MATEMATIKA, 2010, Volume 26, Number 2, 157–165

A Three-Dimension Double-Population Thermal Lattice BGK Model for Simulation of Natural Convection Heat Transfer in a Cube

[1]C. S. Nor Azwadi and [2]T. Tanahashi
[1]Department of Thermo-Fluids, Faculty of Mechanical Engineering
Universiti Technologi Malaysia, 81310 Johour Bahru, Malaysia
[2]Department of Mechanical Engineering, School for Open and Environmental Systems
Keio University, Hiyoshi, Yokohama, 3-1-14 Japan
e-mail: [1]azwadi@fkm.utm.my, [2]taka@mech.keio.ac.jp

Abstract In this paper, a double-population thermal lattice Boltzmann was applied to solve three dimensional, incompressible thermal fluid flow problem. The simplest lattice BGK D3Q6 model was proposed to determine the temperature field while D3Q15 or D3Q19 for the density and velocity fields. The simulation of natural convection in a cubic cavity with Prandtl number 0.71 and Rayleigh number ranging from 10^3 to 10^5 were carried out and compared with the published results in literature. It was observed that the combination of D3Q6 and D3Q19 gave better numerical stability and accuracy compared to D3Q6 with D3Q15 for the simulation at high Rayliegh number.

Keywords Double population; lattice Boltzmann; distribution function; natural convection.

1 Introduction

For more than a decade, lattice Boltzmann method (LBM) has been demonstrated to be a very effective numerical tool for a broad variety of complex fluid flow phenomena that are problematic for conventional methods [1]. Compared with traditional computational fluid dynamics, LBM algorithms are much easier to be implemented especially in complex geometries and multicomponent flows.

Historically, LBM was derived from lattice gas (LG) automata [1]. It utilizes the particle distribution function to describe collective behaviors of fluid molecules. Although promising, the current LBM still have a few shortcomings that limit its general application as a practical computational fluid dynamics tool. One of these shortcomings, which is specifically addressed in this paper, is lack of reliable three dimensional (3D) thermal lattice Boltzmann model with low computational cost.

Generally, there are three types of thermal lattice Boltzmann models that have been proposed; multi-speed model [2], passive scalar model [3] and double-distribution function (DDF) model [4]. Among these models, the passive scalar and DDF model are reported to be numerically stable [5] and widely used in simulating thermal fluid flow problems Azwadi1,Peng,Onishi.

Natural convection heat transfer in a square 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 [6]. However, among the previous numerical studies pertinent to this problem, little works have been done using 3D simulation model.

As far as authors' knowledge, few attempts have been made to predict the phenomenon of natural convection in a cubic cavity using 3D thermal lattice Boltzmann models. Peng et. al [7] proposed and investigated the efficiency and stability of the DDF model using two different particles velocity models of D3Q15 [8] (three-dimension fifteen-particle velocity) and D3Q19. All macroscopic variables such as density, velocity and temperature fields were calculated using the same models whether D3Q15 or D3Q19. They showed that for the simulation at Rayleigh number, $Ra = 10^3$, the results obtained were almost the same for D3Q15 and D3Q19 models. While for $Ra = 10^4$ and 10^5, D3Q19 gave better results than D3Q15 when compared with Navier-Stokes solver. However, these models require high computational cost due to the application of high number of particle velocity for both density and temperature distribution function.

The recent work by Azwadi et. al [9] focused on the development of lattice model for the calculation of temperature field. They found that an eight-particle velocity model, D3Q8 can be developed for internal energy density distribution function if the viscous and compressive heating effect were neglected. Though Azwadi et. al's model has been successfully simulated 3D natural convection problem to a certain degree with low computational cost, this model is limited for the simulation at low Rayleigh numbers. They reported that this was due to the limitation on the value of time relaxation for the internal energy density distribution function where very close to its stability limit at high Rayleigh numbers simulation. However, for real thermal engineering applications, the value of Rayleigh numbers could reach up to 10^5. Therefore, a 3D thermal model which is capable in simulating up to this value of Rayleigh number is expected.

In this research, works have been done on the improvement of passive scalar model. In passive scalar approach, the distribution function for the temperature field is relatively independent of that for the velocity field, so the passive scalar model can use two independent lattices for two distribution functions respectively. Although Peng [7] and Azwadi et. al [9] have developed lattice models based on the double distribution function approach, the proposed final form of governing equations for density and internal energy density were exactly the same as in the passive scalar model if the viscous heat dissipation and the work done by pressure were neglected. In this paper, the simplest pasive scalar model of D3Q6 for the calculation of temperature field is proposed and coupled with D3Q15 or D3Q19 for the calculation of density and velocity field.

The rest of the paper is organized as follows. In the next section, the 3D double-population passive scalar model is constructed. In the subsequent section, the proposed model is employed to simulate the natural convection flow in a cubic cavity with two side walls maintained at different temperatures. The final section concludes this study.

2 Double-Population Thermal Lattice Boltzmann Model

In 3D lattice Boltzmann method, the physical space is divided into cubic lattices, and the evolution of particle population at each lattice site is computed by using particle distribution function. Following the passive scalar approach proposed by Shan [4] and Guo et. al [14], the evolution of particle distribution functions are computed by the following equations

$$f_i\left(x + c_i \Delta x, t + \Delta t\right) - f_i\left(x, t\right) = -\frac{1}{\tau_v}\left(f_i\left(x, t\right) - f_i^{eq}\left(x, t\right)\right) + F_f \tag{1}$$

$$g_i\left(x + c_i\Delta x, t + \Delta t\right) - g_i\left(x, t\right) = -\frac{1}{\tau_c}\left(g_i\left(x, t\right) - g_i^{eq}\left(x, t\right)\right) \tag{2}$$

where density distribution function $f = f\left(x, t\right)$ is used to calculate density and velocity fields and temperature distribution function $g = g\left(x, t\right)$ is used to calculate the temperature field. F_f, τ_v, and τ_c are the external force and the relaxation times for density and temperature distribution function respectively. Note that Bhatnagar-Gross-Krook (BGK) collision model [15] with a single relaxation time is used for the collision term. The macroscopic variables, such as density ρ, velocity u, and temperature T can be evaluated as the moment to the distribution function

$$\rho = \int f dc, \rho u = \int c f dc, \rho T = g dc \tag{3}$$

Suffix i in each evolution equation indicates the number of microscopic velocity applied to density and temperature distribution function. In the present study, D3Q15 and D3Q19 are used for the density while D3Q6 for the temperature distribution function. The configurations of lattice velocities for density distribution functions are shown in Figure 1.

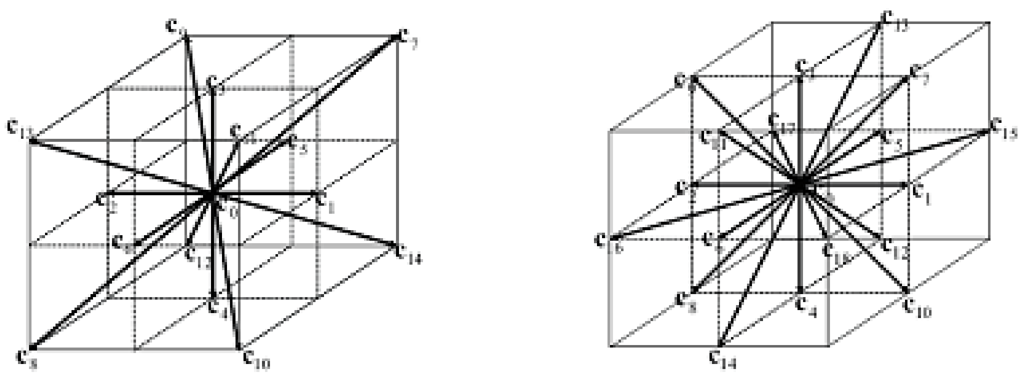

Figure 1: Lattice Structure for D3Q15 (left) and D3Q19 (Right)

The discretised equilibrium distribution function for both D3Q15 and D3Q19 is given as [8].

$$f_i^{eq} = \rho\omega_i\left[1 + 3\frac{c \cdot u}{c^2} + \frac{9\left(c \cdot u\right)^2}{2c^4} - \frac{3u^2}{2c^2}\right] \tag{4}$$

where $\omega_0 = 2/9$, $\omega_{1-6} = 1/9$, and $\omega_{7-14} = 1/72$ for D3Q15 and $\omega_0 = 1/3$, $\omega_{1-6} = 1/18$, and $\omega_{7-18} = 1/36$ for D3Q19. The viscosity in both models is related to the time relaxation through the same equation as

$$\upsilon = \frac{2\tau_v - 1}{6} \tag{5}$$

Through a multiscaling expansion, the mass and momentum equation can be derived from the evolution equation of (1). The detail derivation is given in He and Luo [10] and will not be shown here.

It has been proven in [11, 12] that the effects of heat viscous dissipation and work done by the pressure can be neglected for incompressible flow. Under these assumptions, the temperature field is passively advected by the fluid flows and obeys the so-called passive-scalar equation as

$$\frac{\partial T}{\partial t} + \nabla \cdot (uT) = \chi \nabla^2 T \tag{6}$$

Here, the thermal diffusivity, χ can be related to the time relaxation carried by the energy as follow [13]

$$\chi = \frac{2\tau_c - 1}{6} \tag{7}$$

The lattice structure of D3Q6 for temperature distribution function is shown in Figure 2 and the discretised equilibrium can be written as [4]

$$g_i^{eq} = \frac{1}{6}\rho T \left[1 + 3c \cdot u\right] \tag{8}$$

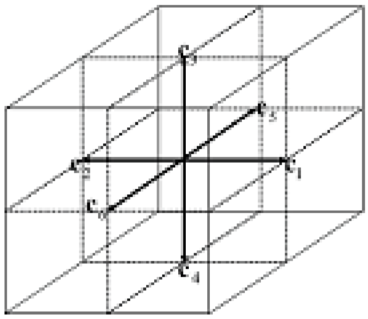

Figure 2: Lattice Structure for D3Q6

3 Natural Convection in a Cubic Cavity

Numerical simulation for the natural convection flow in a cubic cavity was carried out to test the validity of the combination of D3Q15 or D3Q19 with D3Q6 thermal lattice Boltzmann model. Figure 3 shows a schematic diagram of the setup in the simulation.

No-slip boundary conditions for the velocity fields are imposed on all faces of the cubes. The thermal conditions applied on the left and right walls are $T\left(x=0,y,z\right) = T_H$ and $T\left(x=1,y,z\right) = T_C$. 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.

$$\rho G = \rho \beta g_0 \left(T - T_m\right) j \tag{9}$$

where β is the thermal expansion coefficient, g_0 is the acceleration due to gravity, T_m is the average temperature, and j is the vertical direction opposite to that of gravity. So the external force, F_f in Eq. (1) can be written as

$$F_f = 3G\left(c - u\right) f^{eq} \tag{10}$$

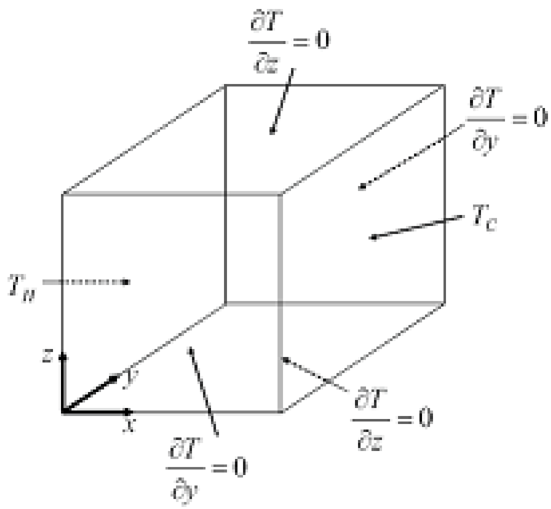

Figure 3: Schematic Geometry for Natural Convection in a Cubic Cavity

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

$$\Pr = \frac{\upsilon}{\chi},\ Ra = \frac{g_0 \beta \Delta T L^3}{\upsilon \chi} \tag{11}$$

Nusselt number, Nu is one of the most important dimensionless numbers in describing the convective transport. Nusselt number at the midplane ($y = 0.5$) is defined by

$$Nu_{mp} = \int_0^1 \frac{\partial T(y,z)}{\partial x} dz \tag{12}$$

In all simulations, Pr is set to be 0.71 and due to the limitation of computer capability (2 GHz and 0.99 GB of RAM), the grid sizes of 101×101 is used for the simulation at all Rayleigh numbers $\left(Ra = 10^3, 10^4, 10^5\right)$. The R. M. S convergence criterion for all the tested cases is

$$\max \left| \left(\left(u^2 + v^2 + w^2\right)^{n+1} \right)^{\frac{1}{2}} - \left(\left(u^2 + v^2 + w^2\right)^{n} \right)^{\frac{1}{2}} \right| \leq 10^{-7} \tag{13}$$

$$\max \left| T^{n+1} - T^n \right| \leq 10^{-7} \tag{14}$$

where the calculation is carried out over the entire system.

4 Numerical Results

The comparisons among D3Q15, D3Q19 and Navier-Stokes solver [13] are held for Rayleigh number 10^3 till 10^5. Among the characteristic numerical values of the flow, the comparisons concern the mean Nusselt number at the mid-plane wall Nu_{mp} , the maximum value for

Table 1: Comparison Among D3Q15, D3Q19 and Navier-Stokes Solver

	Rayleigh Number	10^3	10^4	10^5
$u_{\max}$	D3Q15	0.132	0.199	0.166
	D3Q19	0.132	0.200	0.151
	N-S Solver	0.131	0.201	0.147
x	D3Q15	0.520	0.529	0.490
	D3Q19	0.480	0.510	0.500
	N-S Solver	0.480	0.500	0.500
y	D3Q15	0.186	0.176	0.138
	D3Q19	0.186	0.182	0.142
	N-S Solver	0.200	0.183	0.145
$v_{\max}$	D3Q15	0.132	0.224	0.253
	D3Q19	0.132	0.224	0.248
	N-S Solver	0.132	0.225	0.247
x	D3Q15	0.817	0.882	0.892
	D3Q19	0.814	0.883	0.930
	N-S Solver	0.883	0.883	0.935
y	D3Q15	0.500	0.529	0.510
	D3Q19	0.500	0.500	0.500
	N-S Solver	0.500	0.500	0.500
Nu_{mp}	D3Q15	1.097	2.301	4.975
	D3Q19	1.096	2.301	4.670
	N-S Solver	1.105	2.301	4.646

horizontal and vertical velocity components $u_{\max}$ and $v_{\max}$ with the positions where they occur (x, y).

As can be seen from the table, for the simulation at low Rayleigh number, $Ra = 10^3$, the results obtained were almost the same for D3Q15 and D3Q19 models. However, at high Rayleigh number simulation $\left(Ra = 10^5\right)$ the results show that the D3Q15 cannot give a satisfactory result when compared with the Navier-Stokes solver for this problem. Furthermore, the D3Q15 is already reported to exhibit the velocity oscillation and low computational stability [14]. Therefore, the results which will be presented below were obtained from D3Q19 model.

Streamline and isotherms predicted at mid-plane of the cavity for flows at different Rayleigh numbers are shown in Figure 4 and Figure 5. At $Ra = 10^3$, streamlines are those of a single vortex, with its centre in the centre of the system. As the Rayleigh number increases, $\left(Ra = 10^4\right)$, the central streamline is distorted into an elliptic shape and the effects of convection can be seen in the isotherms. At $Ra = 10^5$, the central streamline is elongated and two secondary vortices appear inside it.

At $Ra = 10^3$, the isotherms are almost vertically parallel to the wall indicating that conduction is the dominant heat transfer mechanism. As the Rayleigh number is increased to 10^4, isotherms start to be horizontally parallel to the wall at the cavity center. This indicates that the heat transfer mechanisms are mixed conduction and convection. For the

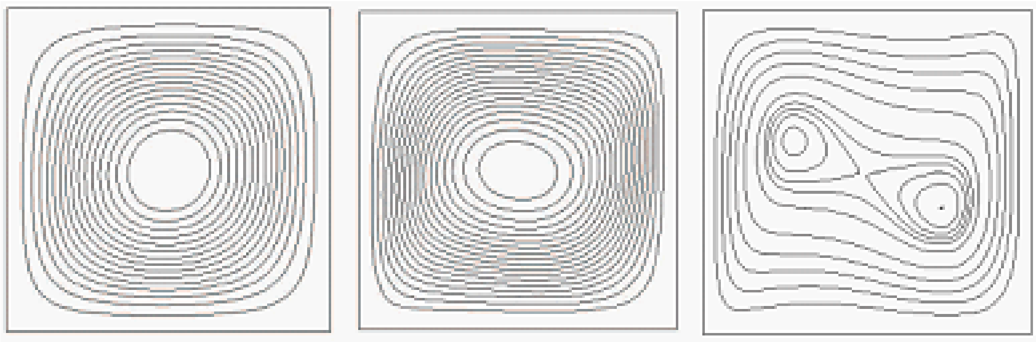

Figure 4: Streamline for Ra = 10^3(left), 10^4(center) and 10^5(right)

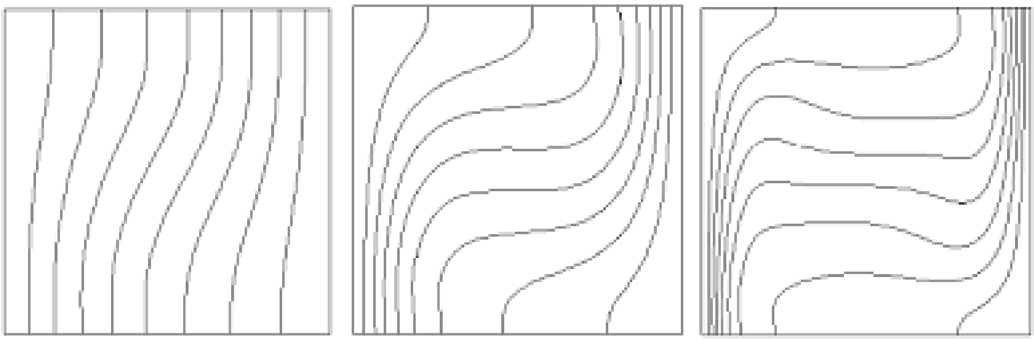

Figure 5: Isotherms for Ra = 10^3(left), 10^4(center) and 10^5(right)

simulation at $Ra = 10^5$, the isotherms become horizontal at the center of the cavity and vertical only in the thin boundary layers near the cold and hot walls indicating that the dominant of heat transfer mechanism is by convection.

The plots of horizontal and vertical velocity components are shown in Figure 6 and Figure 7. 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. These indicate that the fluid motion mainly takes place near the differentially heated walls and the flow in the core of the cavity becomes quasi-motionless. All of these observations are in good agreement with the results reported in previous studies [7, 9, 13, 15].

From the results presented above, it is found that the simplest 3D lattice model, D3Q6 has the capability to solve the thermal flow problems.

5 Conclusion

In this paper, the simplest combination of 3D thermal lattice Boltzmann method is proposed. Computations of natural convection in a cubic cavity correctly predicted the flow feature for different Rayleigh number and gives good agreement with the result of previous studies. The results obtained demonstrate that this new approach in the passive scalar ther-

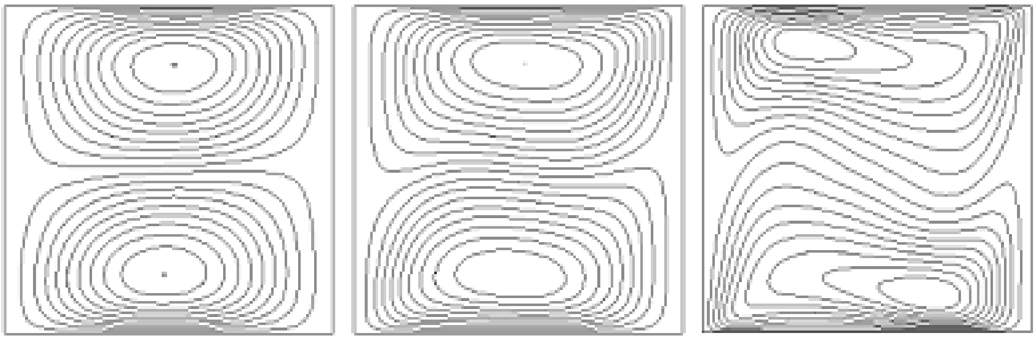

Figure 6: Horizontal Velocity Components for Ra = 10^3(left), 10^4(center) and 10^5(right)

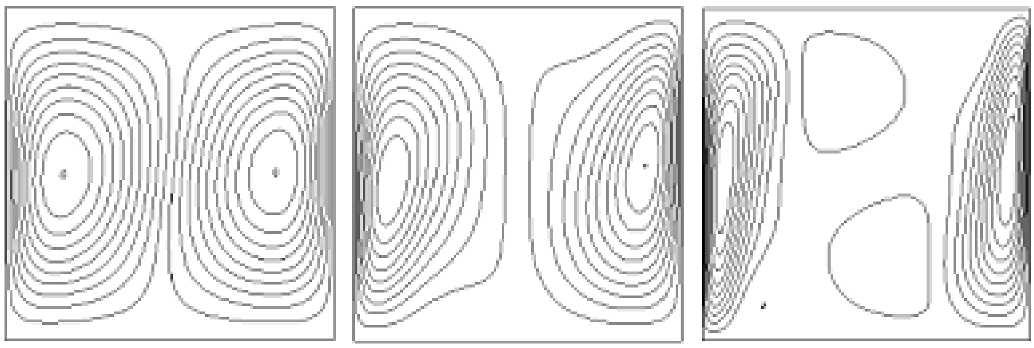

Figure 7: Vertical Velocity Components for Ra = 10^3(left), 10^4(center) and 10^5(right)

mal lattice Boltzmann model is a very efficient procedure to study flow and heat transfer in a differentially heated cubic enclosure.

Acknowledgements

The authors wish to thank Keio University, Universiti Teknologi Malaysia and the Malaysia Government for supporting this research.

References

[1] Bernsdorf, M., Brenner, G. and Durst, F. Numerical Analysis of the Pressure Drop in Porous Media with Lattice Boltzmann (BGK) Automata. *J. Comp. Phys.*, 2000. 129: 247–255.

[2] McNamara and Alder, B. Analysis of the Lattice Boltzmann Treatment of Hydrodynamics. *Physica A*, 1993. 194: 218–228.

[3] Shan, X. Simulation of Rayleigh-Bernard Convection using a Lattice Boltzmann Method. *Phys. Rev. E*, 1997. 55: 2780–2788.

[4] He, X., Chen, S. and Doolen, G. D. Novel Thermal Model for the Lattice Boltzmann Method in Incompressible Limi. *J. Comp. Phys.*, 1998. 146: 282–300.

[5] McNamara, G. and Alder, B. Stabilization of Thermal Lattice Boltzmann Models. *J. Stat. Phys.*, 1995. 81: 395–408.

[6] Davis, D. V. Natural Convection of Air in a Square Cavity: A Benchmark Numerical Solution. *Intl. J. Numer. Meth. Fluid*, 1983. 3: 249–264.

[7] Peng, Y., Shu, C. and Chew, Y. T. A 3D Incompressible Thermal Lattice Boltzmann Model and its Application to Simulate Natural Convection in a Cubic Cavity. *J. Comp. Phys.*, 2003. 193: 260–274.

[8] Qian, Y., Humieres, D. and Lallemand, P. Lattice BGK Models for Navier-Stokes Equation. *Europhys. Lett.*, 1992. 17: 479–484.

[9] Azwadi, C. S. N. and Tanahashi, T. Three Dimensional Thermal Lattice Boltzmann Simulation of Natural Convection in a Cubic Cavity. *Intl. J. Mod. Phys. B*, 2007. 21: 87–96.

[10] He, X. and Luo, L. S. Lattice Boltzmann Model for the Incompressible Navier-Stokes Equation. *J. Stat. Phys.*, 1997. 88: 927–944.

[11] Peng, Y., Shu, C. and Chew, Y. T. Simplified Thermal Lattice Boltzmann Model for Incompressible Thermal Flows. *Phys. Rev. E*, 2003. 68: 026701–026708.

[12] Onishi, J., Chen, Y. and Ohashi, H. Lattice Boltzmann Simulation of Natural Convection in a Square Cavity. *JSME Intl. J. Series B*, 2001. 44: 53–62.

[13] Fusegi, T., Hyun, J., Kuwahara, K. and Farouk, B. A Numerical Study of Three Dimensional Natural Convection in a Differentially Heated Cubical Enclosure. *Intl. J. Heat and Mass Trans.*, 1991. 34: 1543–1557.

[14] Mei, R., Shyy, W., Yu, D. and Luo, L. S. Lattice Boltzmann Method for 3-D Flows with Curved Boundary. *J. Comp. Phys.*, 2000. 161: 680–699.

[15] Tric, E., Labrosse, G. and Betrouni, M. A First Incursion into the 3D Structure of Natural Convection of Air in a Differentially Heated Cubic Cavity, from Accurate Numerical Solution. *Intl. J. Heat and Mass Trans.*, 2000. 43: 4043–4056.