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Accuracy of the viscous stress in the lattice Boltzmann equation with simple boundary conditions

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Based on the theory of asymptotic analysis, we prove that the viscous stress tensor computed with the lattice Boltzmann equation (LBE) in a two-dimensional domain is indeed second-order accurate in space. We only consider simple bounce-back boundary conditions which can be reduced to the periodic boundary conditions by using the method of image. While the LBE with nine velocities on two-dimensional square lattice (i.e., the D2Q9 model) and with the Bhatnagar-Gross-Krook collision model is used as an example in this work, our proof can be extended to the LBE with any linear relaxation collision models in both two and three dimensions.

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The lattice Boltzmann equation (LBE) [1,2] is a numerical method for computational fluid dynamics (CFD) derived from the Boltzmann equation and kinetic theory [3,4]. The lattice Boltzmann (LB) method has become popular recently perhaps because it is rather simple to write an LB code with a second-order accuracy in space [5–8], and because of its successful applications to simulate complex fluids such suspensions [9–14] and interfacial dynamics [15–19]. There have been observations that the LBE is better than its second-order finite-difference (FD) counterparts based on direct discretizations of the Navier-Stokes equations, because of its low numerical dissipation and better isotropy [20–22]. Dellar [23,24] showed that the LBE with the multiple-relaxation-time (MRT) collision model [25] is stable and free of spurious vortices observed in other FD schemes for a double-shear flow in two dimensions (2D). Peng *et al.* [26] demonstrated that the LBE can accurately compute the vorticity in decaying homogeneous isotropic turbulence in three dimensions (3D). More recently, Krüger *et al.* [27] observed that the deviatoric stress tensor computed with the LBE for the decaying Taylor-Green vortex flow in 2D is second-order accurate. These circumstantial evidence indicates that the kinetic modes in the LBE, which have no counterparts in the Navier-Stokes based CFD schemes, may have benefits in terms of accuracy and stability. In this Rapid Communication, we will use the theory of asymptotic analysis [5,7,28–30] to prove that the viscous stress tensor computed with the LBE is indeed second-order accurate in space.

We usually designate an LBE in d-dimensional space and with $q := (N+1)$ discrete velocities, $\mathbb{V} := \{\boldsymbol{c}_i | i = 0,1,\ldots,N\}$, as the D$dQq$ model. The LBE involves q real distribution functions $\{f_i | i = 0,1,\ldots,N\}$ corresponding to q discrete velocities $\{\boldsymbol{c}_i\}$ and evolves on a d-dimensional lattice $\delta x \mathbb{Z}^d$ and discrete time $t_n := n\delta t$, $n \in \mathbb{N}_0$, where δx and δt are the lattice constant (or grid spacing) and the time step size, respectively, and $\mathbb{N}_0 := \{0,1,\ldots\}$. The discrete velocity set $\mathbb{V}$ includes the zero velocity $\boldsymbol{c}_0 = \boldsymbol{0}$ and is symmetric, i.e., $\mathbb{V} = -\mathbb{V}$. The unit of the velocities $\{\boldsymbol{c}_i\}$ is $c := \delta x/\delta t$. The LBE can be concisely written in the following q-dimensional vector form:

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta t, t_{n+1}) = \mathbf{f}(\boldsymbol{x}_j, t_n) + \mathbf{J}[\mathbf{f}(\boldsymbol{x}_j, t_n)] + \mathbf{F}(\boldsymbol{x}_j, t_n), \quad (1)$$

where the following notations have been used:

$$\begin{aligned}
\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta t, t_{n+1}) &:= [f_0(\boldsymbol{x}_j, t_{n+1}), f_1(\boldsymbol{x}_j + \boldsymbol{c}_1\delta t, t_{n+1}), \ldots, \\
&\qquad f_N(\boldsymbol{x}_j + \boldsymbol{c}_N\delta t, t_{n+1})]^\dagger, \\
\mathbf{f}(\boldsymbol{x}_j, t_n) &:= [f_0(\boldsymbol{x}_j, t_n), f_1(\boldsymbol{x}_j, t_n), \ldots, f_N(\boldsymbol{x}_j, t_n)]^\dagger, \\
\mathbf{J}(\boldsymbol{x}_j, t_n) &:= [J_0(\boldsymbol{x}_j, t_n), J_1(\boldsymbol{x}_j, t_n), \ldots, J_N(\boldsymbol{x}_j, t_n)]^\dagger, \\
\mathbf{F}(\boldsymbol{x}_j, t_n) &:= [F_0(\boldsymbol{x}_j, t_n), F_1(\boldsymbol{x}_j, t_n), \ldots, F_N(\boldsymbol{x}_j, t_n)]^\dagger,
\end{aligned}$$

where † denotes the transpose, and $\mathbf{J}$ and $\mathbf{F}$ denote the collision and external forcing terms, respectively. Commonly, the collision term in the LBE, $\mathbf{J}$, is the linear relaxation model with constant relaxation rates, which is based on the linearized Boltzmann collision operator about the local Maxwellian equilibrium [3,4,20,21,25]. The equilibrium in the LBE is usually a linear function of the flow density ρ and polynomial of the flow velocity $\boldsymbol{u}$, which can be obtained by truncating the Taylor expansion of the Maxwellian equilibrium at $\boldsymbol{u} = 0$ [3,4].

To be concrete, we will use the D2Q9 model in the ensuing discussion. The discrete velocities in the D2Q9 model are $\boldsymbol{c}_0 = (0,0)$, $\boldsymbol{c}_1 = (1,0)c = -\boldsymbol{c}_3$, $\boldsymbol{c}_2 = (1,0)c = -\boldsymbol{c}_4$, $\boldsymbol{c}_5 = (1,1)c = -\boldsymbol{c}_7$, and $\boldsymbol{c}_6 = (-1,1)c = -\boldsymbol{c}_8$. For the sake of simplicity, we will use the Bhatnagar-Gross-Krook (BGK) collision model [31]:

$$J_i = -\frac{1}{\tau}\left[f_i - f_i^{(\mathrm{eq})}(\rho,\boldsymbol{u})\right], \quad (2)$$

where the equilibria for incompressible flows (cf., e.g., Ref. [32]) are given by

$$f_i^{(\mathrm{eq})}(\rho,\boldsymbol{u}) = w_i\left[\rho + \frac{\hat{\boldsymbol{c}}_i\cdot\boldsymbol{u}}{\theta} + \frac{1}{2}\left\{\left(\frac{\hat{\boldsymbol{c}}_i\cdot\boldsymbol{u}}{\theta}\right)^2 - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{\theta}\right\}\right], \quad (3a)$$

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$$\rho = \sum_{i=0}^{8} f_i = \sum_{i=0}^{8} f_i^{(\text{eq})}, \tag{3b}$$

$$\boldsymbol{u} = \sum_{i=0}^{8} \hat{\boldsymbol{c}}_i f_i = \sum_{i=0}^{8} \hat{\boldsymbol{c}}_i f_i^{(\text{eq})}, \tag{3c}$$

where $\theta := RT$ is usually set to $1/3$ [20], $\hat{\boldsymbol{c}}_i := \boldsymbol{c}_i/c$, and $w_0 = 4/9$, $w_{1,2,3,4} = 1/9$, and $w_{5,6,7,8} = 1/36$. With the diffusive scaling $\delta t = \delta x^2 = h^2$ in proper units (cf., e.g., Refs. [33,34]) and the following forcing term [35,36],

$$F_i = w_i \frac{\hat{\boldsymbol{c}}_i \cdot \boldsymbol{F}}{\theta} h^3 = 3 w_i \hat{\boldsymbol{c}}_i \cdot \boldsymbol{F} h^3, \tag{4}$$

it can be rigorously proved that the LBE (1) approximates the following incompressible Navier-Stokes equations with a second-order accuracy in space [5–8],

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nu \Delta \boldsymbol{u} + \boldsymbol{F}, \tag{5a}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{5b}$$

where $\boldsymbol{u} := \boldsymbol{u}(\boldsymbol{x},t)$ is the velocity field, $p := p(\boldsymbol{x},t) := \rho(\boldsymbol{x},t)\theta = \rho(\boldsymbol{x},t)/3$ is the hydrostatic pressure, and $\nu = (\tau - 1/2)/3 > 0$ is the shear viscosity, provided that proper initial data $\boldsymbol{u}_0(\boldsymbol{x}) := \boldsymbol{u}(\boldsymbol{x},0)$ and appropriate boundary conditions (BCs) are given. The initial pressure $p_0(\boldsymbol{x}) := p(\boldsymbol{x},0)$ can be consistently determined by $\boldsymbol{u}_0(\boldsymbol{x})$ [37]. It should be noted that the $\boldsymbol{u}$ and p in Eqs. (5) are *not* equal to their counterparts in Eqs. (3).

For the sake of convenience, we split the equilibrium (3a) into the linear and quadratic parts in terms of $\boldsymbol{u}$:

$$f_i^{(\text{eq})}(\rho,\boldsymbol{u}) = L_i^{(\text{eq})}(\rho,\boldsymbol{u}) + Q_i^{(\text{eq})}(\boldsymbol{u},\boldsymbol{u}), \tag{6a}$$

$$L_i^{(\text{eq})}(\rho,\boldsymbol{u}) := w_i\,(\rho + 3\hat{\boldsymbol{c}}_i \cdot \boldsymbol{u}), \tag{6b}$$

$$Q_i^{(\text{eq})}(\boldsymbol{u},\boldsymbol{v}) := \tfrac{1}{2} w_i\,[(3\hat{\boldsymbol{c}}_i \cdot \boldsymbol{u})(3\hat{\boldsymbol{c}}_i \cdot \boldsymbol{v}) - 3\boldsymbol{u} \cdot \boldsymbol{v}]. \tag{6c}$$

Defined on the lattice points $\boldsymbol{x}_j \in \delta x \mathbb{Z}^d$ and at discrete time t_n, the computed distributions $\{f_i\}$ depend on h and can be expanded as an *asymptotic* series of h:

$$f_i(\boldsymbol{x}_j,t_n) \sim \sum_{n=0}^{\infty} f_i^{(n)}(\boldsymbol{x}_j,t_n) h^n, \tag{7}$$

provided that the initial data can be expressed by the same series and the coefficients $\{f_i^{(n)}(\boldsymbol{x}_j,t_n)\}$ are independent of h. Accordingly, both the density ρ and the velocity $\boldsymbol{u}$ can be expanded as asymptotic series of h, too:

$$\rho \sim \sum_{n=0}^{\infty} \rho^{(n)} h^n, \quad \rho^{(n)} := \sum_i f_i^{(n)}(\boldsymbol{x}_j,t_n), \tag{8a}$$

$$\boldsymbol{u} \sim \sum_{n=0}^{\infty} \boldsymbol{u}^{(n)} h^n, \quad \boldsymbol{u}^{(n)} := \sum_i \hat{\boldsymbol{c}}_i f_i^{(n)}(\boldsymbol{x}_j,t_n). \tag{8b}$$

We set $\rho^{(0)} = 1$ and $\boldsymbol{u}^{(0)} = 0$, and thus $f_i^{(0)} := L_i^{(\text{eq})}(\rho^{(0)},\boldsymbol{u}^{(0)}) = w_i \rho^{(0)} = w_i$ in the above expansions.

We now study the properties of the expansion coefficients $\{f_i^{(n)}\}$, and, in turn, $\{\rho^{(n)}\}$ and $\{\boldsymbol{u}^{(n)}\}$. Define

$$\begin{aligned} R_i :=& \sum_n h^n f_i^{(n)}(\boldsymbol{x}_j + \hat{\boldsymbol{c}}_i h, t_k + h^2) - \sum_n h^n f_i^{(n)}(\boldsymbol{x}_j,t_k) \\ &+ \frac{1}{\tau}\left[\sum_n h^n f_i^{(n)} - f_i^{(\text{eq})}\left(\sum_n h^n \rho^{(n)}, \sum_n h^n \boldsymbol{u}^{(n)}\right)\right](\boldsymbol{x}_j,t_k) \\ &- F_i(\boldsymbol{x}_j,t_k), \end{aligned}$$

where $F_i(\boldsymbol{x}_j,t_k)$ is given by Eq. (4). By substituting the Taylor expansion of $f_i^{(n)}(\boldsymbol{x}_j + \hat{\boldsymbol{c}}_i h, t_k + h^2)$ into R_i above, we have

$$\begin{aligned} R_i =& \sum_{k,n>0} h^{n+k} \mathsf{D}_{i,k} f_i^{(n)} + \frac{1}{\tau}\sum_n h^n \big[f_i^{(n)} - L_i^{(\text{eq})}(\rho^{(n)},\boldsymbol{u}^{(n)})\big] \\ &- \frac{1}{\tau}\sum_{n,q+p=n} h^n Q_i^{(\text{eq})}(\boldsymbol{u}^{(p)},\boldsymbol{u}^{(q)}) - F_i, \end{aligned}$$

where

$$\mathsf{D}_{i,k} := \sum_{2m+n=k} \frac{\partial_t^m (\hat{\boldsymbol{c}}_i \cdot \nabla)^n}{m!\,n!}. \tag{9}$$

Obviously, $\mathsf{D}_{\bar{i},k} = (-1)^k \mathsf{D}_{i,k}$ for $\boldsymbol{c}_{\bar{i}} := -\boldsymbol{c}_i$. By equating the coefficient of h^n in R_i to zero, we obtain a hierarchy of equations:

$$L_i^{(\text{eq})}(\rho^{(1)},\boldsymbol{u}^{(1)}) - f_i^{(1)} = 0, \tag{10a}$$

$$L_i^{(\text{eq})}(\rho^{(2)},\boldsymbol{u}^{(2)}) - f_i^{(2)} = \tau \mathsf{D}_{i,1} f_i^{(1)} - Q_i^{(\text{eq})}(\boldsymbol{u}^{(1)},\boldsymbol{u}^{(1)}), \tag{10b}$$

$$\begin{aligned} L_i^{(\text{eq})}(\rho^{(3)},\boldsymbol{u}^{(3)}) - f_i^{(3)} =& \tau\big(\mathsf{D}_{i,1} f_i^{(2)} + \mathsf{D}_{i,2} f_i^{(1)} - F_i/h^3\big) \\ &- 2Q_i^{(\text{eq})}(\boldsymbol{u}^{(1)},\boldsymbol{u}^{(2)}), \end{aligned} \tag{10c}$$

$$\begin{aligned} &L_i^{(\text{eq})}(\rho^{(n)},\boldsymbol{u}^{(n)}) - f_i^{(n)} \\ &\quad = \sum_{k=1}^{n-1} \big[\tau \mathsf{D}_{i,k} f_i^{(n-k)} - Q_i^{(\text{eq})}(\boldsymbol{u}^{(k)},\boldsymbol{u}^{(n-k)})\big], \quad \forall\, n \geqslant 4. \end{aligned} \tag{10d}$$

From Eqs. (10) and using the symmetry of the velocity set $\mathbb{V} = -\mathbb{V}$, we can show (cf. Refs. [5,28]) that

$$\rho^{(2k+1)} = 0, \quad \boldsymbol{u}^{(2k)} = \boldsymbol{0}, \quad \forall\, k \in \mathbb{N}_0, \tag{11}$$

provided that they are so initially and that the boundary conditions are periodic ones. Moreover, the expansion coefficient $f_i^{(n)}$ has the following symmetry property due to the symmetry of $\{\boldsymbol{c}_i\}$ and the structure of $\{f_i^{(\text{eq})}\}$:

$$f_{\bar{i}}^{(n)} = (-1)^n f_i^{(n)} \quad \text{for } \boldsymbol{c}_{\bar{i}} := -\boldsymbol{c}_i. \tag{12}$$

Because of the properties of $\rho^{(2k+1)}$ and $\boldsymbol{u}^{(2k)}$ given by Eq. (11), for odd $n = 2k+1$ we have

$$L_i^{(\text{eq})}(\rho^{(2k+1)},\boldsymbol{u}^{(2k+1)}) = 3 w_i \hat{\boldsymbol{c}}_i \cdot \boldsymbol{u}^{(2k+1)}, \tag{13a}$$

$$\sum_{m=0}^{2k+1} Q_i^{(\text{eq})}(\boldsymbol{u}^{(m)},\boldsymbol{u}^{(2k+1-m)}) = 0, \tag{13b}$$

then we can derive from Eqs. (10b) and (13a) the following result:

$$f_i^{(2)} - \left[L_i^{(\mathrm{eq})}(\rho^{(2)},\boldsymbol{u}^{(2)}) + Q_i^{(\mathrm{eq})}(\boldsymbol{u}^{(1)},\boldsymbol{u}^{(1)})\right] = -3\tau w_i \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i : \nabla \boldsymbol{u}^{(1)}. \tag{14}$$

Now we can compute the second-order moment of the collision term:

$$\begin{aligned}\sum_i \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i\left[f_i - f_i^{(\mathrm{eq})}\right] &= h^2 \sum_i \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i\left[f_i^{(2)} - L_i^{(\mathrm{eq})}(\rho^{(2)},\boldsymbol{u}^{(2)}) - Q_i^{(\mathrm{eq})}(\boldsymbol{u}^{(1)},\boldsymbol{u}^{(1)})\right] + O(h^4)\\ &= -3\tau h^2 \sum_i w_i \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i : \nabla \boldsymbol{u}^{(1)} + O(h^4)\\ &= -\frac{1}{3}\tau h^2[(\nabla \boldsymbol{u}^{(1)}) + (\nabla \boldsymbol{u}^{(1)})^\dagger] + O(h^4).\end{aligned}$$

The above result is a consequence of the fact that

$$\sum_i [f_i^{(3)} - f_i^{(\mathrm{eq})}(\rho^{(3)},\boldsymbol{u}^{(3)})]\hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i = 0$$

because of symmetry of the velocity set $\{\boldsymbol{c}_i\}$ (cf. Ref. [5]). We now arrive at the result that

$$\frac{1}{3}\tau[(\nabla \boldsymbol{u}^{(1)}) + (\nabla \boldsymbol{u}^{(1)})^\dagger] = -\frac{1}{h^2}\sum_i \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i\left[f_i - f_i^{(\mathrm{eq})}\right] + O(h^2). \tag{15}$$

Note that $\boldsymbol{u}^{(1)}$ and $\rho^{(2)}/3 = p^{(2)}$ solve the incompressible Navier-Stokes equations (1). The above result for the viscous stress does not include the Hénon correction term [38], which is obtained easily from the ∇^2 term in the Taylor expansion of $f_i(\boldsymbol{x}_j + \hat{\boldsymbol{c}}_i h, t_k + h^2)$.

We now consider the case with the bounce-back boundary conditions. We will use the method of image and apply it to study the Poiseuille flow in 2D as an example. The flow domain is discretized with a mesh of size of $N_x \times N_y$ with the periodic boundary conditions, where N_y is even. The mesh is divided into two equal parts: $1 \leqslant j_y \leqslant N_y/2$ and $N_y/2 + 1 \leqslant j_y \leqslant N_y$, $\forall\, 1 \leqslant i_x \leqslant N_x$. A positive constant force of magnitude F is exerted along the x direction on the first half of the domain $1 \leqslant j_y \leqslant N_y/2$ while a opposite force $-F$ is applied on the second half $N_y/2 + 1 \leqslant j_y \leqslant N_y$, and thus the system consists of two Poiseuille flows moving in opposite directions along the x axis [39–41]. The boundary conditions for each Poiseuille flow are *equivalent* to the bounce-back boundary conditions,

$$f_{\bar{i}}(\boldsymbol{x}_j,t_n) = f_i(\boldsymbol{x}_j - \hat{\boldsymbol{c}}_{\bar{i}} h,t_n) = f_i(\boldsymbol{x}_j + \hat{\boldsymbol{c}}_i h,t_n), \tag{16}$$

where $\boldsymbol{x}_j$ and $\boldsymbol{x}_j + \hat{\boldsymbol{c}}_i h$ must belong to two different subdomains. Because the periodic boundary conditions are applied to the entire domain, our analysis remains valid for this system. A note of caution: The exact boundary location of the lattice BGK (LBGK) model [42,43] is viscosity dependent [45–48], which is an artifact due to the LBGK model and can be removed by using the MRT model [25], which is imperative to achieve correct boundary conditions for the velocity field $\boldsymbol{u}$ [45–48]. However, the defect of the LBGK model has no bearing in the consistency of our analysis.

In summary, we use the theory of asymptotic analysis to proved that the viscous stress computed with the LBE in a 2D domain with the bounce-back boundary conditions is second-order accurate in space. While our proof uses the lattice BGK model [42,43] as an example, it is straightforward to extend the analysis to the MRT-LBE [20,21,25] and in 3D. Analysis of more complicated LBE models and boundary conditions are left for future work.

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