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Numerical simulation of LBGK model for high Reynolds number flow*

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A principle of selecting relaxation parameter was proposed to observe the limit computational capability of the incompressible LBGK models developed by Guo ZL (Guo model) and He SY (He model) for high Reynolds number flow. To the two-dimensional driven cavity flow problem, the highest Reynolds numbers covered by Guo and He models are in the range 58000–52900 and 28000–29000, respectively, at 0.3 Mach number and 1/256 lattice space. The simulation results also show that the Guo model has stronger robustness due to its higher accuracy.

Keywords: incompressible LBGK model, numerical stability, high Reynolds number
PACC: 4700, 0270, 0520D

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has emerged as a powerful tool for modelling complex fluid dynamics problems.[1] Originally, the LBM was developed as a modification of the lattice gas model.[2] Later derivations [3,4] revealed that the method is a special discretization of the continuous Boltzmann equation. The derivation of the LB method [3] from the Boltzmann equation is essentially based on Grad's moment method,[5] together with the Gauss–Hermite quadrature in the velocity space. The method is developing rapidly in response to recent theoretical advances and the availability of resources for large-scale computation. Applications of LBM to modelling high Reynolds number (Re) flow,[1,6] dynamics of fluid phase separation,[7−9] and multicomponent fluid flow in porous media [10] have proven the capability of LBM as a general purpose computational scheme for modelling complex fluid dynamics problems.

In various flow problems, the driven cavity flow has served as the prototype of complex flow problems for testing and evaluating numerical schemes due to its rich vortex structures and simple geometry. Numerical simulations for the driven cavity flow have been studied by many authors using traditional schemes such as finite difference, multigrid, and finite element methods and their variation.[11,12] Hou *et al* performed the lattice Boltzmann simulation with detailed analysis.[13]. To the LBM, the lattice unit is the smallest captured scale in the LBM and the largest scale depends on the characteristic length scale in simulation. These scales are often determined by the available computer memory. The LBM is consequently able to resolve relatively low Reynolds number flows. Numerical studies have shown that the use of the LBM for high Reynolds number flows, without modelling unresolved small scale effects on large scale dynamics, results in numerical instability.[14] When Re exceeds 5000, the main difficulties encountered in these methods are the increasing CPU time and the cost of computation because of large size of the computational grid employed, and the instability or loss of efficacy of schemes. Therefore, most work was done at low or moderate Reynolds numbers. There is a significant lack of information for the realm of high Reynolds numbers.

The lattice Bhatnagar–Gross–Krook (LBGK) models commonly used in the solution of the incompressible Navier–Stokes equations can be viewed as compressible schemes to simulate incompressible fluid

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flows, and there is the compressible effect which might lead to some undesirable errors in numerical simulations. Some LBGK models have been proposed to reduce or eliminate such errors.[15−18] However, most of the existing LBGK models either can be used only to simulate steady flows or are still of artificial compressible form. So, when used to simulate unsteady incompressible flows, these methods require some additional conditions to eliminate the artificial compressible effect.

Reference [19] proposed a D2G9 LBGK model in two-dimensional space without compressible effect for simulating incompressible flows. Furthermore, Ref.[20] investigated two-dimensional driven cavity flows for a range of Reynolds numbers between 5000 and 20 000. A boundary-processing scheme is introduced in this paper. With this non-equilibrium extrapolation scheme, boundary conditions are easy to implement, which makes LBGK methods suitable for flow problems with complex boundaries.

The main aim of this paper is to investigate the limiting computational capability of the LBGK model presented in Refs.[19–21] for high Re flows (we call it the Guo model for short). This means that we hope to find a critical Reynolds number Re* such that the model is numerically stable when Re≤Re* but blows up at Re>Re*. Note that in Ref.[19] the incompressible Navier–Stokes equations are derived accurate to the order of $O(\Delta t^2)$ in the continuity equation and $O(\Delta t^2 + \Delta t \cdot \mathrm{Ma}^2)$ in the momentum equation, where Δt and Ma are the time step and Mach number, respectively. Therefore, the Guo model can work better for higher Re flows than previous models. For example, a harder restriction on the upper limit of Ma is needed because the accuracy of He model in Ref.[16] is $O(\mathrm{Ma}^2)$ (Ref.[16], Eq.A1-17(a)). If we take Ma=0.3 (an acceptable range of low Mach number is considered about 0.1–0.3.) and Δt=0.002, the error of the He model will be $O(0.3^2)$=$O(0.09)$ but that of the Guo model is only $O(0.002\times0.09)$=$O(0.000\,18)\ll O(0.09)$. This fact suggests that the critical Re of the Guo model would be higher than that of the He model because Re* in fact depends on Ma. In this paper, we take Ma=0.3 to detect the limiting computational capability of the Guo model for high Re flows and pay more attention to the selection of the relaxation time when the lattice size and Re are given. Consequently, a lot of numerical simulations of high Re flows were observed using the Guo model. Furthermore, we also observed the critical Reynolds number of the He model under the same conditions.

This paper is arranged as follows. Section 2 relates briefly the Guo model. How to select the relaxation parameter is proposed in Sec.3. Numerical results are presented in Sec.4. Some concluding remarks are made in Sec.5.

2. Numerical details

2.1. Configuration of flow problem and numerical method

The configuration of the driven cavity flow considered in this paper consists of a two-dimensional square cavity whose top plate moves from left to right with a uniform velocity, while the other three walls are fixed (see Fig.1). The flow is assumed to be a two-dimensional Newtonian fluid described by the incompressible Navier–Stokes equations:

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \upsilon \nabla^2 \boldsymbol{u}, \tag{2}$$

where $\boldsymbol{u} = (u, v)$ is the velocity vector, p is the pressure, $c_s = c/\sqrt{3}$, is the sound speed, and υ is the kinematic viscosity determined by

$$\upsilon = \frac{1}{3}(\tau - 1/2)\frac{(\Delta x)^2}{\Delta t}. \tag{3}$$

In Eq.(3), Δx, Δt, and τ are the lattice grid spacing, the time step and the dimensionless relaxation time, respectively.

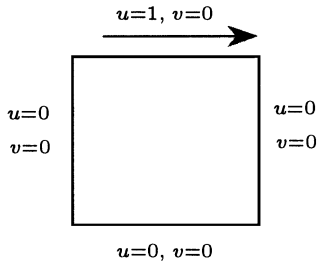


Fig.1. Configuration of flow problem.

The incompressible D2G9 LBGK equation [19] of the system is

$$\begin{aligned} & g_i(\boldsymbol{x} + c\boldsymbol{e}_i\Delta t, t + \Delta t) - g_i(\boldsymbol{x}, t) \\ & = -\tau^{-1}[g_i(\boldsymbol{x}, t) - g_i^{(0)}(\boldsymbol{x}, t)], \end{aligned} \tag{4}$$

where subscript i indicates the velocity direction, and $c = \Delta x/\Delta t$ is the particle velocity. $g_i(\boldsymbol{x}, t)$ is the distribution function at node $\boldsymbol{x}$ and time t with velocity

$\boldsymbol{e}_i$, and $g_i^{(0)}(\boldsymbol{x},t)$ is the corresponding equilibrium distribution defined by

$$\begin{aligned} g_0^{(0)} &= -4\sigma\frac{p}{c^2} + s_0(\boldsymbol{u}), \\ g_i^{(0)} &= \lambda\frac{p}{c^2} + s_i(\boldsymbol{u}), \quad i = 1,2,3,4, \\ g_i^{(0)} &= \gamma\frac{p}{c^2} + s_i(\boldsymbol{u}), \quad i = 5,6,7,8, \end{aligned} \tag{5}$$

where σ, λ, and γ are parameters satisfying $\lambda+\gamma = \sigma$, $\lambda + 2\gamma = 1/2$. $s_i(\boldsymbol{u})$ is

$$s_i(\boldsymbol{u}) = \omega_i\left[3\frac{(\boldsymbol{e}_i\cdot\boldsymbol{u})}{c} + 4.5\frac{(\boldsymbol{e}_i\cdot\boldsymbol{u})^2}{c^2} - 1.5\frac{|\boldsymbol{u}|^2}{c^2}\right] \tag{6}$$

with the weight coefficients

$$\begin{aligned} &\omega_0 = 4/9, \quad \omega_i = 1/9 \quad (i = 1,2,3,4), \\ &\omega_i = 1/36 \quad (i = 5,6,7,8). \end{aligned}$$

The velocity and pressure of flow are given by

$$\boldsymbol{u} = \sum_{i=1}^{8} c\boldsymbol{e}_i g_i \text{ and } p = \frac{c^2}{4\sigma}\left[\sum_{i=1}^{8} g_i + s_0(\boldsymbol{u})\right].$$

At each node of the boundary, the density distribution function is split into two parts: equilibrium and non-equilibrium. For each time step in D2G9 LBGK, the updating of the particle distribution is decomposed into two sub-steps. First is collision,

$$g_i^{+}(\boldsymbol{x},t) = \left(1-\frac{1}{\tau}\right)g_i(\boldsymbol{x},t) + \frac{1}{\tau}g_i^{(0)}(\boldsymbol{x},t), \tag{7}$$

and second streaming,

$$g_i(\boldsymbol{x} + c\boldsymbol{e}_i\Delta t, t+\Delta t) = g_i^{+}(\boldsymbol{x},t). \tag{8}$$

A new type of equilibrium distribution function is introduced to approximate the equilibrium distribution in terms of the specific boundary conditions, while the non-equilibrium distribution is determined by non-equilibrium extrapolation. Thus the distribution function defined is of second-order overall accuracy and the boundary schemes designed have strong stability. The technical details can be found in Refs.[19,21].

2.2. Selection of relaxation parameter

For the LBM, when Mach number Ma of the flow is given, the numerical stability depends on the relaxation time τ and the size of the underlying lattice in use. The Reynolds number used in the problems is Re=LU/υ, where L=1 is the height or width of the cavity, U=1 is the uniform velocity of the top plate. From Eq.(3), we have

$$\upsilon = 1/\mathrm{Re} = c_s^2(\tau - 1/2)\Delta t.$$

The relaxation time is

$$\tau = 1/2 + \frac{1}{\mathrm{Re}c_s^2\Delta t} = 1/2 + \frac{3}{\mathrm{Re}(\Delta x^2/\Delta t)}.$$

Notice that $\tau \to 1/2$ as Re$\to +\infty$, so a high Re will make $\tau - 1/2$ near to 0, which is apt to cause numerical instability.

Let relaxation parameter $s = \tau - 1/2 = 3/\{\mathrm{Re}(\Delta x^2/\Delta t)\}$ and suppose that there exists a threshold value $s_{\min}$, (depending on Re, maybe) for assigning the lattice grid spacing Δx such that when $s \geq s_{\min}$ the model is numerically stable, otherwise it is not. This assumption comes from numerical simulation experiences. Furthermore, let Δt_0, $\bar{s}$ be the upper bounds of time step and s, respectively, i.e.

$$\Delta t \leq \Delta t_0, \quad s_{\min} \leq s = \frac{3\Delta t}{\mathrm{Re}\Delta x^2} \leq \bar{s}. \tag{9}$$

Low Mach number constraint requires $\frac{|u|}{c} \leq \frac{\max|\mathrm{u}|}{\mathrm{c}} \leq \mathrm{Ma} \ll 1$, hence

$$\Delta t \leq \mathrm{Ma}\cdot\Delta x/\overline{u}, \tag{10}$$

where $\overline{u} = \max|\mathrm{u}|$. From Eqs.(9) and (10), we have

$$\begin{aligned} &\frac{1}{3}\Delta x^2\mathrm{Re}\cdot s_{\min} \leq \frac{1}{3}\Delta x^2\mathrm{Re}\cdot s \\ =&\Delta t \leq \min\left\{\frac{1}{3}\Delta x^2\mathrm{Re}\cdot\bar{s},\ \frac{\mathrm{Ma}}{\overline{u}}\Delta x, \Delta t_0\right\}, \end{aligned} \tag{11}$$

or

$$\begin{aligned} s_{\min} \leq s \leq \min\Bigg\{&\bar{s}, \frac{\mathrm{Ma}}{\overline{u}}\Delta x/\left(\frac{1}{3}\Delta x^2\mathrm{Re}\right), \\ &\Delta t_0/\left(\frac{1}{3}\Delta x^2\mathrm{Re}\right)\Bigg\}. \end{aligned} \tag{12}$$

For high Re, we can suppose $\bar{s} \geq 3\cdot\mathrm{Ma}\cdot\Delta x/(\Delta x^2\mathrm{Re}\cdot\overline{u})$ and, furthermore, if $\mathrm{Ma}\cdot\Delta x/\overline{u} \leq \Delta t_0$, then Eq.(12) is reduced to

$$s_{\min} \leq s \leq 3\cdot\mathrm{Ma}\cdot\Delta x/(\Delta x^2\mathrm{Re}\cdot\overline{u}). \tag{13}$$

Let Re* be the root of equation $s_{\min} = 3\cdot\mathrm{Ma}\cdot\Delta x/(\Delta x^2\mathrm{Re}\cdot\overline{u})$. The root Re* is obviously a high Re due to the fact $3\mathrm{Ma}/(\overline{u}\Delta x\cdot\mathrm{Re}) \to 0$ as Re$\to +\infty$. Now if Re$<$ Re*, all s in the interval $[s_{\min}, 3\cdot Ma\cdot\Delta x/(\Delta x^2\mathrm{Re}\cdot\overline{u})]$ will be available parameters to make the model numerically stable, and if Re=Re* the interval only includes the point $s_{\min}$. Finally, if Re$>$Re*, the feasible parameter set $[s_{\min}, 3\cdot\mathrm{Ma}\cdot\Delta x/(\Delta x^2\mathrm{Re}\cdot\overline{u})] = \emptyset$. Therefore Re* is the critical Re of the LBGK model considered.

When Re$\leq$ Re*, the maximum value $s^* = \tau - 1/2 = 3 \cdot \mathrm{Ma}/(\Delta x \mathrm{Re} \cdot \overline{u})$ is obviously a good selection for high Re flows because it corresponds to the largest time stepsize Δt^*, corresponding to the minimum evolution number n for a given evolution time T, hence the lowest computation cost. Furthermore, note that $s_{\min}$ in fact is unknown when an LBGK algorithm is being carried out, so a larger s is easier to maintain the numerical stability than a smaller one. Indeed, s^* is a 'limiting' selection, i.e. no relaxation parameters can make the LBGK model numerically stable if with s^* the model blows up. Therefore, we have to follow the limit selection principle if we hope to compare reasonably the limiting computational capability of two LBGK models on the same basis.

Notice that for a group of parameters (Δx, Ma, α, Δt_0) and s^*, the time step $\Delta t^* = \mathrm{Ma} \cdot \Delta x/\overline{u}$ is independent of Re, so we can say an LBGK model is n-step numerically stable if it has been keeping the numerical stability within the evolution time $T = n\Delta t^*$. In the next section, we shall carry out Guo and He models with 800,000 steps each, to search for their critical Re.

3. Numerical results

Numerical simulations are carried out first using the Guo model for the driven cavity flow on a 256×256 lattice. $\overline{u} = \max|\boldsymbol{u}| = U = 1$ because $|\boldsymbol{u}|$ in the internal cavity can be expected not to exceed U=1. We take Ma=0.3 in the simulations so $\Delta t^* = \mathrm{Ma} \cdot \Delta x/\overline{u}$=0.001 171 875$<$ Δt_0=0.002 and c=3.3333.

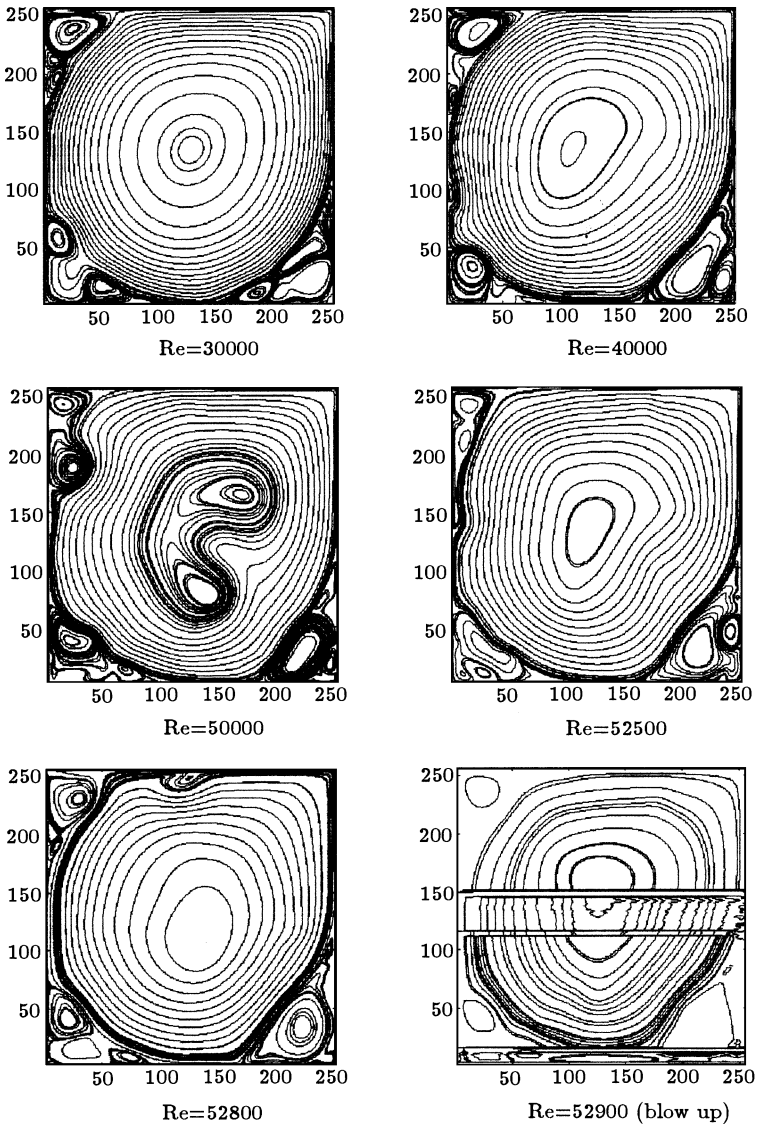


Fig.2. Streamline of the flows from Re=30 000 to 52 900, Guo model, n=500,000, Ma=0.3. When Re=52 900 the algorithm blows up at 274 800 steps.

Figure 2 shows the streamlines of the flows at Re=30 000, 40 000, 50 000, 52 000, 52 500, 52 800 and 52 900. The algorithm is run for 500 000 steps for each of them. We can observe the critical Re lies between 52 800 and 52 900 because the model is 500 000-step numerically stable at Re=52 800 but blows up at Re=52 900.

These plots show clearly the effect of high Re on the flow pattern. It looks like that the centers of the primary vortices are not fixed in the cavity after long time evolution for Re≥40 000. To verify this, Guo model is again carried out for additional 300 000 steps (800 000 steps totally) for the cases of Re≥50 000. Here we only show the streamlines of Re=50 000 in Fig.3. Two characters are observed in the figures: first, the centres of the primary vortexes are changeable in the cavity; second, it seems as if the primary vortex sometimes is collided by the second-class eddy, hence there exists a separating trend to some degree.

The He model can be used for both incompressible steady and unsteady flows. From the model, the incompressible Navier–Stokes equations in artificial compressible form can be derived. However, when used to simulate unsteady incompressible flows, the model requires an additional condition, $T \gg L/c_s$ (T and L are characteristic time and length, respectively), to eliminate the artificial compressible effect. With the same parameters above we also examined the critical Re of He model proposed in Ref.[16]. Figure 4 shows the streamlines of the flows at Re=22 000, 28 000, 29 000 and 30 000. The algorithm is also carried out 800 000 steps for each of them. The critical Re is between 29 000 and 30 000, which is significantly lower than that of the Guo model.

Figure 5 presents the comparison of streamlines of He and Guo models at Re=22 000 and 29000 (Ma=0.3). There are differences between results of the two models. Note that the error between He model and the incompressible Navier–Stokes equations is $O(0.3^2)=O(0.09)$, which is significantly larger than that of Guo model at given parameters $O(0.000\,153)$. Therefore, it is not strange to observe in Fig.5 the distorted and the stable primary vortices of the streamlines of He and Guo model, respectively.

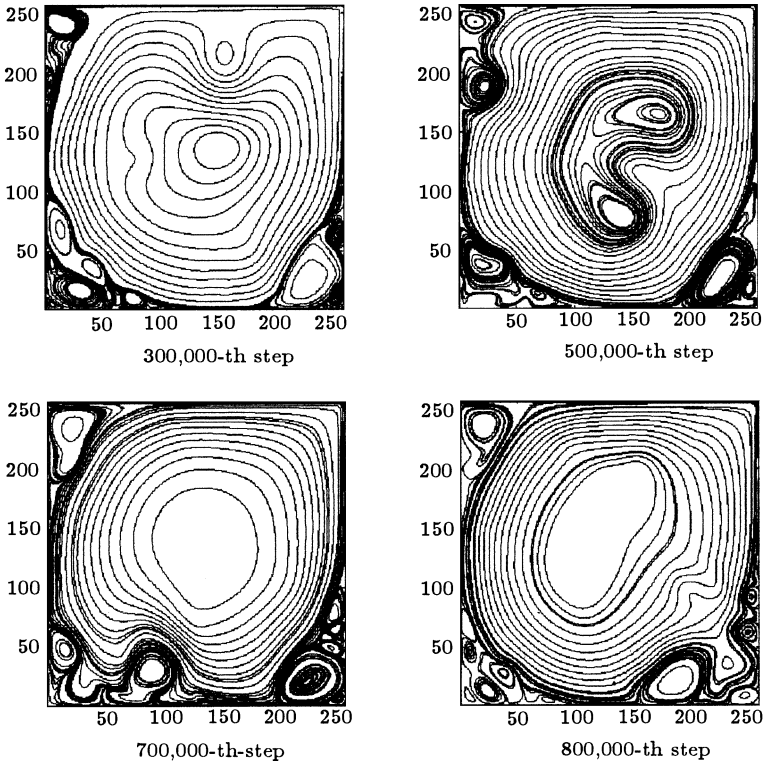


Fig.3. Streamline of the flows in time order series. Guo model, Re=50 000.

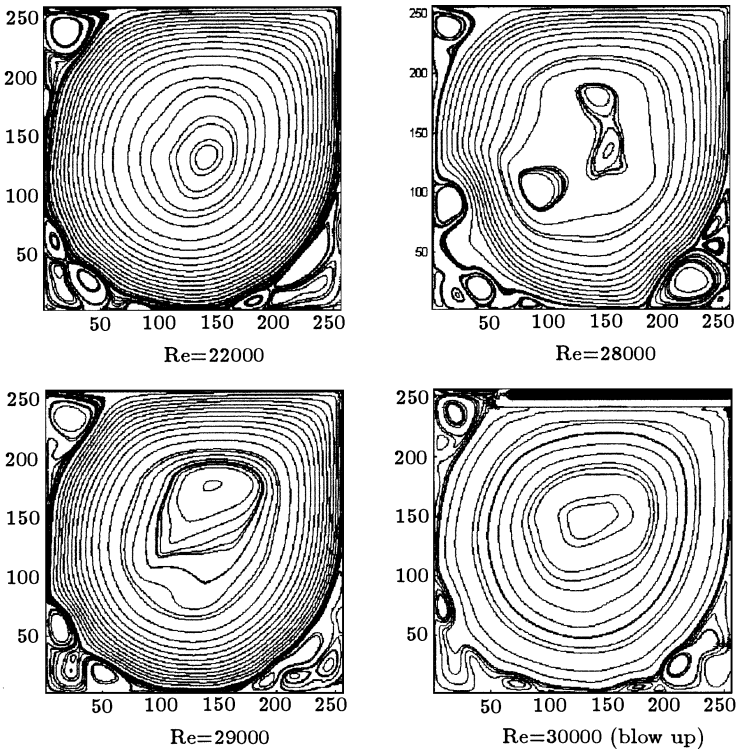


Fig.4. Streamline of the flows from Re=22000 to 30000, He model, n=800,000, Ma=0.3. When Re=30000 the algorithm blows up at 246300th step.

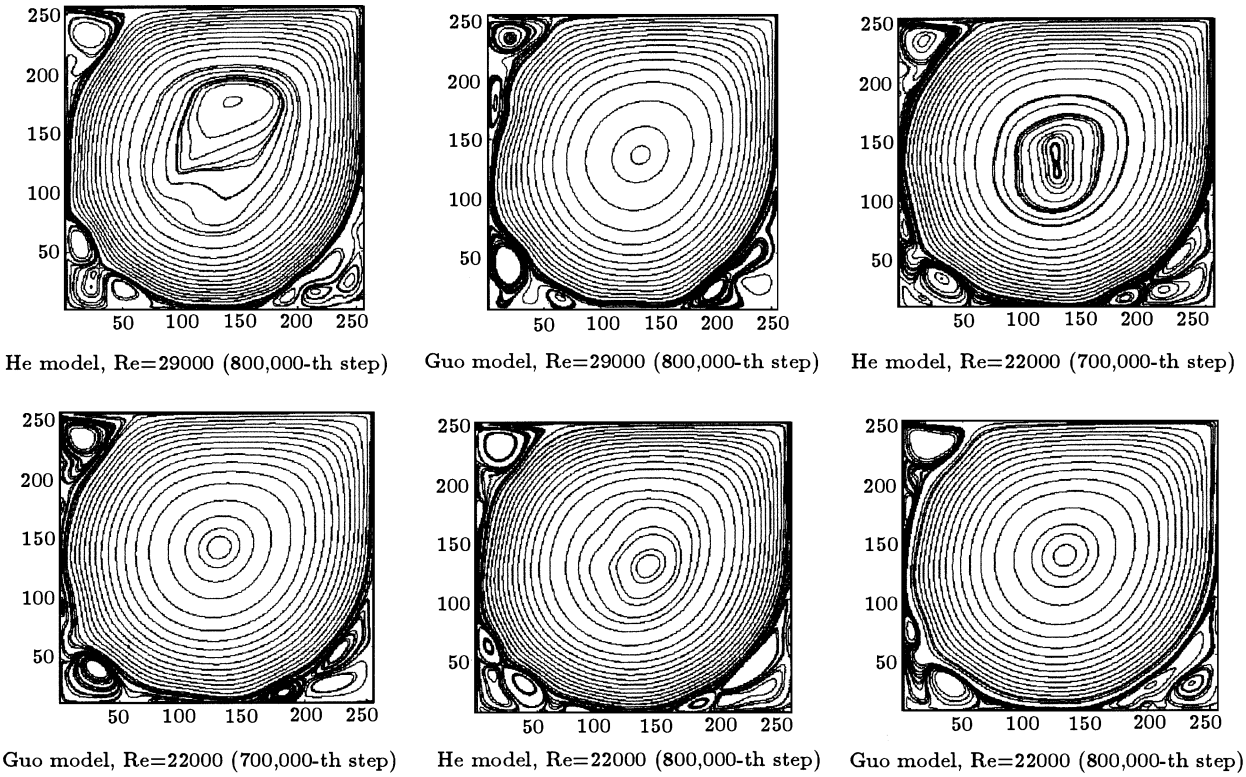


Fig.5. Streamlines of the flow that contrast He and Guo models, Ma=0.3.

We also notice that Ref.[16] claims 0.15 as the upper limit of low Mach number Ma and the comparative simulations of He and Guo models are carried out at Ma=0.125, Re=22 000. Figure 5 shows the comparison of streamlines. In this case, the time stepsize=0.125/256=0.000 488, the total evolutional time T=0.125/256×800 000=390. The errors of He and Guo models (to Navier–Stokes equations) are $O(0.125^2)$=$O(0.0156)$ and $O(0.000\,488\times0.125^2)$=$O(0.000\,007\,625)$, respectively. Therefore, we have strong reason to believe in the simulation results of the Guo model owing to its very small error. In Fig.6 the most similar streamlines of the two models appear at the 300 000th step (evolutional time 146) with smooth primary vortices. However, after that time, the primary vortices of the Guo model have no change but those of the He model are distorted.

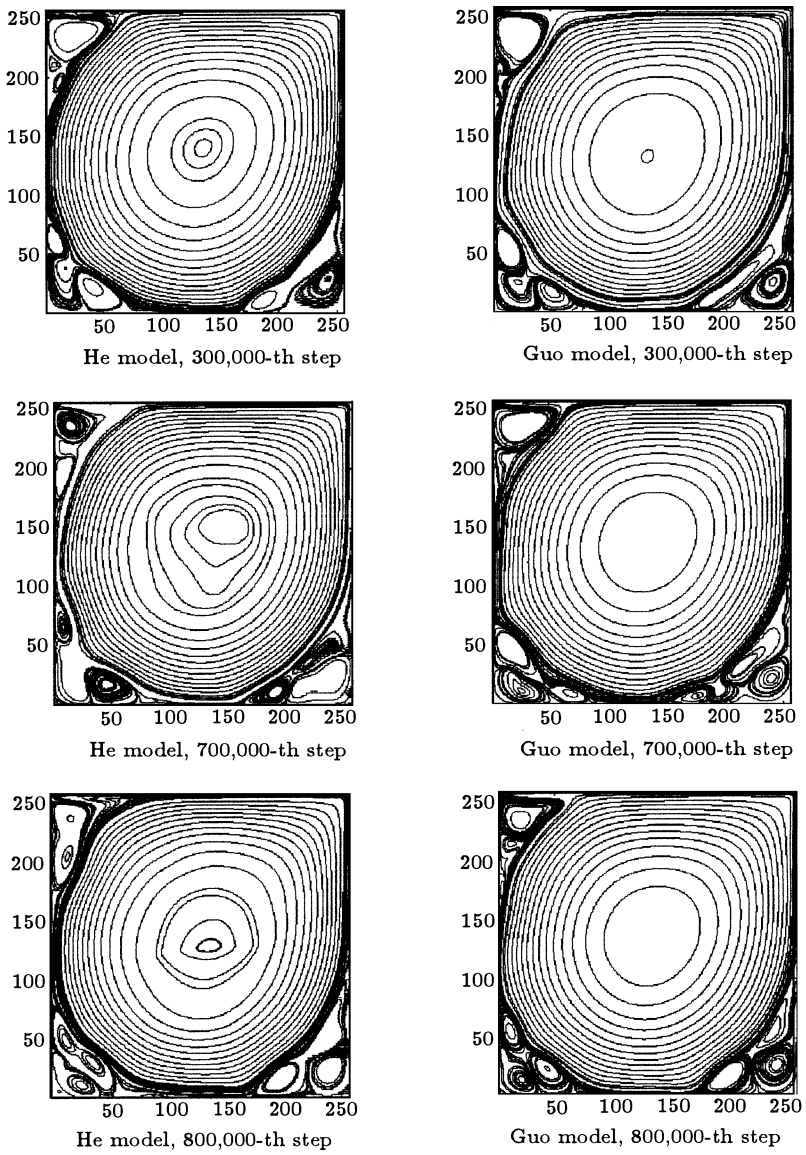


Fig.6. Streamlines of the flow that contrast the He and Guo models, Re=22 000, Ma=0.125.

4. Conclusion and discussion

Both numerical and experimental investigations are important for insight into the complex fluid mechanics of the lid-driven cavity flows. The most comprehensive comparisons between the experimental results obtained in turbulent flow and the corresponding direct numerical simulations (DNS) have been made for a driven cavity. A series of numerical and experimental investigations have been carried out for

Reynolds numbers in the range 1000 to 10 000.[24–29] To our best knowledge, there are few reports in the literature about DNS and experimental investigation of the one-sided lid-driven cavity flow for Re exceeding 22 000. 'A bottleneck that we do see is the paucity of experimental that are available,' observed Shankar and Deshpande in their recent review of the one-sided lid-driven cavity problem.[30] Therefore, to understand the high Re flows, the DNS method is expected to play an increasingly important role.

In the LBGK simulation, designing a reasonable equilibrium distribution is certainly important in theory. However, by our computational experience, some other factors such as dealing with boundary and selecting relaxation parameter also have a strong impact on the numerical stability of an LBGK algorithm, especially in high Re flow cases. Therefore, besides designing a good LBGK algorithm, one should also pay due attention to the factors involved for detecting more high Re flows with the DNS method.

An interesting problem is to examine the limiting computational capability of an LBGK model, i.e. how high Re can be covered by a model when Mach number Ma takes its upper limit. To this aim, selecting the relaxation parameter s as large as possible is a helpful strategy. With this strategy, we can use the critical Re to evaluate the numerical robustness of an LBGK model, and as a consequence compare reasonably the numerical stability between different LBGK models on the same basis.

The research work in this paper is a continuation of Refs.[19,20,21], in which we have investigated the numerical behaviour of the Guo model for Re below 20 000. The results agree well with previous research works. When Re>22 000, it is a little premature to conclude that the Guo model actually provides exact solution of one-side driven cavity flows due to lack of comprehensive comparable materials from DNS and experimental investigation. For this unknown field, we tend to believe in the numerical simulation results of the Guo model to a certain extent owing to the very small error $O(0.000\,153)$ between the model and the incompressible Navier–Stokes equations with given parameters. After all, Navier–Stokes equations are considered as the basis for simulating cavity flows. We expect to do more investigations on high Re cavity flows in the future to check our results.

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