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Consistent initial conditions for lattice Boltzmann simulations

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Abstract

We propose a simple and effective iterative procedure to generate consistent initial conditions for the lattice Boltzmann equation (LBE) for *incompressible* flows with a given initial velocity field $\boldsymbol{u}_0$. Using the Chapman-Enskog analysis we show that not only the proposed procedure effectively solves the Poisson equation for the pressure field p_0 corresponding to $\boldsymbol{u}_0$, it also generates at the same time the initial values for the nonequilibrium distribution functions $\{f_\alpha\}$ in a consistent manner. This procedure is validated for the decaying Taylor–Green vortex flow in two dimensions and is shown to be particularly effective when using the generalized LBE with multiple relaxation times.

1. Introduction

In this work, we intend to address an important issue in the lattice Boltzmann equation (LBE): how to generate consistent initial conditions for the distribution functions in LBE simulations. In the lattice Boltzmann equation, one deals with a set of distribution functions $\{f_\alpha|\alpha = 0,1,2,\ldots,b\}$ corresponding to Q discrete velocities $\{\boldsymbol{c}_\alpha|\alpha = 0,1,2,\ldots,b\}$ at each node occupied by the fluid that is being simulated, as opposed to the hydrodynamic fields (or other primitive quantities). This set of distribution functions can be uniquely transformed into an equivalent set of moments $\{\varrho_\alpha|\alpha = 0,1,2,\ldots,b\}$ by a linear map M [1–4]. Of the moments, the first few are the conserved (hydrodynamic) ones, which are the density ρ and the flow momentum $\boldsymbol{j} = \rho\boldsymbol{u}$ (and the energy density ρe for energy conserving models). Higher order moments are non-conserved (kinetic) ones, which include stresses, heat fluxes and other higher-order fluxes, and the dynamics of which are chosen to yield the desired large scale behavior of the fluid. Hence, to specify the set of nonequilibrium distribution functions $\{f_\alpha\}$ is equivalent to specify the set of the corresponding moments $\{\varrho_\alpha\}$, including the kinetic ones. Henceforth, unique initial and boundary conditions for $\{f_\alpha\}$ in the lattice Boltzmann simulations are equivalent to that for all the moments $\{\varrho_\alpha\}$.

Accurate initial conditions are crucial in the simulations of unsteady, time-dependent problems. In the LBE simulations of *incompressible* flows, a typical approach is to use the equilibrium distribution function $f_\alpha^{(\mathrm{eq})}(\rho,\boldsymbol{j})$ to initialize f_α. Two problems arise immediately. First, in order to fully specify $f_\alpha^{(\mathrm{eq})}$, the initial density field ρ_0 (equivalently the pressure field p_0) is required but often not available. And secondly, the initialization $f_\alpha|_{t=0} = f_\alpha^{(\mathrm{eq})}|_{t=0}$ implies that initially all the kinetic moments are at their equilibrium, which depend only on the hydrodynamic moments. Obviously this is not true when the initial flow fields ρ_0 and $\boldsymbol{u}_0$ have non-vanishing gradients. Proposals have been made to improve the initialization of $\{f_\alpha\}$ by computing the initial density by directly solving the Poisson equation to

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obtain the pressure p and the density ρ via the equation of state, and then the nonequilibrium part of $\{f_\alpha\}$ by using Chapman–Enskog procedure [5]. These computations can be cumbersome and not easy to implement in practice.

In this paper, we propose an iterative initialization procedure to generate consistent initial conditions for $\{f_\alpha\}$ within the framework of the lattice Boltzmann equation along the following general idea: During the initialization procedure the density ρ is the only conserved variable in the system, while the flow momentum $\boldsymbol{j}$ is relaxed to the state prescribed by the initial velocity field $\boldsymbol{u}_0$.

The remaining part of the paper is organized as follows. Section 2 provides a concise and self-contained introduction of the lattice Boltzmann equation and describes the proposed iterative initialization procedure. By using the Chapman–Enskog analysis, we show that the proposed initialization procedure solves the Poisson equation for the pressure. We also show that the multiple-relaxation-time (MRT) LBE is the most efficient model to implement this initialization procedure. Section 3 presents numerical results. The two-dimensional (2D) decaying Taylor–Green vortex flow is used as a test case to validate the procedure, which is shown to be effective. Finally, Section 4 concludes the paper.

2. Consistent initialization for incompressible LBE simulations

We find that it is most convenient to discuss the proposed initialization procedure to generate consistent initial conditions for a given (divergent free) initial velocity field $\boldsymbol{u}_0$ in the LBE simulations within the framework of the generalized lattice Boltzmann equation (GLBE), or the lattice Boltzmann equation with multiple-relaxation-time (MRT) collision model [1–4]. The evolution equation for the MRT–LBE of Q velocities on a D-dimensional lattice $\boldsymbol{x}_i \in \delta_x \mathbb{Z}^D$ with discrete time $t_n \in \delta_t \mathbb{N}_0 := \delta_t\{0,1,\ldots\}$ is

$$\begin{aligned}\mathbf{f}(\boldsymbol{x}_i + \boldsymbol{c}\delta_t, t_n + \delta_t) - \mathbf{f}(\boldsymbol{x}_i, t_n) &= \boldsymbol{\Omega}(\boldsymbol{x}_i, t_n) \\ &= -\mathsf{M}^{-1}\cdot\hat{\mathsf{S}}\cdot[\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}],\end{aligned} \tag{1}$$

where M is a $Q\times Q$ matrix which linearly transforms the distribution functions $\mathbf{f}\in\mathbb{V}\equiv\mathbb{R}^Q$ to the velocity moments $\mathbf{m}\in\mathbb{M}\equiv\mathbb{R}^Q$:

$$\mathbf{m} = \mathsf{M}\cdot\mathbf{f}, \qquad \mathbf{f} = \mathsf{M}^{-1}\cdot\mathbf{m}, \tag{2}$$

the total number of discrete velocities $Q = 1 + b$ or b for model with or without particle of zero velocity, respectively, $\hat{\mathsf{S}}$ is a non-negative $Q\times Q$ diagonal relaxation matrix, and the bold-face symbols denote column vectors:

$$\begin{aligned}&\mathbf{f}(\boldsymbol{x}_i + \boldsymbol{c}\delta_t, t_n + \delta_t) = (f_0(\boldsymbol{x}_i, t_n + \delta_t), \ldots, f_b(\boldsymbol{x}_i + \boldsymbol{c}_b\delta_t, t_n + \delta_t))^{\mathsf{T}},\\ &\mathbf{f}(\boldsymbol{x}_i, t_n) = (f_0(\boldsymbol{x}_i, t_n), f_1(\boldsymbol{x}_i, t_n), \ldots, f_b(\boldsymbol{x}_i, t_n))^{\mathsf{T}},\\ &\mathbf{m} = (m_0(\boldsymbol{x}_i, t_n), m_1(\boldsymbol{x}_i, t_n), \ldots, m_b(\boldsymbol{x}_i, t_n))^{\mathsf{T}},\\ &\mathbf{m}^{(\mathrm{eq})} = (m_0^{(\mathrm{eq})}(\boldsymbol{x}_i, t_n), m_1^{(\mathrm{eq})}(\boldsymbol{x}_i, t_n), \ldots, m_b^{(\mathrm{eq})}(\boldsymbol{x}_i, t_n))^{\mathsf{T}},\end{aligned}$$

where T is the transpose operator.

For the sake of simplicity, we will restrict ourselves to the nine-velocity model in two dimensions (D2Q9 model). The discrete velocities $\{\boldsymbol{c}_\alpha\}$ are

$$\boldsymbol{c}_\alpha = \begin{cases}(0,0), & \alpha = 0,\\ (\pm1,0)c, (0,\pm1)c, & \alpha = 1,2,3,4,\\ (\pm1,\pm1)c, & \alpha = 5,6,7,8,\end{cases} \tag{3}$$

where $c = \delta_x/\delta_t$. A particular order of moments used here is:

$$\mathbf{m} = (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^{\mathsf{T}}, \tag{4}$$

in which ρ is the mass density, and $j_x = \rho u_x$ and $j_y = \rho u_y$ are x and y components of the flow momentum $\boldsymbol{j}$, respectively, which are the conserved moments in the system. Other moments are non-conserved moments and their equilibria are functions of the conserved moments in the system [1–4]. With this particular order of moments given above, the corresponding diagonal relaxation matrix of relaxation rates $\{s_\alpha\}$ is

$$\hat{\mathsf{S}} = \mathrm{diag}(s_\rho, s_e, s_\varepsilon, s_\chi, s_q, s_\chi, s_q, s_\nu, s_\nu). \tag{5}$$

Usually, because ρ, j_x and j_y are conserved quantities, the relaxation rates s_ρ and s_χ have no effect on the system and therefore can assume any value. However, if an external force is present and is included in the equilibria, its effect is influenced by the value of s_χ. The relaxation rates s_ν and s_e determine the shear and bulk viscosities, respectively. In the presence of solid boundaries, s_q affects the exact locations where the noslip boundary conditions are satisfied [6–9].

To reduce round-off errors, we use the density fluctuation $\delta\rho$ and assume the mean density $\bar{\rho} = 1$. The total density is therefore $\rho = \bar{\rho} + \delta\rho$. In addition, we use $\boldsymbol{j} = \bar{\rho}\boldsymbol{u}$ to reduce effects due to compressibility [10]. Thus the conserved quantities in an *athermal* LBE model and the corresponding equilibria are:

$$\delta\rho^{(\mathrm{eq})} = \delta\rho = \sum_\alpha f_\alpha, \tag{6a}$$

$$\boldsymbol{j}^{(\mathrm{eq})} = \boldsymbol{j} := (j_x, j_y) = \bar{\rho}\boldsymbol{u} = \sum_\alpha f_\alpha \boldsymbol{c}_\alpha. \tag{6b}$$

For the *athermal* D2Q9 model in which the (internal) energy is *not* a conserved quantity, the equilibria for non-conserved moments are [2]:

$$e^{(\mathrm{eq})} = -2\alpha_2\delta\rho + 3(j_x^2 + j_y^2), \qquad \varepsilon^{(\mathrm{eq})} = \delta\rho - 3(j_x^2 + j_y^2), \tag{7a}$$

$$\boldsymbol{q}^{(\mathrm{eq})} = (q_x^{(\mathrm{eq})}, q_y^{(\mathrm{eq})}) = -\boldsymbol{j} = -(j_x, j_y), \tag{7b}$$

$$p_{xx}^{(\mathrm{eq})} = j_x^2 - j_y^2, \qquad p_{xy}^{(\mathrm{eq})} = j_x j_y. \tag{7c}$$

With the above equilibria, the LBE system of Eq. (1) leads to the *incompressible* Navier–Stokes equations in the limit of small Mach number and large system size. If we choose $\alpha_2 = 1$ and set all the relaxation rates $\{s_\alpha\}$ to a single value of $1/\tau$, i.e., $s_\alpha = 1/\tau\ \forall\alpha$, then the MRT–LBE reduces to the corresponding lattice Bhatnagar–Gross–Krook [11] (BGK) equation [12,13].

The speed of sound, c_s, for the model is determined by the parameter α_2:

$$c_s^2 = \frac{1}{3}(2-\alpha_2). \tag{8}$$

And the shear viscosity v and the bulk viscosity ζ are:

$$v = \frac{1}{3}\left(\frac{1}{s_v}-\frac{1}{2}\right), \qquad \zeta = \frac{\alpha_2}{6}\left(\frac{1}{s_e}-\frac{1}{2}\right). \tag{9}$$

In LBE simulations, usually the initial velocity field $\boldsymbol{u}_0$ is given, but not the initial pressure field p_0. In practice the initial density ρ_0 (or the initial pressure p_0) is often set to a constant throughout the system. The initial values of the equilibrium moments $\{m_\alpha^{(\mathrm{eq})}\}$ can therefore be computed based upon the initial values of density ρ_0 and $\boldsymbol{j}_0$, and the equilibrium distribution functions $\mathbf{f}^{(\mathrm{eq})} = \mathsf{M}^{-1}\cdot\mathbf{m}^{(\mathrm{eq})}$ are then used as the initial values of the distribution functions $\mathbf{f}$. In what follows we shall demonstrate that such initialization is inadequate because the error of the initial value often persists throughout the entire simulation.

Here we propose a very simple, consistent, and yet effective procedure to initialize $\{f_\alpha\}$ based on hydrodynamic initial conditions of velocity field $\boldsymbol{u}_0$. Given an initial velocity field $\boldsymbol{u}_0$, the density fluctuation field $\delta\rho$ is initialized to 0 for the sake of simplicity. Then, with the velocity field relaxed to the given initial velocity $\boldsymbol{u}_0$, the system is iterated until a steady state of $\{f_\alpha\}$ is obtained, which is then consistent with the velocity field $\boldsymbol{u}_0$. This is accomplished by replacing the original LBE scheme with three conserved quantities by the corresponding generalized diffusion–advection LBE with only one conserved quantity ρ [14,15]. Then the flow momentum is no longer conserved, but relaxes towards the state prescribed by $\boldsymbol{j}_0$ as

$$\boldsymbol{j}^* = \boldsymbol{j} - s_\chi(\boldsymbol{j}-\boldsymbol{j}^{(\mathrm{eq})}), \quad \boldsymbol{j}^{(\mathrm{eq})} := \boldsymbol{j}_0, \tag{10}$$

where the imposed state $\boldsymbol{j}_0$ is related to the given initial velocity field $\boldsymbol{u}_0$ by $\boldsymbol{j}_0 = \bar{\rho}\boldsymbol{u}_0$, assuming the incompressible approximation. Note that a particular value of $s_\chi = 1$ fixes $\boldsymbol{j}$ at the imposed value $\boldsymbol{j}_0 := \bar{\rho}\boldsymbol{u}_0$. After initializing $\boldsymbol{j} = \bar{\rho}\boldsymbol{u}_0$, $\delta\rho = 0$, and $\{m_\alpha^{(\mathrm{eq})}\}$ according to Eq. (7a) with initial $\boldsymbol{j}$ and $\delta\rho$, the steps in the proposed iterative initialization process are:

(1) Relax non-conserved moments according to Eq. (1), starting from $\boldsymbol{j}$ (note that the $\boldsymbol{j}$ in the equilibria given by Eq. (7a) are related to $\boldsymbol{j}_0$ now);
(2) Advect;
(3) Update $\delta\rho$;
(4) Repeat the process until the density approaches to a steady state, which can be measured by, e.g., $\sum_i \|\delta\rho(\boldsymbol{x}_i, t+1) - \delta\rho(\boldsymbol{x}_i, t)\|$.

Note that all the output or measurements should be taken right after the relaxation (collision) process and before the advection process.

Obviously, in the proposed initialization process, there is only one conserved variable in the LBE system—the density ρ. Consequently, the density satisfies the following diffusion equation, which can be obtained by the Chapman–Enskog analysis up to second-order:

$$\partial_t p = \chi\nabla^2 p + \chi\nabla\nabla : \boldsymbol{j}_0\boldsymbol{j}_0 - c_s^2\nabla\cdot\boldsymbol{j}_0, \tag{11}$$

where $p = c_s^2\rho$ has been substituted and the diffusion coefficient χ is given by

$$\chi = c_s^2\left(\frac{1}{s_\chi}-\frac{1}{2}\right). \tag{12}$$

When the density ρ reaches its steady state ρ_0 and the flow moment $\boldsymbol{j}$ reaches the prescribed initial field $\boldsymbol{j}_0 := \bar{\rho}\boldsymbol{u}_0$ through the iteration, the initial pressure field p_0 so obtained satisfies the Poisson equation if $\nabla\cdot\boldsymbol{u}_0 = 0$ and $\bar{\rho} = 1$:

$$\nabla^2 p_0 = -\nabla\cdot(\boldsymbol{u}_0\cdot\nabla\boldsymbol{u}_0). \tag{13}$$

Obviously, the final steady state of the pressure p_0 attained through the iterative procedure is independent of the relaxation rates $\{s_\alpha\}$ in the systems, as indicated by Eq. (13). However, the residual error does depend on the relaxation process (i.e., the relaxation rates), among other factors. Note that, if $\boldsymbol{j}^{(\mathrm{eq})} = \rho\boldsymbol{u}_0$ and $\nabla\cdot\boldsymbol{u}_0 = 0$, Eq. (11) becomes

$$\partial_t\rho + \boldsymbol{u}_0\cdot\nabla\rho = \chi\nabla^2\rho + \chi\nabla\nabla : \boldsymbol{j}_0\boldsymbol{j}_0. \tag{14}$$

The above equation is the general diffusion–advection equation for the passive scalar ρ [14,15].

Since the athermal LBE and the diffusion–advection LBE for initialization procedure obey the same evolution Eq. (1) except the treatment of the flow momentum $\boldsymbol{j}$, that is, $\boldsymbol{j}$ is *identically* equal to $\boldsymbol{j}^{(\mathrm{eq})}$ for the former while $\boldsymbol{j}$ *relaxes* towards $\boldsymbol{j}^{(\mathrm{eq})}$ for the latter, the distribution functions $\{f_\alpha\}$ for the two schemes are the same when the steady state is reached, i.e., when $\boldsymbol{j} = \boldsymbol{j}^{(\mathrm{eq})}$. Therefore the proposed initialization procedure provides not only the correct initial pressure field p_0, but also the nonequilibrium part of the moments (or equivalently, that of the distribution functions). Therefore, the nonequilibria obtained iteratively are also consistent with the Navier–Stokes hydrodynamics obeyed by the conserved moments.

For the lattice BGK equation [12,13], the iterative initialization is described as the following:

$$f_\alpha(\boldsymbol{x}_i + \boldsymbol{c}_\alpha\delta_t, t+\delta_t) = f_\alpha(\boldsymbol{x}_i, t) - \frac{1}{\tau}\left[f_\alpha(\boldsymbol{x}_i, t) - f_\alpha^{(\mathrm{eq})}(\delta\rho, \boldsymbol{u}_0, t)\right], \tag{15}$$

where $\boldsymbol{u}_0$ is the initial velocity field and [10]

$$\delta\rho = \sum_\alpha f_\alpha = \sum_\alpha f_\alpha^{(\mathrm{eq})}, \tag{16a}$$

$$f_\alpha^{(\mathrm{eq})} := w_\alpha\left[\delta\rho + \frac{1}{c_s^2}\bar{\rho}\boldsymbol{c}_\alpha\cdot\boldsymbol{u} + \frac{1}{2c_s^4}\bar{\rho}((\boldsymbol{c}_\alpha\cdot\boldsymbol{u})^2 - c_s^2\boldsymbol{u}\cdot\boldsymbol{u})\right]. \tag{16b}$$

That is, while the velocity field $\boldsymbol{u}$ is fixed at $\boldsymbol{u}_0$ throughout the iterative initialization process, ρ and $\{f_\alpha\}$ are also consistent with the given initial velocity $\boldsymbol{u}_0$. In this case, the diffusion coefficient χ of Eq. (12) is $\chi = v$. Therefore, with a small viscosity as for high-Reynolds number flows, the

relaxation process for the initialization can be rather slow. With the LBGK equation, one does not have the freedom to choose the value of s_χ to accelerate the acoustic relaxation process. In contrast, the MRT–LBE does have the complete freedom to independently choose the relaxation rates relevant for the shear viscosity ν and for the pressure equilibration process, and this is one advantage of the MRT–LBE over the LBGK equation.

3. 2D Taylor–Green vortex flow: A test case

To validate the proposed iterative procedure to generate consistent initial conditions for $\{f_\alpha\}$ with a given initial velocity field $\boldsymbol{u}_0$ in LBE simulations, we study the two-dimensional (2D) decaying Taylor–Green vortex flow as a test case. The Taylor–Green vortex flow has the following analytic solutions to the incompressible Navier–Stokes equation in two dimensions:

$$u_x(x,y,t) = -U_0\cos(k_x x)\sin(k_y y)\mathrm{e}^{-k^2\nu t}, \tag{17a}$$

$$u_y(x,y,t) = \frac{k_x}{k_y}U_0\cos(k_y y)\sin(k_x x)\mathrm{e}^{-k^2\nu t}, \tag{17b}$$

$$p(x,y,t) = -\frac{1}{4}U_0^2\left[\cos(2k_x x) + \left(\frac{k_x}{k_y}\right)^2\cos(2k_y y)\right]\mathrm{e}^{-2k^2\nu t} + P_0, \tag{17c}$$

where U_0 is the initial velocity amplitude, ν is the shear viscosity, $k_x = 2\pi/L_x$ and $k_y = 2\pi/L_y$ are the wave numbers in x and y directions, respectively, $k = \sqrt{k_x^2 + k_y^2}$, and P_0 is an arbitrary constant pressure. For the sake of simplicity, we only consider the case where $k_x = k_y = k_L$ and $P_0 = 0$, therefore the pressure of Eq. (17c) can be rewritten as

$$p(x,y,t) = -\frac{1}{2}U_0^2\cos[k_L(x+y)]\cos[k_L(x-y)]\mathrm{e}^{-2k^2\nu t}. \tag{18}$$

We compute the normalized total kinetic energy

$$K(t) = \frac{2}{N^2U_0^2}\int (u_x^2 + u_y^2)\,\mathrm{d}x\,\mathrm{d}y, \quad x,y \in [0,N] \tag{19}$$

and the normalized projection of the numerical pressure field obtained in the LBE simulations to the analytic solution:

$$P_2(t) = -\frac{16}{U_0^2N^2}\int p(x,y,t)\cos[k_L(x+y)] \times \cos[k_L(x-y)]\,\mathrm{d}x\,\mathrm{d}y. \tag{20}$$

Both $K(t)$ and $P_2(t)$ evolve as $\mathrm{e}^{-2k^2\nu t}$ for the analytic solutions of u_x, u_y and p. Thus $\|P_2(t) - \mathrm{e}^{-2k^2\nu t}\|$ is a measure of global error in pressure field.

We use a 2D system of size N^2 with periodic boundary conditions in both directions. We use three system sizes $N^2 = 32^2$, 64^2 and 128^2, two values of the viscosity, $\nu =$!0.002 ($s_\nu^{-1} = 0.506$) and 0.05 ($s_\nu^{-1} = 0.65$), and $U_0 = 0.05$. Other parameters are: $\alpha_2 = 1$, $s_\chi = 1.0$, $s_q = 1.7$, $s_e = 1.0$, and $s_\varepsilon = 1.4$. The relaxation rates s_q and s_ε have little effect on large scale hydrodynamics, and the choice of their values are determined by linear stability analysis, and $\alpha_2 = 1$, i.e., $c_S^2 = 1/3$, is chosen for optimal linear stability

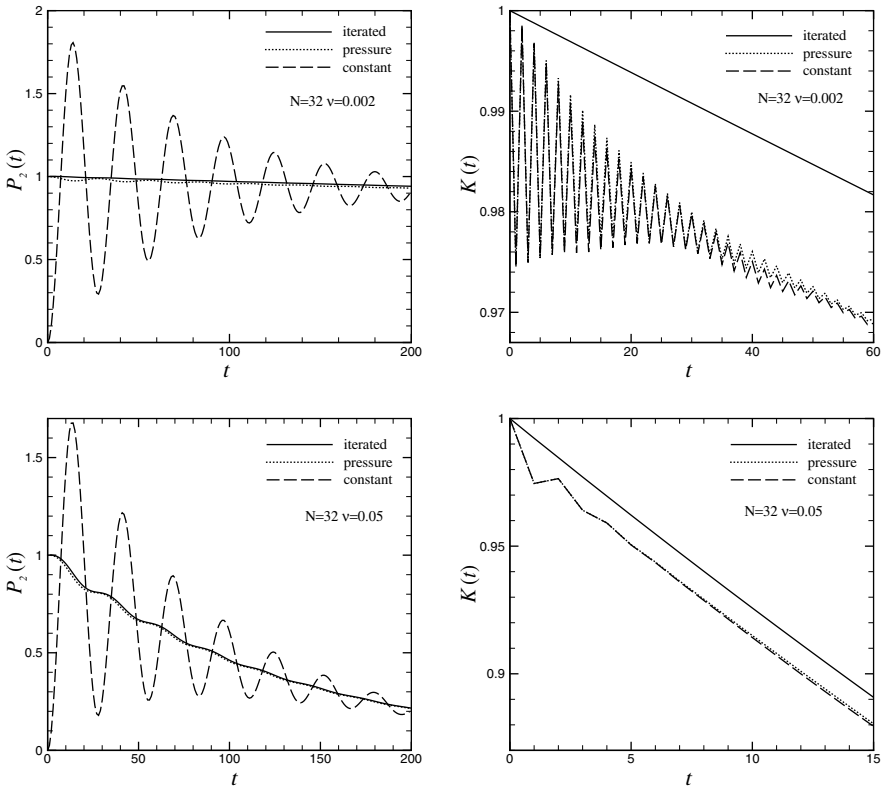

Fig. 1. $P_2(t)$ (left) and $K(t)$ (right) for $N = 32$, $\nu = 0.002$ (top) and $\nu = 0.05$ (bottom). The time t indicates the number of time steps in the LBE simulations.

primarily [2]. A moderate value of $s_e = 1.0$ is chosen so that the system has a moderate amount of bulk viscosity to dissipate the undesirable density (pressure) fluctuations. We choose $s_\chi = 1.0$ ($<s_\nu$) so that $\boldsymbol{j} = \boldsymbol{j}^{(\mathrm{eq})} := \bar{\rho}\boldsymbol{u}_0$, and the velocity field is always the prescribed one after the relaxation step. We compare three initialization schemes with the initial velocity field given by Eqs. (17a) and (17b):

(a) $\{f_\alpha\}$ are initialized through the proposed iterative scheme (labeled iterated);
(b) The pressure field p_0 is initialized with the analytic solution (labeled pressure), and $\{f_\alpha\} = \{f_\alpha^{(\mathrm{eq})}\}$;
(c) The pressure field is initialized with a constant, which is 0 here (labeled constant), and $\{f_\alpha\} = \{f_\alpha^{(\mathrm{eq})}\}$.

In Fig. 1, we show $P_2(t)$ and $K(t)$ for a system of size $N^2 = 32^2$ and $\nu = 0.002$ and 0.05. The number of iteration steps is 1000. We first discuss the behavior of $P_2(t)$. For the case of $\nu = 0.002$, the constant initial pressure field generates severe acoustic oscillations of period $T = N/2c_s$ which persist for a long time. This time scale is of $T_s = [2k^2(\nu + \zeta)]^{-1}$ which is due to the attenuation of acoustic waves with a wave vector along either x or y direction, as indicated by $p(x, y, t)$ of Eq. (17c). It can be shown that in the initialization process the pressure field p approaches its solution with a decay rate of $(2k)^2\chi$, as indicated by Eq. (11) and illustrated by the numerical results of Fig. 1. In the case of constant pressure initialization ("constant"), the magnitude of acoustic waves in $P_2(t)$ due to inaccurate initialization decays as $e^{-(2k)^2\chi t}$. In the cases in which the pressure p_0 is initialized by the iteration ("iterated") or by Eq. (18) ("pressure"), there are no severe acoustic waves; and the small magnitude oscillation reflects the physical acoustic waves in the system unrelated to the initial conditions, as more clearly shown for the case of $\nu = 0.05$.

Although the analytic initial pressure does eliminate severe initial acoustic waves in pressure field, the initial relaxation process leads to a deficit in the total energy $K(t)$, as for the constant pressure initialization. This initial relaxation is a result due to the following two reasons. First, there is an inconsistency between the discretized analytic solution and the true discrete solution for the pressure in the system, because the LBE solution is only a second-order approximation of the continuous one. And second, the nonequilibrium part of $\{f_\alpha\}$ is not properly initialized, they are simply assumed to be 0 in this case. This point will be further addressed later. We also observe that, without the proper initialization, i.e., by using the initializations with the analytic solution for p or a constant p, the total energy $K(t)$ oscillates with period-2. This can be easily understood by linear analysis (cf. [2]). In the large-scale limit ($k \to 0$), the eigenvalues corresponding to kinetic (non-conserved) modes are $(1 - s_\alpha)$ in the leading order, thus the temporal evolution of these kinetic modes behaves as $(1 - s_\alpha)^t$. This leads to the period-2 oscillation approximately as $(-1)^t$ in under relaxed cases (when s_ν close to 2). For a larger viscosity $\nu = 0.05$, everything observed remains the same qualitatively. Quantitatively, the deficit

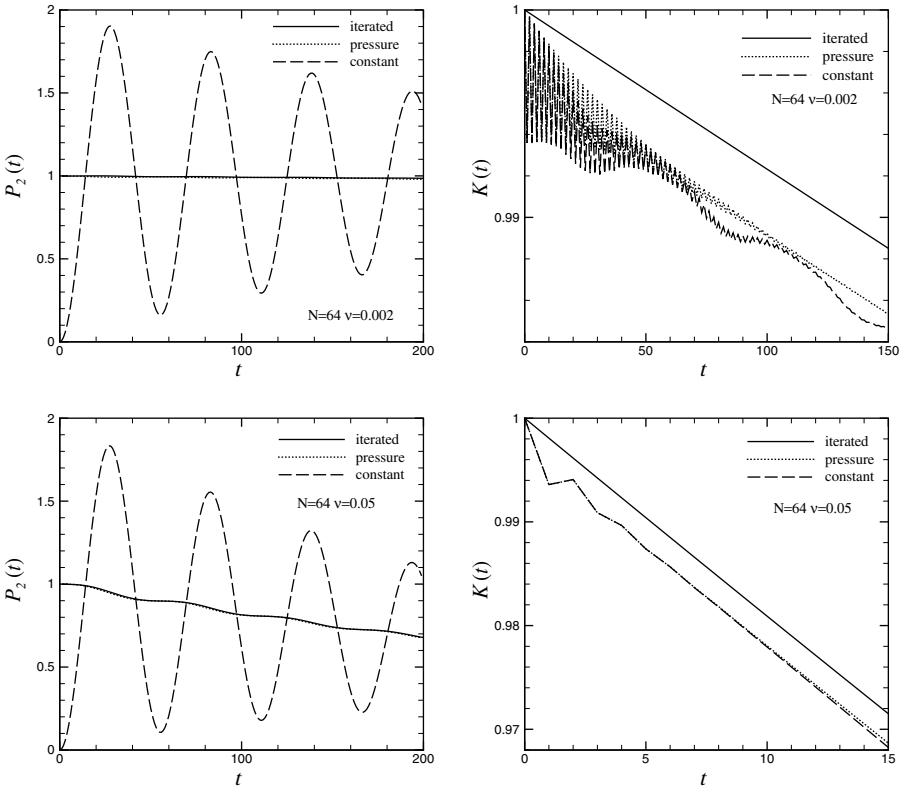

Fig. 2. Same as Fig. 1 for $N = 64$.

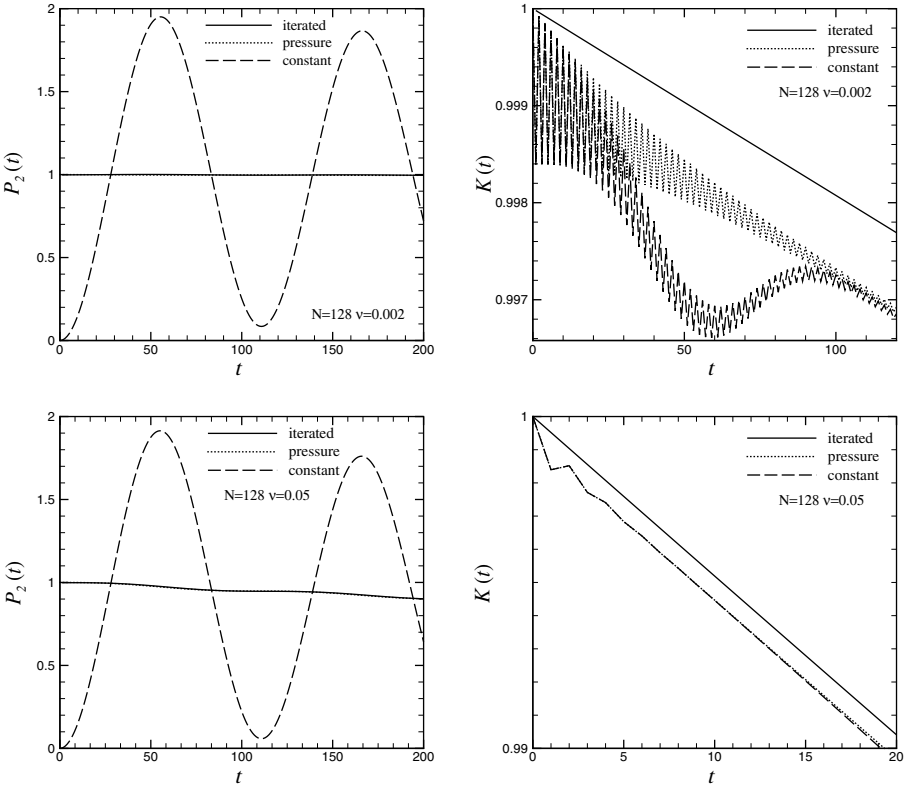

Fig. 3. Same as Fig. 1 for $N = 128$.

in total energy $K(t)$ is much less with the analytic and constant initial pressure fields, and the period-2 oscillation in $K(t)$ is dissipated much faster, because the decay rate is proportional to $\ln|1 - s_\alpha|$.

The same observation can be made for systems of large sizes, $N^2 = 64^2$ and $N^2 = 128^2$, as shown in Figs. 2 and 3, respectively. As the system size enlarges (equivalent to grid refinement), the discrete solution converges to the discretized analytic solution therefore the discrepancy in the total energy $K(t)$ due to the initial relaxation process diminishes.

To further explain what is actually accomplished by the proposed initialization procedure, we conduct the following test. The first-order nonequilibrium part of the second-order moments, e, p_{xx} and p_{xy} are:

$$e^{(1)} = -\frac{1}{s_e}\nabla\cdot\boldsymbol{j}, \tag{21a}$$

$$p_{xx}^{(1)} = -\frac{2}{3s_\nu}(\partial_x j_x - \partial_y j_y), \tag{21b}$$

$$p_{xy}^{(1)} = -\frac{1}{3s_\nu}(\partial_y j_x + \partial_x j_y). \tag{21c}$$

With $\boldsymbol{j} = \bar{\rho}\boldsymbol{u}_0$ and $\boldsymbol{u}_0$ given by Eqs. (17a) and (17b), $p_{xx}^{(1)}$ is the only non-vanishing first-order nonequilibrium in Eq. (21). It is easy to initialize the system with the e and the first-order nonequilibria of Eqs. (21a). The results is shown in Fig. 4. We only test with a system of $N^2 = 64^2$ while other parameters remain the same as in Fig. 2. The total energy $K(t)$ with both the pressure and the first-order

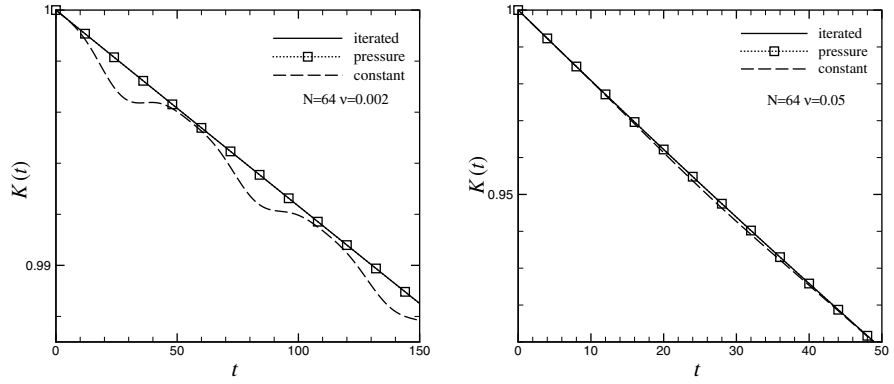

Fig. 4. Corresponding to Fig. 2 for $N = 64$, with p_{xx} initialized up to first-order Chapman–Enskog expansion.

nonequilibria of the second-order moments properly initialized is indistinguishable from that obtained with the proposed iterative initialization procedure. In fact, for both $v = 0.002$ and 0.05 shown in Fig. 4, the total energy with the first-order nonequilibrium and iterative initializations agree with each other at least four digits after the decimal point. If only the first-order nonequilibria are properly initialized, but the pressure is initialized as a constant, the energy deficit is much reduced, however, the equilibration of the pressure induces oscillation in the energy, as clearly shown in Fig. 4. Therefore, we can conclude that inaccurate (zeroth-order) initialization of pressure is responsible for undesirable acoustic oscillations, while inaccurate (first-order) initialization of nonequilibria of the second-order moments is responsible for deficit and period-2 oscillations in the total energy.

Clearly, the proposed iterative scheme works well as intended. The iterative procedure leads to the initial pressure p_0 satisfying the Poisson equation corresponding to the initial velocity $\boldsymbol{u}_0$. In addition, the iterative procedure produces nonequilibrium distribution functions $\{f_\alpha\}$ (or the moments $\{m_\alpha\}$) consistent with the initial velocity $\boldsymbol{u}_0$.

4. Discussions and conclusions

In this paper, we propose an iterative procedure to generate consistent initial conditions for the lattice Boltzmann equation with a given initial velocity field $\boldsymbol{u}_0$. We use the Chapman–Enskog technique to analyze the proposed iterative procedure and show that the pressure field p_0 generated by the proposed initialization procedure indeed satisfies the Poisson equation $\nabla^2 p_0 = -\nabla\nabla : \boldsymbol{u}_0\boldsymbol{u}_0$ for a divergence free $\boldsymbol{u}_0$. The proposed initialization procedure is simple to carry out and effective especially when the MRT–LBE is used. Although the proposed initialization procedure is only tested for a pedagogical case, i.e., the decaying Taylor–Green vortex flow in two dimensions, it has also been successfully applied to direct numerical simulations of decaying homogeneous isotropic turbulence in three dimensions [16–18].

Clearly, for a pedagogical flow with analytic available solution, such as the Taylor–Green vortex flow, in principle one can compute the nonequilibria of the distribution functions $\{f_\alpha\}$ by using the Chapman–Enskog procedure with a given initial velocity field $\boldsymbol{u}_0$, so that $\{f_\alpha\}$ can be properly initialized based on $\boldsymbol{u}_0$, as we have demonstrated here. However, we do not believe this is a useful practice for the following two reasons. First, given the fact that LBE method is only second-order accurate, the discrete solutions of the flow velocity and its derivatives always differs from the corresponding continuous solution, the extent of this difference depends on the accuracy of the LBE method, and is particularly severe at the small scales comparable to grid spacing. To eliminate this inconsistency would be very difficult if possible at all. And second, more importantly, such scheme would be of little use in the cases such as decaying homogeneous isotropic turbulence [16–18], in which the initial velocity is a random field. For these reasons, we believe the proposed initialization procedure is an effective and efficient scheme in the practical sense.

Also, the advantage of using the MRT–LBE, as opposed to the popular lattice BGK equation, is unequivocally demonstrated here. In the setting of the MRT–LBE, the relaxation rates can be chosen freely to accelerate the initialization process, in addition to attain optimal linear stability. While possible [19], it is rather awkward for the lattice BGK equation to achieve the same results. We should also mention that, it has been shown [19] that for the LBGK equation there exists an optimal relaxation time $\tau = 1/2 + 1/\sqrt{6}$, which leads to the elimination of a higher order error in the pressure field. However, this choice of s_χ makes little difference for the overall flow field.

The initial conditions generated by the proposed procedure have an error of the order $O(u^3)$ in the pressure field. This error of cubic velocity is well known [20–23] and is intrinsic to most existing LBE models. The elimination of this error would require an LBE model with more velocity and higher order terms in the equilibria [21,22] and this is left for future research.

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