PROGRESS IN THE DEVELOPMENT AND APPLICATION OF LATTICE BOLTZMANN METHOD

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ABSTRACT: *This paper summarizes our development and application of lattice Boltzmann method. It covers the development of a platform to design lattice velocity model and its associated equilibrium distribution functions, Taylor series expansion- and least square-based lattice Boltzmann method, simplified thermal lattice Boltzmann model, fractional step lattice Boltzmann model for high Reynolds number flows, lattice Boltzmann models for micro flows and multiphase flows with high density ratio, compressible lattice Boltzmann model, and lattice Boltzmann-immersed boundary velocity correction method.*

1. INTRODUCTION

As an alternative computational fluid dynamics approach, the lattice Boltzmann method (LBM) receives more and more attention in recent years [1]. LBM is a particle-based approach, which does not involve the solution of partial differential equations and their resultant algebraic equations. Thus, its implementation and coding are very simple. Currently, LBM has been widely applied to simulate various fluid flow problems. The group in the National University of Singapore also put a lot of effort and made substantial contributions in the development of LBM and exploration of its applications in various areas of heat transfer and fluid flows. This paper summarizes our progress in the development and application of LBM.

2. PLATFORM FOR DEVELOPING NEW LATTICE VELOCITY MODELS

Take the two-dimensional case as an example. The standard lattice Boltzmann equation (LBE) with BGK approximation can be written as

$$f_\alpha(x+e_{\alpha x}\delta t, y+e_{\alpha y}\delta t, t+\delta t) = f_\alpha(x,y,t) + \frac{f_\alpha^{eq}(x,y,t) - f_\alpha(x,y,t)}{\tau}, \alpha = 0,1,...,N, \quad (1)$$

where τ is the single relaxation time; f_α is the density distribution function along the α direction; f_α^{eq} is its corresponding equilibrium state, which depends on the local macroscopic variables such as density ρ and velocity $\boldsymbol{u}$(u, v); δt is the time step and $e_\alpha(e_{\alpha x}, e_{\alpha y})$ is the particle velocity in the α direction; N is the number of discrete particle velocities. The macroscopic density ρ and momentum density $\rho\boldsymbol{u}$ are defined as

$$\rho = \sum_{\alpha=0}^{N} f_\alpha, \qquad \rho\boldsymbol{u} = \sum_{\alpha=0}^{N} f_\alpha e_\alpha \quad (2)$$

The expression of f_α^{eq} depends on the lattice velocity model. Currently, there are many lattice velocity models available in the literature such as D2Q7, D2Q9, D3Q15, D3Q19. These models work very well. However, many users do not know how these models were developed and whether new models can be developed in such a way that Navier-Stokes equations can be recovered. To answer these questions, Zheng et al. [2] proposed a platform which is based on the construction of discrete velocity models that satisfy the isotropic property of lattice tensor, conservation laws, and recover Navier-Stokes equation. From the platform, we can easily determine the equilibrium distribution functions. For details, one can refer to the work of [2].

3. DEVELOPMENT OF EFFICIENT LATTICE BOLTZMANN SOLVERS

In this section, we will introduce three efficient lattice Boltzmann solvers for the application of LBM on irregular domains and at high Reynolds numbers.

3.1 Taylor series expansion- and least square-based lattice Boltzmann method (TLLBM)

The standard LBM is usually limited to the application on the regular domain with the use of uniform mesh. In order to implement LBM more efficiently for flows with arbitrary geometry, the Taylor series expansion- and least square-based lattice Boltzmann method (TLLBM) [3] was proposed. TLLBM is actually based on the standard LBE, the well-known Taylor series expansion, the idea of developing Runge-Kutta method, and the least squares optimization. It is free of lattice models. Theoretical analysis for one-dimensional case showed that TLLBM could recover the Navier-Stokes equations with the second order of accuracy. At a mesh point (x_0, y_0), the density distribution function along the α direction at the time level $t+\delta t$ can be updated by TLLBM as

$$f_\alpha(x_0, y_0, t+\delta t) = \sum_{k=1}^{M+1} a_{1,k}^\alpha g_{k-1}^\alpha(t) \tag{3}$$

where $a_{1,k}^\alpha$ are the coefficients, which only depend on the coordinates of mesh points and lattice velocity, and are pre-computed before the TLLBM is applied, g_k^α is the post-collision distribution function at the neighboring mesh point (x_k, y_k), which can be written as

$$g_k^\alpha = f_\alpha(x_k, y_k, t) + \left[f_\alpha^{eq}(x_k, y_k, t) - f_\alpha(x_k, y_k, t) \right] / \tau \tag{4}$$

The application of TLLBM is very simple. The coefficients $a_{1,k}^\alpha$ are only computed once and stored for the following computations. Fig. 1 shows the streamlines in a polar cavity at Re=350 obtained by TLLBM using a non-uniform mesh of 81×81. Clearly, the TLLBM results compare excellently well with those from a Navier-Stokes solver. Good agreement was achieved in the size of the vortices and location of the separation and reattachment points.

TLLBM result N-S solution

Fig. 1 Comparison of streamlines between TLLBM result and N-S solution

3.2 Simplified Thermal Lattice Boltzmann Model

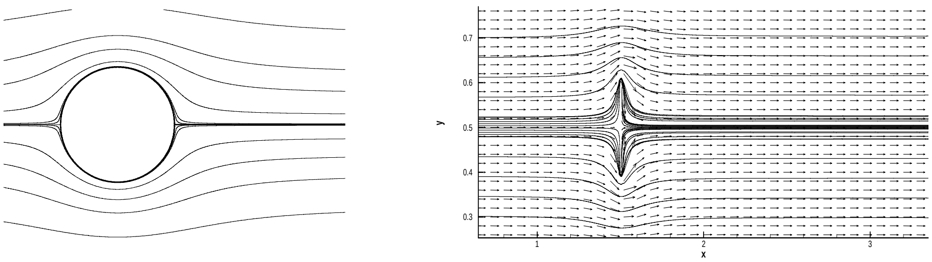
As compared to the application of LBM for isothermal flows, there are very few applications of LBM for thermal flows. The main reason is due to severe numerical instability for the thermal models. Among various thermal lattice Boltzmann models, the double distribution function model proposed by He et al. [4] is the most popular one. However, there exist some shortcomings for this thermal model. On one hand, it contains one complicated gradient operator term in the evolution equation for the temperature, and thus the simplicity property of LBM is lost. On the other hand, since the viscosity is involved not only in the momentum equation but also in the energy equation, the new variables for the double distribution functions are introduced so as to keep the viscosity consistent in the governing equations for the double distribution model and to avoid the implicitness of the scheme. The governing equations are transformed to the forms whose variables are the new density distributions. On the other hand, the simple bounce-back condition for the non-equilibrium functions is the relationship for the old density distributions. Such relationship becomes very complicated after changing to the new forms for the new variables, since the evolution equations are for the new variables. This leads to the loss of one good feature for LBM that boundary condition can be easily implemented. To remove these drawbacks, Peng et al. [5] proposed a simplified double distribution thermal model, which is based on the assumption that in real incompressible applications, the compression work done by the pressure and the viscous heat dissipation can be neglected. Numerical study found that the complicated gradient operator term in the original double distribution thermal model is mainly used to recover the compression work and the viscous heat dissipation. So this term is intentionally thrown away by the simplified model. After this simplification, there is no viscous term in the evolution equation for the new density distribution function, thus, there is no need to introduce new variables to keep the viscosity the same for both governing equations. As a result, the above mentioned two shortcomings for the original double distribution model can be overcome. The details of the simplified thermal model can be found in [5]. In the application, the idea of TLLBM is also incorporated in the simplified thermal model so that thermal problems with curved boundary and the use of non-uniform mesh can be easily resolved. Fig. 2 shows the streamlines and isotherms obtained by the simplified thermal model for natural convection in a concentric annulus between an outer square cylinder and an inner circular cylinder at $Ra=10^6$ and aspect ratio of 1.67. The results are compared well with those from Navier-Stokes solvers.

Streamlines Isotherms

Fig. 2 Streamlines and isotherms for $Ra=10^6$ and rr=1.67

3.3 Fractional Step Lattice Boltzmann Model for High Reynolds Number Flow

The application of LBM is very simple as it only involves algebraic operation. On the other hand, it also suffers some drawbacks. One of them is the poor stability condition at high Reynolds number. According to the stability analysis, the relaxation parameter $\tau = 0.5$ is the margin of instability. When the Reynolds number is large, the viscosity ν is very small. As a consequence, τ will approach to 0.5 if the number of mesh points is not very large. In addition, as compared with the N-S solvers, more memory is needed in LBM to store the density distributions. To improve LBM for the application at high Reynolds numbers, Shu et al. [6] proposed the fractional step lattice scheme, where the efficient fractional step method is introduced into LBM, and the computation is taken by two steps. In the first step, the relaxation parameter τ is fixed as 1, which is well in the stability region of LBM computation. The viscosity in this step is fixed. Then in the second step, the real viscosity is compensated by using the fractional step method to solve a linear diffusion equation. In the scheme, the dependent variables are macroscopic density and velocity. So, the physical boundary conditions can be directly and easily implemented. The details of fractional step lattice Boltzmann model can be found in [6]. Fig. 3 shows numerical results of an extreme case of zero value of viscosity (Reynolds number is infinity) obtained by the fractional step LBM. Obviously, the flow attaches to the surface, and there is no vortex developed behind the cylinder or vertical plate.



Flow past a circular cylinder Flow past a vertical plate

Fig. 3 Simulation of inviscid flows by fractional step LBM

4. LATTICE BOLTZMANN MODEL FOR MICRO FLOWS

The key factor in the LBM is the relaxation parameter τ, which can be determined from the viscosity ν by the following relationship,

$$\upsilon = \left(\tau - 1/2\right) c_s^2 \delta t \qquad (5)$$

Note that the above relation is derived through the Chapman-Enskog multi-scale expansion in such a way that the obtained macroscopic variables from LBM satisfy Navier-Stokes equations. This means that equation (5) is implicitly based on the continuum assumption. As we know, the reference length in micro flows is very small, and the continuum assumption may not be valid. So, to apply LBM for simulation of micro flows, we have to abandon equation (5) and set up a new relationship between τ and the Knudsen number, Kn. Another important issue is that there are velocity slip and temperature jump in micro flows. Therefore, the bounce back rule used in the conventional LBM cannot be applied. From the kinetic theory, Lim et al. [7] and Niu et al. [8] established a new relationship between τ and Kn and proposed the diffuse scattering boundary condition to account for the slip condition on the wall. These new ways enable LBM to simulate micro flows effectively. Fig. 4 shows the non-linear pressure distribution along a micro channel obtained by the new LBM solver. Clearly, the LBM results compare very well with the experimental data of UCLA group both in the slip flow and transition regimes.

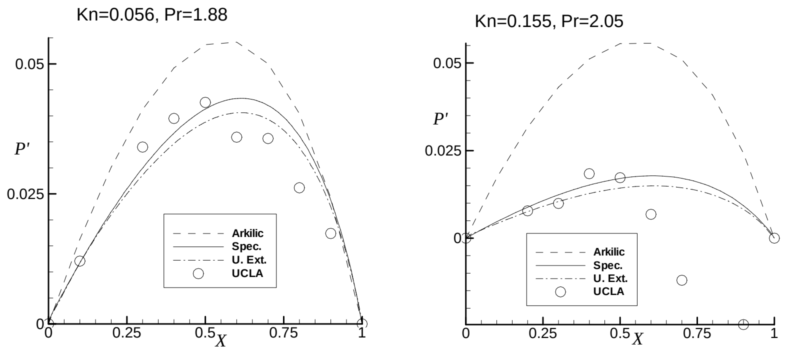
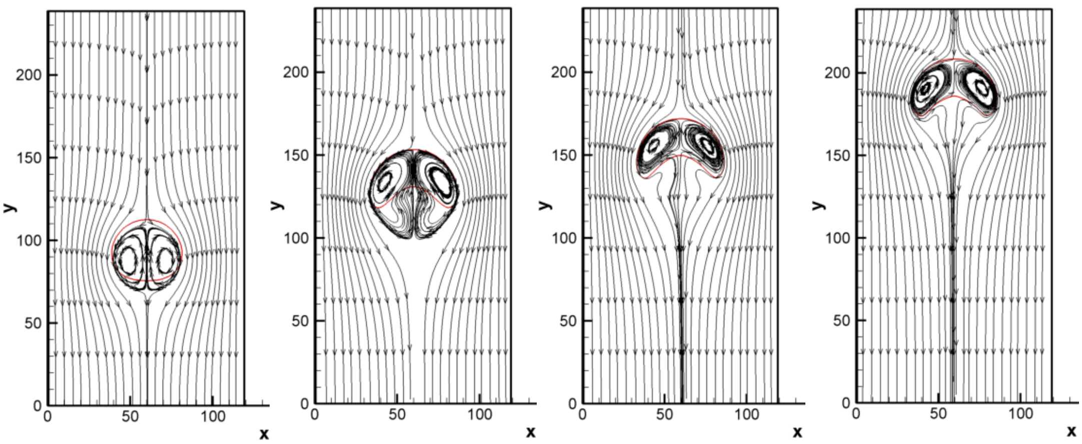


Fig. 4 Comparison of non-linearity of pressure distribution for a micro channel flow

5. LATTICE BOLTZMANN MODEL FOR MULTIPHASE FLOWS WITH HIGH DENSITY RATIO



(a) Step=1000 (b) step=3000 (c) step=4000 (d) step=6000

Fig. 5 The flow pattern of a bubble rising under buoyancy with density ratio of 1000

As LBM is very simple in implementation, it is a natural demanding to develop a lattice Boltzmann model to simulate multiphase flows. Currently, there are several models developed for multiphase and multi-component flows. They are color method, potential method and free energy method. All these methods regard the interface as a transition layer (diffuse interface). The color and potential methods do not explicitly describe the evolution of the interface. They regard the region with non-zero gradient of density difference as the interface. In contrast, the free energy method captures the interface by solving a convection-diffusion equation. A distribution function is designed to solve this equation. By using the Chapman-Enskog expansion, it was found that all the existing methods did not completely recover the lattice Boltzmann equation for interface to the Cahn-Hilliard equation. The efficiency is also not good. In addition, all the methods use the nine bits discrete velocity model in 2D interface capturing and fifteen or even more bits discrete velocity model in 3D interface capturing. To solve these problems, Zheng et al. [9, 10] proposed a new lattice Boltzmann interface capturing method, which can recover the lattice Boltzmann equation to the Cahn-Hilliard equation without any additional terms and it can keep the Galilean invariance property. In addition, the potential form of the surface tension related term is applied to reduce the spurious currents. As a consequence, the large density difference is incorporated in the interface capturing equation. Thus, it can be used to model multiphase flows with large density ratio which can be above 1000. Fig. 5 shows the flow pattern of a bubble rising under buoyancy with density ratio of 1000, where the red curves represent the bubble shapes (interfaces), which are defined as the position of zero value of order parameter. These results are in line with the experimental findings. For all the cases, a pair of vortex is first formed inside the bubble at beginning. Due to buoyancy force, the bubble will move upwards. In the meantime, the middle part of the bubble will encounter a larger deformation due to the hit of surrounding water.

6. LATTICE BOLTZMANN MODEL FOR COMPRESSIBLE FLOWS WITH STRONG SHOCK WAVES

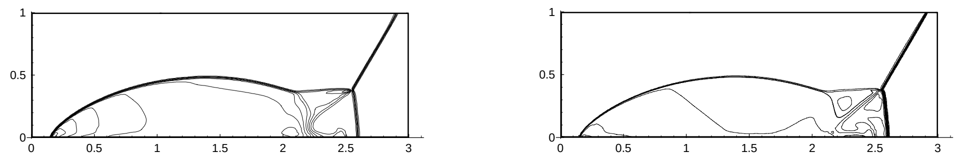
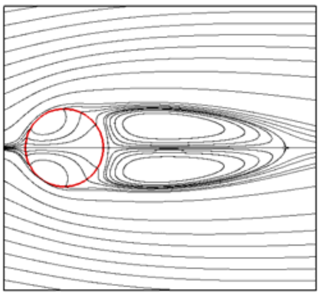


Fig. 6 Density (left) and internal energy (right) contours of the double Mach reflection problem

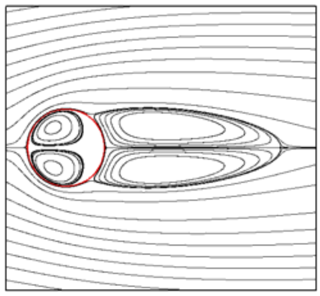
In the LBM application, one of the key issues is the determination of the equilibrium distribution function. For isothermal flows, it can be simplified from the Maxwellian distribution function by the Taylor series expansion in terms of Mach number. The coefficient in the equilibrium distribution function depends on the temperature (T). For the incompressible isothermal flow, T can be considered as a constant. Thus, the coefficient will not generate temperature gradient when the Chapman-Enskog expansion is applied. As a result, Navier-Stokes equations can be well recovered. However, when the compressible flow is considered where the temperate is changed, the coefficient in the equilibrium distribution function will generate additional terms of temperature gradient in the process of Chapman-Enskog expansion, which do not exist in the macroscopic governing equations. This is one of reasons why the conventional equilibrium distribution function cannot be applied to the compressible flow. Another reason is the limitation of small Mach number resulted from the Taylor series expansion in terms of Mach number. To apply the technique of LBM for simulation of compressible flows, Qu et al. [11] proposed an innovative way to construct the equilibrium distribution function for compressible flows by using the simple circular function. With this scheme, some supersonic flows with weak and strong shock waves were simulated successfully. Fig. 6 displays the density and internal energy contours of double Mach reflection at Mach number of 10. The results agree well with those obtained from the Euler solvers.

7. LATTICE BOLTZMANN-IMMERSED BOUNDARY VELOCITY CORRECTION METHOD (LB-IBVCM)

The immersed boundary method (IBM) is an efficient approach for simulation of flows around complex geometry and moving bodies. It comes from the concept that the deformation or moving of the boundary will yield a force that tends to restore the boundary to its original shape or position. The restoring forces on the boundary are in turn distributed into the surrounding nodes and the flow field with a body force is solved over the whole domain including both the inside and outside of immersed body. From the solution process, it is obvious that IBM is an iterative procedure to satisfy both the governing equation and the boundary condition. However, due to numerical errors, at the converged state, the non-slip condition is only approximately satisfied. As a result, some streamlines may pass through the solid body. This is not true in physics. To remove this drawback, Shu et al. [12] proposed the immersed boundary velocity correction method (IBVCM), in which, the velocity correction is made in the vicinity of the boundary point to enforce the non-slip boundary condition, and the ad hoc coefficient and the force calculation are not required. Due to common feature of using Cartesian mesh, IBVCM can be effectively combined with LBM to simulate incompressible viscous flows. Fig. 7 shows the streamlines of flow past a circular cylinder at Reynolds number of 40. As shown in the figure, the conventional LB-IBM results clearly reveal the penetration of streamlines to the cylinder surface. In contrast, the LB-IBVCM results do not have any penetration at all boundary points since the non-slip condition is accurately satisfied.



(a) Conventional LB-IBM



(b) Present LB-IBVCM

Fig. 7 Streamlines for the flow over cylinder at *Re* = 40

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