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*Published in:*  
Applied Mathematics Letters

*DOI:*  
[10.1016/j.aml.2020.106304](https://doi.org/10.1016/j.aml.2020.106304)

*Publication date:*  
2020

*Licence:*  
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*Document Version*  
Peer reviewed version

[Link to publication in Discovery Research Portal](#)

*Citation for published version (APA):*

Guo, C., Zhao, W., & Lin, P. (2020). On the collision matrix of the lattice Boltzmann method for anisotropic convection–diffusion equations. *Applied Mathematics Letters*, 105, 1-7. [106304].  
<https://doi.org/10.1016/j.aml.2020.106304>

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# On the collision matrix of the lattice Boltzmann method for anisotropic convection-diffusion equations

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## Abstract

In this work, we are concerned with the lattice Boltzmann method for anisotropic convection-diffusion equations (CDEs). We prove that the collision matrices of many widely used lattice Boltzmann models for such equations admit an elegant property, which guarantees the second-order accuracy of the half-way anti-bounce-back scheme. Numerical experiments validated our results for both two- and three-dimensional anisotropic CDEs.

*Keywords:* anisotropic convection-diffusion equations, lattice Boltzmann method, collision matrix, half-way anti-bounce-back scheme, second-order accuracy

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## 1. Introduction

The lattice Boltzmann method (LBM), originated from lattice-gas automata [1, 2, 3], is a popular mesoscopic approach for the Navier-Stokes equations [4]. As a discrete kinetic scheme, the LBM solves the macroscopic equations by realizing the propagation and collision of distribution functions associated with discrete velocities on a regular lattice. It is simple in formulation and easy for parallelization, can deal effectively with complex boundaries, and thus has been successfully used in various complex flows [4, 5].

Besides its successful applications in flow simulations, the LBM has also been developed for convection-diffusion equations (CDEs) in recent years; see *e.g.*, [6, 7, 8, 9, 10, 11, 12, 13, 14]. Among them, most LB models are limited to isotropic CDEs and those for anisotropic ones can be found in [7, 8, 9, 10, 11, 12, 13]. In [8, 9], a series of equilibrium- and link-type models are designed to handle the anisotropic diffusions in two and three dimensions. Different from this, multiple-relaxation-time (MRT) models are used in [11, 12] to recover the anisotropic diffusion-coefficient tensors as they have sufficient tunable parameters. It is shown in [10] that these MRT models can not produce precise macroscopic equations under the convective scaling and thus several modified models are proposed therein for both two- and three-dimensional problems. Furthermore, MRT models and appropriate equilibrium distributions are combined in [7] to solve general nonlinear anisotropic CDEs. Recently, a single-relaxation-time LB model is proposed in [13] for anisotropic CDEs based on a diffusion velocity formulation.

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In this paper, we consider the MRT models developed in [10, 12]. To correctly recover the anisotropic CDEs, their collision matrices (particularly those in [10]) are more complicated than the traditional ones [15]. Nevertheless, we show that the collision matrices of all these MRT models admit an elegant property formulated in [16]. With this property, the half-way anti-bounce-back scheme can be justified to be second-order accurate [17]. Numerical experiments validate our analysis for both two- and three-dimensional anisotropic CDEs. We would also like to point out that the property in [16] is different from the symmetry requirement proposed in [3], which can not guarantee the second-order accuracy of the half-way anti-bounce-back scheme. Additionally, we note that while the collision matrix of a MRT model in [10] is not symmetric, it still produces good computational results [10].

The rest of the paper is organised as follows. Section 2 introduces three MRT LB models for the anisotropic CDEs. It is proved in Section 3 that the collision matrices of all these models admit an elegant property. Numerical validations are provided in Section 4 and finally Section 5 concludes the paper.

## 2. LB models for the anisotropic CDE

Consider an anisotropic CDE with source term

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \nabla \cdot (\mathbf{D} \nabla \phi) + F, \quad (2.1)$$

where  $\phi := \phi(\mathbf{x}, t)$  is a scalar variable of spatial coordinate  $\mathbf{x} \in \mathbb{R}^n$  ( $n$  is the dimension of space) and time  $t$ ,  $\mathbf{u}$  is the velocity vector which may vary with space or time,  $\mathbf{D}$  is the symmetric positive definite matrix, and  $F := F(\mathbf{x}, t)$  is the source term. For the CDE (2.1), a general MRT LB model reads as [10, 12, 15]

$$f_i(\mathbf{x} + \mathbf{e}_i \delta_x, t + \delta_t) - f_i(\mathbf{x}, t) = - \sum_j (\mathbf{M}^{-1} \mathbf{S} \mathbf{M})_{ij} (f_j - f_j^{(eq)}) + \delta_t \omega_i F, \quad i = 0, 1, 2, \dots, N-1. \quad (2.2)$$

Here  $f_i := f_i(\mathbf{x}, t)$  is the  $i$ -th distribution function with discrete velocity  $\mathbf{e}_i$  at position  $\mathbf{x}$  and time  $t$ ,  $\delta_x$  and  $\delta_t$  are the lattice size and time step, respectively,  $\mathbf{M} \in \mathbb{R}^{N \times N}$  is the transformation matrix,  $\mathbf{S}$  is the relaxation matrix,  $f_i^{(eq)}$  is the equilibrium distribution function, and  $\omega_i$  is the  $i$ -th weight.

In this paper, we consider three MRT LB models from [10, 12]. The corresponding discrete velocities, equilibrium distribution functions, the transformation matrix and the relaxation matrix are detailedly introduced as follows.

### 2.1. HW-1 model in [10]

The discrete velocities of this model are the D2Q9 (two dimensions and nine discrete velocities) lattice model with  $\mathbf{e}_0 = (0, 0)$ ,  $\mathbf{e}_1 = -\mathbf{e}_3 = (1, 0)$ ,  $\mathbf{e}_2 = -\mathbf{e}_4 = (0, 1)$ ,  $\mathbf{e}_5 = -\mathbf{e}_7 = (1, 1)$  and  $\mathbf{e}_6 = -\mathbf{e}_8 = (-1, 1)$ . The equilibrium distribution functions are

$$f_i^{(eq)} = \omega_i \phi + \frac{\mathbf{e}_i \cdot \mathbf{u}}{\beta_i c} \phi, \quad i = 0, 1, \dots, 8, \quad (2.3)$$

where  $\omega_0 = 5/9$ ,  $\omega_{1-4} = 1/18$ ,  $\omega_{5-8} = 1/18$ ,  $\beta_{1-4} = 3$ ,  $\beta_{5-8} = 12$  and  $c = \delta_x / \delta_t$ . The transformation matrix  $\mathbf{M}_1$  and the relaxation matrix  $\mathbf{S}_1$  are defined as

$$\mathbf{M}_1 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}, \quad \mathbf{S}_1 = \begin{pmatrix} s_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & s_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{xx} & 0 & s_{xy} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & s_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{yx} & 0 & s_{yy} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & s_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_8 \end{pmatrix}, \quad (2.4)$$

where  $\begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix} := \mathbf{a}_1$  is related to the diffusion matrix  $\mathbf{D}$  via  $\mathbf{D} = \frac{1}{3}(\mathbf{I} - \frac{\mathbf{a}_1}{2})\mathbf{a}_1^{-1}(\mathbf{I}$  is the  $2 \times 2$  unit matrix).

## 2.2. HW-2 model in [10]

In this model, the discrete velocities, equilibrium distribution functions, and the transformation matrix  $\mathbf{M}_2$  are the same with those of HW-1 model above. The only difference is that the relaxation matrix is replaced by

$$\mathbf{S}_2 = \begin{pmatrix} s_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & s_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{xx} & (\frac{s_{xx}}{2} - 1)s_4 & s_{xy} & \frac{s_{xy}}{2}s_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & s_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{yx} & \frac{s_{yx}}{2}s_4 & s_{yy} & (\frac{s_{yy}}{2} - 1)s_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & s_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_8 \end{pmatrix}. \quad (2.5)$$

## 2.3. YN model in [12]

The third model we consider is from [12], which is very efficient as it only uses 7 velocities for three dimensional problems. The discrete velocities are  $\mathbf{e}_0 = (0, 0, 0)$ ,  $\mathbf{e}_1 = -\mathbf{e}_2 = (1, 0, 0)$ ,  $\mathbf{e}_3 = -\mathbf{e}_4 = (0, 1, 0)$ ,  $\mathbf{e}_5 = -\mathbf{e}_6 = (0, 0, 1)$ , and the equilibrium distribution functions are

$$f_i^{(eq)} = \omega_i \phi \left( 1 + 4 \frac{\mathbf{e}_i \cdot \mathbf{u}}{c} \right), \quad (2.6)$$

where  $\omega_0 = 1/4$  and  $\omega_{1-6} = 1/8$ . The transformation matrix  $\mathbf{M}_2$  and the relaxation matrix  $\mathbf{S}_3$  are given by

$$\mathbf{M}_2 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 6 & -1 & -1 & -1 & -1 & -1 & -1 \\ 0 & 2 & 2 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 1 & 1 & -1 & -1 \end{pmatrix}, \quad \mathbf{S}_3^{-1} = \begin{pmatrix} s_0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{s}_{xx} & \bar{s}_{xy} & \bar{s}_{xz} & 0 & 0 & 0 \\ 0 & \bar{s}_{xy} & \bar{s}_{yy} & \bar{s}_{yz} & 0 & 0 & 0 \\ 0 & \bar{s}_{xz} & \bar{s}_{yz} & \bar{s}_{zz} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & s_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & s_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & s_6 \end{pmatrix} \quad (2.7)$$

with  $\bar{s}_{ij} = \frac{1}{2}\delta_{ij} + 4D_{ij}$  and  $\delta_{ij}$  the Kronecker delta function.

## 3. Property of the collision matrices

Though the above MRT models seem complicated, we prove that the collision matrices  $\mathbf{A} := [\mathbf{A}_{ij}] = \mathbf{M}^{-1}\mathbf{S}\mathbf{M}$  of all the three MRT models admit an elegant property formulated in [16]:

$$\mathbf{A}_{ij} = \mathbf{A}_{\bar{i}\bar{j}}, \quad \forall i, j, \quad (3.8)$$

where  $\bar{i}$  is defined such that  $\mathbf{e}_i = -\mathbf{e}_{\bar{i}}$ . To see this, we introduce

**Definition 3.1.** *The  $i$ -th row of the transformation matrix  $\mathbf{M}$  is said to be odd if  $\mathbf{M}_{ij} = -\mathbf{M}_{i\bar{j}}$  for all  $j$ .*

**Lemma 3.2.** *If the  $\alpha$ - and  $\beta$ -th rows of the transformation matrix  $\mathbf{M}$  are odd, then  $\mathbf{M}_{\alpha i}\mathbf{M}_{\beta j} = \mathbf{M}_{\alpha\bar{i}}\mathbf{M}_{\beta\bar{j}}$ ,  $\forall i, j$ .*

*Proof.* According to Definition 3.1, the oddness of the  $\alpha$ - and  $\beta$ -th rows of  $\mathbf{M}$  indicates that  $\mathbf{M}_{\alpha i} = -\mathbf{M}_{\alpha\bar{i}}$  and  $\mathbf{M}_{\beta j} = -\mathbf{M}_{\beta\bar{j}}$ . Thus  $\mathbf{M}_{\alpha i}\mathbf{M}_{\beta j} = \mathbf{M}_{\alpha\bar{i}}\mathbf{M}_{\beta\bar{j}}$  immediately follows.  $\square$

On the other hand, we denote by  $T$  the transpose operator and recall the following fact from [16].

**Lemma 3.3.** *For the transformation matrix  $\mathbf{M}$  satisfying  $\mathbf{M}_{li}\mathbf{M}_{lj} = \mathbf{M}_{\bar{l}i}\mathbf{M}_{\bar{l}j}$ ,  $\forall i, j, l$  and any diagonal matrix  $\Lambda$ , it holds that  $(\mathbf{M}^T\Lambda\mathbf{M})_{ij} = (\mathbf{M}^T\Lambda\mathbf{M})_{\bar{i}\bar{j}}$  for all  $i$  and  $j$ .*

Then our main finding reads as

**Theorem 3.4.** *The collision matrices of all the three MRT models (HW-1, HW-2 and YN) above satisfy the property (3.8).*

*Proof.* First, we denote  $\mathbf{H} := (\mathbf{M}\mathbf{M}^T)^{-1}$  and rewrite the collision matrix as

$$\mathbf{A} = \mathbf{M}^{-1}\mathbf{S}\mathbf{M} = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^{-1}\mathbf{S}\mathbf{M} = \mathbf{M}^T\mathbf{H}\mathbf{S}\mathbf{M}.$$

Then we decompose the relaxation matrix as  $\mathbf{S} = \hat{\mathbf{S}} + \mathbf{S}'$  with  $\hat{\mathbf{S}}$  the diagonal part of  $\mathbf{S}$ . Thus the collision matrix can be decomposed as

$$\mathbf{A} = \mathbf{M}^T\hat{\mathbf{H}}\hat{\mathbf{S}}\mathbf{M} + \mathbf{M}^T\mathbf{H}\mathbf{S}'\mathbf{M}. \quad (3.9)$$

Observe that the transformation matrices  $\mathbf{M}_1$  and  $\mathbf{M}_2$  of the three MRT models are orthogonal, *i.e.*,  $\mathbf{H}$  is diagonal, and thereby  $\hat{\mathbf{H}}\hat{\mathbf{S}}$  is diagonal, too. Additionally, it is easy to see that they satisfy the condition of Lemma 3.3, namely,  $\mathbf{M}_{li}\mathbf{M}_{lj} = \mathbf{M}_{\bar{l}\bar{i}}\mathbf{M}_{\bar{l}\bar{j}}, \forall i, j, l$ . Then it follows from Lemma 3.3 that

$$(\mathbf{M}^T\hat{\mathbf{H}}\hat{\mathbf{S}}\mathbf{M})_{ij} = (\mathbf{M}^T\hat{\mathbf{H}}\hat{\mathbf{S}}\mathbf{M})_{\bar{i}\bar{j}}. \quad (3.10)$$

If we can further show

$$(\mathbf{M}^T\mathbf{H}\mathbf{S}'\mathbf{M})_{ij} = (\mathbf{M}^T\mathbf{H}\mathbf{S}'\mathbf{M})_{\bar{i}\bar{j}}, \quad (3.11)$$

then (3.8) holds true. We prove this relation for each model in the following. Denote  $\mathbf{R}' := \mathbf{H}\mathbf{S}'$  and note that  $\mathbf{R}'_{ij} \neq 0$  if and only if  $\mathbf{S}'_{ij} \neq 0$  since  $\mathbf{H}$  is diagonal. With this, we see that for the HW-1 model with  $\mathbf{M} = \mathbf{M}_1$  and  $\mathbf{S} = \mathbf{S}_1$ , the only nonzero entries of  $\mathbf{R}'$  are  $\mathbf{R}'_{35}$  and  $\mathbf{R}'_{53}$ . Thus we directly compute

$$\begin{aligned} (\mathbf{M}^T\mathbf{R}'\mathbf{M})_{ij} &= \sum_k \mathbf{M}_{ik}^T(\mathbf{R}'\mathbf{M})_{kj} = \sum_{k,l} \mathbf{M}_{ik}^T\mathbf{R}'_{kl}\mathbf{M}_{lj} \\ &= \mathbf{M}_{i3}^T\mathbf{R}'_{35}\mathbf{M}_{5j} + \mathbf{M}_{i5}^T\mathbf{R}'_{53}\mathbf{M}_{3j} = \mathbf{M}_{3i}\mathbf{R}'_{35}\mathbf{M}_{5j} + \mathbf{M}_{5i}\mathbf{R}'_{53}\mathbf{M}_{3j}. \end{aligned} \quad (3.12)$$

Moreover, note that the 3- and 5-th rows of  $\mathbf{M}_1$  are odd, thus we deduce from Lemma 3.2 that

$$\mathbf{M}_{3i}\mathbf{M}_{5j} = \mathbf{M}_{3\bar{i}}\mathbf{M}_{5\bar{j}}, \quad \forall i, j.$$

Combining the above two equations yields (3.11). Similarly, for the HW-2 model with  $\mathbf{M} = \mathbf{M}_1$  and  $\mathbf{S} = \mathbf{S}_2$ , the only nonzero entries of  $\mathbf{R}'$  are  $\mathbf{R}'_{34}, \mathbf{R}'_{35}, \mathbf{R}'_{36}, \mathbf{R}'_{53}, \mathbf{R}'_{54}$  and  $\mathbf{R}'_{56}$ , and the 3-, 4-, 5- and 6-th rows of  $\mathbf{M}_1$  are odd, thus (3.11) also holds true.

For the YN model,  $\mathbf{M} = \mathbf{M}_2$ ,  $\mathbf{S} = \mathbf{S}_3$ , the nonzero entries of  $\mathbf{R}'$  are  $\mathbf{R}'_{12}, \mathbf{R}'_{13}, \mathbf{R}'_{21}, \mathbf{R}'_{23}, \mathbf{R}'_{31}, \mathbf{R}'_{32}$ , and the 1-, 2-, 3-th rows of  $\mathbf{M}_2$  are odd, then (3.11) can be derived in the same fashion as for the two dimensional models above. Therefore, we have shown (3.11) for all the three models. Then the property (3.8) immediately follows from (3.11) and (3.10). This completes the proof.  $\square$

**Remark 1.** *It is shown in [17] that under the property (3.8) the second-order accuracy of the half-way anti-bounce-back scheme*

$$f_i(\mathbf{x}_f, t + \delta_t) = -f'_i(\mathbf{x}_f, t) + 2\omega_i\psi(\mathbf{x}_b, t) \quad (3.13)$$

*can be justified for the Dirichlet boundary condition  $\phi(\mathbf{x}_b, t) = \psi(\mathbf{x}_b, t)$ ,  $\mathbf{x}_b \in \partial\Omega$  of the isotropic CDE, where  $f'_i(\mathbf{x}_f, t) := f_i(\mathbf{x}_f, t) - \sum_j (\mathbf{M}^{-1}\mathbf{S}\mathbf{M})_{\bar{i}\bar{j}}(f_j - f_j^{(eq)})\mathbf{x}_f + \delta_t\omega_i F(\mathbf{x}_f, t)$  is the post-collision distribution. Since the LB model of the isotropic CDE has the same form as (2.2) for the anisotropic ones, the second-order accuracy of the scheme (3.13) can be justified in the same way as in [17] for the anisotropic CDE (2.1).*

**Remark 2.** *The property (3.8) is different from the symmetry condition proposed in [3], which cannot ensure the second-order accuracy of the half-way anti-bounce-back scheme. Moreover, it is easy to see that the collision matrix of the HW-2 model is not symmetric, but it still produces good computational results [10].*

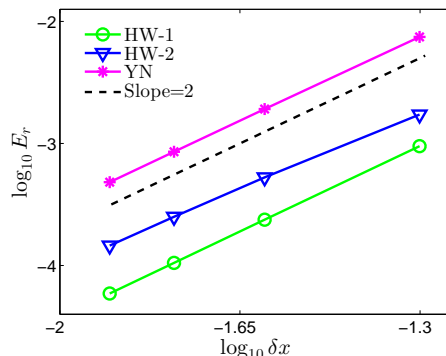


Figure 1: Convergence order of the MRT models with the half-way anti-bounce-back scheme for the anisotropic CDEs.

#### 4. Numerical validations

Since the property (3.8) guarantees the second-order accuracy of the half-way anti-bounce-back scheme (3.13), we verify this scheme to support our analysis results. Specifically, we construct two problems in both two- and three-dimensions. The first problem has analytical solution  $\phi(\mathbf{x}, t) = \cos(x - y + t)$ ,  $\mathbf{x} := (x, y) \in \Omega = \{(x, y) \mid 0 \leq x, y \leq 1\}$  with vector field  $\mathbf{u} = (1, 2)$  and diffusion matrix

$$D = \begin{pmatrix} 0.2 & 0.1 \\ 0.1 & 0.2 \end{pmatrix}.$$

Then the source term  $F = 0.2\phi$  can be computed from the CDE (2.1). Similarly, the analytical solution for the three dimensional case is taken as  $\phi(\mathbf{x}, t) = \cos(x - y + z + t)$ ,  $\mathbf{x} = (x, y, z) \in \Omega = \{(x, y, z) \mid 0 \leq x, y, z \leq 1\}$ . The diffusion matrix, the vector field and the source term are given by

$$D = \begin{pmatrix} 0.2 & 0.1 & 0.1 \\ 0.1 & 0.2 & 0.1 \\ 0.1 & 0.1 & 0.1 \end{pmatrix}, \quad \mathbf{u} = (1, 3, 1), \quad F = 0.3\phi.$$

The initial and boundary conditions are determined by the analytical solutions.

In the computation, the free relaxation coefficients are taken as  $s_0 = 1.0, s_1 = s_2 = 1.1, s_4 = s_{xx}, s_6 = s_{yy}, s_7 = s_8 = 1.2$  and  $s_0 = 1.0, s_4 = s_5 = s_6 = 1.1$  for the two- and three-dimensional models, respectively. All the boundaries are set to be located at the middle of two grid points and the scheme (3.13) is used for the boundary treatment. Additionally, we take  $\delta_t = \delta_x^2$  with  $\delta_x = 1/20, 1/40, 1/60, 1/80$  for both cases. The accuracy is computed with  $L^2$ -error  $E_r$  at time  $t = 0.5$ . Fig. 1 shows the convergence behaviors for the three MRT models. It is clear that second-order convergence is achieved for all the models. These verify the second-order accuracy of the half-way anti-bounce-back scheme as well as our results in Theorem 3.4.

#### 5. Conclusions and remarks

In this paper, we consider three MRT LB models from [10, 12] for the anisotropic CDEs. Though the collision matrices of these MRT models are more complicated than the traditional ones [15], we show that they all admit an elegant property formulated in [16]. With this property, the half-way anti-bounce-back scheme can be justified to be second-order accurate [17]. Numerical experiments validate our analysis for both two- and three-dimensional anisotropic CDEs. We would also like to point out that the property in [16] is different from the symmetry requirement proposed in [3], which can not guarantee the second-order accuracy of the half-way anti-bounce-back scheme. Moreover, we note that while the collision matrix of a MRT model in [10] is not symmetric, it still produces good computational results [10].

## Acknowledgements

This work was supported by the National Natural Science Foundation of China (Nos. 11771040, 11801030 and 11861131004).

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