Double MRT thermal lattice Boltzmann method for simulating convective flows

Ahmed Mezrhab,1,*, Mohammed Amine Moussaoui,1 Mohammed Jami,1 Hassan Najib2, M’hamed Bouzidi3

1 Laboratoire de Mécanique & Énergétique, Département de Physique, Faculté des Sciences, Université Mohammed Ier, 60000 Oujda, Morocco
2 Université Lille Nord de France, F-59000 Lille, and LML UMR CNRS 8107, F-59655 Villeneuve d’Ascq cedex, France
3 Université Clermont 2, LaMI EA 3867, IUT de Montlucon, Av. A. Briand, BP 2235, F-03101 Montlucon cedex, France

ARTICLE INFO

Article history:
Received 26 January 2010
Received in revised form 24 June 2010
Accepted 25 June 2010
Communicated by F. Porcelli

Keywords:
Double distribution function
Thermal lattice Boltzmann equation
Natural convection
Laminar flow
Square cavity

ABSTRACT

A two-dimensional double Multiple Relaxation Time-Thermal Lattice Boltzmann Equation (2-MRT-TLBE) method is developed for predicting convective flows in a square differentially heated cavity filled with air (Pr = 0.71). In this Letter, we propose a numerical scheme to solve the flow and the temperature fields using the MRT-D2Q9 model and the MRT-D2Q5 model, respectively. Thus, the main objective of this study is to show the effectiveness of such model to predict thermodynamics for heat transfer. This model is validated by the numerical simulations of the 2-D convective square cavity flow. Excellent agreements are obtained between numerical predictions. These results demonstrate the accuracy and the effectiveness of the proposed methodology.

© 2010 Elsevier B.V. All rights reserved.

1. Introduction

During recent years, the Lattice Boltzmann Equation (LBE), which was derived from Lattice Gas Automata (LGA), has received considerable attention by researchers in all scientific domains and it has been developed as an alternative approach for solving various fluid flow problems. Unlike traditional computational fluid dynamics (CFD) based on a macroscopic continuum equation, the LBE is based on solving the discrete-velocity Boltzmann equation in statistical physics. Historically, the first two-dimensional model allowing the simulation of the hydrodynamic phenomena was proposed by Frisch et al. [1]. Further works on the LGA have led to the elaboration of the lattice Boltzmann model first proposed by McNamara and Zanetti [2], then to the linearized collision operator presented by Higuera et al. [3,4], who used a linearized expression for the collision term; and lastly to the use of BGK operator by Chen and Qian [5,6]. The LBE has proved its ability to simulate complex fluid flows such as multiphase flows [7,8], porous media flows, diffusion and dispersion [9,10], flows of suspensions [11,12], compressible flows [13,14], magnetohydrodynamics [15], and reaction–diffusion system [16].

Because of the advantages of the LBE and simply boundary treatment, this method has been used for thermal flows. Four kinds of thermal LBE models have been implemented: the passive scalar approach, the multispeed approach (MS), the hybrid approach, and the double population distribution function (DDF) approach. In the passive scalar approach, the temperature is considered as a passive scalar, which is only advected by the flow [17,18]. The MS approach, which is a simple extension of the athermal LBE, consists in using only one particle distribution function for treating all thermo-hydrodynamic equations [19,20]. In the hybrid approach, the momentum conservation equations are solved by using the LBE scheme whereas the diffusion–advection equation for the temperature is solved separately by using other conventional numerical techniques such as finite-difference, finite volume and finite element methods [21,22]. The DDF approach can be regarded as another version of the hybrid scheme. Nevertheless, it leans on two different distributions function, the first for the momentum equations and the second for the energy equation [23,24]. As a result, it has been extensively adopted by researchers to solve various hydro-thermodynamics problems.

Most works based on the DDF approach to model convective flows utilizes the Lattice Boltzmann Bhatnagar–Gross–Krook (LBGK) method, which is approximated by a relaxation process with a single relaxation time (SRT-LBE). Because of its extreme simplicity, the LBGK method has become the most popular lattice Boltzmann model in spite of its well-known deficiencies. However, this simplicity comes at the expense of numerical instability (see Lallemand and Luo [25]) and inaccuracy in implementing boundary conditions (Ginzburg and d’Humières [26]). These deficiencies in
the BGK models can be easily addressed by using the multiple relaxation-time (MRT) models introduced by d’Humières [27]. Because of their advantages compared to the BGK method, the MRT-LBE models have been successfully applied to a variety of isothermal and non-isothermal flows [28–30]. Thus, the present article aims at presenting a novel DDF approach leaning on the multiple relaxation time-lattice Boltzmann equation (MRT-LBE) with D2Q9 lattice model for solving the mass and momentum conservation equations, and the MRT-LBE with D2Q5 lattice model for computing the temperature. The method is validated and its accuracy is demonstrated by solving 2-D convective square cavity flow, since literature is abundant about this subject.

The remainder of this Letter is organized as follows. Section 2 presents the MRT-LBE associated to the D2Q9 lattice model to simulate the fluid flow and to the D2Q5 lattice model to solve the energy equation. Section 3 presents numerical simulations of the 2-D incompressible flow inside a differentially heated square cavity. The obtained results are compared with available computational results. The last section is dedicated to the concluding remarks.

2. D2Q9-MRT LBE model for fluid problem

Any Lattice Boltzmann Equation (LBE) model leans on three ingredients. The first ingredient is a discrete phase consisting of a regular lattice space \( \delta_x \mathbb{Z} \times \delta_y \mathbb{Z} \) with a lattice constant \( \delta_x \) and a finite set of symmetric discrete velocities \( \{e_\alpha \mid 0 \leq \alpha \leq N \} \) associated with a set of a velocity distribution functions \( \{f^{eq}_\alpha \in \mathbb{V} = \mathbb{R}^9 \mid 0 \leq \alpha \leq N \} \). These later are functions of the local conserved quantities. The third ingredient consists of a time evolution equation, with discrete time \( t_n = \delta t N = \delta t \{0, 1, 2, \ldots \} \):

\[
\mathbf{f}(r_j + \delta t, t_n + \delta t) - \mathbf{f}(r_j, t_n) = -S(\mathbf{f}(r_j, t_n) - \mathbf{f}^{eq}(r_j, t_n))
\]

where \( S \) is the collision matrix. The collision sub-step is not easy to carry out in the velocity space since \( S \) is usually a full matrix. As shown in Refs. [22,25,27], it rather convenient to accomplish the collision process in the moment space. Therefore, the above equation can be written as follows:

\[
\mathbf{f}(r_j + \delta t, t_n + \delta t) - \mathbf{f}(r_j, t_n) = -M^{-1} S^*(\mathbf{m}(r_j, t_n) - \mathbf{m}^{eq}(r_j, t_n))
\]

where \( \mathbf{m}(r, t) \) and \( \mathbf{m}^{eq}(r, t) \) are \((N + 1)\)-tuple vectors of moments and their corresponding equilibria:

\[
\mathbf{m} = (m_0, m_1, \ldots, m_N)^T \in \mathbb{M}(= \mathbb{R}^9)
\]

where the superscript \( T \) denotes transverse vector.

The mapping between discrete velocity space and \( \mathbb{V} \) and moment space \( \mathbb{M} \) is achieved by the transformation matrix \( M \) which maps the vector \( f(r, t) \) to the vector \( m(r, t) \):

\[
\mathbf{m} = M \mathbf{f} \quad \text{and} \quad \mathbf{f} = M^{-1} \mathbf{m}
\]

The relaxation matrix \( S^* \) in moment space is a diagonal matrix given by \( S = \text{diag}(s_\alpha) \), where \( s_\alpha \) are relaxation time. Note that the transformation matrix \( M \) is an orthogonal one and it can be constructed via the Gram–Schmidt orthogonalisation [22,25,27,31]. From these references, and for the nine velocity-model in two dimensions \((N = 8)\), i.e., the D2Q9 model (here D2Q9 denotes the model with 9 velocities in 2 dimensions), the matrix \( M \) can be written as:

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

The row vectors of \( M \) are mutually orthogonal, i.e., \( MM^T \) is a diagonal matrix non-normalized. This allows to easily computing \( M^{-1} \) according to the formula [29]:

\[
M^{-1} = M^T (MM^T)^{-1}
\]

In the present work, we use the D2Q9 model (see Fig. 1), and the nine discrete velocities are given by

\[
e_\alpha = \begin{cases}
0.0, & \alpha = 0 \\
\cos((\alpha - 1)\pi/2), & 1 \leq \alpha < 4 \\
\sqrt{2}\cos((2\alpha - 9)\pi/4), & 5 \leq \alpha \leq 8
\end{cases}
\]

where \( e = \delta v / \delta t \) is the particle velocity and the lattice spacing \( \delta t \) is set to equal 1, as is the time step \( \delta t = \delta t = 1 \). In what follows all quantities are given in dimensionless units, normalized by the spacing \( \delta x \) and time step \( \delta t \).
The nine components of the moment vector \( \mathbf{m} \) are arranged in the following order: \( m_0 = \rho \) is the fluid density, \( m_1 = e \) is related to the energy, \( m_2 = \varepsilon \) is related to the energy square, \( m_{3,5} = j_{x,y} \) are components of the momentum \( \mathbf{f} = (j_x, j_y) \), \( m_{4,6} = q_{x,y} \) are related to components of the energy flux and \( m_{7,8} = p_{xx,xy} \) are related to the components of the symmetric and traceless strain rate tensor. So, for the D2Q9 model, the nine macroscopic moments of this model are:

\[
\mathbf{m} = (\rho, e, j_x, j_y, q_x, q_y, p_{xx}, p_{xy})^T
\]

among which the conserved variables of athermal fluid are only density, \( \rho \), and momentum, \( \mathbf{f} = (j_x, j_y) = \rho (u, v) \). The corresponding equilibrium moments \( \mathbf{m}^{eq}(\rho, j) \) for the non-conserved moments are [25]:

\[
\begin{align*}
    m_{1}^{eq} &= e^{eq} = -2\rho + 3(j_x^2 + j_y^2) \\
    m_{2}^{eq} &= e^{eq} = \rho - 3(j_x^2 + j_y^2)/\rho_m \\
    m_{4}^{eq} &= q_x^{eq} = -j_x \\
    m_{6}^{eq} &= q_y^{eq} = -j_y \\
    m_{7}^{eq} &= p_{xx}^{eq} = (j_x^2 - j_y^2)/\rho_m \\
    m_{8}^{eq} &= p_{xy}^{eq} = j_{x,y}/\rho_m
\end{align*}
\]

The constant \( \rho_m \) is the mean density in the system and is usually set to be unity in simulations. With the above equilibrium moments, the sound speed of the lattice is \( c_s = 1/\sqrt{3} \).

As suggested by Lallemand and Luo [25], the non-conserved moments relax linearly towards their equilibrium values. Therefore, for the D2Q9 model, the collision process of the MRT method is accomplished as follows:

\[
\mathbf{m}^+ = \mathbf{m} - S^+ (\mathbf{m} - \mathbf{m}^{eq})
\]

where \( \mathbf{m}^+ \) denotes the post-collision state. The post-collision vector \( \mathbf{f}^+ \) is carried out as

\[
\mathbf{f}^+ = \mathbf{f} - M^{-1} S^+ \mathbf{M} (\mathbf{f} - \mathbf{f}^{eq})
\]

It should be stressed that the relaxation parameters \( s_\alpha \) can be determined by a linear stability analysis [25], and in the present simulation, they are chosen as the following: \( s_1 = s_2 = 1.4, s_4 = s_6 = 1.2 \) and \( s_7 = s_8 = 2/(1 + 2v/\delta x^2) \), \( v \) being the kinematic viscosity of the fluid. What should be mentioned here is that it is possible to recover the SRT-LBE, also called LBGK after its authors Bhatnagar–Gross–Krook [32], by setting \( s_1 = s_2 = s_4 = s_6 = s_7 = s_8 = 1/\tau \).

The macroscopic fluid variables, density \( \rho \) and velocity \( \mathbf{u} \), are obtained from the moments of the distribution functions as follows:

\[
\rho = \sum_{i=0}^{8} f_i \\
\mathbf{J}(j_x, j_y) = \rho \mathbf{u} = \sum_i f_i \mathbf{e}_i - G/2
\]

where \( G \) is the external force acting per unit mass: \( G = -\rho \beta g(T - T_m) \).

The bounce-back condition is applied at all walls [33]. This type of condition locates the physical wall at the half grid spacing beyond the last fluid node \( x_f \) as shown in Fig. 2. This figure shows that the particle moves from \( x_f \) toward \( x_m \), then it comes back to its place after being reflected by the stationary wall. This is expressed by the following equation:

\[
f_j (x_f, t + 1) = f_j (x_f + e_j, t + 1)
\]

where \( f_j \) is the distribution function of the velocity \( e_j \equiv -e_i \).

### 3. D2Q5-MRT LBE model for thermal problem

As in our previous works [34–36], we could have used the simple finite difference approach to compute the temperature since it reduces the computational cost. However, in this Letter, we have chosen to use the double-distribution function (DDF) model in the goal to prove the effectiveness of the model D2Q5 for solving the energy equation. Furthermore, Rasin et al. [37] have presented some test simulations to validate the kinetic scheme and compare it with a finite-difference Modified Lax–Wendroff (MLW) scheme. For the isotropic diffusion, their numerical results show satisfactory agreement with the analytical solution, with a fast decay of the error with the time-step followed by saturation when the amplitude falls below \( 10^{-3} \), and the timing data indicate that the kinetic LB scheme can compute significantly faster than MLW. Mishra et al. [38] have used alternatively a finite volume method (FVM) and a lattice Boltzmann method to solve the energy equation in 2-D transient conduction and radiation heat transfer problems. They highlighted that LBM is accurate and requires slightly fewer steps to converge to the steady-state. Otherwise, it has been established in hydrodynamic applications that LBM schemes have computational advantages in multi-dimensional and complex geometries. In this context, the present 2-MRT-TLBE can be viewed as a possible alternative to finite difference methods (FDM) or finite volume methods (FVM) for computing heat transfer in such geometries. Hence, in order to take thermal effects into account, we introduced the D2Q5 LBE model to solve the advection–diffusion equation for the temperature by using a second set of a velocity distribution functions \( \{g_\alpha \in \mathbb{V}(= \mathbb{R}^2) \mid 0 \leq \alpha \leq 4 \} \) defined on each node \( r_j \) of the regular lattice parameterized by a space step \( \delta x, \delta y \in (\delta x, \delta z)^2 \). We define \( \delta t \) as the time step of the evolution of LBE and let the celerity \( c = \alpha_0/\delta t \). We choose the velocities \( c_i, i \in (0, \ldots, 4) \), such that \( c_i = e_i/\delta x, \delta y \), where \( e_i \) are the vectors connecting neighboring nodes of the regular lattice. In this work, we use the five-velocity model whose the labelling is depicted in Fig. 3. The discrete velocities are:

\[
e_\alpha = \begin{cases} 
(0,0), & \alpha = 0 \\
(\cos((\alpha - 1)\pi/2), \sin((\alpha - 1)\pi/2))c, & 1 \leq \alpha \leq 4
\end{cases}
\]
A LBE with multiple relaxation times for distributions \( g_j \) can be expressed as [39]:

\[
g_j(r_i + c_i \delta_t, t + \delta_t) = g_j^\dagger(r_i, t)
\]

(14)

where the superscript * denotes post-collision quantities. Therefore, during each time increment \( \delta_t \), there are two fundamental substeps, i.e. the collision process and the advection process. In the advection substep, the “particles” move from a lattice node \( r_i \) to either itself with the velocity \( c_0 = 0 \), one of the four nearest neighbors with the velocity \( c_i, i \in (1, \ldots, 4) \). As for the collision substep, it consists in the redistribution of the populations \( g_j \) at each node \( r_i \), and it is modeled by the operator \( g_j^\dagger(r_i, t) \) (see Eq. (14)). The collision substep is not easy to carry out in the velocity space. As shown in Ref. [27], it becomes convenient when this substep is carried out in the moment space. To this end, one define some moments \( m_k \) based on the distribution \( g_j \) through a linear transformation,

\[
m_k = \sum_{j=0}^{4} M_{kj} g_j, \quad 0 \leq k \leq 4
\]

(15)

The transformation matrix \( M \) matrix for this model can be explicitly given by:

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

(16)

Note that matrix \( M \) is invertible and orthogonal.

To simulate diffusion problems, we conserve only the first moment

\[
m_0 = T = \sum_{j=0}^{4} g_j
\]

(17)

In the collision substep and obtain one macroscopic scalar equation. For the non-conserved moments, we assume that they relax towards equilibrium \( m^{eq}_k \) that are nonlinear functions of conserved quantities and set:

\[
m^*_k = (1 - s_k) m_k + s_k m^{eq}_k, \quad 1 \leq k \leq 4
\]

(18)

where \( s_k = \delta_t / \tau_k \) is a relaxation rate which satisfy the constraint \( 0 < s_k < 2 \) to get a numerically stable scheme. The relaxation rates \( s_k \) are not necessarily identical as in the so-called BGK method [40]. Choosing \( m^{eq}_0 = 0, m^{eq}_1 = 0, m^{eq}_2 = aT, m^{eq}_3 = 0 \) and using Taylor expansion [39] or Chapman–Enskog procedure [41], we find the diffusion equation up to order three in \( \delta_t \):

\[
\frac{\partial T}{\partial t} - \frac{c_2^2 \delta_t}{10} \left( \frac{1}{s_1} - \frac{1}{2} \right) \frac{\partial^2 T}{\partial x^2} + \left( \frac{1}{s_2} - \frac{1}{2} \right) \frac{\partial^2 T}{\partial y^2} = 0 (\delta_t^3)
\]

(19)

Eq. (19) reduces to the standard isotropic diffusion equation for \( s_1 = s_2 = s, \delta_x = \delta_y = 1, a = -2 \), and whose the diffusion coefficient is

\[
\alpha = \left( \frac{1}{s} - \frac{1}{2} \right) / 5
\]

(20)

With a given velocity field \((u, v)\), if we take \( m^{eq}_0 = uT \) and \( m^{eq}_1 = vT \), the LBE scheme describes the following advection–diffusion equation:

\[
\frac{\partial T}{\partial t} + \mathbf{u} \nabla T - \alpha \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) = 0 (\delta_t^3)
\]

(21)

4. Application of the 2-MRT-LBE to convective square cavity flow

To demonstrate the applicability of this method, we have carried out simulations for the convective flow in a 2-D differentially heated square cavity, which is a benchmark problem. The horizontal walls (top and bottom) are perfectly insulated while the vertical walls (left and right) are isothermal and maintained at different temperatures \( T_h \) and \( T_c \) (\( T_h > T_c \)), respectively, as depicted in Fig. 4. The present flow is considered steady, laminar, incompressible and two-dimensional. The momentum equations are simplified using Boussinesq approximation, in which all fluid properties are assumed constant except the density whose variation with the temperature is allowed in the buoyancy term. The dimensionless parameters governing this problem are the Prandtl number \( Pr \) and the Rayleigh number \( Ra \) defined by \( Pr = v/\alpha \) and \( Ra = \beta g(T_h - T_c) H^3 Pr/\nu^2 \).

4.1. Boundary conditions

The implementation of boundary conditions is of great importance for the simulation. A difficulty of the lattice Boltzmann equation is that the unknown distribution functions pointing to fluid zone at the boundaries nodes must be specified.

The box size is \( N_x \times N_y = N \times N \). For the lattice Boltzmann part, the bounce-back boundary conditions [33] are applied for all walls. The effective boundaries are \( x = 1/2 \) and \( x = N + 1/2 \) (because of the bounce-back boundary conditions). The macroscopic boundary conditions for the temperature are:
We assume that the node function term. Important are the features of the flow and heat transfer (\(umax\)). For this, we need to compute the maximum horizontal velocity \(u_{\text{max}}\), the maximum vertical velocity \(v_{\text{max}}\) and the maximum stream function \(\psi_{\text{max}}\). For this, we need to compute the maximum horizontal velocity \(u_{\text{max}}\), the maximum vertical velocity \(v_{\text{max}}\) and the maximum stream function \(\psi_{\text{max}}\).

For this test case, the main quantitative results that can be obtained for a wide range of Rayleigh numbers \((10^3 \leq Ra \leq 10^8)\). Let us note that due to its practical importance in many general science and engineering applications, natural convection flows in a cavity has been the subject of many theoretical, experimental and numerical studies [42–44]. The fluid flow and the heat transfer generated in the square cavity are characterized by two distinct thermal regimes: laminar flow \(10^3 \leq Ra \leq 10^5\) and transitional to the turbulent flow \(10^5 < Ra \leq 10^8\). In the following, streamline and isotherm plots as well as the average Nusselt number \((Nu)\), \(u_{\text{max}}\), \(v_{\text{max}}\) and \(\psi_{\text{max}}\) are provided to simplify the description of this physical phenomena. Also, we indicate that in all the streamline and isotherm plots, the contour lines correspond to equi-spaced absolute values of the dimensionless stream function \(\psi/\alpha\) and the dimensionless temperature \(\theta\), respectively.

4.3. Choice of grid

At first, we have performed the calculations for different meshes to determine the number of points \(N^2\) which allows a good compromise between precision and computing time. Table 1 presents the average Nusselt number \((Nu)\), the maximum horizontal velocity \((u_{\text{max}})\), the maximum vertical velocity \((v_{\text{max}})\) and the maximum stream function \((\psi_{\text{max}})\) as a function of the mesh size \(N^2\) for \(Ra = 10^8\) and \(Ra = 10^9\) taking as two examples. As can be seen, the solutions become grid independent at an \(N^2 = 161 \times 161\) mesh for \(Ra = 10^8\) and at an \(N^2 = 181 \times 181\) mesh for \(Ra = 10^9\). When \(N\) further increases from 181 to 201, there is not much improvement for the results. Consequently, far the computations, grids with \(161 \times 161\) for \(Ra \leq 10^7\) and \(181 \times 181\) points are chosen for \(Ra > 10^7\) to optimize the relation between accuracy and computing time.

In all simulations, \(Pr\) is set to be 0.71. These have been carried out for a wide range of Rayleigh numbers \((10^3 \leq Ra \leq 10^8)\). Let us note that due to its practical importance in many general science and engineering applications, natural convection flows in a cavity has been the subject of many theoretical, experimental and numerical studies [42–44]. The fluid flow and the heat transfer generated in the square cavity are characterized by two distinct thermal regimes: laminar flow \(10^3 \leq Ra \leq 10^5\) and transitional to the turbulent flow \(10^5 < Ra \leq 10^8\). In the following, streamline and isotherm plots as well as the average Nusselt number \((Nu)\), \(u_{\text{max}}\), \(v_{\text{max}}\) and \(\psi_{\text{max}}\) are provided to simplify the description of this physical phenomena. Also, we indicate that in all the streamline and isotherm plots, the contour lines correspond to equi-spaced absolute values of the dimensionless stream function \(\psi/\alpha\) and the dimensionless temperature \(\theta\), respectively.

4.4. The laminar flow \((10^3 \leq Ra \leq 10^5)\)

Table 2 shows the numerical results of the average Nusselt number through the cavity \(Nu\), the maximum horizontal velocity \(u_{\text{max}}\), the maximum vertical velocity \(v_{\text{max}}\), and the maximum stream function \(\psi_{\text{max}}\) for a wide range of Rayleigh numbers. Numerical results given by many authors [45–49] are included for comparison. Among these authors include De Vahl Davis [45] who was among the first to consider the natural convection in a square cavity. He used a stream function-vorticity finite difference method with grids up to \(81 \times 81\) points, and employed Richardson extrapolation to obtain more accurate benchmark solutions for Rayleigh numbers up to \(10^6\). Another benchmark solution for this problem is one that has been presented by Hortmann et al. [46] using

### Table 1
Grid dependence study for \(Ra = 10^8\) and \(Ra = 10^9\).

<table>
<thead>
<tr>
<th>(N = N_x \times N_y)</th>
<th>(Ra = 10^8)</th>
<th>(Ra = 10^9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N_x \times N_y)</td>
<td>(Nu)</td>
<td>(u_{\text{max}})</td>
</tr>
<tr>
<td>61 \times 61</td>
<td>8.805</td>
<td>64.212</td>
</tr>
<tr>
<td>81 \times 81</td>
<td>8.812</td>
<td>64.497</td>
</tr>
<tr>
<td>101 \times 101</td>
<td>8.814</td>
<td>64.633</td>
</tr>
<tr>
<td>121 \times 121</td>
<td>8.816</td>
<td>64.708</td>
</tr>
<tr>
<td>141 \times 141</td>
<td>8.817</td>
<td>64.758</td>
</tr>
<tr>
<td>161 \times 161</td>
<td>8.817</td>
<td>64.793</td>
</tr>
<tr>
<td>181 \times 181</td>
<td>8.818</td>
<td>64.824</td>
</tr>
<tr>
<td>201 \times 201</td>
<td>8.818</td>
<td>64.843</td>
</tr>
</tbody>
</table>

4.2. Quantities to be determined

For this test case, the main quantitative results that can be important are the features of the flow and heat transfer \((u_{\text{max}}, v_{\text{max}}, \psi_{\text{max}}\) and \(Nu\)). For this, we need to compute the maximum horizontal velocity \(u_{\text{max}}\), the maximum vertical velocity \(v_{\text{max}}\) obtained at \(N_x/2\), the maximum stream function \(\psi_{\text{max}}\) on the whole domain, and the average Nusselt number \(Nu\) which is the major control parameter of the thermal transfer enhancement.

It is worth mentioning that the stream function is determined from

\[
\nabla^2 \psi(x, y) = \frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial y}
\]
a finite volume multi-grid method with much finer grids up to $640 \times 640$. Mayne et al. [47] used an h-adaptive finite element code for solving coupled Navier–Stokes and energy equations. Shu et al. [48] carried out the numerical simulation using the Taylor series expansion- and least-squares-based lattice Boltzmann method (TL-LBM) with both uniform and non-uniform grids. Their values presented in Table 2 are taken from non-uniformed results. Guo et al. [49] developed a thermal lattice BGK model for Boussinesq incompressible fluids. The basic idea was to solve the velocity field and the temperature field using two independent lattice BGK equations, respectively, and then combine them into one coupled model for the whole system. The lattice grid used was $N_x \times N_y = 128 \times 128$. Dixit et al. [23] applied a thermal lattice Boltzmann method based on the BGK to simulate high Rayleigh number (up to $10^{10}$). They introduce a double populations interpolation supplemented lattice Boltzmann method. For Rayleigh numbers ranging from $10^3$ to $10^6$, they used $64 \times 64$, $64 \times 64$, $128 \times 128$, $256 \times 256$ and $512 \times 512$, respectively. Kuznik et al. [24] implemented a Taylor series expansion and a least-square-based lattice Boltzmann method (TLLBM) with a non-uniform mesh.

It can be seen from Table 2 that, the results agree well with each other, indicating that the present method can indeed be used for simulating natural convective flows. Also, we can see that as, the Rayleigh number increases the difference between the present results and those of Davis [45] decreases. Hence, we can say that the 2-MRT-LBE come to be more accurate as Ra increases.

Fig. 6 and 7 show respectively the isotherms and streamlines predicted by the present 2-MRT-LBE for Rayleigh number ranging from $10^3$ to $10^6$ characterising the laminar flow regime. From these figures, it seen that for low Ra, the heated fluid rises along the left wall, encounters the top adiabatic wall, travels towards the cold wall, comes down and recirculates inducing a steady clockwise rotational flow that form a single vortex with its centre in the middle of the cavity as a typical feature of the flow. The vortex tends to become elliptic as Ra increases ($Ra = 10^4$), and breaks up into two vortices that will appear inside a central elongated streamline at $Ra = 10^5$. As Ra reaches $10^6$, the two vortices move to take place near the differentially heated walls and a third vortex will appear in the core of the cavity. Note that the streamlines become more packed next the walls as the Ra increases. This suggests that the flow moves faster as natural convection is intensified. The maximum absolute value of stream function can be viewed as a measure of the intensity of natural convection in the cavity. The maximum absolute value of the stream function is enhanced with Rayleigh increasing as listed in Table 2, with those published. This leads to the increase of the maximum stream function value and Nusselt number Nu, which can also be seen in Table 2.

The isotherm lines vortex indicate the change of the dominant heat transfer mechanism with Rayleigh number. For small Rayleigh number $Ra$, isotherms are parallel to the heated walls and slightly deformed by the flow, and the heat is transferred mainly by heat conduction between the hot and cold walls. As $Ra$ increases to $10^4$, the dominant heat transfer mechanism changes from conduction to convection, the shape of isotherms begin to bend in the bulk region. When $Ra$ reaches $10^5$, the isotherm lines flatten in the central region of the cavity, and are vertical only in the thin boundary layers near the hot and cold walls. With increasing $Ra$ up to $10^6$, the fluid is thermally stratified. In other words, the isotherms become horizontal occupying the majority of the cavity, and the temperature gradients near the top right and bottom left corners are much steeper than those observed at low values of Rayleigh numbers. To sum up, these observations agree well with those reported in previous studies [23,24,45–49].

4.5. The transitional flow ($10^3 < Ra \leq 10^6$)

It worth recalling that one of the main interests of this Letter is to prove that the transitional flow can be simulated using Multiple Relaxation Time-Lattice Boltzmann Equation with D2Q9 model for the fluid velocity variables and D2Q5 for the temperature.

Table 3 contains the numerical values of $Nu$, $umax$, $vmax$ and $psi_{max}$ compared with literature results. The results gathered by Markatos and Pericleous [50], Le Quéré [51] and Wan et al. [52] are also brought to enrich the comparison.

Markatos and Pericleous [50] were the first to introduce a turbulence model in their calculations. They performed two-dimensional simulations for Rayleigh numbers up to $10^{10}$. Le Quéré [51] used a pseudo-spectral Chebyshev algorithm by increasing the spatial resolution up to $128 \times 128$ polynomial expansion for natural convection in a square 2-D differentially heated cavity with adiabatic top and bottom walls. Wan et al. [52] introduced a high-accuracy discrete singular convolution (DSC) for the numerical simulation of coupled convective heat transfer problems.

From the results presented in Table 3, the numerical values are in good agreement with those from literature: the relative errors, compared with the results of Le Quéré [51], are less than 0.6%, 1%, 1.5% and 0.7% for $Nu$, $umax$, $vmax$ and $psi_{max}$ respectively. This allows us to say that the 2-MRT-LBE has the capability to solve the transitional flow.

Streamlines and isotherms plots predicted for $Ra = 10^7$ and $10^8$ and characterizing the transitional flow are shown in Fig. 8.
Fig. 6. Streamlines of the laminar flow for four different Rayleigh numbers.

Fig. 7. Isotherm contours of the laminar flow for four different Rayleigh numbers.
Table 3
Comparison of transitional flow with previous works for the square heated cavity

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^7$</td>
<td>$Nu$</td>
<td>16.523</td>
<td>no data</td>
<td>13.860</td>
<td>no data</td>
<td>16.408</td>
<td>16.790</td>
<td>16.510</td>
</tr>
<tr>
<td></td>
<td>$u_{\text{MAX}}$</td>
<td>148.580</td>
<td>145.266</td>
<td>145.060</td>
<td>148.768</td>
<td>164.236</td>
<td>148.400</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_{\text{MAX}}$</td>
<td>999.236</td>
<td>703.250</td>
<td>714.470</td>
<td>no data</td>
<td>702.029</td>
<td>701.922</td>
<td>998.300</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\text{MAX}}$</td>
<td>30.170</td>
<td>no data</td>
<td>no data</td>
<td>no data</td>
<td>no data</td>
<td>no data</td>
<td>30.140</td>
</tr>
<tr>
<td>$10^8$</td>
<td>$Nu$</td>
<td>30.225</td>
<td>23.670</td>
<td>32.045</td>
<td>29.819</td>
<td>30.506</td>
<td>30.303</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$u_{\text{MAX}}$</td>
<td>321.876</td>
<td>283.689</td>
<td>295.670</td>
<td>14.300</td>
<td>321.457</td>
<td>389.877</td>
<td>305.332</td>
</tr>
<tr>
<td></td>
<td>$v_{\text{MAX}}$</td>
<td>2222.390</td>
<td>2223.4424</td>
<td>2259.080</td>
<td>1812.000</td>
<td>2243.360</td>
<td>2241.374</td>
<td>2169.562</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\text{MAX}}$</td>
<td>53.700</td>
<td>no data</td>
<td>no data</td>
<td>no data</td>
<td>53.760</td>
<td>53.323</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 8. Isotherms (left) and streamlines (right) of the transitional flow for four different Rayleigh numbers.

At $Ra = 10^7$, it can be observed on the stream function patterns that wavy perturbations occur close to the horizontal adiabatic boundary specially at upper-left and bottom right corners. These perturbations intensify with increasing $Ra$ to $10^8$ and secondary eddies develop. This process could be the main source of the onset of unsteady flow. The temperature field becomes more and more stratified. The isotherms near the hot wall stretch upward due to the warm fluid wake. They are dense near the lower portion of the hot wall and the upper portion of the cold wall, indicating the presence of a strong heat flux. It should be noted that in general, the convection within the cavity is very weak at low $Ra$, and the streamlines are almost regular and stratified throughout all the $Ra$ range.

5. Conclusion

In this Letter, we have developed a novel thermal lattice Boltzmann method to simulate thermo-hydrodynamics. The key point in this method is the use of two sets of distribution functions. What should be mentioned is that this method leans on the use of multiple relaxation times with the D2Q9 model for fluid velocity variables and the D2QS for the temperature. A two-dimensional air flow and heat transfer in differentially heated square cavity was considered as a test validation review. The numerical results for a wide range of Rayleigh numbers show that this method is suitable and numerically stable at high Rayleigh numbers. Computations of the laminar and transitional flow features are well predicted. It is also found that the results predicted by the present 2-MRT-TLBE method are in good agreement with other numerical results. Finally, the proposed method can be readily extended to the 3-D case and the relevant work will be reported in the future.

References