THREE-DIMENSIONAL THERMAL LATTICE BOLTZMANN SIMULATION OF NATURAL CONVECTION IN A CUBIC CAVITY

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In this paper, a three-dimensional (3D) thermal lattice Boltzmann model is proposed to simulate 3D incompressible thermal flow problem. Our model is based on the double-distribution function approach. We found that a new and simple lattice type of eight-velocity model for the internal energy density distribution function can be developed, where the viscous and compressive heating effects are negligible. Numerical results of 3D natural convection flow in a cubic cavity are presented.

Keywords: 3D thermal lattice Boltzmann; double-distribution function; natural convection flow.

1. Introduction

Natural convection heat transfer in a cavity has attracted much attention in recent years due to its wide applications such as cooling of radioactive waste containers, ventilation of rooms, solar energy collectors and crystal growth in liquids. A comprehensive review was presented by Davis. However, among the previous numerical studies pertinent to this problem, little work has been done using the 3D simulation model.

In recent years, the lattice Boltzmann method, a method based on mesoscopic kinetic equation for the particle distribution function, has attracted much interest in the physics and engineering communities. The lattice Boltzmann method is considerably an alternative approach to the well-known finite difference, finite element and finite volume techniques for solving the Navier–Stokes equations. Although a newcomer in numerical scheme, the lattice Boltzmann approach has proven to be a versatile tool for simulating a wide variety of fluid dynamical applications. These include turbulent single-phase flow, transport in porous media and multiphase flows in several scientific and industrial applications. However, the simulation of flows with heat transfer turned out to be much more difficult.
Currently, a few thermal lattice Boltzmann models have been proposed. The earliest model which is known as multispeed model, uses the same distribution function in defining the macroscopic velocity. However, this model is reported to suffer numerical instability and has a demerit that it can simulate thermal fluid flows only at a fixed Prandtl number.

As an alternative approach, Shan proposed the so-called passive-scalar model. This model applies that the flow fields (velocity and density) and the temperature are represented by two different distribution functions. The macroscopic temperature is assumed to satisfy the same evolution equation as a passive scale, which is advected by the flow velocity but does not affect the flow field.

The work of Luo and He showed that the isothermal lattice Boltzmann equation can be directly obtained by properly discretizing the continuous Boltzmann equation in both time and space phases. Following the same procedure, He et al. proposed the double-distribution function model, where the thermal lattice Boltzmann evolution equation can be derived by discretizing the continuous Boltzmann equation for the internal energy distribution. It has been shown that this model is simple and applicable to problems with different Prandtl numbers. More importantly, this model requires low order moment and thus provides higher numerical stability than the passive-scalar model. However, on the other hand, the analysis of thermal fluid phenomena using the 3D thermal lattice Boltzmann method is scarcely performed.

In this paper, following the double-distribution function idea, we extend the newly developed 2D four-velocity model to a 3D model. We found that a new and simple lattice type of eight-velocity model for the internal energy density distribution function can be developed, where the viscous and compressive heating effects are negligible. In order to validate this new model, we present the numerical results for the natural convection heat transfer in a cubic cavity.

The rest of the paper is organized as follows. In the next section, we show the theory of the internal energy density distribution function, the discretization procedure of continuous Boltzmann equation which will lead to developing of our new type of eight-velocity lattice model and the derivation of macroscopic equations via Chapman–Enskog expansion procedure. In the subsequent section, we employ our model to simulate the natural convection flow in a cubic cavity. The final section concludes this study.

2. Internal Energy Density Distribution Function

Following the double-distribution function approach proposed by He and Azwadi, we get the governing equations for these two functions:

\[
\frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = -\frac{1}{\tau_f} (f - f^{eq}) + F_f ,
\]

\[
\frac{\partial g}{\partial t} + c \frac{\partial g}{\partial x} = -\frac{1}{\tau_c} (g - g^{eq}) ,
\]
where the density distribution function \( f \equiv f(x, c, t) \) is used to simulate the density and velocity fields, and the internal energy density distribution function \( g \equiv g(x, c, t) \) is used to simulate the macroscopic temperature field. The macroscopic variables, such as the density \( \rho \), velocity \( \mathbf{u} \) and temperature \( T \), can be evaluated as the moment to the distribution function

\[
\rho = \int f \, dc, \quad \rho \mathbf{u} = \int c f \, dc, \quad \rho T = \int g \, dc.
\]

The \( f^{\text{eq}} \) and \( g^{\text{eq}} \) in Eqs. (1) and (2) are the equilibrium distribution function for density and internal energy, respectively, given by

\[
f^{\text{eq}} = \rho \left( \frac{1}{2\pi RT} \right)^{D/2} \exp \left\{ -\frac{c^2}{2RT} \right\} \left[ 1 + \frac{c \cdot \mathbf{u}}{RT} + \frac{(c \cdot \mathbf{u})^2}{2(2RT)^2} - \frac{u^2}{2RT} \right].
\]

\[
g^{\text{eq}} = \rho T \left( \frac{1}{2\pi RT} \right)^{D/2} \exp \left\{ -\frac{c^2}{2RT} \right\} \left[ 1 + \frac{c \cdot \mathbf{u}}{RT} \right].
\]

Equation (5) is obtained by assuming that at low-Mach-number flow (incompressible flow), the higher order of \( u^2 \) and viscous heat dissipation can be neglected.\(^{10}\) It also has been proved\(^ {11}\) that the above simplification does not alter the corresponding macroscopic equation of energy. The only change is the value of the constant parameter in the thermal conductivity, which can be absorbed by manipulating the parameter \( \tau_c \).

We have also recently shown that the discretized equilibrium distribution function for both density and internal energy density distribution function can be obtained by applying the Gauss-Hermite quadrature procedure for the calculation of \( f^{\text{eq}} \) and \( g^{\text{eq}} \) velocity moments. As a result, a 3D 27-velocity, D3Q27 lattice model as shown in Fig. 1 (left) is obtained, and the corresponding discretized equilibrium density distribution function is given by

\[
f_{i}^{\text{eq}} = \rho \omega_i \left[ 1 + 3 \frac{c \cdot \mathbf{u}}{c^2} + \frac{9 (c \cdot \mathbf{u})^2}{2c^4} - \frac{3u^2}{2c^2} \right],
\]

where \( c = (3RT)^{1/2} \) and the weights are \( \omega_0 = 8/27, \omega_{1-6} = 2/27, \omega_{7-18} = 1/54 \) and \( \omega_{19-26} = 1/216 \).

While the lattice type for energy model is shown in Fig. 1 (right), the corresponding discretized internal energy density equilibrium distribution function is given by

\[
g_{1-8}^{\text{eq}} = \frac{1}{8} \rho T \left[ 1 + \frac{c \cdot \mathbf{u}}{c^2} \right].
\]

Through a multiscaling expansion, the mass and momentum equation can be derived for 3DQ27 as below. The details derivation is given by Luo\(^ {12}\) and will not be shown here.

\[
\nabla \cdot \mathbf{u} = 0,
\]
where $p = c_s^2$ is the pressure, $c_s^2 = c/3^{1/2}$ is the sound speed and the kinematic viscosity is given by

$$\nu = \frac{2\tau_v - 1}{6}.$$  

Following the same procedure, the macroscopic temperature equation can also be derived. To see this, we first apply the first order forward Euler scheme in time and first order upwind scheme to Eq. (2), which gives

$$g_i(t + \Delta t, x + c_i \Delta t) - g_i(t, x) = \frac{\Delta t}{\tau_c} (g_i(t, x) - g_i^{eq}(t, x)).$$  

Taylor series expansion to $O(\Delta t^2)$ results in

$$\Delta t (\partial_t + c_i \cdot \nabla) g_i + \frac{\Delta t^2}{2} (\partial_t + (c_i \cdot \nabla))^2 g_i = \frac{\Delta t}{\tau_c} (g_i - g_i^{eq}).$$

Next, we assume that the mean free path is of the same order as that of Knudsen number $\varepsilon$ and we expand $g_i$ as

$$g = g_i^{eq} + \varepsilon g_i^{(1)} + \varepsilon^2 g_i^{(2)} + \cdots$$

and the time derivative as

$$\partial_t = \partial_{t0} + \varepsilon \partial_{t1} + \varepsilon^2 \partial_{t2} + \cdots,$$

where $\varepsilon$ is assumed to be a small parameter. Substituting Eqs. (13) and (14) into Eq. (12) and collecting the terms of order $\varepsilon$ and $\varepsilon^2$, respectively, we have

$$(\partial_{t0} + c_i \cdot \nabla) g_i^{eq} = -\frac{1}{\tau_c} g_i^{(1)}$$

and

$$\partial_{t1} g_i^{eq} + (\partial_{t0} + c_i \cdot \nabla) \left( 1 - \frac{1}{2\tau_c} \right) g_i^{(1)} = -\frac{1}{\tau_c} g_i^{(2)}.$$
Summation over $i$ for Eqs. (15) and (16) leads to
\begin{align}
\partial_t \rho T + \nabla \cdot \rho \mathbf{u} T &= 0, \\
\partial_t \Pi^{(1)} + \left( + \frac{1}{2 \tau_c} \right) \Pi^{(1)} &= 0,
\end{align}
where $\Pi^{(1)} = (\tau_c/8) \nabla^2 (\rho T)$. Combining Eqs. (17) and (18), we get
\begin{align}
\partial_t \rho T + \nabla \cdot \rho \mathbf{u} T &= \chi \nabla^2 (\rho T).
\end{align}
The thermal diffusivity $\chi$ for this model is determined by
\begin{align}
\chi &= \tau_c - 0.5.
\end{align}

From above derivations, we can see that the evolution equation of Eqs. (1) and (2) can lead to the Navier–Stokes and energy equations through the Chapman–Enskog expansion.

3. Numerical Simulations

Numerical simulation for the natural convection flow in a cubic cavity was carried out to test the validity of the 3D eight-velocity, 3DQ8 thermal lattice Boltzmann model. Figure 2 shows a schematic diagram of the setup in the simulation. No-slip boundary conditions are imposed on all the faces of the cubes. The thermal conditions applied on the left and right wall are $T(x = 0, y, z) = T_H$ and $T(x = 1, y, z) = T_C$. The other faces being adiabatic, $\partial T/\partial n = 0$, where $\partial T/\partial n$ is the appropriate normal derivative.
The temperature difference between the left and right walls introduces a temperature gradient in a fluid, and the consequent density difference induces a fluid motion, that is, convection.

In the simulation, the Boussinesq approximation is applied to the buoyancy force term.

\[ \rho \mathbf{G} = \rho \beta g_0 (T - T_m) \mathbf{j}, \]  

where \( \beta \) is the thermal expansion coefficient, \( g_0 \) is the acceleration due to gravity, \( T_m \) is the average temperature and \( \mathbf{j} \) is the vertical direction opposite to that of gravity. So the external force in Eq. (1) is

\[ F_f = 3 \mathbf{G}(\mathbf{c} - \mathbf{u}) f^{eq}. \]  

The dynamical similarity depends on two dimensionless parameters: the Prandtl number \( Pr \) and the Rayleigh number \( Ra \),

\[ Pr = \frac{\nu}{\chi}, \quad Ra = \frac{g_0 \beta T L^3}{\nu \chi}. \]  

We carefully choose the characteristic speed \( v_c = \sqrt{g_0 LT} \) so that the low-Mach-number approximation holds. The Nusselt number \( Nu \) is one of the most important dimensionless numbers in describing the convective transport. The Nusselt number at the mid-plane is defined by

\[ Nu_{mp} = \int_0^1 \frac{\partial T (y, z)}{\partial x} dz. \]  

In all simulations, \( Pr \) is set to be 0.71, and due to the limitation of computer capability, the grid sizes of 101 \( \times \) 101 is used for \( Ra = 10^3 \) and \( Ra = 10^4 \). The grid dependence study has to be done before the comparison for \( Ra = 10^3 \). The result is given in Table 1. It can be clearly seen that as we increase the size of the mesh grid, the calculated variables converge to a constant value.

<table>
<thead>
<tr>
<th>Table 1. Characteristic values, ( Ra = 10^3 ).</th>
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<tbody>
<tr>
<td>Grid</td>
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<tr>
<td>( u_{max} )</td>
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<tr>
<td>( y )</td>
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<tr>
<td>( z )</td>
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<td>( x )</td>
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<tr>
<td>( y )</td>
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<td>( z )</td>
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<tr>
<td>( w_{max} )</td>
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<tr>
<td>( x )</td>
</tr>
<tr>
<td>( y )</td>
</tr>
<tr>
<td>( z )</td>
</tr>
<tr>
<td>( Nu_{mp} )</td>
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</table>
Streamlines and isotherms predicted for flows at different Rayleigh numbers are shown in Figs. 3 and 4. The velocity components for $Ra = 10^3$ and $Ra = 10^4$ are shown in Figs. 5 and 6. It can be seen from these figures that as the Rayleigh number increases, the velocity maximum moves closer to the wall and its amplitude increases. At $Ra = 10^3$, streamlines are those of a single vortex, with its center in the center of the system. The corresponding isotherms are parallel to the heated walls, indicating that most of the heat transfer is by heat conduction. As the Rayleigh number increases, ($Ra = 10^4$), the central streamline is distorted into an elliptic shape and the effects of convection can be seen in the isotherms.

For the simulation at $Ra = 10^5$, we used the D3Q27 lattice type for the internal energy density distribution function in order to avoid the stability problem reported by Azwadi.\textsuperscript{9} The corresponding equilibrium internal energy density distribution function is given by

$$g^e_i = \rho T \omega_i \left[ 1 + 3 \frac{c \cdot u}{c^2} \right],$$

where the weights are $\omega_0 = 8/27$, $\omega_{1-6} = 2/27$, $\omega_{7-18} = 1/54$ and $\omega_{19-26} = 1/216$. 
Fig. 5. Contour maps of horizontal velocity components for $Ra = 10^3$ (left) and $Ra = 10^4$ (right).

Fig. 6. Contour maps of vertical velocity components for $Ra = 10^3$ (left) and $Ra = 10^4$ (right).

Fig. 7. Streamlines (left) and isotherms (right) of natural convection for $Ra = 10^5$.

The numerical results for the simulation at $Ra = 10^5$ are shown in Figs. 7 and 8. At $Ra = 10^5$, the central streamline is elongated and two secondary vortices appear inside it. The isotherms become horizontal at the center of the cavity indicating that
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Fig. 8. Contour maps of horizontal (left) and vertical (right) velocity components for $Ra = 10^5$.

Table 2. Comparison of numerical results between the present work and the "benchmark solution" gathered by Tric.

<table>
<thead>
<tr>
<th>$Ra = 10^3$</th>
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<td>Present work</td>
</tr>
<tr>
<td>$Tric^{14}$</td>
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</tr>
<tr>
<td>3.564</td>
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<td></td>
<td></td>
<td>16.719</td>
</tr>
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<td>45.370</td>
<td>43.900</td>
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<tr>
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<tr>
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<td>$y = 0.52$</td>
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<tr>
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<td>$z = 0.73$</td>
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<tr>
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<td>$w_{max}$</td>
<td>$w_{max}$</td>
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</tr>
<tr>
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<td>$y = 0.85$</td>
<td>$y = 0.85$</td>
</tr>
<tr>
<td>$z = 0.25$</td>
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<tr>
<td>$N_{u_{mp}}$</td>
<td>$N_{u_{mp}}$</td>
<td>$N_{u_{mp}}$</td>
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<tr>
<td>1.093</td>
<td>1.087</td>
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<td></td>
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<td>2.250</td>
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<tr>
<td>4.988</td>
<td>4.612</td>
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</table>

the dominant of heat transfer mechanism is convection. A "benchmark solution" gathered by Tric$^{14}$ is brought for comparison and shown in Table 2. The table contains the numerical result of the maximum of each velocity component in the cavity, with its location and the Nusselt number at the mid-plane ($y = 0.5$). Note that the velocity shown in the table is normalized by the reference velocity of $\chi/H$, where $\chi$ is the thermal diffusivity and $H$ is the height of the cavity.

From the results presented above, we can say that our new 3D thermal lattice Boltzmann model has the capability to solve the thermal flow problems.

4. Conclusion

In this paper, we have developed a new type of lattice model which only uses eight-velocity for internal energy density distribution function in incompressible limit. Both of the evolution equations have been derived from the continuous Boltzmann
equation and Maxwell–Boltzmann equilibrium distribution function. (Computations of natural convection in a cubic cavity correctly predicted the flow features for different Rayleigh numbers. The results are also in good agreement with those of previous studies.) This shows that our model has the capability to solve the thermal flow problems.

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References