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THE IMPROVEMENT AND REALIZATION OF FINITE-DIFFERENCE LATTICE BOLTZMANN METHOD

The Lattice Boltzmann Method (LBM) is a numerical method developed in recent decades. It has the characteristics of high parallel efficiency and simple boundary processing. The basic idea is to construct a simplified dynamic model so that the macroscopic behavior of the model is the same as the macroscopic equation. From the perspective of micro-dynamics, LBM treats macro-physical quantities as micro-quantities to obtain results by statistical averaging. The Finite-difference LBM (FDLBM) is a new numerical method developed based on LBM. The first finite-difference LBE (FDLBE) was perhaps due to Tamura and Akinori and was examined by Cao et al. in more detail. Finite-difference LBM was further extended to curvilinear coordinates with nonuniform grids by Mei and Shyy. By improving the FDLBE proposed by Mei and Shyy, a new finite difference LBM is obtained in the paper. In the model, the collision term is treated implicitly, just as done in the Mei-Shyy model. However, by introducing another distribution function based on the earlier distribution function, the implicitness of the discrete scheme is eliminated, and a simple explicit scheme is finally obtained, such as the standard LBE. Furthermore, this trick for the FDLBE can also be easily used to develop more efficient FVLBE and FELBE schemes. To verify the correctness and feasibility of this improved FDLBM model, which is used to calculate the square cavity model, and the calculated results are compared with the data of the classic square cavity model. The comparison result includes two items: the velocity on the centerline of the square cavity and the position of the vortex center in the square cavity. The simulation results of FDLBM are very consistent with the data in the literature. When $Re=400$, the velocity profiles of u and v on the centerline of the square cavity are consistent with the data results in Ghia's paper, and the vortex center position in the square cavity is also almost the same as the data results in Ghia's paper. Therefore, the verification of FDLBM is successful and FDLBM is feasible. This improved method can also serve as a reference for subsequent research.

Keywords: Lattice Boltzmann Method (LBM); Finite-difference LBM (FDLBM); Square cavity.

Introduction

Lattice Boltzmann Method (LBM) is a flow field simulation method from micro to macro developed in the 1980s, which can reflect the interrelationship between macroscopic physical quantities and meso-structure motion. The basic idea is to construct a simplified dynamic model so that the macroscopic behavior of the model is the same as the macroscopic

equation. From the perspective of micro-dynamics, LBM treats macro-physical quantities as micro-quantities to obtain results by statistical averaging [1, 2]. Therefore, it has been successfully applied in related fields such as multiphase flow, chemical reaction diffusion, percolation, and particle suspension flow.

Historically, LBM evolved from the lattice-gas automata (LGA) method. Later it was realized that the lattice Boltzmann equation (LBE) could also be derived

from the continuous Boltzmann equation by choosing an appropriate set of discrete velocities based on some special discretization schemes. And it provides a solid theoretical foundation for LBM. The idea that LBE is a discrete scheme of the continuous Boltzmann equation also provides a way to improve the computational efficiency and accuracy of LBM. From this idea, the discretization of the phase space and the configuration space can be done independently. Once the phase space is discretized, any standard numerical technique can serve the purpose of solving the discrete velocity Boltzmann equation (DVBE).

It is not surprising that the finite-difference, finite-volume, and finite-element methods have been introduced into LBM in order to increase computational efficiency and accuracy by using nonuniform grids. The first finite-difference LBE (FDLBE) was perhaps due to Reider and Sterling [3], and was examined by Chen *et al.* [4, 5] in more detail. The study of FDLBE is still in progress. A high-order upwind compact finite difference lattice Boltzmann method (UCDLBM) was developed by Sun [6], which effectively solves the problem of viscous incompressible flow. Mei and Shyy [7] further extended the finite difference LBM to curvilinear coordinates with non-uniform grids, and suggested using the second extrapolation method to determine the unknown collision term of the curvilinear coordinate system at the new time level in FDLBE. Mostafa [8] proposed a numerical framework based on multiple relaxation time lattice Boltzmann (LB) model and novel discretization techniques for simulating compressible flows. Highly efficient finite difference lattice Boltzmann methods are employed to simulate one- and two-dimensional compressible flows. Qiu [9] simulates the two-dimensional cover-driven cavity flow on a non-uniform grid, and discusses the impact of the implicit-explicit Runge-Kutta scheme and the non-uniform grid of the current lattice Boltzmann method. And a hybrid Lattice Boltzmann (LB) -finite difference (FD) numerical scheme for the simulation of reacting flows at low Mach numbers is presented by Hosseini [10].

In this work, we present an improved version of the FDLBE first proposed by Mei and Shyy [7]. In our model, the collision term is treated implicitly, just as

done in the Mei-Shyy model. However, the implicitness of the discrete scheme is completely removed by introducing another distribution function based on the earlier distribution function, and we finally obtain a simple explicit scheme like the standard LBE. Furthermore, this trick for the FDLBE can also be easily used to develop more efficient FVLBE and FELBE schemes.

1. Numerical Model of FDLBM

The starting point of the FDLBE proposed by Mei and Shyy [7] is the continuous discrete velocity Boltzmann equation

$$\frac{\partial \hat{f}_i}{\partial t} + \hat{\xi}_i \cdot \nabla \hat{f}_i = \Omega_i, \quad (1-1)$$

where $\hat{\xi}_i$ is the discrete particle velocity, \hat{f}_i is the distribution function (DF) associated with $\hat{\xi}_i$, and Ω_i is the collision operator. In the kinetic theory, the collision operator is very complicated and is usually approximated by the simple single-relaxation-time Bhatnagar-Gross-Krook (BGK) Model in LBM,

$$\Omega_i = \frac{\hat{f}_i^e - \hat{f}_i}{\hat{\tau}}, \quad (1-2)$$

where $\hat{\tau}$ is the relaxation time and \hat{f}_i^e is the local equilibrium distribution function (EDF). The equation (1-2) is integrated on $[t_n, t_{n+1}]$ to get the new equation as follows

$$\hat{f}^{n+1} = \hat{f}^n - \Delta t \hat{\xi}_i \cdot \nabla \hat{f}_i^n + \frac{\Delta t}{2} [\Omega_i^{n+1} + \Omega_i^n]. \quad (1-3)$$

In order to remove the implicit term in the collision term of equation (1-3), a new distribution function is introduced as follows

$$\hat{g}_i = \hat{f}_i + \frac{\Delta t}{2\hat{\tau}} (\hat{f}_i - \hat{f}_i^e). \quad (1-4)$$

By applying this DF to equation (1-3), we obtain the following semi-discretized Boltzmann equation:

$$\hat{g}_i^{n+1} = \left[1 - \frac{\Delta t}{2\hat{\tau}} \right] \hat{f}_i^n + \frac{\Delta t}{2\hat{\tau}} \hat{f}_i^{e,n} - \Delta t \hat{\xi}_i \cdot \nabla \hat{f}_i^n, \quad (1-5)$$

where

$$\hat{f}_i = \frac{2\hat{\tau}}{2\hat{\tau} + \Delta t} (\hat{g}_i + \frac{\Delta t}{2\hat{\tau}} \hat{f}_i^e). \quad (1-6)$$

Once the gradient operator is discretized, the DF \hat{g}_i can evolve according to equation (1-5), given that \hat{g}_i

is initialized. The macroscopic density ρ and velocity \mathbf{u} of the fluid can be determined from the DF \hat{g}_i directly. In fact, from equation (1-4) we can obtain

$$\rho = \sum \hat{g}_i, \quad \rho \mathbf{u} = \sum \hat{\xi}_i \hat{g}_i. \quad (1-7)$$

2. Numerical model of FDLBM with external force term

After adding an external force term $\hat{\mathbf{a}} \cdot \nabla_{\hat{\xi}} \hat{f}_i$ to equation (1-1), the new discrete velocity Boltzmann equation is obtained as follows

$$\frac{\partial \hat{f}_i}{\partial t} + \hat{\xi}_i \cdot \nabla \hat{f}_i + \hat{\mathbf{a}} \cdot \nabla_{\hat{\xi}} \hat{f}_i = \Omega_i. \quad (2-1)$$

After $-\hat{\mathbf{a}} \cdot \nabla_{\hat{\xi}} \hat{f}_i$ is replaced by the symbol S_i , Equation (2-1) changes to:

$$\frac{\partial \hat{f}_i}{\partial t} + \hat{\xi}_i \cdot \nabla \hat{f}_i = \Omega_i + S_i. \quad (2-2)$$

The equation (2-2) is integrated on $[t_n, t_{n+1}]$ to get the new equation as follows

$$\begin{aligned} \hat{f}^{n+1} &= \hat{f}^n - \Delta t \hat{\xi}_i \cdot \nabla \hat{f}_i + \frac{\Delta t}{2} [\Omega_i^{n+1} + \Omega_i^n] + \\ &+ \frac{\Delta t}{2} [S_i^{n+1} + S_i^n], \end{aligned} \quad (2-3)$$

where

$$S_i = \frac{2\hat{\mathbf{a}} \cdot (\hat{\xi}_i - \hat{\mathbf{u}})}{\tau} \hat{f}_i^e, \quad (2-4)$$

$$\sum S_i = 0, \quad \sum \hat{\xi}_i S_i = \hat{\mathbf{a}}. \quad (2-5)$$

In order to remove the implicit term at the right end of equation (2-3), a new distribution function is introduced as follows

$$\hat{g}_i = \hat{f}_i + \frac{\Delta t}{2\tau} (\hat{f}_i - \hat{f}_i^e) - \frac{\Delta t}{2} S_i. \quad (2-6)$$

By applying this DF to equation (2-3), we obtain the following semi-discretized Boltzmann equation:

$$\begin{aligned} \hat{g}_i^{n+1} &= \left[1 - \frac{\Delta t}{2\tau} \right] \hat{f}_i^n + \frac{\Delta t}{2\tau} \hat{f}_i^{e,n} - \\ &- \Delta t \hat{\xi}_i \cdot \nabla \hat{f}_i^n + \frac{\Delta t}{2} S_i^n, \end{aligned} \quad (2-7)$$

where

$$\hat{f}_i = \frac{2\hat{\tau}}{2\hat{\tau} + \Delta t} \left(\hat{g}_i + \frac{\Delta t}{2\hat{\tau}} \hat{f}_i^e + \frac{\Delta t}{2} S_i \right). \quad (2-8)$$

The macroscopic density ρ and velocity \mathbf{u} of the fluid can be determined from the DF \hat{g}_i directly. In fact, from equation (2-6) we can obtain

$$\rho = \sum \hat{g}_i, \quad \rho \mathbf{u} = \sum \hat{\xi}_i \hat{g}_i + \frac{\rho \hat{\mathbf{a}} \Delta t}{2}. \quad (2-9)$$

3. Boundary conditions

Initial and boundary conditions are usually given in terms of macroscopic physical variables such as ρ and \mathbf{u} . But in LBM, the initial and boundary conditions should be implemented through the distribution function \hat{f}_i . How to determine the initial and boundary values of the DF is an important issue in LBM.

In this paper, the boundary conditions of the two types of distribution functions are processed by the non-equilibrium extrapolation method proposed by Guo [11]. The basic principle is to decompose the distribution function at the boundary point into two parts: equilibrium and non-equilibrium. Part of it is approximated by the definition of boundary conditions, while the non-equilibrium part is determined by non-equilibrium extrapolation.

4. Solving steps of FDLBM

The steps to solve the finite difference LBM are shown in the following Fig. 1. In these steps, the most important thing is to use the second-order upwind and center difference hybrid format differential convection term. Among them, the convection term is differentiated to obtain the following formula (4-1) by using the second-order upwind formula

$$\frac{\partial f_i}{\partial \xi_\beta} \Big|_{\mathbf{u}} = \begin{cases} \frac{1}{2\Delta \xi_\beta} \begin{bmatrix} 3f_i(\xi_\beta) - \\ -4f_i(\xi_\beta - \Delta \xi_\beta) + \\ +f_i(\xi_\beta - 2\Delta \xi_\beta) \end{bmatrix} & \text{if } c_{i\beta} \geq 0, \\ -\frac{1}{2\Delta \xi_\beta} \begin{bmatrix} 3f_i(\xi_\beta) - \\ -4f_i(\xi_\beta + \Delta \xi_\beta) + \\ +f_i(\xi_\beta + 2\Delta \xi_\beta) \end{bmatrix} & \text{if } c_{i\beta} < 0. \end{cases} \quad (4-1)$$

And the convection term is differentiated to obtain the following formula (3-2) by using the central difference format

$$\frac{\partial f_i}{\partial \xi_\beta} \Big|_{\mathbf{c}} = \frac{1}{2\Delta \xi_\beta} [f_i(\xi_\beta + \Delta \xi_\beta) + f_i(\xi_\beta - \Delta \xi_\beta)]. \quad (4-2)$$

Therefore, the convection term is differentiated to

obtain the following formula (4-3) by using a second-order upwind and central difference hybrid format

$$\left. \frac{\partial f_i}{\partial \xi_\beta} \right|_{\text{mix}} = \varepsilon \left. \frac{\partial f_i}{\partial \xi_\beta} \right|_u + (1 - \varepsilon) \left. \frac{\partial f_i}{\partial \xi_\beta} \right|_c, \quad \text{where } 0 \leq \varepsilon \leq 1. \quad (4-3)$$

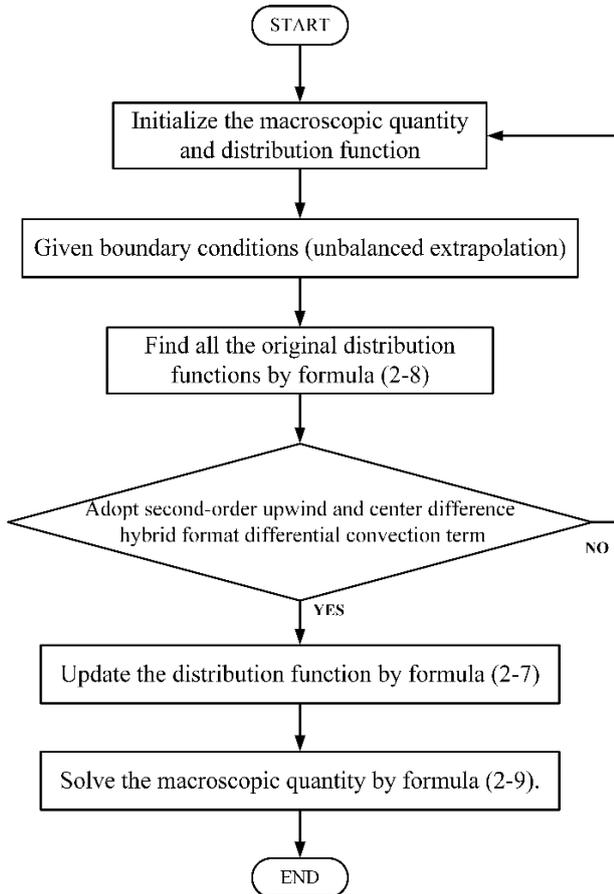


Fig. 1 Solving steps of FDLBM

5. Verification of FDLBM-Square cavity

It is a benchmark problem that the air flow in the square cavity is driven by the cavity cover. The reliability of FDLBM was verified by comparison with the data results in Ghia's paper [12]. This is mainly verified by comparing the velocity on the center line of the cavity and the position of the vortex center. In Ghia's paper, the velocity on the center line of the cavity is shown in Fig. 2 and Fig. 3 below. And When Re=400, the position of the vortex center in the cavity is shown in Table 1 below. If the results of the vortex center position obtained by the FDLBM method are consistent

with the results of the vortex center in Table 1, then FDLBM can be considered to be feasible.

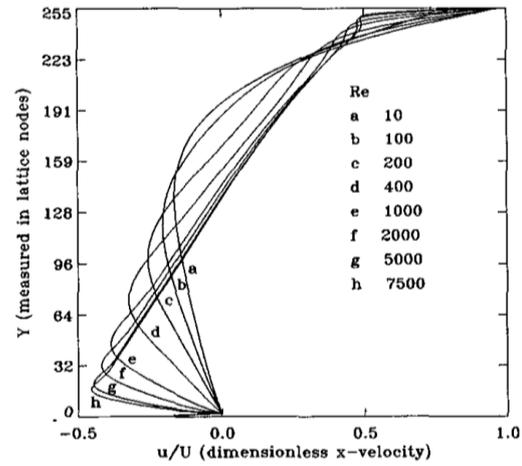


Fig. 2. Velocity type u on centerline of square cavity

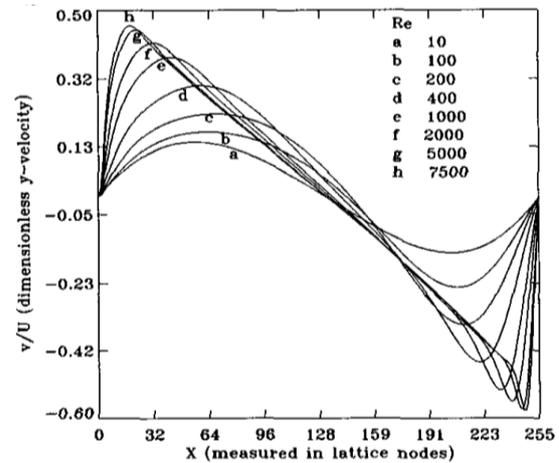


Fig. 3. Velocity type v on centerline of square cavity

Where u is the velocity component on the x-axis, and v is the velocity component on the y-axis.

Table 1

The position of the vortex center in Ghia's paper (Re=400)

Vortex center position	In Ghia's paper [12]	
	Coordinates	
Primary vortex	x	0.5547
	y	0.6055
Lower left vortex	x	0.0508
	y	0.0469
Lower right vortex	x	0.8906
	y	0.1250

5.1. Square cavity model

The square cavity model used in this article is consistent with the model in Ghia's paper. This article simulates the sliding of the plate on the square cavity to the right, driving the air flow in the square cavity. The calculation area and boundary types are shown in Fig. 4. The width and height of the square cavity are H , all walls are fixed walls, and the cavity is filled with air.

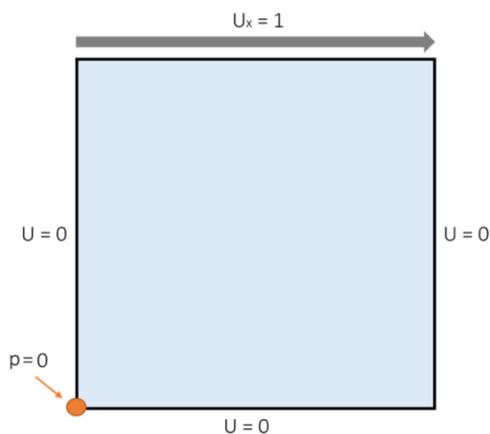


Fig. 4. Physical model of the square cavity

The problem considered is two-dimensional viscous flow in a cavity. An incompressible fluid is bounded by a square enclosure and the flow is driven by a uniform translation of the top. The present simulation uses Cartesian coordinates with the origin located at lower left corner. The top boundary moves from left to right with velocity $U_x=1$.

The calculation conditions are shown in Table 2 as follows.

Table 2

The calculation conditions

Conditions	Re	Ma	H(m)
Values	400	0.1	1

5.2. Numerical simulation results

The non-uniform grid used in the calculation is shown in Fig. 5. The grid is non-uniformly distributed in the x and y directions.

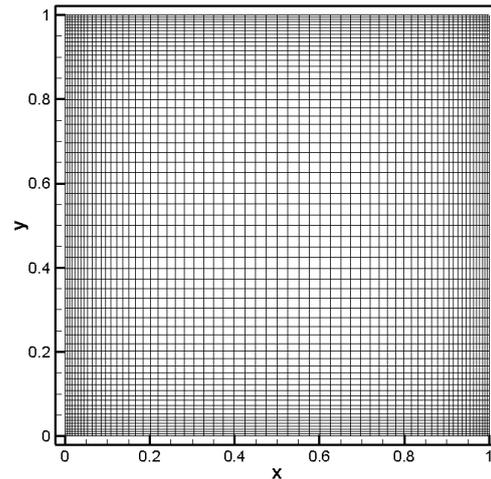


Fig. 5. Non-uniform mesh (64×64)

Fig. 6 shows the velocity flow field in the x direction and Fig. 7 shows the velocity flow field in the y direction through numerical calculation. Fig. 8 is a streamline diagram inside the square cavity.

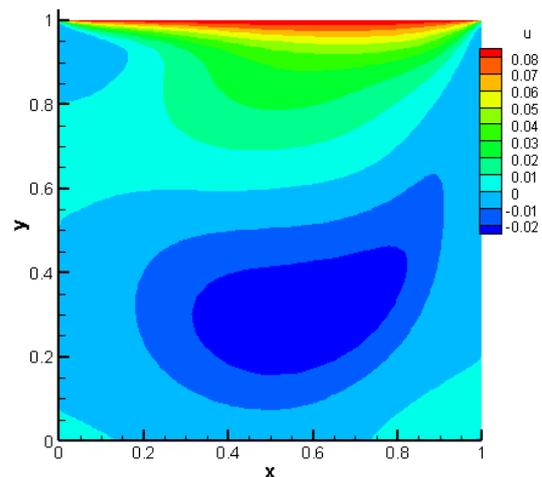


Fig. 6. Velocity flow field in the x direction

Where u is the velocity component on the x -axis, and v is the velocity component on the y -axis.

5.3. Analysis of numerical simulation results

The first is the velocity in the cavity drawn by the rainbow color table (Fig. 6 and Fig. 7), and the flow direction indicated by the vector diagram (Fig. 8). It can be seen that the velocity at the top of the cavity is close to $U_x=1$, where the fluid flow is driven by the moving wall. After the fluid is pushed to the wall on the right, it

flows down first, and then returns to the left side of the cavity. The movement creates a large vortex in the center of the cavity.

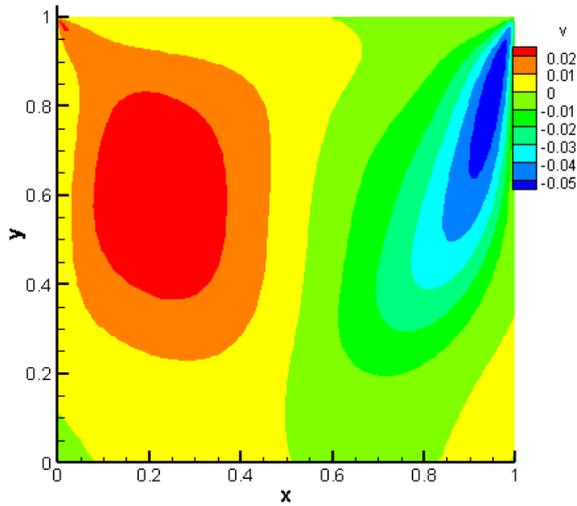


Fig. 7. Velocity flow field in y direction

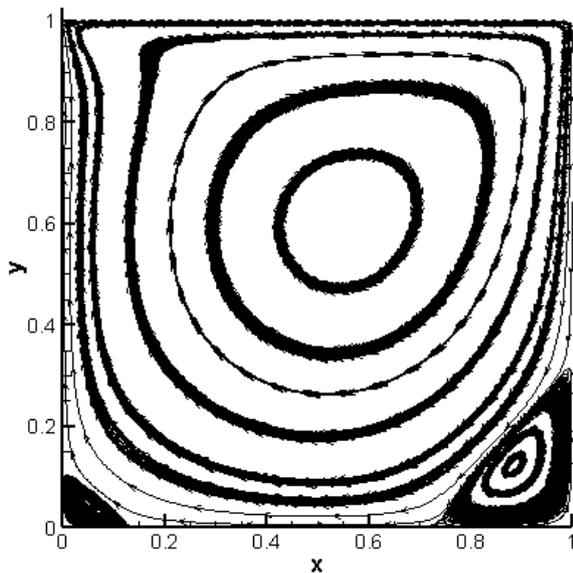


Fig. 8. Streamline diagram

From the flow velocity flow results in Fig. 6 and Fig. 7, the velocity profile of u and v on the center line of the square cavity were obtained as shown in Fig. 9. The circles in the figure represent the data In Ghia's paper, and the curves represent the result of the FDLBM calculation.

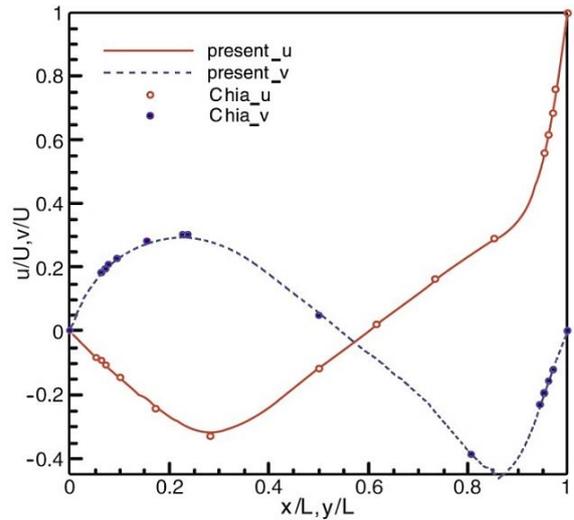


Fig. 9 The velocity profile of u and v on the center line of the square cavity

From the above streamline diagram, it can be concluded that the vortex center position in the square cavity calculated by FDLBM is shown in Table 3.

Table 3

Data comparison

Vortex center position	In Ghia's paper [12]		Present simulation		Error rate
	Coordinates	Coordinates	Coordinates	Coordinates	
Primary vortex	x	0.5547	x	0.5563	<0.3%
	y	0.6055	y	0.6045	<0.2%
Lower left vortex	x	0.0508	x	0.0512	<0.8%
	y	0.0469	y	0.0473	<0.9%
Lower right vortex	x	0.8906	x	0.8851	<0.7%
	y	0.1250	y	0.1239	<0.9%

It can be seen from Fig. 9 that the velocity profiles of u and v on the center line of the square cavity are very consistent with the results in Ghia's paper.

It can be seen from Table 3 above that the vortex center position calculated by FDLBM is consistent with the vortex center position calculated by Ghia, and the error range is less than 1%.

Conclusion

The top cover drive cavity is a benchmark problem. The simulation results of FDLBM are very consistent with the data in the literature by comparing with the literature (Ref. 12). When $Re=400$, the velocity profiles of u and v on the center line of the square cavity are consistent with the data results in Ghia's paper, and the vortex center position in the square cavity is also almost the same as the data results in Ghia's paper. Therefore, the verification of FDLBM is successful and FDLBM is feasible.

It can be concluded that compared with traditional computational fluid dynamics methods (such as finite difference, finite element method, finite volume method, etc.), the lattice Boltzmann method has the following advantages:

- 1) the algorithm is simple, a simple linear operation plus a relaxation process can simulate various complex nonlinear macroscopic phenomena;
- 2) able to handle complex boundary conditions;
- 3) the pressure in the lattice Boltzmann method can be directly solved by the equation of state;
- 4) programming is easy, and the pre- and post-processing of calculation is also very simple;
- 5) it has high parallelism;
- 6) it can directly simulate the flow field of connected domains such as porous media with complex geometric boundaries, without the need for calculation grid conversion.

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ВДОСКОНАЛЕННЯ ТА РЕАЛІЗАЦІЯ МЕТОДА КОНЦЕВО-РІЗНИЦЕВОЇ РЕШІТКИ БОЛЬЦМАНА

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Решітчастий метод Больцмана (LBM) - це числовий метод, розроблений в останні десятиліття. Він має характеристики високої паралельної ефективності та простої граничної обробки. Основна ідея полягає в побудові спрощеної динамічної моделі, щоб макроскопічна поведінка моделі була такою ж, як і макроскопічне рівняння. З точки зору мікродинаміки, LBM трактує макрофізичні величини як мікро величини для отримання результатів шляхом статистичного усереднення. Кінцево-різницевий LBM (FDLBM) - це новий чисельний метод, розроблений на основі LBM. Перший кінцево-різничий LBE (FDLBE), можливо, був обумовлений Тамурою та Акінорі, і його досліджували Сао et al. більш детально. Кінцево-різницевий LBM був додатково розширений до криволінійних координат з неоднорідними сітками Мей і Ший. Удосконалюючи FDLBE, запропонований Мей та Шей, у роботі отримано нову кінцеву різницю LBM. У моделі термін зіткнення трактується неявно, як це робиться в моделі Мей-Ший. Однак, вводячи іншу функцію розподілу на основі попередньої функції розподілу, неявність дискретної схеми повністю усувається, і нарешті отримується проста явна схема, така як стандартний LBE. Крім того, цей фокус для FDLBE також можна легко використовувати для розробки більш ефективних схем FVLBE та FELBE. Для того, щоб перевірити правильність і доцільність цієї вдосконаленої моделі FDLBM, яка використовується для розрахунку моделі квадратної порожнини, а обчислені результати порівнюються з даними класичної моделі квадратної порожнини. Результат порівняння включає два пункти: швидкість на центральній лінії квадратної порожнини та положення центра вихру в квадратній порожнині. Результати моделювання FDLBM дуже узгоджуються з літературними даними. Коли $Re = 400$, профілі швидкості u і v на центральній лінії квадратної порожнини відповідають результатам даних у статті Ghia, а положення центрального вихру в квадратній порожнині також майже однакове з результатами даних розрахунках Ghia. Отже, перевірка FDLBM є успішною, і FDLBM є можливою. Цей вдосконалений метод може також служити еталоном для подальших досліджень.

Ключові слова: Решітчастий метод Больцмана (LBM); Кінцево-різницевий LBM (FDLBM); Квадратна порожнина.

УЛУЧШЕНИЕ И РЕАЛИЗАЦИЯ МЕТОДА КОНЕЧНО-РАЗНОСТНОЙ РЕШЕТКИ БОЛЬЦМАНА

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Решеточный метод Больцмана (LBM) - это численный метод, разработанный в последние десятилетия. Он обладает характеристиками высокой параллельной эффективности и простой обработки границ. Основная идея состоит в том, чтобы построить упрощенную динамическую модель, чтобы макроскопическое поведение модели было таким же, как и макроскопическое уравнение. С точки зрения микродинамики LBM рассматривает макрофизические величины как микровеличины для получения результатов путем статистического усреднения. Конечно-разностная LBM (FDLBM) - это новый численный метод, разработанный на основе LBM. Первая конечно-разностная LBE (FDLBE), возможно, возникла благодаря Тамуре и Акинори и была исследована Сао и другими более детально. Конечно-разностная LBM была дополнительно расширена до криволинейных координат с неоднородными сетками Мей и Ши. Путем улучшения FDLBE, предложенного Mei и Shyu, в статье получена новая конечно-разностная LBM. В модели термин столкновения обрабатывается неявно, как и в модели Мей-Шай. Однако путем введения другой функции распределения, основанной на более ранней функции распределения, неявность дискретной схемы полностью устраняется, и, наконец, получается простая явная схема, такая как стандартная LBE. Кроме того, этот прием для FDLBE также можно легко использовать для разработки более эффективных схем FVLBE и FELBE. Чтобы проверить правильность и осуществимость этой улучшенной модели FDLBM, которая

используется для расчета модели квадратной полости, и результаты расчетов сравниваются с данными классической модели квадратной полости. Результат сравнения включает два параметра: скорость на центральной линии квадратной полости и положение центра вихря в квадратной полости. Результаты моделирования FDLBM очень согласуются с данными в литературе. Когда $Re = 400$, профили скорости u и v на центральной линии квадратной полости согласуются с результатами данных в статье Ghia, а положение центра вихря в квадратной полости также почти такое же, как данные, полученные в расчетах Ghia. Следовательно, проверка FDLBM успешна и FDLBM выполнима. Этот улучшенный метод также может служить справочным материалом для последующих исследований.

Ключевые слова: решеточный метод Больцмана (LBM); Конечно-разностная LBM (FDLBM); Квадратная полость.

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