Designing Correct Fluid Hydrodynamics on A Rectangular Grid using MRT Lattice Boltzmann Approach

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Abstract

While the lattice Boltzmann method (LBM) has become a powerful numerical approach for solving complex flows, the standard LBM typically uses a square lattice grid in two spatial dimensions and cubic lattice grid in three dimensions. For inhomogeneous and anisotropic flows, it is desirable to have a LBM model that utilizes a rectangular grid. There were two previous attempts to extend the multiple-relaxation-time (MRT) LBM to a rectangular lattice grid in 2D without altering the number of microscopic velocities, however, the resulting hydrodynamic momentum equation was not fully consistent with the Navier-Stokes equation, due to anisotropy of the transport coefficients. In the present work, a new MRT model with an additional degree of freedom is developed in order to match precisely the Navier-Stokes equation when a rectangular lattice grid is used. We first revisit the previous attempts to understand the origin and nature of anisotropic transport coefficients by conducting an inverse design analysis within the Chapman-Enskog procedure. Then an additional adjustable parameter that governs the relative orientation in the energy-normal stress subspace is introduced. It is shown that this adjustable parameter can be used to fully eliminate the anisotropy of transport coefficients, thus the exact Navier-Stokes equation can be derived on a rectangular grid. Our theoretical findings are confirmed by numerical solutions using two benchmark problems. The numerical results also demonstrate that the proposed model shows remarkably good performance with appropriate choice of model parameters.

Keywords: Rectangular grid, multiple-relaxation time, lattice Boltzmann method, Navier-Stokes equations

1. Introduction

As an alternative numerical method based on the kinetic theory, the lattice Boltzmann method (LBM) has attracted a great deal of attention since its inception about 25 years ago [1, 2]. The basic idea is to design a fully discrete version of the Boltzmann equation, with a minimum set of discrete microscopic velocities, that can yield the exact Navier-Stokes equation through the Chapman-Enskog analysis. From the computational viewpoint, the advantages of LBM include its algorithm simplicity, intrinsic data locality (thus straightforward to perform parallel computation), and capability to conveniently incorporate complex fluid-solid and fluid-fluid boundary conditions. Hence, LBM has been widely employed in simulations of complex fluid systems, such as multiphase flows [3, 4], complex viscous flows with deformable boundary and complex geometry such as porous media [5, 6, 7], and micro-scale flows [9, 10], etc.

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Despite of the tremendous success of LBM, the standard LBM is restricted to square grid or hexagonal grid in two spatial dimensions (2D) and cubic grid in three spatial dimensions (3D). This restriction is aligned with the set of microscopic velocities used and is desirable for model isotropy. However, this could result in a low computational efficiency when the flow field is highly nonuniform, inhomogeneous, and anisotropic, such a boundary layer flow where the velocity gradients in one spatial dimension is much stronger than the other directions. To alleviate this problem within LBM, different approaches have been developed to allow the use of a nonuniform grid. One approach is to employ an interpolation method to decouple the grid associated with lattice Boltzmann microscopic velocities, from the numerical mesh. Pioneering work in this direction includes the studies of Filippova and Hänel [11, 12] who reconstruct distribution functions at arbitrary locations using spatial and temporal interpolations. Another approach is to introduce local grid refinement or use different mesh densities for different regions of the flow (i.e., multi-block methods) [13]. Methods to communicate distribution functions, defined on coarse and fine grids, at the block interfaces have been developed. Other methods to use a non-uniform grid typically utilize a local interpolation scheme [14, 15]. While these approaches have been actively extended and applied in many applications, their accuracy is limited by the interpolation scheme which may also introduce additional numerical viscosity and artificial dissipation. Therefore, it is desirable to construct a lattice Boltzmann method with a more flexible grid that is free of interpolation.

Inspired by the work of Koelman [16], Bouzidi et al. [17] made a first attempt to construct a multiple-relaxation-time (MRT) LBM on a two-dimensional rectangular grid. The model showed a good performance with appropriate choice of model parameters, but the resulting hydrodynamic momentum equation is not fully consistent with the Navier-Stokes equation. Another attempt was made by Zhou [18] who redefined the moments so that the transformation matrix for a rectangular grid was identical to that for a standard MRT on a square grid. However, the modifications suggested in Zhou [18] led to anisotropic fluid viscosity. In Section 2, we will revisit the models of Bouzidi et al. [17] and Zhou [18] using a consistent inverse design framework, and show, once again, that their models are unable to recover exactly the Navier-Stokes equations. Hegele et al. [19] indicated some extra degrees of freedom should be employed to satisfy the isotropy conditions for rectangular lattice Boltzmann scheme. There are three possible approaches: decoupling the discretization of the velocity space from spatial and temporal discretization, modification a collision operator with additional parameter, and adoption more discrete microscopic velocities. They introduced two extra microscopic velocities to extend the D3Q19 model with BGK collision operator and were able to restore, on a rectangular grid, the isotropy condition required for the Navier-Stokes equation. They also suggested that four new velocities are needed in order to correctly extend the D3Q19 model onto a noncubic 3D grid.

In the present work, we explore the possibility to restore the isotropy condition on a 2D rectangular grid, without introducing any additional microscopic velocity. We take advantage of some of the flexibility within the MRT LBM scheme [20, 21]. For this purpose, we will introduce an additional parameter in the energy-normal stress moment subspace. Before presenting our novel MRT LBM scheme on a rectangular grid, previous MRT schemes on a rectangular grid are firstly reviewed in Section 2. An inverse design analysis will be used to derive the equilibrium moments and the anisotropy of the transport coefficients for a rectangular grid is revealed. In section 3, our new scheme with additional free parameter is constructed in order to restore the isotropy for a rectangular grid, namely, the usual Navier-Stokes hydrodynamic equation is derived using a rectangular grid. Also, the coupling relationships between relaxations times and determination of computational parameters are re-interpreted, which enables the flexibility to choose computational parameters according to different flow problems. In Section 4, numerical validation of our new scheme is provided using a channel flow and a lid-driven cavity flow. Concluding remarks are provided in Section 5.

2. An analysis of previous MRT LBM schemes on a rectangular grid

2.1. The model of Bouzidi et al. [17]

We begin with the MRT LBM scheme [20] in 2D, which has been shown to provide more flexibility in relaxing different moments and to significantly improve computational stability and accuracy, while simplicity and computational efficiency of LBM are retained. However, we consider a rectangular grid as shown in Fig. 1, where the non-zero lattice velocity in the \( x \) direction is one, and in the \( y \) direction is \( a (a < 1) \). Following the spirit of the D2Q9 model but with the different velocities in \( x \) and \( y \) directions, the discrete velocities are defined as
The distribution functions in MRT LBM evolve as

$$f_i(x + e_i \delta t) - f_i(x, t) = \Omega_i$$

where \(f_i\) is the distribution function associated with the molecular velocity \(e_i\) at position \(x\) and time \(t\), \(\Omega_i\) is the collision operator.

In MRT LBM, the streaming process takes place in the physical space while the collision process is performed in the moment space. The nine distribution functions define nine degrees of freedom, which implies that nine independent moments can be constructed. We first adopt the moments introduced in Bouzidi et al. [17] through a transformation matrix \(M\)

$$m = Mf$$

where \(f = (f_0, f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8)^T\). The transformation matrix \(M\) specifies the nature of the moments and is given as [17]

$$M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -2r_1 & r_2 & r_3 & r_2 & r_3 & r_1 & r_1 & r_1 & r_1 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & a & 0 & -a & a & a & -a & -a \\ 0 & 0 & -2a & 0 & 2a & a & a & -a & -a \\ -2r_4 & r_5 & r_6 & r_5 & r_6 & r_4 & r_4 & r_4 & r_4 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}$$

where \(r_1 = 1 + a^2, r_2 = 1 - 2a^2, r_3 = -2 + a^2, r_4 = -1 + a^2, r_5 = 2 + a^2, r_6 = -1 - 2a^2\). The row vectors are orthogonal and they define the following nine moments

$$m = (\rho, e, \epsilon, j_x, q_{xx}, j_y, q_{yy}, p_{xx}, p_{xy})^T,$$

where \(\rho\) is the density, \(e\) is the kinetic energy, \(\epsilon\) is the kinetic energy squared, \(j_x\) and \(j_y\) are the momentum density in the \(x\) and \(y\) directions, respectively, \(q_x\) and \(q_y\) are the \(x\) and \(y\) components of the energy flux, \(p_{xx}\) and \(p_{xy}\) are related to the diagonal and off-diagonal components of the viscous stress tensor.
The MRT collision operator $\Omega$, is expressed as

$$\Omega = -M^{-1} S \Gamma \left[ f(x, t) - F^q(x, t) \right]$$  \hspace{1cm} (6)

where $S$ is a non-negative diagonal relaxation matrix,

$$S = \text{diag} \left( s_\rho, s_\rho, s_\rho, s_j, s_j, s_j, s_q, s_q, s_q, s_q, s_i \right)$$  \hspace{1cm} (7)

where $s_\rho$ and $s_j$ are the relaxation times for $p_{\text{xx}}$ and $p_{\text{xy}}$, respectively. When all the relaxation times are set to be equal, the usual BGK model is recovered.

We shall now perform the Chapman-Enskog multiscaling analysis in order to derive the macroscopic hydrodynamic equations. To this end, we first expand the distribution function $f_i$, the derivatives in time and space as \cite{[1, 22]}

$$m = m^{(0)} + \epsilon m^{(1)} + \epsilon^2 m^{(2)} + \cdots$$  \hspace{1cm} (8a)

$$\frac{\partial}{\partial t} = \epsilon \partial_{\alpha} + \epsilon^2 \partial_{\beta},$$  \hspace{1cm} (8b)

$$\frac{\partial}{\partial x_{\alpha}} = \epsilon \partial_{\alpha \alpha},$$  \hspace{1cm} (8c)

where $\epsilon$ is a small parameter which is proportional to the ratio of the lattice spacing to a characteristic macroscopic length.

Performing Taylor expansion of Eq. (2) and substituting the above expansions, the following equations at zeroth-, first- and second-order in $\epsilon$ can be obtained

$$O(\epsilon^0) : \quad m^{(0)} = m^{(eq)},$$  \hspace{1cm} (9a)

$$O(\epsilon^1) : \quad \left( \hat{I} \partial_{\alpha} + \hat{C}_\alpha \partial_{\alpha} \right) m^{(0)} = -\frac{S}{\delta t} m^{(1)},$$  \hspace{1cm} (9b)

$$O(\epsilon^2) : \quad \partial_{\alpha} m^{(0)} + \left( \hat{I} \partial_{\alpha} + \hat{C}_\alpha \partial_{\alpha} \right) \left( t - \frac{S}{2} \right) m^{(1)} = -\frac{S}{\delta t} m^{(2)},$$  \hspace{1cm} (9c)

where $\hat{C}_\alpha = M_{\text{diag}}(\epsilon_{0\alpha}, \epsilon_{1\alpha}, \cdots, \epsilon_{n\alpha}) M^{-1}$. Eq. (9c) has already been simplified by making use of Eq.(9b).

The first, fourth and sixth components of Eq. 9(b) are

$$\partial_{t, \rho} + \partial_{1, x} f^{(eq)}_x + \partial_{1, y} f^{(eq)}_y = 0 \quad (10a)$$

$$\partial_{1, x} f^{(eq)}_x + \partial_{1, y} \left[ \frac{2}{3} \rho + \frac{e^{(eq)}}{3(a^2 + 1)} + \frac{a^2}{3(a^2 + 1)} p^{(eq)}_{xx} \right] + \partial_{1, y} \left( a p^{(eq)}_{xy} \right) = 0 \quad (10b)$$

$$\partial_{1, x} f^{(eq)}_y + \partial_{1, y} \left( a p^{(eq)}_{xy} \right) + \partial_{1, y} \left[ \frac{2a^2}{3} \rho + \frac{a^2 e^{(eq)}}{3(a^2 + 1)} - \frac{a^2}{3(a^2 + 1)} p^{(eq)}_{xx} \right] = 0 \quad (10c)$$

The design target at $O(\epsilon)$ is the Euler equations

$$\partial_{t, \rho} + \partial_{1, x} (\rho u_x) + \partial_{1, y} (\rho u_y) = 0, \quad (11a)$$

$$\partial_{1, x} (\rho u_x) + \partial_{1, y} (\rho c_y^2 + \rho u_y^2) + \partial_{1, y} (\rho u_x u_y) = 0, \quad (11b)$$

$$\partial_{1, y} (\rho u_y) + \partial_{1, y} (\rho u_x u_y) + \partial_{1, y} (\rho c_y^2 + \rho u_y^2) = 0, \quad (11c)$$

where the pressure has been written as $p = \rho c_y^2$. Comparing Eq. (10) to Eq. (11), we obtain

$$f^{(eq)}_x = \rho u_x, \quad f^{(eq)}_y = \rho u_y, \quad (12a)$$

$$\frac{2}{3} \rho + \frac{e^{(eq)}}{3(a^2 + 1) + \frac{a^2}{3(a^2 + 1)} p^{(eq)}_{xx}} = \rho (c_x^2 + u_x^2), \quad (12b)$$

$$\frac{2a^2}{3} \rho + \frac{a^2 e^{(eq)}}{3(a^2 + 1) - \frac{a^2}{3(a^2 + 1)} p^{(eq)}_{xx}} = \rho (c_y^2 + u_y^2), \quad (12c)$$

$$a p^{(eq)}_{xy} = \rho u_x u_y, \quad (12d)$$
At this point, the remaining three equilibrium moments, \( q_{x}^{(eq)} \) and \( q_{y}^{(eq)} \), are to be determined. As we will realize soon that \( e^{(eq)} \) doesn’t affect the Navier-Stokes equation, it can be defined somewhat arbitrarily. \( q_{x}^{(eq)} \) and \( q_{y}^{(eq)} \) will be determined by the hydrodynamic equation at \( O(e^{2}) \).

At \( O(e^{2}) \), the first, fourth, and sixth components of Eq. (9c) yield

\[
\partial_{1}\rho = 0, \\
\partial_{1}(\rho u_{x}) = \frac{a^{2}(1 - 0.5 s_{0})}{3(a^{4} + 1)} \partial_{11} p_{xs}^{(1)} - a(1 + 0.5 s_{x}) \partial_{1y} p_{ys}^{(1)} - \frac{1 - 0.5 s_{y}}{3(a^{4} + 1)} \partial_{11} \epsilon^{(1)}, \\
\partial_{2}(\rho u_{y}) = \frac{a^{2}(1 - 0.5 s_{0})}{3(a^{4} + 1)} \partial_{11} p_{ys}^{(1)} - a(1 - 0.5 s_{x}) \partial_{1y} p_{ys}^{(1)} - \frac{a^{2}(1 - 0.5 s_{y})}{3(a^{4} + 1)} \partial_{11} \epsilon^{(1)}.
\]

The design target at \( O(e^{2}) \) is to potentially match the Navier-Stokes equation which may be stated in a more general form as:

\[
\partial_{1}(\rho u_{x}) = \partial_{11} \left[ \rho \zeta_{x} \left( \partial_{11} u_{x} + \partial_{11} u_{y} \right) + \rho \nu_{x} \left( \partial_{11} u_{x} - \partial_{11} u_{y} \right) \right] + \partial_{1y} \left[ \rho \zeta_{y} \left( \partial_{11} u_{x} + \partial_{11} u_{y} \right) \right], \\
\partial_{2}(\rho u_{y}) = \partial_{11} \left[ \rho \nu_{y} \left( \partial_{11} u_{x} + \partial_{11} u_{y} \right) \right] + \partial_{1y} \left[ \rho \zeta_{y} \left( \partial_{11} u_{x} + \partial_{11} u_{y} \right) \right] + \rho \nu_{y} \left( \partial_{11} u_{x} - \partial_{11} u_{y} \right),
\]

where \( \zeta_{x} \) and \( \zeta_{y} \) are bulk viscosity in \( x \) and \( y \) directions, respectively; \( \nu_{x} \) and \( \nu_{y} \) are two viscosities associated with normal viscous stress components, and \( \nu \) is the shear viscosity.

At this point, we need the explicit expressions for \( e^{(1)} \), \( p_{xs}^{(1)} \), and \( p_{ys}^{(1)} \) which can be obtained from Equation 9(b). They are

\[
- s' e^{(1)} = \partial_{11} \left[ 2\rho \left( 3c_{x}^{2} - r_{1} \right) + 3a \nu_{x}^{2} \right] + \partial_{1x} \left( j_{x}^{(eq)} + a^{2} q_{x}^{(eq)} \right) + \partial_{1y} \left( a^{2} j_{y}^{(eq)} + q_{y}^{(eq)} \right), \\
- s' \rho u_{x}^{(1)} = \partial_{11} \left[ \frac{\rho r_{x}}{a^{4}} \left( 3r_{1} c_{x}^{2} - 2a^{2} \right) + 3\rho \left( a^{2} \nu_{x}^{2} - \frac{a^{2}}{a^{2}} \right) \right] + \partial_{1x} \left( a^{2} j_{y}^{(eq)} - q_{x}^{(eq)} \right) + \partial_{1y} \left( - j_{y}^{(eq)} + a^{2} q_{y}^{(eq)} \right), \\
- s' \rho u_{y}^{(1)} = \partial_{11} \left( \frac{\rho u_{x} u_{y}}{a} \right) + \partial_{1y} \left( \frac{2j_{x}^{(eq)} + 1}{3a} q_{y}^{(eq)} \right) + \partial_{1y} \left( \frac{2}{3} j_{y}^{(eq)} + \frac{a}{3} q_{y}^{(eq)} \right)
\]

where \( s' \) is the spatial derivative. It is noted that the \( \partial_{1}[\ldots] \) terms in the above equations involve \( \partial_{1}(\rho u_{x} u_{y}) \), which can be converted to spatial derivatives using Euler equations as

\[
\partial_{1} \left( \rho u_{a} u_{b} \right) = -u_{a} \partial_{b} p - u_{b} \partial_{a} p + O(a^{2}).
\]

Since, at low Mach number, \( p = O(Ma^{2}) \), we conclude that \( \partial_{1}(\rho u_{a} u_{b}) = O(a^{2}) \) and thus can be neglected.

Comparing Eq. (15) with Eq. (16), it is obvious that only \( p_{xs}^{(1)} \) contributes to the cross shear stress term. To match the form of \( \partial_{1} u_{x} + \partial_{1} u_{y} \) required by the Navier-Stokes equation, we must demand that \( q_{x}^{(eq)} = \gamma_{1} j_{x}^{(eq)} = \frac{\gamma_{1}}{2} \rho u_{x} \) and \( q_{y}^{(eq)} = \gamma_{2} j_{y}^{(eq)} = \frac{\gamma_{2}}{2} \rho u_{y} \), where \( \gamma_{1} \) and \( \gamma_{2} \) are constants to be determined. Furthermore, the net coefficients for the \( \partial_{1} u_{x} \) term and \( \partial_{1} u_{y} \) term must be made identical, namely,

\[
\frac{2}{3a} + \frac{1}{6a} \gamma_{2} = \frac{2a}{3} + \frac{a}{6} \gamma_{1}
\]
This implies that $\gamma_1$ can be determined in terms of $\gamma_2$ as

$$\gamma_1 = \frac{\gamma_2 + 4(1 - a^2)}{a^2}$$  

(19)

This is identical to Eq. (3.6) in Bouzidi et al. [17] since our $\gamma_1$ and $\gamma_2$ are denoted by $c_1$ and $c_2$ in their paper. In the following, we denote $\gamma_2$ by $\gamma$. At this point, we have determined all necessary equilibrium moments which could affect the hydrodynamics equations.

Substituting Eq. (16) into Eq. (14) with the forms of the equilibrium moments already determined, we can derive the explicit expression of each transport coefficient that appears in Eq. (15). The results are

$$v_s = \frac{\delta t}{2(a^2 + 1)} (1 - a^2) \left(\frac{1}{s_e} - 0.5\right) + \frac{a^2 \delta t}{6(a^2 + 1)} \left(a^2 - \frac{\gamma}{2a^2} - \frac{a^2 \gamma}{2} + 3\right) \left(\frac{1}{s_n} - 0.5\right).$$  

(20a)

$$\xi_s = \frac{\delta t}{6(a^2 + 1)} (7 + \gamma + 3a^2 - 12c_1^2) \left(\frac{1}{s_e} - 0.5\right) + \frac{a^2 \delta t}{6(a^2 + 1)} \left(5a^2 - \frac{2}{a^2} - \frac{\gamma}{2a^2} - 6a^2 c_1^2 + 6 \frac{c_1^2}{a^2} + \frac{a^2 \gamma}{2} - 3\right) \left(\frac{1}{s_n} - 0.5\right).$$  

(20b)

$$v_y = \frac{a^2 \delta t}{2(a^2 + 1)} (a^2 - 1) \left(\frac{1}{s_e} - 0.5\right) + \frac{a^2 \delta t}{6(a^2 + 1)} \left(a^2 - \frac{2}{a^2} - \frac{a^2 \gamma}{2} + 3\right) \left(\frac{1}{s_n} - 0.5\right).$$  

(20c)

$$\xi_y = \frac{a^2 \delta t}{6(a^2 + 1)} (7 + \gamma + 3a^2 - 12c_1^2) \left(\frac{1}{s_e} - 0.5\right) - \frac{a^2 \delta t}{6(a^2 + 1)} \left(5a^2 - \frac{2}{a^2} - \frac{\gamma}{2a^2} - 6a^2 c_1^2 + 6 \frac{c_1^2}{a^2} + \frac{a^2 \gamma}{2} - 3\right) \left(\frac{1}{s_n} - 0.5\right).$$  

(20d)

$$v = \frac{\gamma + 4}{6} \left(\frac{1}{s_e} - 0.5\right) \delta t.$$  

(20e)

It can be seen from Eq. (20), the hydrodynamic transport coefficients on a rectangular grid depend on parameters $c_1, \gamma, s_e, s_n, s_c$ and the grid parameter $a$. The question here is whether we can achieve the isotropy conditions required by the Navier-Stokes equation: $\nu = v_x = v_y$ and $\xi_x = \xi_y$ (together they represent three conditions). Since the relaxation parameters are directly related to the various transport coefficients, Bouzidi et al. [17] attempted to approach the isotropy conditions by relating $s_x$ and $s_n$ to $s_c$, using a linearized dispersion analysis. Here we shall derive the same relationships from a very different perspective.

First, we define an average bulk viscosity as

$$\zeta \equiv \frac{\xi_x + \xi_y}{2} = \frac{(7 + \gamma + 3a^2 - 12c_1^2)}{12} \left(\frac{1}{s_e} - 0.5\right) \delta t$$  

(21)

which is identical to the expression of bulk viscosity in Bouzidi et al. [17]. In order to construct the coupling relationships between the relaxation parameters, we impose the following two conditions

$$\nu = \frac{v_x + v_y}{2},$$  

(22a)

$$\frac{\xi_x - \xi_y}{2} + \frac{v_x - v_y}{2} = 0.$$  

(22b)

The first condition states that the average normal shear viscosity should be the same as the cross shear viscosity, which represents one step towards the isotropy conditions. The second condition amounts to $v_x + \xi_x = v_y + \xi_y$, namely, the net normal viscosities in the x and y directions are the same. Herein, we can build two coupling relationships between $s_e, s_n$ and $s_c$. The true isotropy involves three conditions, here we impose two conditions first.

Substituting the expressions of the transport coefficients in Eq.(20) into Eq.(22), we can express $s_e$ and $s_n$ in terms of $s_c$ as follows

$$\frac{1}{s_c} - \frac{1}{2} = \frac{2(4 + \gamma) \left[(12c_1^2 - \gamma)(1 + a^2) - 2(5a^2 + 2)\right]}{(1 + a^2)(1 + \gamma - 3a^2)(\gamma + 10 - 12c_1^2) + 6[a^4(\gamma - 2) - 3(a^2 - 1)]} \left(\frac{1}{s_c} - \frac{1}{2}\right).$$  

(23)

$$\frac{1}{s_n} - \frac{1}{2} = \frac{2(4 + \gamma) \left[(12c_1^2 - \gamma)(1 + a^2) - 2(3a^4 + 5a^2 + 5)\right]}{(1 + a^2)(1 + \gamma - 3a^2)(\gamma + 10 - 12c_1^2) + 6[a^4(\gamma - 2) - 3(a^2 - 1)]} \left(\frac{1}{s_c} - \frac{1}{2}\right).$$  

(24)
which are precisely the two relationships proposed in Bouzidi et al. [17] based on the linearized dispersion analysis. An important detail should be noted. In the above derivation the limit of \( a \to 1 \) is a singular limit. In this limit, the first condition, Eq. (22a), will yield

\[
\frac{(2 - \gamma) \Delta t}{12} \left( \frac{1}{s_n} - 0.5 \right) = \frac{(4 + \gamma) \Delta t}{6} \left( \frac{1}{s_c} - 0.5 \right)
\]

(25)

The second condition, Eq. (22b), leads to a condition

\[
(1 - a^2) \left\{ \left[ (12c_1^2 - \gamma - 4)(1 - a^2) - 6a^2 \right] \left( \frac{1}{s_n} - 0.5 \right) + \left[ (7 + \gamma + 3a^2 - 12c_1^2)(1 + a^2) + 3(1 + a^2) \right] \left( \frac{1}{s_c} - 0.5 \right) \right\} = 0
\]

which is automatically satisfied when \( a = 1 \). In deriving the relationships, Eqs. (23) and (24), however, we did not use the condition of \( a = 1 \) but instead set

\[
\left[ (12c_1^2 - \gamma - 4)(1 - a^2) - 6a^2 \right] \left( \frac{1}{s_n} - 0.5 \right) + \left[ (7 + \gamma + 3a^2 - 12c_1^2)(1 + a^2) + 3(1 + a^2) \right] \left( \frac{1}{s_c} - 0.5 \right) = 0.
\]

(27)

Therefore, we could have two possible routes to satisfy the Navier-Stokes equation in the limit of \( a = 1 \). The first possibility is to use the condition Eq. (25) only. This condition implies that \( \gamma \) can be left as a free parameter so that Eq.(25) becomes a required condition between \( s_n \) and \( s_c \). A special case is to set \( s_n = s_c \), then we have

\[
\frac{2 - \gamma}{12} = \frac{4 + \gamma}{6},
\]

(28)

which leads to a specific requirement that \( \gamma \) must to be set to \(-2\). The second possibility to achieve the Navier-Stokes equations in the limit of \( a = 1 \) is to use the conditions Eqs. (23) and (24), which with \( a = 1 \) become

\[
\frac{1}{s_c} - \frac{1}{2} = \frac{2(4 + \gamma)}{(2 - \gamma)} \left( \frac{\gamma + 7 - 12c_1^2}{(2 - \gamma)} \right) \left( \frac{1}{s_c} - \frac{1}{2} \right)
\]

(29)

\[
\frac{1}{s_n} - \frac{1}{2} = \frac{2(4 + \gamma)}{(2 - \gamma)} \left( \frac{1}{s_c} - \frac{1}{2} \right)
\]

(30)

Eq.(30) is identical to Eq. (25), but Eq.(29) imposes a condition between \( s_c \) and \( s_n \) that depends on both \( \gamma \) and \( c_1 \), which is really unnecessary for \( a = 1 \). Still, Eq. (29) indicates the limiting relationship between \( s_c \) and \( s_n \) when \( a \) is close to one, namely, on a rectangular grid, the relaxation of energy must be linked to the relaxation of cross shear stress moment. With Eqs. (23) and (24), we can show that the transport coefficients can now be simply written as

\[
\nu_x = \nu + \Delta^B, \quad \nu_y = \nu - \Delta^B, \quad \zeta_x = \zeta - \Delta^B, \quad \zeta_y = \zeta + \Delta^B,
\]

(31a-31d)

where the only remaining deviation \( \Delta^B \) from isotropy is

\[
\Delta^B = \frac{1 - a^2}{4} \left( \frac{1}{s_c} - 0.5 \right) \Delta t.
\]

(32)

Several observations can be made. First, when \( a = 1 \) or when the square grid is used, the isotropy conditions are automatically satisfied and the Navier-Stokes equation is recovered. Second, when \( a < 1 \) and \( 0 < s_c < 2 \), it is not possible to rigorously satisfy the Navier-Stokes equation or restore the isotropy. The bulk viscosity in the \( x \) direction is always less than that in the \( y \) direction, and the normal shear viscosity in the \( x \) direction is always larger than that in the \( y \) direction. Therefore, we have shown that the Bouzidi et al.’s model does not satisfy the Navier-Stokes equation. Third, if \( a \) is close to one or if \( s_c \) is close to 2, the deviation from the Navier-Stokes equation is not significant.
2.2. The model of Zhou [18]

Next, we briefly re-visit the model proposed by Zhou [18] also intended for a rectangular grid. He simply used
the transformation matrix that is identical to what is used for a square grid, namely,

\[
M = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 \\
0 & 0 & 1 & 0 & -1 & 1 & -1 & -1 \\
0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
\end{pmatrix}
\]

(33)

This amounts to a different set of definitions for the moments. Compared with the model of Bouzidi et al. [17], energy
and normal shear stress moments were defined differently in Zhou [18], while the remaining 7 moments are essentially
the same up to a constant factor. In these two-dimensional moment subspace, the energy and normal stress moments
between the two models can be related to each other as

\[
e^B = \frac{a^2 + 1}{2} e^Z + \frac{1 - a^2}{2} \cdot 3 p_{xx}^{Z(eq)} ,
\]

(34a)

\[
3 p_{sx}^B = \frac{a^3 - 1}{2} e^Z + \frac{1 + a^2}{2} \cdot 3 p_{sx}^{Z(eq)},
\]

(34b)

where \(e^B, p_{sx}^B\) and \(e^Z, p_{sx}^{Z(eq)}\) refer to the energy and shear stress moments in Bouzidi’s model and Zhou’s model, respec-
tively. Without the consideration of the external forcing term, the leading-order multiscaling expansion of Zhou’s
model leads to the following hydrodynamic equations

\[
\partial_t \rho + \partial_{1x}(\rho u_x) + \partial_{1y}(\rho u_y) = 0,
\]

(35a)

\[
\partial_t (\rho u_x) + \partial_{1x} \left( \frac{2}{3} \rho + \frac{1}{6} e^{Z(eq)} + \frac{1}{2} p_{xx}^{Z(eq)} \right) + \partial_{1y}(\rho u_x u_y) = 0,
\]

(35b)

\[
\partial_t (\rho u_y) + \partial_{1y} \left( \frac{2 a^2}{3} \rho + \frac{a^2}{6} e^{Z(eq)} - \frac{a^2}{2} p_{sx}^{Z(eq)} \right) + \partial_{1x}(\rho u_x u_y) = 0.
\]

(35c)

The hydrodynamic equations at \(O(e^2)\) are

\[
\partial_t (\rho u_x) + \partial_{1x} \left[ \frac{1}{6} (1 - 0.5 s_x) e^{Z(1)} + \frac{1}{2} (1 - 0.5 s_x) p_{xx}^{Z(1)} \right] + a \partial_{1y} \left[ (1 - 0.5 s_x) p_{sy}^{Z(1)} \right] = 0, \tag{36a}
\]

\[
\frac{1}{a} \partial_t (\rho u_y) + a \partial_{1y} \left[ \frac{1}{6} (1 - 0.5 s_x) e^{Z(1)} - \frac{1}{2} (1 - 0.5 s_x) p_{sx}^{Z(1)} \right] + \partial_{1x} \left[ (1 - 0.5 s_x) p_{sy}^{Z(1)} \right] = 0. \tag{36b}
\]

Applying the similar inverse design analysis as done in Section 2.1, the following equilibrium moments are ob-
moments in Eq. (37) are identical to those in Zhou [18]. Substituting the above derived equilibrium moments into the incorrect according to the requirements of self-consistency, which was set as \( -\omega \). However, the definition of \( \omega \) where \( \omega = 2 \frac{\sigma}{a} \) is related to the speed of sound as \( 2\omega a = c_s^2 \). It is noted that our inverse design analysis provides the best scenario of the model towards satisfying the correct hydrodynamics. However, the definition of \( q_i^{eq} \) in Zhou’s work is incorrect according to the requirements of self-consistency, which was set as \(-\rho u_i\). While the remaining equilibrium moments in Eq. (37) are identical to those in Zhou [18]. Substituting the above derived equilibrium moments into the Eqs. (36), we obtain

\[
\begin{align*}
\partial_t \rho u_x &= \partial_{x_1} \left[ \rho \xi_x \left( \partial_{x_1} u_x + \partial_{x_1} u_y \right) + \rho \nu_x \left( \partial_{x_1} u_y - \partial_{x_1} u_x \right) \right] + \partial_{x_1} \left[ \rho \nu_x \left( \partial_{x_1} u_x + \partial_{x_1} u_y \right) \right], \\
\partial_t \rho u_y &= \partial_{x_1} \left[ \rho \nu_x \left( \partial_{x_1} u_x + \partial_{x_1} u_y \right) \right] + \partial_{x_1} \left[ \rho \nu_x \left( \partial_{x_1} u_y - \partial_{x_1} u_x \right) \right],
\end{align*}
\]

where \( \xi_x, \nu_x \) and \( \nu_y \) are bulk and shear viscosities for \( x \) and \( y \) moment equation, respectively. Their explicit expressions are

\[
\begin{align*}
\xi_x &= \left( \frac{1}{s_x} - 0.5 \right) \left( \frac{1}{12a^2} + \frac{7}{12} - \omega a - \frac{\omega}{a} \right) \delta t + \left( \frac{1}{s_n} - 0.5 \right) \left( \frac{\omega}{a} - \omega a + \frac{3a^2 - 1}{12a^2} \right) \delta t, \\
\nu_x &= \left( \frac{1}{s_x} - 0.5 \right) \left( \frac{1}{12a^2} + \frac{7}{12} - \omega a - \frac{\omega}{a} \right) \delta t - \left( \frac{1}{s_n} - 0.5 \right) \left( \frac{\omega}{a} - \omega a + \frac{3a^2 - 1}{12a^2} \right) \delta t, \\
\nu_y &= \frac{1}{12a^2} \left( \frac{1}{s_x} - 0.5 \right) \left( 1 - a^2 \right) \delta t + \frac{1}{12a^2} \left( \frac{1}{s_n} - 0.5 \right) \left( 7a^2 - 1 \right) \delta t, \\
\nu_y &= \frac{1}{12a^2} \left( \frac{1}{s_x} - 0.5 \right) \left( 1 - a^2 \right) \delta t + \frac{1}{12a^2} \left( \frac{1}{s_n} - 0.5 \right) \left( 7a^2 - 1 \right) \delta t, \\
\nu_x &= \frac{1}{3a} \left( \frac{1}{s_x} - 0.5 \right) \delta t.
\end{align*}
\]

We note that by setting \( a = 1 \), the standard model for the square grid can be recovered.

Since the shear and bulk transfer coefficients in \( x \) and \( y \) moment equation are not identical, it is impossible to achieve isotropy when \( a < 1 \). The assumptions Zhou proposed in Eq. (62) and Eq. (63) of his paper for the relaxation parameters also fail to satisfy the Navier-Stokes equation when \( a < 1 \).

If the same conditions, Eqs. (22a) and (22b), are imposed, we can obtain the following coupling relationships between the relaxation parameters

\[
\begin{align*}
\frac{1}{s_x} - 0.5 &= \frac{4a \left( 12\omega a - 12\omega a^3 + 3a^2 - 1 \right)}{\left( 1 - a^2 \right) \left( 1 - 7a^2 \right)} \left( \frac{1}{s_x} - 0.5 \right), \\
\frac{1}{s_n} - 0.5 &= \frac{4a}{7a^2 - 1} \left( \frac{1}{s_x} - 0.5 \right).
\end{align*}
\]
With these relationships, we can then express the transport coefficients

\[ \nu_x' = \nu_x + \Delta Z, \]  
\[ \nu_y' = \nu_y - \Delta Z, \]  
\[ \zeta_x' = \zeta_x - \Delta Z, \]  
\[ \zeta_y' = \zeta_y + \Delta Z, \]

where the deviation from isotropy is

\[ \Delta Z = \frac{1 - a^2}{12a^2} \left( \frac{1}{s_e} - 0.5 \right) \delta t \]  

and the bulk viscosity is

\[ \zeta^B = \frac{\zeta_x + \zeta_y}{2} = \left( \frac{7}{12} + \frac{1}{12a^2} - \omega a - \frac{\omega a}{a} \right) \left( \frac{1}{s_e} - 0.5 \right) \delta t \]  

The presence of the extra term \( \Delta Z \) indicates again that it is impossible to satisfy the full isotropy conditions as required by the Navier-Stokes equation with Zhou’s definitions of moments.

In summary, without introducing a new degree of freedom, it is impossible for MRT LBM to satisfy the Navier-Stokes equation when a rectangular grid is used.

3. A new MRT LBM model for a rectangular lattice grid

From the above analysis, it becomes clear that both the values and the anisotropy of the hydrodynamic transport coefficients result mainly from their dependence on the definition and relaxation parameters of energy and stress moments. Inspired by the above inverse analysis, our new rectangular MRT scheme introduces a more flexible coupling between the energy moment and normal stress moment. Specifically, we modify the definitions of these two moments by a coordinate rotation of the Bouzidi et al.’s definitions, as illustrated in Fig. 2. Such rotation will not change the orthogonality property of the nine moments. The relative orientation angle becomes a new adjustable parameter.

The new energy and normal stress moments are defined in terms of Bouzidi et al.’s definitions as

\[ e = e^B + \theta p_{xx}^B \]  
\[ p_{xx} = p_{xx}^B - \theta e^B \]

where \( \theta \sim - \tan \phi \) with \( \phi \) is the angle of rotation, \( e \) and \( p_{xx} \) refer to the new energy and normal viscous stress moments, respectively, while \( e^B \) and \( p_{xx}^B \) represent the corresponding moments defined in Bouzidi et al. [17] for a rectangular grid, as indicated by the transformation matrix, Eq. (4). The other 7 moments are kept the same as that defined by Bouzidi et al. [17].
With these new definitions, the second and eighth row of the transformation matrix will be modified accordingly

\[
M = \begin{bmatrix}
\langle \rho \rangle & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\langle e \rangle & -2R_1 & R_2 & R_3 & R_4 & R_5 & R_6 & R_7 \\
\langle s \rangle & 4 & -2 & -2 & -2 & 1 & 1 & 1 \\
\langle f_1 \rangle & 0 & 1 & 0 & -1 & 0 & 1 & -1 \\
\langle q_1 \rangle & 0 & 0 & -2a & 0 & 2a & a & -a \\
\langle f_2 \rangle & 0 & 0 & a & 0 & -a & a & -a \\
\langle q_2 \rangle & 0 & 0 & -2a & 0 & 2a & a & -a \\
\langle 3p_n \rangle & -2R_4 & R_5 & R_6 & R_7 & R_8 & R_9 & R_{10} \\
\langle p_c \rangle & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & -1
\end{bmatrix}
\]

(45)

where \( R_1 = r_1 + \theta r_4, R_2 = r_2 + \theta r_5, R_3 = r_3 + \theta r_6, R_4 = r_4 - \theta r_1, R_5 = r_5 - \theta r_2, R_6 = r_6 - \theta r_3, \) and \( r_1, r_2, r_3, r_4, r_5, r_6 \) have been defined previous in Section 2.

By the same inverse design process using the Chapman Enskog analysis presented in Section 2.1, it is found that two equilibrium moments (i.e., energy and normal viscous stress) are modified and the others are the same as in Section 2.1. The updated equilibrium moments are

\[
n^{(eq)} = \rho 
\]

\[
\begin{bmatrix}
2 \left( 3c_1^2 - n_1 \right) + 3 \left( u_x^2 + u_y^2 \right) + \theta \left[ \frac{u_x}{\alpha} \left( 3r_1 c_2^2 - 2a^2 \right) + 3 \left( a^2 u_x^2 - \frac{u_x^4}{\alpha} \right) \right] \\
\frac{u_x}{\alpha} \left( 3r_1 c_2^2 - 2a^2 \right) + 3 \left( a^2 u_x^2 - \frac{u_x^4}{\alpha} \right) - \theta \left[ \frac{u_y}{\alpha} \left( 3c_1^2 - n_1 \right) + 3 \left( u_x^2 + u_y^2 \right) \right]
\end{bmatrix}
\]

(46)

The macroscopic equations for the new MRT scheme is structurally identical to that of those given in Section 2.1. The Euler equation is satisfied at \( O(\epsilon) \). The explicit expressions for the transport coefficients resulting from the \( O(\epsilon^2) \)
analysis, as defined in Eqs. (15a) and (15b), are

\[
v_x = \frac{\delta t}{6(a^2 + 1)} \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{\alpha_\gamma}{2} - \frac{2}{a^2} \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1} + \frac{1}{s_e} - 0.5 \right) \frac{\theta(a^2 + 1)}{\theta^2 + 1}.
\]

\[
v_y = \frac{\alpha_\gamma^2 \delta t}{6(a^2 + 1)} \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{\alpha_\gamma}{2} - \frac{2}{a^2} \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1} - \theta \left( \frac{1}{s_e} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1}.
\]

\[
v_z = \frac{\alpha_\gamma^2 \delta t}{6(a^2 + 1)} \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{\alpha_\gamma}{2} - \frac{2}{a^2} \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1} + \theta \left( \frac{1}{s_e} - 0.5 \right) \frac{\theta(a^2 + 1)}{\theta^2 + 1}.
\]

\[
\xi_x = \frac{\delta t}{6(a^2 + 1)} \left( 7 + \gamma + 3a^2 - 12c_2^2 \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{\theta(a^2 + 1)}{\theta^2 + 1} - \theta \left( \frac{1}{s_e} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1}.
\]

\[
\xi_y = \frac{\delta t}{6(a^2 + 1)} \left( 7 + \gamma + 3a^2 - 12c_2^2 \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{\theta(a^2 + 1)}{\theta^2 + 1} + \theta \left( \frac{1}{s_e} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1}.
\]

\[
\xi_z = \frac{\delta t}{6(a^2 + 1)} \left( 7 + \gamma + 3a^2 - 12c_2^2 \right) \left( \frac{1}{s_n} - 0.5 \right) \frac{\theta(a^2 + 1)}{\theta^2 + 1} + \theta \left( \frac{1}{s_e} - 0.5 \right) \frac{a^2 - \theta}{\theta^2 + 1}.
\]

\[
v = \frac{\gamma + 4}{6} \left( \frac{1}{s_e} - 0.5 \right) \delta t.
\]

At this moment, they look rather complicated. Clearly, when \( \theta = 0 \), Eqs. 47(a-e) reduces to Eqs. 20(a-e) as expected.

We adopt the same procedure by first imposing part of the isotropy requirements, given by Eqs. (22a) and (22b). The following coupling relationships can then be derived,

\[
\left( \frac{1}{s_n} - 0.5 \right) = \frac{2(\gamma + 4)(a^2 + 1)(1 + \theta^2)c_{22}}{C_{11}C_{22} - C_{12}C_{21}} \left( \frac{1}{s_e} - 0.5 \right)
\]

\[
\left( \frac{1}{s_n} - 0.5 \right) = \frac{2(\gamma + 4)(a^2 + 1)(1 + \theta^2)c_{21}}{C_{11}C_{22} - C_{12}C_{21}} \left( \frac{1}{s_e} - 0.5 \right)
\]

where

\[
C_{11} = \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a_\gamma}{2} - \frac{2}{a^2} \right) (2\theta^2a^2 + \theta - a^4\theta) + 3(1 - a^2)(2\theta^2a^2 + 1 - a^4),
\]

\[
C_{12} = \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a_\gamma}{2} - \frac{2}{a^2} \right) (2a^2 - \theta + a^4\theta) + 3(1 - a^2)(\theta^2 - 2a^2\theta - 4a^4\theta),
\]

\[
C_{21} = 2a^2\theta \left( 7 + \gamma + 3a^2 - 12c_2^2 \right) + (1 - a^4)(7 + \gamma + 3a^2 - 12c_2^2) + (a^4 + 1) \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a_\gamma}{2} - \frac{2}{a^2} \right) \theta + 3(a^4 + 1)(1 - a^2) + (1 - a^4)(1 - a^2) \left[ \frac{2}{a^2} - 5 + (6a^2 - \frac{\gamma}{2})(1 + \frac{1}{a^2}) \right] \theta + (1 - a^2) \left[ (12c_2^2 - \gamma - 4)(1 + a^2) - 6a^2 \right] \theta,
\]

\[
C_{22} = -2a^2\theta \left( 7 + \gamma + 3a^2 - 12c_2^2 \right) + (1 - a^4)(7 + \gamma + 3a^2 - 12c_2^2)\theta - (a^4 + 1) \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a_\gamma}{2} - \frac{2}{a^2} \right) \theta + 3(a^4 + 1)(1 - a^2)\theta - (1 - a^4)(1 - a^2) \left[ \frac{2}{a^2} - 5 + (6a^2 - \frac{\gamma}{2})(1 + \frac{1}{a^2}) \right] \theta + (1 - a^2) \left[ (12c_2^2 - \gamma - 4)(1 + a^2) - 6a^2 \right]
\]

It is important to note that the coefficients \( C_{11}, C_{12}, C_{21}, \) and \( C_{22} \) are functions of \( a, c, \gamma, \theta \) only, they do not depend on the relaxation parameters. When \( \theta = 0 \), the coupling relationships in Eqs. 48(a-b) reduce precisely to the coupling relationships Eq. (23) and (24). Furthermore, with the above conditions, the transport coefficients can now
be rewritten in the similar way as in Eq. (25) and Eq. (34) as

\[ \begin{align*}
v_x &= v + \frac{v_y - v_z}{2} \\
v_y &= v - \frac{v_x - v_z}{2} \\
\xi_x &= \xi - \frac{v_x - v_z}{2} \\
\xi_y &= \xi + \frac{v_x - v_z}{2}
\end{align*} \] (49a-d)

where

\[ \frac{v_x - v_y}{2} = \frac{\theta \delta t}{12 (1 + \theta^2)} \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a^2}{2a^2} \right) \left( \frac{1}{s_x} - \frac{1}{s_y} \right) + \frac{(1 - a^2) \delta t}{4 (1 + \theta^2)} \left( \frac{1}{s_x} - 0.5 \right) + \theta^2 \left( \frac{1}{s_y} - 0.5 \right) \] (50)

Now the final condition for matching the Navier-Stokes equation is simply to require

\[ \frac{v_x - v_y}{2} = 0 \] (51)

which leads to

\[ \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a^2}{2a^2} \right) \left( \frac{1}{s_x} - \frac{1}{s_y} \right) + 3(1 - a^2) \left( \frac{1}{s_x} - 0.5 \right) + \theta^2 \left( \frac{1}{s_y} - 0.5 \right) = 0 \] (52)

Now recall Eq. (48), which states the coupling relationship: \((s_x^{-1} - 0.5) \sim (s_y^{-1} - 0.5)\) and \((s_y^{-1} - 0.5) \sim (s_x^{-1} - 0.5)\). This implied that all the relaxation parameters \(s_x, s_y, s_c\) can be removed from Eq. (52) if we substitute Eqs. (48) into it. The relationship between \(a, c, \gamma, \theta\) is

\[ \left( 3 + a^2 - \frac{\gamma}{2a^2} - \frac{a^2}{2a^2} \right) (C_{21} + C_{22}) \theta + 3(1 - \theta^2)(C_{22} - C_{21}) \theta^2 = 0. \] (53)

Substituting the expressions of \(C_{11}, C_{12}, C_{21}, \) and \(C_{22}\), we can rewrite Eq. (53) in the following form

\[ (1 - a^2) \left( 1 + \theta^2 \right) (A \theta^2 + B \theta - A) = 0, \] (54)

where

\[ A = 3(a^2 - 1) \left[ (\gamma - 12c^2)(1 + a^2) + 2(5a^2 + 2) \right], \]

\[ B = a^2(12\gamma - 108c^2 + 66) + 18\theta^2(c^2 - 1) + 18c^2 + 18(a^4 - 1). \]

Several interesting observations are now in order. First, in the limit of \(a \to 1\), Eq. (54) is automatically satisfied for any \(\theta\). Namely, the Navier-Stokes equation emerge. In this limit, any value of \(\theta\) would work, with the formulation of Bouzidi et al. [17] and Zhou [18] as two special examples. In this limit, the coupling relationships, Eqs. (48a-b), are not related with \(\theta\) and become \(s_x = s_y = s_c\). Second, when \(a \neq 1\), then we must require

\[ A \theta^2 + B \theta - A = 0, \] (55)

which is a surprising simple second-order equation for setting \(\theta\) in terms of \(a, c, \gamma\), so that the full isotropy can be realized on a rectangular grid to yield the Navier-Stokes equation. This equation has two solutions \(\theta_1\) and \(\theta_2 = -1/\theta_1\). The relationship \(\theta_2 = -1/\theta_1\) stems from the fact that the last coefficient \((-A)\) differs from the first coefficient \((A)\) by a sign. The second solution \(\theta_2\) represents the result of rotating the direction of the \(e - p_{xx}\) axes in the first solution by 90 degrees. Therefore, without the loss of generality, we may restrict our discussions below to only the solution of \(\theta > 0\), which is given as

\[ \theta_1 = -\frac{B}{2A} + \sqrt{\frac{4A^2 + B^2}{2A}} \] (56)
The above analysis indicates that the free parameter $\theta$ provides the feasibility to eliminate the anisotropy in the transport coefficients. Such feasibility does not exist in the models of Bouzidi et al. [17] and Zhou [18], which is the reason why their models fail to rigorously satisfy the Navier-Stokes equation. We have derived the explicit requirement for setting this parameter in terms of the model parameters $c_s, \gamma, a$.

We stress that, in principle, for a given lattice aspect ratio $a$, $c_s$ and $\gamma$ are two free parameters in the model, which can be tuned to achieve the best numerical stability of our proposed MRT LBM model on a rectangular grid.

4. Numerical validations

We shall now confirm our new MRT LBM scheme on a rectangular grid, by considering two flow problems: a 2D channel flow and a 2D lid-driven cavity flow. For a given value of $a \neq 1$, the values of the model parameters should be chosen to keep the simulation numerically stable. The range of the relaxation parameters should be $0 < s_i < 2$. Here we consider steady-state flows. The simulation ends when the following condition

$$\frac{\sum_i [u_x(i, j, t + dt) - u_x(x, y, t)]^2 + [u_y(i, j, t + dt) - u_y(x, y, t)]^2}{\sum_i [u_x(x, y, t)^2 + u_y(x, y, t)^2]} < 10^{-8}$$

is reached.

4.1. The 2D channel flow

In this cases, the numerical simulations are conducted by the new MRT LBM model with several different values of the grid aspect ratio $a$ and the results are compared with the exact solution. The periodic boundary conditions are applied to the flow inlet and outlet, the half-way bounce back conditions are imposed on the channel walls. The model parameters are listed in Table 1. Note that the value of $\theta$ is determined from Eq. (56) after $c_s$ and $\gamma$ are chosen. The relaxation parameter $s_\epsilon$ are chosen according to the set-up of the flow problem, and $s_p$ and $s_j$ are obtained by Eqs.(48a-b). Besides, for all the cases studied here, the relaxation times $s_p, s_j$ are set to be 0, the other two relaxation times are chosen to be $s_\epsilon = 1.4, s_\gamma = 1.5$.

Fig. 3 shows the dimensionless velocity profiles (normalized by the channel center velocity) for 4 different values of the grid aspect ratio $a$, as well as the theoretical velocity profile. We observe that the results from our new model
are in excellent agreement with the exact solution. Next, in Figure 4, we compare the relative errors at the same \( U \) between the computed and exact results at different resolutions (\( N_y \)) in the \( y \) direction for \( a = 0.8 \) and \( a = 0.5 \).

The relative error is defined as: \( \frac{\mathbf{U}_{\text{LBM, y}} - \mathbf{U}_{\text{theory, y}}}{U} \), where \( \mathbf{U}_{\text{theory, y}} \) is the theoretical velocity of the poiseuille flow. The two dash-dotted lines denote the slope of \(-2\). Clearly, it proves the new scheme is of the second-order accuracy for \( a = 0.8 \) though the error seems to be larger if a smaller \( a \) is used. It is well known that mid-way bounce back boundary results to the second-order accuracy for standard LBM models [23, 24]. Here we confirm that the same is true on a rectangular grid.

### 4.2. The 2D lid-driven cavity flow

The 2D lid-driven cavity flow (Fig. 5) has been a standard benchmark flow to test many numerical methods. Depending on the flow Reynolds number, the flow pattern and the number of corner vortices are different. This flow has also been extensively used to study the performance of LBM solutions [25, 26, 27]. We consider a square cavity of width \( H \). At the top boundary, \( u_t = 0 \) and \( u_x = U \). Since the equilibrium distributions depend on \( a \), we need to obtain \( \mathbf{f}^{(eq)} \) from \( \mathbf{m}^{(eq)} \) by \( \mathbf{f}^{(eq)} = M^{-1} \mathbf{m}^{(eq)} \). The lattice node is placed half-way from the top wall, and the bounce back
where the nearly incompressible formulation is used, with the departure is around 0.015, which is significantly less than the shear viscosity which can be explained by the deviation term of the transport coefficients in Eq. (32). When \( a = 0.8 \) and \( Re = 100 \), this departure is around 0.015, which is significantly less than the shear viscosity \( \nu = 0.1 \). For \( a = 0.5 \), the departure term is 0.024, again is relatively small when compared to \( \nu = 0.1 \). It also found \( \Delta^0 \) should be less than a certain value

<table>
<thead>
<tr>
<th>( a )</th>
<th>( \gamma )</th>
<th>( c_1^2 )</th>
<th>( \theta )</th>
<th>( Re )</th>
<th>( s_x )</th>
<th>( s_y )</th>
<th>( s_u )</th>
<th>( U )</th>
<th>( N_x \times N_y )</th>
<th>Viscosity</th>
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<td>0.026</td>
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<td>1.1724</td>
<td>1.8878</td>
<td>1.0665</td>
<td>0.1</td>
<td>4 ( \times ) 125</td>
<td>0.10</td>
</tr>
<tr>
<td>0.65</td>
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<td>0.3333</td>
<td>0.421</td>
<td>100</td>
<td>1.2500</td>
<td>1.2508</td>
<td>0.3652</td>
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<td>4 ( \times ) 154</td>
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<tr>
<td>0.50</td>
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<td>0.16</td>
<td>0.298</td>
<td>100</td>
<td>0.9091</td>
<td>1.2859</td>
<td>0.3155</td>
<td>0.1</td>
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<tr>
<td>0.30</td>
<td>-3.8</td>
<td>0.04</td>
<td>0.076</td>
<td>100</td>
<td>0.2857</td>
<td>1.4796</td>
<td>0.2526</td>
<td>0.03</td>
<td>4 ( \times ) 334</td>
<td>0.03</td>
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<table>
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<th>( \gamma )</th>
<th>( c_1^2 )</th>
<th>( s_c )</th>
<th>( s_x )</th>
<th>( s_y )</th>
<th>( s_u )</th>
<th>( \Delta^0 )</th>
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<td>1.4889</td>
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<tr>
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<td>0.9091</td>
<td>1.6317</td>
<td>0.5630</td>
<td>0.021</td>
<td></td>
</tr>
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</table>

on the top wall is implemented as

\[
\begin{align*}
    f_4(x_f, t + \delta t) &= \tilde{f}_4(x_f, t) - \left[ f_2^{eq} - f_4^{eq} \right] = \tilde{f}_4(x_f, t) \\
    f_5(x_f, t + \delta t) &= \tilde{f}_5(x_f, t) - \left[ f_5^{eq} - f_4^{eq} \right] = \tilde{f}_5(x_f, t) - \rho \left( \frac{\gamma + 4}{12 a^2} \right) U \\
    f_6(x_f, t + \delta t) &= \tilde{f}_6(x_f, t) - \left[ f_6^{eq} - f_5^{eq} \right] = \tilde{f}_6(x_f, t) + \rho \left( \frac{\gamma + 4}{12 a^2} \right) U
\end{align*}
\]

where the nearly incompressible formulation is used, with \( \rho = \rho_0 + \delta \rho \) and \( \rho_0 = 1 \). Note that the above half-way bounce-back relations for a moving wall reduce to the standard forms when \( a = 0 \) and \( \gamma = -2 \). The value of \( \rho \) in the above is simply set to \( \rho_0 \). On the other three walls, the half-way bounce back scheme is applied. The governing parameter of the flow is the Reynolds number defined as \( Re = UH/\nu \). The number of lattice nodes in x direction is fixed to 100 and that in y direction is adjusted according to different grid aspect ratio \( a \).

In Fig. 6 and Fig. 7 we show the steady-state velocity profiles at \( x = 0.5D \) and \( y = 0.5H \) respectively, using both our new model and the model of Bouzidi et al., for the cavity flow at \( Re = 100 \). The computational parameters for the former are listed in Table 2. For the latter case the parameters are listed in Table 3 which are taken from the Table 4.1 in Bouzidi et al. [17] and the coupled relaxation times are obtained from Eq. 23 and Eq.24. The other relaxation times are set as: \( s_o = 0, s_x = 1.4, s_y = 0, s_u = 1.5 \). The results from a previous study [28] is also shown for comparison which employed the multigrid procedure and finite-difference solution.

In Fig. 6(a) and 7(a), the steady-state \( u_x \) and \( u_y \) velocity profiles along the centerline from our new model for four different values of \( a \) are plotted. The smallest \( a \) is 0.3 and the new model is still numerically stable. These clearly demonstrate that the results are not affected by \( a \), and are in excellent agreement with the work of Ghia et al. [28]. The corresponding results for the model of Bouzidi et al. [17] are shown in Figs. 6(b) and 7(b). The code based on their model became unstable at \( a = 0.3 \), so no results for \( a = 0.3 \) are shown. Interesting, for \( a \geq 0.5 \), their results are also in good agreement with one another and with those of Ghia et al. [28], although a closer inspection shows some minor differences in the \( u_x \) profiles. The good agreement for the model of Bouzidi et al. [17] is somewhat coincidental, which can be explained by the deviation term of the transport coefficients in Eq. (32).
Figure 5. A schematic of lid-driven cavity flow in a square cavity

Figure 6. Comparison of $u_x$ at the mid-plane with $Re=100$. (a) new model; (b) Bouzidi et al.'s scheme
Figure 7. Comparison of $u_y$ at the mid-plane with $Re=100$. (a) new model; (b) Bouzidi et al.’s scheme
in order to keep the numerical stability and accuracy, otherwise the computation by Bouzidi et al. scheme will be unstable. Further study is need to investigate the effect of the departure term on the simulation.

Furthermore, the computation based on the Bouzidi’s scheme was found to be unstable when the Reynolds number is higher. By comparison, our model works fine for higher Reynolds numbers. Fig. 8 shows velocity profiles at $x = 0.5H$ and $a = 0.8$ with different Reynolds number. The parameters are listed in Table 2. In general, the agreement for the new model is good at most of the flow Reynolds number, except at $Re = 3200$, which may be due to the low resolution adopted in the simulation. For Bouzidi et al. scheme, the computation became unstable when $Re > 1000$. These tests show that the new model with additional parameter $\theta$ can improve numerical stability, in addition to rigorous consistency with the Navier-Stokes equation. A full discussion of the optimization of the model parameters and their impact on numerical stability is beyond the scope of the current paper, and will be reported in a separate paper.

In Fig. 9 we plot the velocity contours and streamlines for the cavity flows at four different Reynolds numbers by the new model. The structure of the flow depends on the flow Reynolds number. With increasing flow Reynolds number, the primary vortex moves towards the left and downward gradually and becomes increasing circular. The size, number, and intensity of the corner vortices all increase with $Re$. The secondary corner eddies appear initially
Figure 9. Velocity contour and streamline for the flows with different Reynolds numbers. (a) $Re = 100$, (b) $Re = 400$, (c) $Re = 1000$, (d) $Re = 3200$
near the corners. Their centers move slowly toward the cavity center with the increase of Reynolds number. Finally, in Fig. 10 we compare the location of the primary vortex center at different Reynolds numbers against the data from Ghia et al. The agreement is satisfactory. These tests validate our new model on a rectangular grid, in terms of both accuracy and numerical stability.

5. Summary and concluding remarks

In this paper, we have shown, for the first time, that the D2Q9 MRT LBM model can be used on a rectangular grid to produce viscous flows that are fully consistent with the Navier-Stokes equations. The basic idea is to introduce a new adjustable parameter into the previous model of Bouzidi et al. [17]. This parameter amounts to a rotation in the 2D energy-normal stress moment subspace. We first re-derived the hydrodynamic equations of the two previous models [17, 18] intended for a rectangular grid. By inverse design using the Chapman-Enskog multi-scaling analysis, we showed that these two previous models are unable to satisfy all isotropy conditions of the transport coefficients. At the Euler equation level, the two previous models are equivalent. Zhou’s model could also be viewed as a rotation in the 2D energy-normal stress moment subspace relative to Bouzidi et al. [17]. But such rotation was fixed by Zhou’s definition of the moments in order to use the $a$-independent transformation matrix. In our model, this rotation does not fix the transformation matrix, which provides the necessary flexibility to restore the full isotropy of transport coefficients as required by the Navier-Stokes equation. Clearly, the success of our new model rests in part on the flexibility of relaxation parameters in the MRT LBM approach. Namely, the BGK LBM uses the same relaxation parameter for all moments, and is clearly unable to produce the necessary isotropy on a rectangular grid.

We showed, by the inverse design, that all equilibrium moments can be determined, except that for the energy squared moment which plays no role in the Navier-Stokes equation. Two conditions required to partially meet isotropy (the full isotropy has three conditions) are identified, and are shown to yield the two coupling relationships derived previously in Bouzidi et al. [17] using a very different approach. These partial conditions allow all departures from isotropy be expressed in terms of a single quantity. The additional parameter $\theta$ in our model is then used to eliminate this term. We believe our inverse design and the partial isotropy conditions provide new insights to previous models as well as to better explain how our new model works from the theoretical perspective.
Our new model contains two adjustable parameters, the speed of sound $c_s$, and a parameter $\gamma$ defining the energy flux. Their values can be optimized for the use of smaller aspect ratio $a$, the best numerical stability, or for achieving a higher flow Reynolds number. The discussions and demonstration of such optimization and capability are beyond the scope of this paper, and will be reported in a future paper.

We have also validated our new model using the 2D channel flow and the 2D lid-driven cavity flow. We showed that the new model yields excellent results that are independent of the value of the grid aspect ratio $a$. For the channel flow, the second-order accuracy is confirmed with half-way bounce back. For the cavity flow, we showed how to treat a moving wall within our new model. Again our results are in excellent agreement with those reported in the literature. Numerical tests show that our model is numerically stable for small $a$ and for high flow Reynolds numbers.

Finally, we note that there are alternative methods to restore isotropy. For example, by using two more microscopic velocities, Hegele et al. [19] were able to meet this goal in 2D. However, our model does not require any addition of microscopic velocities. We also believe that our idea can be apply in 3D to allow the use of non-cubic grids, instead of the cubic grid for standard models. This possibility will be reported in the near future.

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References