Theory of the Lattice Boltzmann method: Derivation of macroscopic equations via the Maxwell iteration

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We propose using the Maxwell iteration to derive the hydrodynamic equations from the lattice Boltzmann equation (LBE) with an external forcing term. The proposed methodology differs from existing approaches in several aspects. First, it need not explicitly introduce multiple-timescales or the Knudsen number, both of which are required in the Chapman–Enskog analysis. Second, it need not use the Hilbert expansion of the hydrodynamic variables, which is necessary in the asymptotic analysis of the LBE. The proposed methodology assumes the acoustic scaling (or the convective scaling) $\delta_t \sim \delta_x$, thus δ_t is the only expansion parameter in the analysis of the LBE system, and it leads to the Navier–Stokes equations in compressible form. The forcing density derived in this work can reproduce existing forcing schemes by adjusting appropriate parameters. The proposed methodology also analyzes the numerical accuracy of the LBE. In particular, it shows the Mach number Ma should scale as $O(\delta_t^{1/3})$ to maintain the truncation errors due to Ma and δ_t in balance when $\delta_t \to 0$, so that the LBE can converge to the expected hydrodynamic equations effectively and efficiently.

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I. INTRODUCTION

There are several ways and means to derive the macroscopic equations from the lattice Boltzmann equation (LBE). The first is the Chapman–Enskog (CE) analysis [1,2]. The CE analysis appears naturally as the means to study the LBE because the LBE is derived from kinetic equations [3,4]. The CE analysis requires an explicit introduction of multiple timescale expansion with the expansion parameter to be the Knudsen number $\varepsilon := \mathrm{Kn} := \ell/L$, which is the ratio between the mean-free-path ℓ and a characteristic macroscopic length L. However, the Knudsen number Kn cannot be derived in the LBE and has to be introduced artificially [5–7]. The CE analysis usually assumes the convective (or acoustic) scaling, i.e., $\delta_t \sim \delta_x$, where δ_t and δ_x are the time-step size and the grid spacing, respectively, and yields the compressible Navier–Stokes equations.

The second approach is the asymptotic analysis [8–11]. In the asymptotic analysis of the LBE, the expansion parameters are both the time-step size δ_t and the grid spacing δ_x. The asymptotic analysis usually assumes the diffusive scaling $\delta_t \sim \delta_x^2$ and must use the Hilbert expansion for the conserved hydrodynamic variables. The asymptotic analysis leads to the incompressible Navier–Stokes equations.

The third approach is the equivalent-equation analysis [12–16]. In this approach, solutions of the LBE are assumed to be smooth thus they can be approximated by their Taylor expansions. This approach also assumes the convective scaling $\delta_t \sim \delta_x$. However, this approach must rely on the Chapman–Enskog procedure to relate the time derivatives of the macroscopic variables to their spatial derivatives in order to derive the Navier–Stokes equations. This approach has also been used to analyze the LBE with a forcing term [16].

In this work we propose to use the Maxwell iteration [17–23] as a means to derive the macroscopic equations from the LBE. In this approach, one also uses the Taylor expansion of the distribution function (cf., e.g., Ref. [24]) and assumes the convective scaling $\delta_t \sim \delta_x$, thus the time-step size δ_t is the only expansion parameter, and the compressible Navier–Stokes equations are derived. It will be seen that the Maxwell iteration is much more straightforward and logically clearer than the existing approaches, including the Chapman–Enskog procedure, for the analysis of the LBE. In addition to obtaining the hydrodynamic equations, the Maxwell iteration also provides a numerical analysis of the LBE for its numerical accuracy. In particular, our analysis shows that the Mach number Ma should be scaled as $O(\delta_t^{1/3})$ in the limit of $\delta_t \to 0$ to maintain the truncation errors due to Ma and δ_t in the balance so to optimize the efficiency of the lattice Boltzmann simulation.

The remainder of this paper is organized as follows: Section II provides a brief introduction of the LBE in its moment representation [25–28]. Specifically, the lattice Boltzmann model with nine velocities on a two-dimensional square lattice (D2Q9 model) with the multiple-relaxation-time (MRT) collision model is analyzed in this work. Section III describes the detailed procedure of the Maxwell iteration for the LBE. Section IV presents the main results of this work. The compressible Navier–Stokes equations with a forcing term are derived from the LBE through the Maxwell iteration. The force density derived from our analysis is given in both the discrete velocity space $\mathbb{V}$ and the moment space $\mathbb{M}$ and can be related to various forcing schemes derived previously. The derived force density is consistent with the second-order accuracy of the LBE for solving the Navier–Stokes equations under the condition that $\mathrm{Ma} = O(\delta_t^{1/3})$ as $\delta_t \to 0$. Finally, Sec. V discusses our results and concludes the paper. There are also two appendixes. Appendix A discusses the treatment

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of the singular relaxation matrix S in which the relaxation rates corresponding to the conserved moments can be set to zero. Appendix B shows the stress tensor computed from the nonequilibrium momentum flux, which is identical to the one obtained with the Maxwell iteration.

II. LATTICE BOLTZMANN EQUATION IN MOMENT REPRESENTATION

The lattice Boltzmann equation has its kinetic root and can be directly derived from kinetic equations [3,4]. The LBE evolves in a coupled discrete phase space with discrete time $\{t_n|n = 0, 1, 2, \ldots\}$ with time-step size δ_t, i.e., $t_n = n\delta_t$, $n \in \mathbb{N}_0 := \{0, 1, 2, \ldots\}$. The coupled phase space consists of a finite and symmetric discrete set $\mathbb{V} := \{\boldsymbol{c}_i\} = \{-\boldsymbol{c}_i\}$ and a d-dimensional lattice space $\mathbb{Z}^d$ with a lattice constant δ_x. The lattice $\mathbb{Z}^d$, the discrete velocity set $\mathbb{V}$, and discrete time are coupled as follows:

$$\boldsymbol{x}_j + \boldsymbol{c}_i\delta_t \in \mathbb{Z}^d \ \forall\, \boldsymbol{x}_j \in \mathbb{Z}^d \quad \text{and} \quad \boldsymbol{c}_i \in \mathbb{V}, \tag{1}$$

such that particle transport term in the Boltzmann equation, $\partial_t f + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f = \partial_t f + \boldsymbol{\nabla}\cdot(\boldsymbol{\xi} f)$, is modeled by hopping from one lattice point $\boldsymbol{x}_j$ to another $\boldsymbol{x}_j + \boldsymbol{c}_i\delta_t$. The collision term in the Boltzmann equation is modeled as a linear relaxation process in the LBE. It is particularly illuminating to write linear relaxation processes in the LBE in terms of the relaxation process of moments [25], for it can be seen as a discrete counterpart of the truncated Gross–Jackson model [29].

The lattice Boltzmann equation can be concisely written in a vector form:

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta_t, t_n + \delta_t) - \mathbf{f}(\boldsymbol{x}_j, t_n) = \boldsymbol{\Omega}(\boldsymbol{x}_j, t_n) + \delta_t\mathbf{G}(\boldsymbol{x}_j, t_n), \tag{2}$$

where $\mathbf{f}$, $\boldsymbol{\Omega}$, and $\mathbf{G}$ are Q-dimensional vectors denoting the discrete-velocity particle distribution, the collision term, and the force density to be determined, respectively. Specifically, they are defined as

$$\begin{aligned}
\mathbf{f}(\boldsymbol{x}_j+\boldsymbol{c}\delta_t,t_n+\delta_t) &:= (f_0(\boldsymbol{x}_j,t_n+\delta_t),\ f_1(\boldsymbol{x}_j+\boldsymbol{c}_1\delta_t,t_n+\delta_t),\\
&\qquad \ldots, f_q(\boldsymbol{x}_j+\boldsymbol{c}_q\delta_t,t_n+\delta_t))^\dagger,\\
\mathbf{f}(\boldsymbol{x}_j,t_n) &:= (f_0(\boldsymbol{x}_j,t_n), f_1(\boldsymbol{x}_j,t_n), \ldots, f_q(\boldsymbol{x}_j,t_n))^\dagger,\\
\boldsymbol{\Omega}(\boldsymbol{x}_j,t_n) &:= (\Omega_0(\boldsymbol{x}_j,t_n), \Omega_1(\boldsymbol{x}_j,t_n), \ldots, \Omega_q(\boldsymbol{x}_j,t_n))^\dagger,\\
\mathbf{G}(\boldsymbol{x}_j,t_n) &:= (G_0(\boldsymbol{x}_j,t_n), G_1(\boldsymbol{x}_j,t_n), \ldots, G_q(\boldsymbol{x}_j,t_n))^\dagger,
\end{aligned}$$

where $q := (Q-1)$ is the number of nonzero velocities and $\dagger$ denotes the transpose; and it is always assumed that $\boldsymbol{c}_0 := \mathbf{0}$.

It is natural to carry out the transport process in physical space, while to execute the collision process in moment space $\mathbb{M}$, because the relaxation of moments is directly related to dissipative processes in nonequilibrium systems. To cast the collision in terms of relaxation process of moments is the essence the multiple-relaxation-time (MRT) collision model for the LBE proposed by d'Humières [25]. In the MRT model, the collision term in the LBE (2) can be written in general as follows:

$$\boldsymbol{\Omega} = -\mathsf{M}^{-1}\cdot\mathsf{S}\cdot[\mathbf{m} - \mathbf{m}^{(0)}], \tag{3}$$

where $\mathbf{m}$ and $\mathbf{m}^{(0)}$ are Q-dimensional vectors of moments and their equilibria, respectively, S is a diagonal matrix, whose elements are the relaxation rates s_i, and $s_i \in (0, 2)$ [10,26,30]; and M is the transformation matrix which maps the distribution functions $\{f_i\}$ to the moments $\{m_i\}$, i.e.,

$$\mathbf{m} := \mathsf{M}\cdot\mathbf{f}, \quad \mathbf{f} = \mathsf{M}^{-1}\cdot\mathbf{m}. \tag{4}$$

It should be mentioned that, for any discrete velocity model, the number of linearly independent moments is equal to the number of discrete velocities [26,28].

To be concrete, we use the nine-velocity model on a two-dimensional square lattice, i.e., the D2Q9 model, as a specific model in what follows. We should stress that our methodology is model independent and can be applied to analyze any lattice-Boltzmann model. For the D2Q9 model, the discrete velocities are $\boldsymbol{c}_0 = (0,0)c$, $\boldsymbol{c}_1 = -\boldsymbol{c}_3 = (1,0)c$, $\boldsymbol{c}_2 = -\boldsymbol{c}_4 = (0,1)c$, $\boldsymbol{c}_5 = -\boldsymbol{c}_7 = (1,1)c$, and $\boldsymbol{c}_6 = -\boldsymbol{c}_8 = (-1,1)c$, where $c := \delta_x/\delta_t$. Specific to the D2Q9 model, the nine moments are chosen to be [26]

$$\mathbf{m} := (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^\dagger, \tag{5}$$

where ρ is the zeroth-order moment and the mass density, e is the second-order moment related to energy, ε is the fourth-order moment related to the energy squared; j_x and j_y are the first-order moments corresponding to the x and y components of momentum, respectively, q_x and q_y are the third-order moments corresponding to the x and y components of energy flux, respectively, and p_{xx} and p_{xy} are the second-order moments related to the diagonal and off-diagonal components of the stress tensor, respectively [26]. Note that the ordering of moments in Eq. (5) is arbitrary. With the ordering of the moments specified by Eq. (5), the transformation matrix M is given by [26]

$$\mathsf{M} = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1\\
-4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2\\
4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1\\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1\\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1\\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1\\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1\\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1
\end{pmatrix}. \tag{6}$$

It is directly to check that M is orthogonal—all row vectors, which project distributions $\{f_i\}$ to moments $\{m_i\}$, are mutually orthogonal [26]; therefore $\mathsf{M}\cdot\mathsf{M}^\dagger$ is diagonal and hence M^{-1} can be easily calculated. Also, the elements of M are integers, which makes the computation involving M simple and easy. Because the moments are cast in an orthogonal basis, change in one moment does not affect any other moment at the same space point. These features of M makes the algorithm of the MRT-LBE rather efficient. When row vectors of M are normalized, it becomes the unitary matrix U, i.e., $\mathsf{U}^\dagger = \mathsf{U}^{-1}$.

It should be noted that the construction of the moments is not unique in addition to the arbitrary ordering of the moments given in Eq. (5). First of all, the normalization of moments can be arbitrary (cf., e.g., Refs. [31,32]); we choose not to normalize the moments so the elements in M are integers. We also note that the basis for the D2Q9 model need not include $\boldsymbol{c}_i^3$ and $\boldsymbol{c}_i^4$ [31,32], for they are in fact linear combinations of the lower-order monomials. However, $\boldsymbol{c}_i^3$ and $\boldsymbol{c}_i^4$ do appear in three-dimensional models (cf., e.g., Ref. [27]). Second, the moments of equal order can be subjected to a rotation due to a rotation of coordinate system. For example, the first-order modes $\{c_{i,x}\}$ and $\{c_{i,y}\}$, corresponding to the fourth row and sixth row of M given by Eq. (6), respectively, assume that $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$ are parallel to the x axis and the y axis, respectively. Of course, if the coordinate system is rotated clockwise through an arbitrary constant angle θ, then the first-order modes in the rotated coordinates become $\{\|\boldsymbol{c}_i\|\cos\theta\}$ and $\{\|\boldsymbol{c}_i\|\sin\theta\}$; and replacing the fourth row and sixth row of M given by Eq. (6) respectively with $\{\|\boldsymbol{c}_i\|\cos\theta\}$ and $\{\|\boldsymbol{c}_i\|\sin\theta\}$ would not change the orthogonality among the rows of M. And third, the orthogonality among the moments, encoded by the mutual orthogonality among the rows of M of Eq. (6), is with respect to a weight of unity. If the orthogonality of the moments is with respect to the weight $w_i \propto \exp(-\boldsymbol{c}_i\cdot\boldsymbol{c}_i/2RT)$ [3,4], then the kinetic moments have no project to the equilibrium distribution with such basis [31,32].

For *athermal* LBE *without* external forcing, the density ρ and flow momentum $\boldsymbol{j} := \rho\boldsymbol{u} := (j_x, j_y)$ are the only conserved moments in the system and, as defined in the transformation matrix M of Eq. (6), they are given by

$$\rho = \sum_i f_i = \sum_i f_i^{(0)}, \tag{7a}$$

$$\rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i = \sum_i \boldsymbol{c}_i f_i^{(0)}, \tag{7b}$$

where $\boldsymbol{u} := (u_x, u_y)$ is the flow velocity. By definition, the equilibria of the conserved moments are themselves, i.e., $\rho^{(0)} = \rho$ and $\boldsymbol{j}^{(0)} = \rho\boldsymbol{u}$. When external forcing $\boldsymbol{F} := (F_x, F_y)$ is present, the equilibrium of the momentum $\boldsymbol{j}$ should include the effect of the forcing; that is,

$$\rho\boldsymbol{u} := \boldsymbol{j}^{(0)} = \sum_i \boldsymbol{c}_i f_i^{(0)} = \sum_i \boldsymbol{c}_i f_i + b\delta_t \boldsymbol{F}, \tag{8}$$

where b is a parameter to be determined later through analysis. Because the forcing $\boldsymbol{F}$ is included in the equilibria of momentum $\boldsymbol{j}^{(0)}$ given above, thus is considered in the collision process. It has been well known that, to correctly account for its effect, the forcing has to be included in the collision process [33,34]. In fact, numerical analysis of correct implementation of forcing in the LBE has been carried out previously [35], and it has been shown that correct implementation of forcing is crucial to obtain second-order accuracy for the lattice Boltzmann scheme [35]. We show that correct forcing schemes can be derived easily and naturally through the Maxwell iteration.

In what follows, we restrict ourselves to the equilibria which are linear in ρ and second-order in $\boldsymbol{u}$. Specifically, the equilibrium moments for the D2Q9 model are given by

$$m_0^{(0)} = \rho, \quad m_{3,5}^{(0)} = j_{x,y}^{(0)} := \sum_i \boldsymbol{c}_i f_i + b\delta_t F_{x,y}, \tag{9a}$$

$$m_1^{(0)} = -2\rho + 3\frac{\boldsymbol{j}^{(0)}\cdot\boldsymbol{j}^{(0)}}{\rho}, \quad m_2^{(0)} = \rho - 3\frac{\boldsymbol{j}^{(0)}\cdot\boldsymbol{j}^{(0)}}{\rho}, \tag{9b}$$

$$m_{4,6}^{(0)} = -j_{x,y}^{(0)}, \tag{9c}$$

$$m_7^{(0)} = \frac{1}{\rho}\left[\left(j_x^{(0)}\right)^2 - \left(j_y^{(0)}\right)^2\right], \quad m_8^{(0)} = \frac{1}{\rho} j_x^{(0)} j_y^{(0)}, \tag{9d}$$

where $\boldsymbol{j}^{(0)}\cdot\boldsymbol{j}^{(0)} := (j_x^{(0)})^2 + (j_y^{(0)})^2$. It should be pointed out that the equilibria given above is equivalent to the second-order Taylor expansion of the Maxwellian in terms of small velocity $u := \|\boldsymbol{u}\|$ [3,4], because

$$\mathbf{m}^{(0)} := \mathsf{M}\cdot\mathbf{f}^{(0)}, \quad \mathbf{f}^{(0)} = \mathsf{M}^{-1}\cdot\mathbf{m}^{(0)}.$$

Thus, u is a small quantity in this setting. It should also be mentioned that the number of adjustable parameters is predetermined by the number of discrete velocities [26,28]. For this reason, it is pointless to include terms higher than second order in u for the D2Q9 model in the equilibria (9).

With the ordering of moments given by Eq. (5), the diagonal matrix S composed of the relaxation rates $\{s_i\}$ is given in the following form:

$$\mathsf{S} := \mathrm{diag}(s_0, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8). \tag{10}$$

The linear stability requires that $0 \leqslant s_i \leqslant 2$ for nonconserved moments, i.e., $i = 1, 2, 4, 6, 7,$ and 8 [26,30]. Later, we further discuss the constraints on the values of the relaxation rates $\{s_i | 0 \leqslant i \leqslant 8\}$.

The form of the force density in the discrete velocity space consistent with the equilibria given by Eq. (9) has been derived previously [36,37]:

$$\begin{aligned} w_i\left[\frac{\boldsymbol{c}_i}{c_s^2} + \left(\frac{\boldsymbol{c}_i\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^4} - \frac{\boldsymbol{u}}{c_s^2}\right)\right]\cdot\boldsymbol{F} \\ = w_i[\mathsf{H}^{(1)}(\hat{\boldsymbol{c}}_i)\cdot\hat{\boldsymbol{F}} + \mathsf{H}^{(2)}(\hat{\boldsymbol{c}}_i) : \hat{\boldsymbol{u}}\hat{\boldsymbol{F}}], \end{aligned} \tag{11}$$

where $w_0 = 4/9$, $w_1 = w_2 = w_3 = w_4 = w_0/4 = 1/9$, $w_6 = w_7 = w_8 = w_9 = w_0/16 = 1/36$, $c_s := c/\sqrt{3}$, $\hat{\boldsymbol{c}}_i := \boldsymbol{c}_i/c_s$, $\hat{\boldsymbol{u}} := \boldsymbol{u}/c_s$, $\hat{\boldsymbol{F}} := \boldsymbol{F}/c_s$, and $\mathsf{H}^{(n)}(\hat{\boldsymbol{c}}_i)$ denotes the nth-order tensorial Hermite polynomial on discrete velocity set $\{\hat{\boldsymbol{c}}_i\}$ in d-dimensional space: specifically,

$$\mathsf{H}^{(1)}(\hat{\boldsymbol{c}}_i) = \hat{\boldsymbol{c}}_i, \tag{12a}$$

$$\mathsf{H}^{(2)}(\hat{\boldsymbol{c}}_i) = \hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i - \mathsf{I}. \tag{12b}$$

The force density in the form given by Eq. (11) can be projected to the moment space as follows:

$$\begin{pmatrix} 0 \\ 6\boldsymbol{u}\cdot\boldsymbol{F} \\ -6\boldsymbol{u}\cdot\boldsymbol{F} \\ F_x \\ -F_x \\ F_y \\ -F_y \\ 2(u_x F_x - u_y F_y) \\ u_y F_x + u_x F_y \end{pmatrix}. \tag{13}$$

Based on expression (13), we assume the forcing in moment space $\boldsymbol{\Phi} := \mathsf{M}\cdot\mathbf{G}$, as follows:

$$\boldsymbol{\Phi} := \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \end{pmatrix} = \begin{pmatrix} 0 \\ h_1\boldsymbol{u}\cdot\boldsymbol{F} \\ h_2 6\boldsymbol{u}\cdot\boldsymbol{F} \\ h_3 F_x \\ -h_4 F_x \\ h_5 F_y \\ -h_6 F_y \\ h_7(u_x F_x - u_y F_y) \\ h_8(u_y F_x + u_x F_y) \end{pmatrix}, \tag{14}$$

where h_i, $i = 1,2,\ldots,8$, are the parameters to be determined later through analysis. The above moments of the forcing term are given in the most general form without considering symmetries of the system. Once the parameters $\{h_i | i = 1,2,\ldots,8\}$ are determined, the force density in the LBE (2) is obtained as $\mathbf{G} = \mathbf{M}^{-1} \cdot \boldsymbol{\Phi}$.

The physical significance of the force density projected to the moment space is rather clear. First, $\Phi_0 = 0$ simply means the forcing does not affect mass conservation. The effect of the forcing on the velocity should be proportional to $\delta_t \boldsymbol{F}$, as indicated by $\Phi_3 = h_3 F_x$ and $\Phi_5 = h_5 F_x$. The effect of forcing on the energy mode should be be proportional to the work done by the force, i.e., $\boldsymbol{u}\cdot\boldsymbol{F}$, as indicated by $\Phi_1 = h_1 \boldsymbol{u}\cdot\boldsymbol{F}$. The effect of forcing on the stresses is determined by the off-diagonal second-order moments of $\boldsymbol{F}$, as given by Φ_7 and Φ_8. The projection of forcing to the fourth-order moment Φ_2 should be similar to Φ_1, the energy mode, because Φ_2 and Φ_1 have the same symmetry and in the equilibria, only terms up to u^2 (energy) are retained. By the same reasoning, the third-order moments, Φ_4 and Φ_6, should be similar to Φ_3 and Φ_5, respectively.

III. THE MAXWELL ITERATION

As mentioned previously, we choose the convective scaling $\delta_t = \delta_x$ in our analysis, so that $c = \delta_x/\delta_t = 1$. In this setting, δ_t is the *only* small parameter in the LBE (2).

With the Taylor expansion of the left-hand side in terms of δ_t, the LBE (2) can be written as

$$\mathbf{L}(\delta_t \mathbf{D}) \cdot \mathbf{f} = -\mathbf{M}^{-1} \cdot \mathbf{S} \cdot [\mathbf{m} - \mathbf{m}^{(0)}] + \delta_t \mathbf{G}, \tag{15}$$

where $\mathbf{L}(\delta_t \mathbf{D})$ is the linear differential operator defined as

$$\mathbf{L}(\delta_t \mathbf{D}) := e^{\delta_t \mathbf{D}} - \mathbf{I} = \sum_{k=1}^{\infty} \frac{(\delta_t \mathbf{D})^k}{k!} = \sum_{k=1}^{\infty} \frac{\delta_t^k}{k!} \mathbf{D}^k,$$

where $\mathbf{D}$ is the diagonal matrix-valued operator with the diagonal elements $\partial_t + \boldsymbol{c}_i \cdot \nabla$, i.e.,

$$\mathbf{D} := \mathbf{I}\partial_t + \mathbf{C}_x \partial_x + \mathbf{C}_y \partial_y, \tag{16a}$$

$$\mathbf{C}_x := \mathrm{diag}(0,1,0,-1,0,1,-1,-1,1), \tag{16b}$$

$$\mathbf{C}_y := \mathrm{diag}(0,0,1,0,-1,1,1,-1,-1), \tag{16c}$$

where $\mathbf{I}$ denotes the 9×9 identity matrix. Multiplying its two sides with $\mathbf{M}$, Eq. (15) can be written entirely in terms of moments:

$$\mathbf{L}(\delta_t \tilde{\mathbf{D}}) \cdot \mathbf{m} = -\mathbf{S} \cdot [\mathbf{m} - \mathbf{m}^{(0)}] + \delta_t \boldsymbol{\Phi}, \tag{17}$$

where $\boldsymbol{\Phi} = \mathbf{M} \cdot \hat{\mathbf{F}}$, and $\tilde{\mathbf{D}} := \mathbf{M} \cdot \mathbf{D} \cdot \mathbf{M}^{-1} = \partial_t \mathbf{I} + \tilde{\mathbf{C}}_x \partial_x + \tilde{\mathbf{C}}_y \partial_y$ with $\tilde{\mathbf{C}}_{x,y} := \mathbf{M} \cdot \mathbf{C}_{x,y} \cdot \mathbf{M}^{-1}$ given explicitly as

$$\tilde{\mathbf{C}}_x := \frac{c}{6}\begin{pmatrix} 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 2 & 2 & 0 & 0 & 0 & 0 & -6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 2 & 0 & 0 \end{pmatrix},$$

$$\tilde{\mathbf{C}}_y := \frac{c}{6}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 4 & 1 & 0 & 0 & 0 & 0 & 0 & -3 & 0 \\ 0 & 2 & 2 & 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 2 & 0 & 0 \\ 0 & 0 & 0 & 4 & 2 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Assume for now that all the relaxation rates in Eq. (10) are positive, i.e., $s_i > 0$ with $0 \leqslant i \leqslant 8$, such that $\mathbf{S}$ is invertible (the singular case of $\mathbf{S}$ is discussed in Appendix A). Then Eq. (17) can be rewritten as

$$\mathbf{m} = \mathbf{m}^{(0)} - \mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}}) \cdot \mathbf{m} + \delta_t \mathbf{S}^{-1} \cdot \boldsymbol{\Phi}. \tag{18}$$

The above equation can be formally solved by the Maxwell iteration [17–23] by setting $\mathbf{m} = \mathbf{m}^{[k-1]}$ in the right-hand side to obtain $\mathbf{m} = \mathbf{m}^{[k]}$ on the right-hand side:

$$\mathbf{m}^{[k]} = \mathbf{m}^{(0)} - \mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}}) \cdot \mathbf{m}^{[k-1]} + \delta_t \mathbf{S}^{-1} \cdot \boldsymbol{\Phi}, \tag{19}$$

with $k \geqslant 1$ and $\mathbf{m}^{[0]} = \mathbf{m}^{(0)}$.

The first-order iteration with $k = 1$ is

$$\begin{aligned} \mathbf{m}^{[1]} &= [\mathbf{I} - \mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}})] \cdot \mathbf{m}^{(0)} + \delta_t \mathbf{S}^{-1} \cdot \boldsymbol{\Phi} \\ &= \mathbf{m}^{(0)} + O(\delta_t). \end{aligned} \tag{20}$$

The above result of $\mathbf{m}^{[1]}$ immediately leads to the result for the second-order iteration with $k = 2$ in Eq. (19):

$$\begin{aligned} \mathbf{m}^{[2]} &= \{\mathbf{I} - \mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}}) + [\mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}})]^2\} \cdot \mathbf{m}^{(0)} \\ &\quad + \delta_t [\mathbf{I} - \mathbf{S}^{-1} \cdot \mathbf{L}(\delta_t \tilde{\mathbf{D}})] \cdot \mathbf{S}^{-1} \cdot \boldsymbol{\Phi} \\ &= \mathbf{m}^{[1]} + O\big(\delta_t^2\big), \end{aligned} \tag{21}$$

and more generally,

$$\mathbf{m}^{[k]} = \mathbf{m}^{[k-1]} + O\big(\delta_t^k\big), \tag{22}$$

simply because $\mathbf{L}(\delta_t \tilde{\mathbf{D}}) = O(\delta_t)$. Through k iterations, we can obtain $\mathbf{m}^{[k]}$ in terms of $\mathbf{m}^{(0)}$ and $\boldsymbol{\Phi}$. Moreover, it is obvious that the accuracy of the solution by iteration is

$$\mathbf{m} = \mathbf{m}^{[k]} + O\big(\delta_t^{k+1}\big). \tag{23}$$

With the first-order result $\mathbf{m}^{[1]}$ of Eq. (20), Eq. (23) becomes

$$\mathbf{m} = [\mathbf{I} - \delta_t \mathbf{S}^{-1} \cdot \tilde{\mathbf{D}}] \cdot \mathbf{m}^{(0)} + \delta_t \mathbf{S}^{-1} \cdot \boldsymbol{\Phi} + O\big(\delta_t^2\big), \tag{24}$$

and with the second-order result $\mathbf{m}^{[2]}$ of Eq. (21), Eq. (23) is

$$\begin{aligned} \mathbf{m} &= \mathbf{m}^{(0)} - \delta_t \mathbf{S}^{-1} \cdot \tilde{\mathbf{D}} \cdot \left[\mathbf{I} - \delta_t \left(\mathbf{S}^{-1} - \frac{1}{2}\mathbf{I}\right) \cdot \tilde{\mathbf{D}}\right] \cdot \mathbf{m}^{(0)} \\ &\quad + \delta_t (\mathbf{I} - \delta_t \mathbf{S}^{-1} \cdot \tilde{\mathbf{D}}) \cdot \mathbf{S}^{-1} \cdot \boldsymbol{\Phi} + O\big(\delta_t^3\big). \end{aligned} \tag{25}$$

Equations (24) and (25) will be used to derive the hydrodynamic equations in the ensuing section.

It can be seen from both Eqs. (24) and (25) that $\tilde{\mathbf{D}} \cdot \mathbf{m}^{(0)}$, i.e., the gradient of the equilibrium moments, will be an important centerpiece in the ensuing analysis, thus it is given explicitly as

$$\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)} := \partial_t\begin{pmatrix}\rho\\ e^{(0)}\\ \varepsilon^{(0)}\\ j_x^{(0)}\\ -j_x^{(0)}\\ j_y^{(0)}\\ -j_y^{(0)}\\ p_{xx}^{(0)}\\ p_{xy}^{(0)}\end{pmatrix}+\partial_x\begin{pmatrix}\rho u_x\\ 0\\ -\rho u_x\\ J_x\\ T_x\\ \rho u_x u_y\\ \rho u_x u_y\\ \frac{2}{3}\rho u_x\\ \frac{1}{3}\rho u_y\end{pmatrix}+\partial_y\begin{pmatrix}\rho u_y\\ 0\\ -\rho u_y\\ \rho u_x u_y\\ \rho u_x u_y\\ J_y\\ T_y\\ -\frac{2}{3}\rho u_y\\ \frac{1}{3}\rho u_x\end{pmatrix}, \tag{26}$$

where $e^{(0)} := m_1^{(0)}$, $\varepsilon^{(0)} := m_2^{(0)}$, $p_{xx}^{(0)} := m_7^{(0)}$, and $p_{xy}^{(0)} := m_8^{(0)}$ are defined in Eq. (9), and

$$J_{x,y} := \frac{2}{3}\rho + \frac{1}{6}e^{(0)} \pm \frac{1}{2}p_{xx}^{(0)}, \tag{27a}$$

$$T_{x,y} := \frac{1}{3}e^{(0)} + \frac{1}{3}\varepsilon^{(0)} \mp p_{xx}^{(0)}. \tag{27b}$$

Some comments regarding the iteration are in order here. First of all, as will be shown later, the second-order iteration of Eq. (25) is both necessary and sufficient to derive the Navier–Stokes equations. Second, the iterations higher than second order are useless for the given model, i.e., D2Q9, because the equilibria of the D2Q9 model are the second-order Taylor expansion in $\boldsymbol{u}$ of the Boltzmann–Maxwell distribution. Third, to use higher-order iteration means increasing the order of accuracy of the model, which requires higher order of the Taylor expansion of the Boltzmann–Maxwell distribution in terms of $\boldsymbol{u}$ [3,4] and, in turn, a large velocity set accordingly. And fourth and last, using the higher-order iteration *alone* will not improve the accuracy of the LBE, nor its capability to solve kinetic equations beyond the hydrodynamic regime.

IV. DERIVATION OF HYDRODYNAMIC EQUATIONS

A. Euler equations

The derivation of the hydrodynamic equations is carried out in two stages. The first is to obtain the Euler equations and the second is to obtain the Navier–Stokes equations. To obtain the Euler equations, it is sufficient to use the first-order iteration $\mathbf{m}^{[1]}$ because the Euler equations only include first-order derivatives. From the first-order iteration of $\mathbf{m}$ of Eq. (24), the equations for the density ρ and momenta ρu_x and ρu_y are derived:

$$\partial_t\rho + \nabla\cdot(\rho\boldsymbol{u}) - \Phi_0 = O(\delta_t), \tag{28a}$$

$$\partial_t(\rho u_x)+\partial_x\left(p+\rho u_x^2\right) + \partial_y(\rho u_x u_y) = (h_3+bs_3)F_x+O(\delta_t), \tag{28b}$$

$$\partial_t(\rho u_y)+\partial_x(\rho u_x u_y)+\partial_y\left(p+\rho u_y^2\right) = (h_5+bs_5)F_y+O(\delta_t), \tag{28c}$$

where $p := \rho/3$ and the substitution of $(\Phi_3,\Phi_5) = (h_3F_x, h_5F_y)$ has been made. Because $\Phi_0 = 0$, the above equations become the Euler equations:

$$\partial_t\rho + \nabla\cdot(\rho\boldsymbol{u}) = O(\delta_t), \tag{29a}$$

$$\partial_t(\rho\boldsymbol{u}) + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \boldsymbol{F} + O(\delta_t), \tag{29b}$$

provided that

$$h_3 + bs_3 = 1, \quad h_5 + bs_5 = 1. \tag{30}$$

B. Navier–Stokes equations

To derive the Navier–Stokes equations, we use some results concerning the moments up to second order as given in Eq. (26) for $\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)}$, i.e., $(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_i$ with $i = 0, 1, 3, 5, 7, 8$:

$$(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_0 \equiv \partial_t\rho + \nabla\cdot(\rho\boldsymbol{u}) = O(\delta_t), \tag{31a}$$

$$(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_3 \equiv \partial_t(\rho u_x) + \nabla\cdot(\rho\boldsymbol{u}u_x) + \partial_x p = F_x + O(\delta_t), \tag{31b}$$

$$(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_5 \equiv \partial_t(\rho u_y) + \nabla\cdot\left(\rho\boldsymbol{u}u_y\right) + \partial_y p = F_y + O(\delta_t), \tag{31c}$$

$$(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_1 \equiv \partial_t e^{(0)} = 6(\boldsymbol{F} + p\nabla)\cdot\boldsymbol{u} + O(\delta_t) + O(u^3), \tag{31d}$$

$$\begin{aligned}(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_7 &\equiv \partial_t p_{xx}^{(0)} + 2[\partial_x(pu_x) - \partial_y(pu_y)]\\ &= 2[p(\partial_x u_x - \partial_y u_y) + (u_xF_x - u_yF_y)]\\ &\quad + O(\delta_t) + O(u^3),\end{aligned} \tag{31e}$$

$$\begin{aligned}(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_8 &\equiv \partial_t p_{xy}^{(0)} + \partial_x(pu_y) + \partial_y(pu_x)\\ &= p(\partial_x u_y + \partial_y u_x) + u_xF_y\\ &\quad + u_yF_x + O(\delta_t) + O(u^3).\end{aligned} \tag{31f}$$

To derive the above equations, the following results have been used:

$$\partial_t(\rho u_x u_y) + u_x(\partial_y p - F_y) + u_y(\partial_x p - F_x) = O(u^3), \tag{32a}$$

$$\partial_t\left(\rho u_x^2\right) + 2u_x(\partial_x p - F_x) = O(u^3), \tag{32b}$$

$$\partial_t\left(\rho u_y^2\right) + 2u_y(\partial_y p - F_y) = O(u^3). \tag{32c}$$

The Euler equations (29) have been used to obtain the above equations. Obviously, the equations of $(\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)})_i$, for $i = 0$, 3, and 5, i.e., the first three equations of (31), are simply the Euler equations (29).

The terms $O(u^3)$ in Eqs. (31) are to be ignored because the equilibria (9) are the second-order Taylor expansion of the Boltzmann–Maxwell distribution in $\boldsymbol{u}$, and $u = O(\mathrm{Ma})$, where $\mathrm{Ma} := u/c_s$ is the Mach number and c_s is the speed of sound in the system. The errors in Eq. (31) are $O(\mathrm{Ma}^3) + O(\delta_t)$; therefore $O(u^3)$ terms in Eq. (31) should be of the same order as the truncation errors in the equilibria. If we *require* the truncation errors due to both u and δ_t to be of the same size, i.e.,

$$\mathrm{Ma} = O\left(\delta_t^{1/3}\right), \tag{33}$$

then all the errors can be combined together, and the errors are all of $O(\delta_t)$. This point will be further discussed later.

1. The mass equation

The equation for the density derived from the result of the second-order iteration, Eq. (25), is

$$\begin{aligned}&\tau_0\delta_t[\partial_t\rho+\nabla\cdot(\rho\boldsymbol{u})]\\&\quad=\tau_0\delta_t^2\{\partial_t[\tilde{\tau}_0(\tilde{\mathbf{D}}\cdot\mathbf{m}^{(0)})_0-\tau_0\Phi_0]+\partial_x[\tilde{\tau}_3(\tilde{\mathbf{D}}\cdot\mathbf{m}^{(0)})_3-\tau_3\Phi_3]\\&\qquad+\partial_y[\tilde{\tau}_5(\tilde{\mathbf{D}}\cdot\mathbf{m}^{(0)})_5-\tau_5\Phi_5]\}+\tau_0\delta_t\Phi_0+O\big(\delta_t^3\big),\end{aligned}\tag{34}$$

where $\tau_i := 1/s_i$ and $\tilde{\tau}_i := (1/s_i - 1/2)$. Bear in mind that, in the presence of a forcing $\boldsymbol{F}$, the momentum is given by Eq. (8), i.e.,

$$\big(m_3^{(0)},m_5^{(0)}\big)=\sum_i \boldsymbol{c}_i f_i + b\delta_t\boldsymbol{F}.$$

By substituting Φ_i given in Eq. (14), the mass conservation equation at the Euler order, Eq. (29a), and the conditions (30) on h_3 and h_5 into the right-hand side of the above equation, we obtain the mass conservation equation at the Navier–Stokes order:

$$\partial_t\rho+\nabla\cdot(\rho\boldsymbol{u})=\left(b-\frac{1}{2}\right)\delta_t\nabla\cdot\boldsymbol{F}+O\big(\delta_t^2\big),\tag{35}$$

where constant b is introduced in Eq. (8) for the definition of momentum $\rho\boldsymbol{u}$ in presence of the forcing $\boldsymbol{F}$. Obviously, we must set $b = 1/2$ in order to have a correct equation for mass conservation. With $b = 1/2$ fixed, Eq. (30) becomes

$$h_3=1-\frac{1}{2}s_3,\quad h_5=1-\frac{1}{2}s_5;\tag{36}$$

that is, the coefficients h_3 and h_5 are determined by the relaxation rates s_3 and s_5, respectively.

2. The momentum equations

The equation for the x momentum ρu_x derived from Eq. (25) is

$$\begin{aligned}&\delta_t\tau_3[\partial_t(\rho u_x)+\nabla\cdot(\rho\boldsymbol{u}u_x)+\partial_x p]-\delta_t bF_x\\&\quad=\delta_t^2\tau_3\bigg[\partial_t(\tilde{\tau}_3\rho u_x-\tau_3\Phi_3)+\frac{2}{3}\partial_x(\tilde{\tau}_0\rho-\tau_0\Phi_0)\\&\qquad+\frac{1}{6}\partial_x(\tilde{\tau}_1e^{(0)}-\tau_1\Phi_1)+\frac{1}{2}\partial_x\big(\tilde{\tau}_7p_{xx}^{(0)}-\tau_7\Phi_7\big)\\&\qquad+\partial_y\big(\tilde{\tau}_8p_{xy}^{(0)}-\tau_8\Phi_8\big)\bigg]+\delta_t\tau_3\Phi_3+O\big(\delta_t^3\big),\end{aligned}\tag{37}$$

where $e^{(0)} := m_1^{(0)} := \rho(-2+3u^2)$, $p_{xx}^{(0)} := m_7^{(0)} := \rho(u_x^2 - u_y^2)$, and $p_{xy}^{(0)} := m_8^{(0)} := \rho u_x u_y$, which are defined in Eq. (9). Substitution of Eqs. (31) and (14) for $\{\Phi_i\}$ into the left-hand side of above equation leads to the following equation for the x momentum ρu_x:

$$\begin{aligned}&\partial_t(\rho u_x)+\nabla\cdot(\rho\boldsymbol{u}u_x)+\partial_x p-(s_3b+h_3)F_x\\&\quad=\partial_x[\rho\zeta\nabla\cdot\boldsymbol{u}+\rho\nu_{xx}(\partial_x u_x-\partial_y u_y)]\\&\qquad+\partial_y[\rho\nu_{xy}(\partial_x u_y+\partial_y u_x)]+\delta_t R_x+O\big(\delta_t^2\big),\end{aligned}\tag{38}$$

where ζ, ν_{xx}, and ν_{xy} are the dissipation coefficients for the moments $m_1 := e$, $m_7 = p_{xx}$, and $m_7 = p_{xy}$, respectively, and they are given by

$$\zeta=\frac{1}{3}\left(\frac{1}{s_1}-\frac{1}{2}\right)c\delta_x,\tag{39a}$$

$$\nu_{xx}=\frac{1}{3}\left(\frac{1}{s_7}-\frac{1}{2}\right)c\delta_x,\tag{39b}$$

$$\nu_{xy}=\frac{1}{3}\left(\frac{1}{s_8}-\frac{1}{2}\right)c\delta_x,\tag{39c}$$

where $c := \delta_x/\delta_t$. The first-order term R_x in Eq. (38) is

$$\begin{aligned}R_x&=\tilde{\tau}_1\partial_x(\boldsymbol{u}\cdot\boldsymbol{F})+\tilde{\tau}_7\partial_x(u_xF_x-u_yF_y)+\tilde{\tau}_8\partial_y(u_xF_y+u_yF_x)\\&\quad-\frac{1}{6}\tau_1\partial_x\Phi_1-\frac{1}{2}\tau_7\partial_x\Phi_7-\tau_8\partial_y\Phi_8\\&=\left(\frac{\tilde{\tau}_1}{h_1}-\frac{\tau_1}{6}\right)\partial_x\Phi_1+\left(\frac{\tilde{\tau}_7}{h_7}-\frac{\tau_7}{2}\right)\partial_x\Phi_7+\left(\frac{\tilde{\tau}_8}{h_8}-\tau_8\right)\partial_y\Phi_8.\end{aligned}\tag{40}$$

Similarly, the momentum equation for the y momentum ρu_y can be derived from Eq. (25):

$$\begin{aligned}&\partial_t(\rho u_y)+\nabla\cdot(\rho\boldsymbol{u}u_y)+\partial_y p-(h_5+s_5b)F_y\\&\quad=\partial_x[\rho\nu_{xy}(\partial_x u_y+\partial_y u_x)]+\partial_y[\rho\zeta\nabla\cdot\boldsymbol{u}\\&\qquad-\rho\nu_{xx}(\partial_x u_x-\partial_y u_y)]+\delta_t R_y+O\big(\delta_t^2\big),\end{aligned}\tag{41}$$

where

$$\begin{aligned}R_y&=\tilde{\tau}_8\partial_x(u_xF_y+u_yF_x)+\tilde{\tau}_1\partial_y(\boldsymbol{u}\cdot\boldsymbol{F})-\tilde{\tau}_7\partial_y(u_xF_x-u_yF_y)\\&\quad-\frac{1}{6}\tau_1\partial_y\Phi_1+\frac{1}{2}\tau_7\partial_y\Phi_7-\tau_8\partial_x\Phi_8\\&=\left(\frac{\tilde{\tau}_1}{h_1}-\frac{\tau_1}{6}\right)\partial_y\Phi_1-\left(\frac{\tilde{\tau}_7}{h_7}-\frac{\tau_7}{2}\right)\partial_y\Phi_7+\left(\frac{\tilde{\tau}_8}{h_8}-\tau_8\right)\partial_x\Phi_8.\end{aligned}\tag{42}$$

Combining Eq. (38) and for ρu_x and Eq. (41) for ρu_y yields

$$\partial_t(\rho\boldsymbol{u})+\nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u})=-\nabla p+\nabla\cdot\boldsymbol{\sigma}+\boldsymbol{F}+\delta_t\boldsymbol{R}+O\big(\delta_t^2\big),\tag{43a}$$

$$\boldsymbol{\sigma}:=\rho\nu[(\nabla\boldsymbol{u})+(\nabla\boldsymbol{u})^\dagger-\mathbf{I}(\nabla\cdot\boldsymbol{u})]+\rho\zeta(\nabla\cdot\boldsymbol{u})\mathbf{I},\tag{43b}$$

where $\boldsymbol{R} := (R_x, R_y)$, and $\nu = \nu_{xx} = \nu_{xy}$, which means $s_7 = s_8$ due to Eq. (39).

3. Discrete forcing moments

For Eq. (43) to be the Navier–Stokes equation up to $O(\delta_t^2)$, the first-order terms R_x and R_y must be eliminated simultaneously, which can be achieved by the following three conditions:

$$h_1=3(2-s_1),\tag{44a}$$

$$h_7=(2-s_7),\tag{44b}$$

$$h_8=\frac{1}{2}(2-s_8).\tag{44c}$$

So far, only h_0, h_1, h_3, h_5, h_7, and h_8 have been determined. The third-order moments (Φ_4, Φ_6) and the forth-order moments Φ_2 do not enter the analysis, for they are higher-order terms which only appear as truncation errors. To have the maximum degrees of freedom of the model, we retain all possible relaxation rates $\{s_i|i=1,2,\ldots,8\}$ in $\{\Phi_i\}$.

The forcing term in moment space is given by

$$\Phi_0 = 0, \tag{45a}$$

$$\Phi_1 = 3(2-s_1)\boldsymbol{u}\cdot\boldsymbol{F}, \quad \Phi_2 = -h_2\boldsymbol{u}\cdot\boldsymbol{F}, \tag{45b}$$

$$\Phi_3 = \frac{1}{2}(2-s_3)F_x, \quad \Phi_5 = \frac{1}{2}(2-s_5)F_y, \tag{45c}$$

$$\Phi_4 = -h_4F_x, \quad \Phi_6 = -h_6F_y, \tag{45d}$$

$$\Phi_7 = (2-s_\nu)(u_xF_x - u_yF_y),$$

$$\Phi_8 = \frac{1}{2}(2-s_\nu)(u_yF_x + u_xF_y), \tag{45e}$$

where $s_7 = s_8 := s_\nu$ has been substituted and h_2, h_4, and h_6 are yet to be determined.

The symmetry requires that the relaxation rates of the third-order moments must be equal, i.e., $s_4 = s_6 := s_q$ [26], and to ensure accurate realization of the Dirichlet boundary condition for the velocity $\boldsymbol{u}$, the relaxation rate of the third-order moment s_q is required to satisfy the following relationship [7,31,38,39]:

$$s_q = 8\frac{(2-s_\nu)}{(8-s_\nu)}. \tag{46}$$

Note that boundary condition on moments different from the velocity, such as the pressure (equivalently the density ρ), will lead different relationship $s_q(s_\nu)$ [15].

The linear analysis of the LBE [26] can determine the parameters h_2, h_4, and h_6:

$$h_2 = 3(2-s_\epsilon), \tag{47a}$$

$$h_{4,6} = \frac{1}{2}(2-s_q), \tag{47b}$$

where $s_\epsilon := s_2$. Consequently, we arrive in the following expressions of the forcing term in the moment space:

$$\Phi_1 = 3(2-s_e)\boldsymbol{u}\cdot\boldsymbol{F}, \quad \Phi_2 = -3(2-s_\epsilon)\boldsymbol{u}\cdot\boldsymbol{F}, \tag{48a}$$

$$\Phi_3 = \frac{1}{2}F_x, \quad \Phi_5 = \frac{1}{2}F_y, \tag{48b}$$

$$\Phi_4 = -\frac{1}{2}(2-s_q)F_x, \quad \Phi_6 = -\frac{1}{2}(2-s_q)F_y, \tag{48c}$$

$$\Phi_7 = (2-s_\nu)(u_xF_x - u_yF_y),$$

$$\Phi_8 = \frac{1}{2}(2-s_\nu)(u_yF_x + u_xF_y), \tag{48d}$$

where $s_e := s_1$ and $s_3 = s_5 = 1$. The relaxation rates s_e and s_ν determine the bulk and shear viscosity, respectively, as given in Eq. (39); the relaxation rate s_ϵ determines a dissipation through the forth-order moment, and the relaxation rate s_q has to satisfy Eq. (46) in order to maintain the accuracy of Dirichlet boundary conditions [7,31,38,39].

Some comments are in order here. First, one of our goals is to derive desired hydrodynamic equations for the moments. To this end, the moments $\mathbf{m}$ satisfying Eq. (25) are both necessary and sufficient the derive the Navier–Stokes equations, as can be shown in the preceding derivation. Second, this method can be used to carry out numerical analysis of the LBE. The D2Q9 model with the equilibria of Eq. (9) is second-order accurate, thus its analysis requires only a second-order Taylor expansion in Eq. (25). For the LBE with an accuracy higher than second order, its analysis would require an appropriate higher-order expansion.

C. Forcing in discrete velocity space

To understand the connections between various models derived previously, we project the moments of the forcing term back to the velocity space by using its most general form given in Eq. (45) for $\mathbf{G} = \mathbf{M}^{-1}\cdot\boldsymbol{\Phi}$:

$$\begin{aligned} G_i &= w_i\left[\hat{\boldsymbol{C}}_i\cdot\hat{\boldsymbol{F}} + \frac{1}{2}(\hat{\boldsymbol{c}}_i\hat{\boldsymbol{c}}_i - \mathbf{I}):\hat{\mathbf{W}}\right] \\ &= w_i\left[\mathbf{H}^{(1)}(\hat{\boldsymbol{C}}_i')\cdot\hat{\boldsymbol{F}} + \frac{1}{2}\mathbf{H}^{(2)}(\hat{\boldsymbol{c}}_i):\hat{\mathbf{W}}\right], \end{aligned} \tag{49a}$$

$$\hat{\boldsymbol{C}}_i = \begin{pmatrix} (1-\frac{1}{2}s_3)\hat{c}_{ix} \\ (1-\frac{1}{2}s_5)\hat{c}_{iy} \end{pmatrix} - \left(\frac{3}{4}\frac{\boldsymbol{c}_i\cdot\boldsymbol{c}_i}{c^2} - 1\right)\begin{pmatrix} (s_3-\tilde{s}_4)\hat{c}_{ix} \\ (s_5-\tilde{s}_6)\hat{c}_{iy} \end{pmatrix}, \tag{49b}$$

$$\begin{aligned} \hat{\mathbf{W}} &= \left(1-\frac{1}{2}s_\nu\right)(\hat{\boldsymbol{u}}\hat{\boldsymbol{F}} + \hat{\boldsymbol{F}}\hat{\boldsymbol{u}}) \\ &\quad + \left[\frac{1}{4}(s_\nu - \tilde{s}_2) + \frac{36\boldsymbol{c}_i\cdot\boldsymbol{c}_i(\boldsymbol{c}_i\cdot\boldsymbol{c}_i - c^2) + c^4}{2(3\boldsymbol{c}_i\cdot\boldsymbol{c}_i - 2c^2)c^2}(s_1 - \tilde{s}_2)\right] \\ &\quad \times (\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{F}})\mathbf{I}, \end{aligned} \tag{49c}$$

where $\hat{\boldsymbol{c}}_i = (\hat{c}_{ix},\hat{c}_{iy}) := \boldsymbol{c}_i/c_s$, $c_s = c/\sqrt{3}$, $c := \delta_x/\delta_t$, $\tilde{s}_2 = 2 - h_2/3$, and $\tilde{s}_{4,6} = 2(1-h_{4,6})$. The formulas above do not consider the symmetry of the system. When the symmetry of the system is considered, i.e., $s_3 = s_5$, $s_4 = s_6$, and Eq. (47) for h_2, h_4, and h_6 are used, the above formula for G_i reduced to the model derived by Guo *et al.* [40].

Two other models deserve special attention: the two-relaxation-time (TRT) model [41–43] and the lattice Bhatnagar–Gross–Krook (LBGK) model [or the single-relaxation-time (SRT) model] [44,45]. It is known that the TRT model enforces the Dirichlet boundary conditions in $\boldsymbol{u}$ exactly and minimizes the truncation error for the Poiseuille flow [39,41–43]. The TRT model can be efficiently implemented in the velocity space without using the projection to the moment space. In the TRT model, there are two relaxation rates: one for the even-order moments and the other for the odd-order moments, i.e., $s_1 = s_2 = s_\nu$ and $s_3 = s_4 = s_5 = s_6 = s_q$, but s_q must satisfy Eq. (46). The forcing for the TRT model is given by

$$\begin{aligned} G_i = w_i\Bigg[&\left(1-\frac{1}{2}s_q\right)\mathbf{H}^{(1)}(\hat{\boldsymbol{c}}_i)\cdot\hat{\boldsymbol{F}} \\ &+ \frac{1}{2}\left(1-\frac{1}{2}s_\nu\right)\mathbf{H}^{(2)}(\hat{\boldsymbol{c}}_i):(\hat{\boldsymbol{u}}\hat{\boldsymbol{F}} + \hat{\boldsymbol{F}}\hat{\boldsymbol{u}})\Bigg]. \end{aligned} \tag{50}$$

Because of the relationship $s_q(s_\nu)$ given by Eq. (46), the TRT model effectively has only one adjustable parameter s_ν which is determined by the viscosity ν or the Reynolds number Re of a flow. In contrast, the MRT-LBE model allows $s_1 = s_e$ and $s_2 = s_\varepsilon$ to be independent adjustable parameters, which affect numerical dissipation [7,26].

For the LBGK model, $s_i = 1/\tau$, then the forcing term reduces to the following simple form:

$$G_i = w_i\left(1 - \frac{1}{2\tau}\right)\left[\frac{(\boldsymbol{c}_i - \boldsymbol{u})\cdot\boldsymbol{F}}{c_s^2} + \frac{\boldsymbol{c}_i\boldsymbol{c}_i : (\boldsymbol{u}\boldsymbol{F} + \boldsymbol{F}\boldsymbol{u})}{2c_s^4}\right]$$
$$= w_i\left(1 - \frac{1}{2\tau}\right)\left[\mathsf{H}^{(1)}(\hat{\boldsymbol{c}}_i)\cdot\hat{\boldsymbol{F}} + \frac{1}{2}\mathsf{H}^{(2)}(\hat{\boldsymbol{c}}_i) : (\hat{\boldsymbol{u}}\hat{\boldsymbol{F}} + \hat{\boldsymbol{F}}\hat{\boldsymbol{u}})\right], \tag{51}$$

which has been previously derived by Guo *et al.* [46]. We note that the above formula is the same as Eq. (11), apart from the factor $[1 - 1/(2\tau)]$.

D. Implementation of forcing scheme

We now discuss the implementation of forcing in lattice Boltzmann (LB) algorithm. As usual, the forcing is included in the collision part of the LB algorithm, which can be decomposed into the following three steps [33–35,47]:

(i) The first step in the collision process, as indicated by Eq. (8), is to compute the proper local equilibrium momentum affected by the forcing, i.e., $\boldsymbol{j}^{(0)} := \sum_i \boldsymbol{c}_i f_i + \delta_t \boldsymbol{F}/2$.

(ii) The second step is to use the equilibrium momentum including the forcing $\boldsymbol{j}^{(0)}$ to compute other moments due the collision process, which is modeled by relaxation.

(iii) The third and final step is to add the remaining part of forcing effect either in moment space according to formula Eq. (45) or its variations, or in velocity space according to Eq. (49) or its variations.

The forcing scheme described in this work differs from the existing one [33–35,47] only slightly: the first and third steps described above are identical in the existing forcing scheme, but not in the present one. If $\Phi_i = 0$ for $i = 1, 2, 4, 6, 7$, and 8, and $s_3 = s_5 = 1$, then the present forcing scheme given in Eq. (48) is equivalent to the existing one [33–35,47], which is symmetric, i.e., the forcing term $\boldsymbol{F}$ is split into two equal halves of $\boldsymbol{F}/2$, one half is added before the collision (or relaxation) and the other is added after [35,47]. The implementation of the forcing term by splitting has also been applied to the case of Coriolis forces [48,49] and a similar splitting is also derived in Ref. [50].

V. DISCUSSION AND CONCLUSIONS

In this work, we propose using the Maxwell iteration [18–23] to derive the hydrodynamic equations from the lattice Boltzmann equation. This approach does *not* require artificial introduction of the Knudsen number as the expansion parameter in the LBE. Instead, the only expansion parameter in the present approach is the discrete time-step size δ_t or, equivalently, the lattice spacing δ_x, because of the acoustic scaling. This procedure not only derives the hydrodynamic equations but also provides a numerical analysis of the accuracy of the LBE as a numerical scheme. It should also be noted that the Maxwell iteration is a nonlinear process, while the asymptotic and Taylor expansions themselves are linear processes.

The choice of the convective (or acoustic) scaling leads to the athermal compressible Navier–Stokes equations; that is, only the mass and momentum-conservation equations are obeyed, and the energy is not a conserved quantity in the LBE. Under convective scaling, we derive the forcing scheme which can recover all the existing ones by choosing the appropriate combinations of relaxation rates. Because the analysis requires no specific knowledge of the forcing term, it is valid for the forcing term with arbitrary spatial-temporal dependence, such as Coriolis and Poincaré forces, so long as the spatial-temporal variations are adequately resolved with given δ_x and δ_t.

It is important to stress that, while the hydrodynamic equations we derive here are compressible in form, this does *not* imply by any means that the LBE can be used to solve the fully compressible Navier–Stokes equations with shocks or other effects associated with high-speed flows. Furthermore, to maintain the second-order accuracy of the lattice-Boltzmann equation as a flow solver, one must impose the scaling relationship between the Mach number Ma and the time-step size δ_t (or grid spacing δ_x) in the limit of $\delta_t \to 0$, $\delta_x/\delta_t = 1$:

$$\mathrm{Ma} = O\left(\delta_t^{1/3}\right) \quad \text{or} \quad \mathrm{Ma}^3 = O(\delta_t). \tag{52}$$

The underlying reason for the above scaling between Ma and δ_t is that there are two sources of numerical error in the LBE: one is due to the approximation of the Boltzmann–Maxwell distribution by its Taylor expansion in $\boldsymbol{u}$, and the other is due to the spatiotemporal discretization. In the LBE, the errors due to the Mach number truncation of the equilibrium must be kept in a balance in the discretization errors in the limit of $\delta_t \to 0$; otherwise the error due to the low-order Mach number expansion will become dominant, so the refinement of mesh and time-step size would not reduce the overall numerical error of the LBE simulation.

Based on the preceding analysis and discussion, for a lattice Boltzmann with an nth-order Taylor expansion of the Boltzmann–Maxwell distribution and a corresponding discrete velocity set, we may generalize the relationship (52) to the following conjecture:

$$\mathrm{Ma} = O\left(\delta_t^{\,1/(n+1)}\right). \tag{53}$$

It indicates whether the compressibility error starts to become dominant over the discretization errors for a given Mach number and mesh resolution. Not surprisingly, with a given Ma < 1, the LB model with a higher-order truncation in Ma, i.e., larger n in Eq. (53), will be able to use finer grid spacing δ_x and time step δ_t before the truncation error due to Ma becomes dominant.

Since the LBE does not solve the compressible Navier–Stokes equations with shocks or other physical effects due to Ma $\geqslant 1$, the role of the Mach number Ma in the LBE deserves to be further clarified, beyond Ma being a measure of the compressible effect *per se*. First, Ma indicates the size of truncation error due to the Taylor expansion of the equilibrium [3,4], which is an error in the LB model. And second and more importantly, the scaling (53) shows that Ma is explicitly connected to the time step size δ_t, thus suggesting that Ma indeed plays the role of the Courant–Friedrichs–Lewy (CFL) number.

We can also discuss another scaling related to the Reynolds number Re in the lattice Boltzmann simulation. The Reynolds number is defined as

$$\mathrm{Re} := \frac{UL}{\nu} = \frac{\sqrt{3}\times \mathrm{Ma}\times N}{\tilde{\tau}_\nu}, \tag{54}$$

where $N := L/\delta_x$, $\nu := \tilde{\tau}_\nu c_s^2\delta_t$, $\tilde{\tau}_\nu := (1/s_\nu - 1/2)$, $\mathrm{Ma} := U/c_s$, and $c_s = c/\sqrt{3}$ and $c := \delta_x/\delta_t$ are used. Should we assume the acoustic scaling $\delta_x/\delta_t = 1$ and consequently the scaling $\mathrm{Ma} = O(\delta_t^{1/3})$, then we can see from the above relationship (54) between Re and Ma that $\mathrm{Re} \sim O(\delta_t^{-2/3})$ when $\tilde{\tau}_\nu$ remains constant. To maintain a constant Re under the acoustic scaling, $\tilde{\tau}_\nu$ has to scale as $O(\delta_t^{2/3})$ in the limit of $\delta_t \to 0$. The significance of the scaling of $\mathrm{Re} \sim O(\delta_t^{-2/3})$ is clear: In the lattice-Boltzmann simulation, if the grid Reynolds number $\mathrm{Re}^* := U\delta_x/\nu$ is maintained constant, then, for a system with the characteristic length L and corresponding mesh size $N := L/\delta_x$, the Reynolds number $\mathrm{Re} = N\mathrm{Re}^* \to \infty$ as $\delta_x \to 0$. In the diffusive scaling $\delta_t \sim \delta_x^2$, $\mathrm{Ma} = O(\delta_x)$ as $\delta_x \to 0$ [8,9,11]; thus, Re remains as a constant in the limit. However, in practice, the acoustic scaling is usually used in the lattice Boltzmann simulations (cf., e.g., Refs. [7,33,34]). Unless the rigorous incompressible limit is required, the diffusive scaling is not necessary, for the number of time steps would grow rather rapidly as the mesh is refined in the diffusive scaling.

In summary, we propose to use the Maxwell iteration to derive the macroscopic equation from the lattice Boltzmann equation with convective scaling. We demonstrate the efficacy of this approach by deriving the Navier–Stokes equations from the D2Q9 lattice Boltzmann model with multiple-relaxation-time collision term and an external forcing. This approach is simple and direct without the necessity to artificially introduce the Knudsen number, nor does it need the Hilbert expansion of the conserved quantities which are required in the asymptotic analysis. More importantly, the analysis shows the scaling between the truncation error due to the Mach number Ma and that due to time step size δ_t in the limit of $\delta_t \to 0$. This analysis can also be extended to analyze the lattice Boltzmann model for more general fluids [11].

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APPENDIX A: SINGULAR CASE OF RELAXATION MATRIX S

In the derivation of the hydrodynamic equations, the relaxation matrix S is assumed to be invertible, i.e., $s_i > 0$. For the sake of completeness, we can show that this assumption is unnecessary.

The only relaxation rates can be set to zero are those for the conserved modes, i.e., $s_i = 0$ for $i = 0$, 3, and 5, for ρ, j_x, and j_y, respectively. In this case, the relaxation matrix is

$$\mathsf{S}' = \mathrm{diag}(0,s_1,s_2,0,s_4,0,s_6,s_7,s_8). \tag{A1}$$

To handle the singular relaxation matrix S', we introduce the new moments in the presence of the forcing:

$$\mathbf{m}' = \mathbf{m} + \delta_t\mathbf{G}', \tag{A2}$$

$$\mathbf{G}' = b(0,0,0,F_x,0,F_y,0,0,0)^\dagger, \tag{A3}$$

so that $m_i' = m_i^{(0)}$ for $i = 0$, 3, and 5. With $\mathbf{m}'$ and S', Eq. (17) becomes

$$\mathsf{L}(\delta_t\tilde{\mathsf{D}})\cdot\mathbf{m}' = -\mathsf{S}'\cdot[\mathbf{m}' - \mathbf{m}^{(0)}] + \delta_t\mathbf{\Phi} + \delta_t\mathsf{L}(\delta_t\tilde{\mathsf{D}})\cdot\mathbf{G}', \tag{A4}$$

where we have used the fact that $\mathsf{S}'\cdot\mathbf{G}' = \mathbf{0}$.

Because $[m_i' - m_i^{(0)}] = 0$ for $i = 0$, 3, and 5, the corresponding relaxation rates s_i for $i = 0, 3$, and 5 can be arbitrary. Hence, in Eq. (A4) the singular relaxation matrix S' can be replaced by the regular one S of Eq. (10) with $s_i > 0$ for $i = 0$, 3, and 5. Consequently, Eq. (A4) becomes

$$\mathbf{m}' = \mathbf{m}^{(0)} - \mathsf{S}^{-1}\cdot\mathsf{L}(\delta_t\tilde{\mathsf{D}})\cdot\mathbf{m}' + \delta_t\mathsf{S}^{-1}\cdot\mathbf{\Phi}', \tag{A5a}$$

$$\mathbf{\Phi}' := \mathbf{\Phi} + \mathsf{L}(\delta_t\tilde{\mathsf{D}})\cdot\mathbf{G}'. \tag{A5b}$$

Note that Eq. (A5a) is identical to Eq. (18) in form. It can be shown that the hydrodynamic equations obtained with the Maxwell iterations of Eq. (A5a) are indeed identical to the ones obtained with Eq. (18).

The above analysis is to address the singular case when $s_i = 0$ for the conserved moments. However, we can argue that s_i should be set to 1, instead of 0, for the conserved moments in the LBE. Consider the following spatially uniform relaxation system (cf., e.g., Ref. [19] and [51, Eq. (41)]):

$$\partial_t\varrho_i = \lambda_i\varrho_i, \quad \varrho_i(t) = e^{\lambda_i t}\varrho_i(0). \tag{A6}$$

In the case of discrete time $t_n = n\delta_t$, $n \in := \{0,1,\ldots\}$,

$$\varrho_i(t_n) = e^{\lambda_i n\delta_t}\varrho_i(0) := s_i^n\varrho(0), \tag{A7}$$

where $s_i := e^{\lambda_i\delta_t}$. For the conserved modes, $\lambda_i = 0$, thus $s_i = 1$. It should also be mentioned that, because the dissipation of nonconserved moments is proportional to $(1/s_i - 1/2)$, numerically it requires that $s_i > 0$ for any nonconserved moment. Therefore, the consideration of a singular S is not necessary.

APPENDIX B: NONEQUILIBRIUM MOMENTUM FLUX

The stress tensor can also be obtained from the nonequilibrium momentum flux, which can be computed from the nonequilibrium part of the distribution function as follows [47,52]:

$$\mathbf{\Sigma} = \sum_i \boldsymbol{c}_i\boldsymbol{c}_i\frac{\left(f_i - f_i^{(0)}\right) + \left(f_i^* - f_i^{(0)}\right)}{2}, \tag{B1}$$

where f_i and f_i^* denote the precollision and postcollision distribution, respectively. The moments corresponding to f_i^* are given by

$$\mathbf{m}^* = \mathbf{m} - \mathsf{S}\cdot(\mathbf{m} - \mathbf{m}^{(0)}) + \delta_t\mathbf{\Phi}.$$

We analyze the momentum flux tensor $\mathbf{\Sigma}$ by using the results obtained with the Maxwell iteration. We first dissect $\mathbf{\Sigma}$ into two parts, $\mathbf{\Sigma}' := \sum_i \boldsymbol{c}_i\boldsymbol{c}_i(f_i - f_i^{(0)})$ and $\mathbf{\Sigma}'' := \sum_i \boldsymbol{c}_i\boldsymbol{c}_i(f_i^* - f_i^{(0)})$. Denote the elements of $\mathbf{\Sigma}'$ by σ'_{ij}, then

$$\begin{aligned}(\sigma'_{11},&\sigma'_{12},\sigma'_{21},\sigma'_{22})^\dagger\\ &:= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot(\mathbf{m}-\mathbf{m}^{(0)})\\ &= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot[-\delta_t\mathsf{S}^{-1}\cdot\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)} + \delta_t\mathsf{S}^{-1}\cdot\mathbf{\Phi}] + O(\delta_t^2)\\ &= -\delta_t\mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot\mathsf{S}^{-1}\cdot[\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)} - \mathbf{\Phi}] + O(\delta_t^2),\end{aligned}$$

where $\mathbf{m} = \mathbf{m}^{[1]}$ of Eq. (24) has been substituted in the above calculation, $\mathbf{\Phi}$ is given by Eq. (45), and

$$\mathbf{\Pi} := \begin{pmatrix}0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1\\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1\\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1\\ 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1\end{pmatrix}. \tag{B2}$$

The elements of $\mathbf{\Pi}$ in the first and fourth rows are $c_{i,x}c_{i,x}$ and $c_{i,y}c_{i,y}$, respectively, and the elements in the second and third rows are $c_{i,x}c_{i,y}$. In terms of moments, the first and fourth rows correspond to the modes J_x and J_y defined in Eq. (27a), and the second and third row correspond to the mode p_{xy}. By using the results of $\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)}$ given in Eq. (31), we obtain

$$\begin{aligned}\mathbf{\Sigma}' = -\boldsymbol{\sigma}' - \frac{1}{2}\delta_t\{p[(\nabla\boldsymbol{u}) + (\nabla\boldsymbol{u})^\dagger] + (\boldsymbol{uF} + \boldsymbol{Fu})\}\\ +\delta_t O(u^3) + O(\delta_t^2),\end{aligned} \tag{B3}$$

$$\boldsymbol{\sigma}' := \rho\begin{pmatrix}\nu_{xx}(\partial_x u_x - \partial_y u_y) & \nu_{xy}(\partial_x u_y + \partial_y u_x)\\ \nu_{xy}(\partial_x u_y + \partial_y u_x) & \nu_{xx}(\partial_y u_y - \partial_x u_x)\end{pmatrix} + \rho\zeta(\nabla\cdot\boldsymbol{u})\mathsf{I}, \tag{B4}$$

where ν_{xx}, ν_{xy}, and ζ are defined in Eq. (39), and $p := \rho c_s^2$. Similarly to $\mathbf{\Sigma}'$, we have

$$\begin{aligned}(\sigma''_{11},&\sigma''_{12},\sigma''_{21},\sigma''_{22})^\dagger\\ &:= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot(\mathbf{m}^* - \mathbf{m}^{(0)})\\ &= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot[\mathbf{m} - \mathsf{S}\cdot(\mathbf{m}-\mathbf{m}^{(0)}) + \delta_t\mathbf{\Phi} - \mathbf{m}^{(0)}]\\ &= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot[(\mathsf{I}-\mathsf{S})\cdot(\mathbf{m}-\mathbf{m}^{(0)}) + \delta_t\mathbf{\Phi}]\\ &= \mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot(\mathsf{I}-\mathsf{S})\cdot[-\delta_t\mathsf{S}^{-1}\cdot\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)} + \delta_t\mathsf{S}^{-1}\cdot\mathbf{\Phi}]\\ &\quad +\delta_t\mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot\mathbf{\Phi} + O(\delta_t^2)\\ &= -\delta_t\mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot(\mathsf{S}^{-1}-\mathsf{I})\cdot[\tilde{\mathsf{D}}\cdot\mathbf{m}^{(0)} - \mathbf{\Phi}]\\ &\quad +\delta_t\mathbf{\Pi}\cdot\mathsf{M}^{-1}\cdot\mathbf{\Phi} + O(\delta_t^2),\end{aligned}$$

and

$$\begin{aligned}\mathbf{\Sigma}'' = -\boldsymbol{\sigma}' + \frac{1}{2}\delta_t\{p[(\nabla\boldsymbol{u}) + (\nabla\boldsymbol{u})^\dagger] + (\boldsymbol{uF} + \boldsymbol{Fu})\}\\ +\delta_t O(u^3) + O(\delta_t^2).\end{aligned} \tag{B5}$$

Therefore,

$$\frac{1}{2}(\mathbf{\Sigma}' + \mathbf{\Sigma}'') = -\boldsymbol{\sigma}' + \delta_t O(u^3) + O(\delta_t^2),$$

and, under the conditions that $\nu_{xx} = \nu_{xy} = \nu$ and $\delta_t = O(\mathrm{Ma}^3)$, we have $\boldsymbol{\sigma}' = \boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ is the desired stress tensor given by Eq. (43). Thus,

$$\mathbf{\Sigma} = -\boldsymbol{\sigma} + O(\delta_t^2);$$

that is, the stress tensor obtained by Eq. (B1) is in fact accurate to second-order in both δ_t and δ_x under the convective scaling [53].

We note that the stress tensor directly computed from the second-order iteration of $\mathbf{m}$ given by Eq. (25) yields the same result for the stress tensor $\boldsymbol{\sigma}$ as that obtained with the nonequilibrium momentum flux given by Eq. (B1), as shown in Sec. IV B 2 [cf. Eq. (43) and the derivation].

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