearity of propagation), a way to solve Eq. (16) (and similar equations in higher dimensions) is the following: (a) Neglecting the nonlinearity in P^{eq}, we note that the solution q^{lin} of (16) can be found exactly, following the route of exact summation of the Chapman-Enskog expansion [25,26]. (b) Once the renormalized linear closure q^{lin} is obtained, it can be refined to take into account the nonlinearities. Substituting q^{lin} into (16), we compute the defect of invariance $\Delta^{\mathrm{lin}} = \Delta(q^{\mathrm{lin}})$. With this, a refinement can be written, $q \approx q^{\mathrm{lin}} + a\Delta^{\mathrm{lin}}$, where a can be estimated via a relaxation method [24].

(iii) Importantly, the simple OSR or nonperturbative linear renormalization should be sufficient for most of the cases of interest in microflow simulations. In fact, the nonlinearity of P^{eq} is mainly responsible for the hydrodynamic behavior of the model (advection term in the Navier-Stokes equations), whereas the task of renormalization is to remove lattice constraints and restore such features as Knudsen layers, slip velocity, etc. With this, the renormalized kinetic equations retaining the full P^{eq} are still nonlinear, as in the case of Couette flow considered above.

(iv) As a final remark, in the standard kinetic theory, the one-step renormalization was first introduced in [27] as a correction to Grad's moment systems and received some attention after in the work [28]. However, this approach cannot compete with the LB method both in terms of computational efficiency and (more restrictively) because of the lack of well-defined boundary conditions, especially for nonstationary problems.

In conclusion, the traditional viewpoint of the LB hierarchy treats each level separately, without any relation across the levels. Here, an alternative viewpoint is suggested according to which bare kinetic equations of the form (1) on the lower and computationally attractive levels appear as closures of the higher-level kinetic equations. Based on this, we suggested to renormalize the low-order LB equations in such a way that physics beyond the standard hydrodynamics is correctly reported from the higher levels to the lower levels. We demonstrated analytically that the renormalized lattice Boltzmann model on a standard velocity set reproduces the Knudsen layer in the Couette flow which otherwise is possible only with the higher-level models. In this sense, the renormalized kinetic equations on standard lattices are *the* LB equations, and not the bare ones, written by a plain analogy with kinetic theory. We mention that in three dimensions the reduction of the higher-order models to the standard $D3Q27$ lattice is done in the same way as described above. We note that the renormalization discussed in this Rapid Communication concerns propagation of nonhydrodynamic effects down the LB hierarchy and not a renormalization or sub-grid modeling of the Navier-Stokes' turbulence, as in [29,30]. We are, however, optimistic that the present methods can also be useful in the latter problem.

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