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COMPRESSIBLE LATTICE BOLTZMANN METHOD AND APPLICATIONS

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Abstract. Lattice Boltzmann Method (LBM) is a novel numerical method for flows simulations. Compared with classic methods of Finite Difference Method, Finite Volume Method and Finite Element Method, LBM has numerous advantages, including inherent parallelization and simplicity of boundary condition treatment. The LBM usually has a constraint of incompressible fluid (Mach number less than 0.4). A variant of the LBM is studied and used to deal with compressible fluid with Mach number up to 0.9 in this paper. Special emphasis is placed on mesh generation of 3-D complete geometry in Cartesian coordinate system. Numerical experiments are fulfilled in 2-D and 3-D compressible flows. Performance evaluation of the algorithm demonstrates high parallel efficiency and prefect scalability. Numerical results indicate that the LBM is successful with the simulation of compressible fluid.

Key words. Lattice Boltzmann Method, Compressible fluid, Cartesian Mesh generation.

1. Introduction

There are two different ways to numerically simulate fluid flow, i.e., one based on macro-continuous model from top to button and one of micro-discrete model from button to top. From Euler equations and Navier-Stokes equations, classical numerical methods of finite different method, finite volume method and finite element discretize the equations, obtain the liner systems and solve the systems. While such from top to button approaches intuitive, there are still many deficiencies. For example, in such method, often focus on analysis from the continuous differential equations to the discrete algebraic equations of the truncation error, but ignored the discrete process of conservation of certain physical quantities. Furthermore, in dealing with complex flow systems, to solve this type of nonlinear differential equations is very difficult or impossible.

In recent years, much attention of the Lattice Boltzmann method[1, 2] (hereinafter referred to as LBM) belong to micro-discrete model based on from button to top approach. In the LBM method, the fluid is an abstract for a large number of micro-particles, and these micro-particles in a discrete lattice migrate and collide in accordance with a simple movement rules. By the statistical particle can get the macro movement of fluid characteristics. This particle properties of LBM method also make the conventional numerical methods do not have many unique advantages, such as the physical image is clear, the boundaries treat easier and the computing is nature of parallel processing and so on. LBM method also provides the possibility and the reality of macro and micro. It is both a direct calculation of

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the viscous fluid, and also approximate Navier-Stokes equations under certain conditions. At the same time, LBM modeling is achieved with a simple mathematical modeling of complex systems, it also breaks the traditional concept of modeling for other complex systems and provides a new way. The evolution process of LBM method (in particular, LBGK model) is very simple and clear, its program more concise. Lattice Boltzmann method involved in the calculations are localized, with the natural parallelism, very suitable for large-scale parallel computer. Because of these advantages, LBM method is considered a promising method of calculation and raised a strong interest.

Currently, LBM has been in the multi-phase flow, porous media flow, particulate flow, reacting flow, magnetic fluid mechanics and bio-mechanics have achieved great success, their efficiency, accuracy and robustness have been widely confirmed. The traditional LBM methods can only handle low-speed incompressible fluid flow, can not be used for high-speed moving objects such as aircraft simulation, thereby limiting the application of the method. To calculate the high-speed compressible fluid flow, researchers have begun a new model of research, such as Alexander et al [7] approaches such as the use of controlled speed of sound; Yu and Zhao [4] introduce magnetism to reduce the speed of sound, thus alleviating the constraints of small Mach number impact, but these methods do not restore the energy equation, and apply to a limited extent. Palmer and Rector et al [9, 10] made the thermal LBM model, but still do not reflect the high Mach number phenomenon; Qu et al [7] proposed to use a circle function instead of using the Maxwell distribution function; Li et al [8] proposed a pairs of distribution function method; Sun et al [9] made the locally adaptive LB model, the speed of his model can get a very wide speed unlimited size; Yan Guang-wu [10] proposed multi-level multi-speed compressible model. These methods are the methods of changing the model of LBM proceed to find a distribution function and lattice model of a suitable compressible problem, in order to solve compressible fluid flow problems. These models themselves are some shortcomings, such as some models require large amount of computing, and some itself is complex, and some lack of rigorous theoretical derivation, and some extended to three-dimensional problem more difficult, reducing the usefulness.

Recently, Shan Xiao-wen et al [11] introduced Hermite functions and derived distribution function, and made theoretically the LBM method for solving compressible fluid flow problems, this method has a more rigorous mathematical derivation. This paper will use this method to study high speed compressible fluid problems.

2. The Lattice Boltzmann Method

Qian [2, 3, 4] and Chen [5, 6] et al used independently Bhatnagar-Gross-Krook (BGK) collision relaxation model, and proposed lattice BGK (Lattice BGK, LBGK) model, the complex collision operation transformed into a simple relaxation process:

$$f_i(\mathbf{x}+\mathbf{e_i}, t+1) = (1-\omega) f_i(\mathbf{x}, t) + \omega f_i^{eq}(\mathbf{x}, t), \tag{1}$$

where $f_i(\mathbf{x}, t)$ is defined in the discrete velocity set $\mathbf{e_i}$, is particle density distribution function at time t in the space grid points $\mathbf{x}$, $f_i^{eq}(\mathbf{x}, t)$ is the amount by the system's current macro-constructed local dynamic equilibrium distribution function, relaxation factor ω depends on the physical properties (such as fluid viscosity, thermal conductivity coefficient, mass diffusion coefficient). In LBGK model, The macrosystem state is constructed by the micro-particle group, on the other hand, the micro-particle group movement is controlled by the local macro-state of dynamics system. This reflects the individual partial discipline and adaptability. The local dynamic equilibrium distribution function $f_i^{eq}(\mathbf{x},t)$ is like a "Wizard" lead dynamically the system towards the state in line with objective laws. This relaxation technique makes the computational efficiency is very high.

Currently, LBM is no longer a pure fluid computing method, it is the design and modeling of complex systems provides a new way and means. The simplest and most commonly used LB model is the LBGK model using relaxation BGK collision model. The evolution equation of the LBGK model is:

$$f_i(\mathbf{x}+\mathbf{c_i}\triangle t, t+\triangle t) - f_i(\mathbf{x},t) = \Omega_i(f) = \omega(f_i^{(0)}(\mathbf{x},t) - f_i(\mathbf{x},t), \tag{2}$$

where$f_i(\mathbf{x},t)$ is particle density distribution function at time t in the space grid points $\mathbf{x}$ along the direction $\mathbf{e_i}$, $f_i^0(\mathbf{x},t)$is the corresponding local dynamic distribution function, $\mathbf{c} = \Delta\mathbf{x}/\Delta t$ is particle speed, the relaxation factor $\omega = 1/\tau$, τ said the relaxation time that particle distribution function reach the equilibrium state. The macro-density and macro-velocity of fluid determined by the following formula:

$$\begin{cases} \rho = \sum_{i=0}^{n} f_i = \sum_{i=0}^{n} f_i^{eq}, \\ \rho\mathbf{u} = \sum_{i=0}^{n} f_i\mathbf{c}_i = \sum_{i=0}^{n} f_i^{eq}\mathbf{c}_i, \end{cases} \tag{3}$$

The pressure is calculated by $p = C_s^2\rho$ The evolution of LBGK model is a relaxation process, through the micro-particle density distribution function f_i and the equilibrium state f_i^{eq} to speed up relaxedly,allowing the system to quickly evolve to meet the objective laws of the state. LBGK model is a class of high-efficient computing models, since it has been proposed, due to the high computational efficiency, the strong parallel, and the easy implement of program, as well as the advantages of the boundary handling simple, it is made the most significant LBM and used most widely model, was applied to many complex flow simulation. In LBGK model, The most common is Qian[2] made DdQq series model,see fig.1 where d is the space dimension, q represents the number of discrete speeds. The local dynamic equilibrium distribution functions of such models usually take the following format:

$$f_i^{eq} = \omega_i\rho\{1 + \frac{3(\mathbf{e}_i\cdot\mathbf{u})}{c^2} + \frac{9(\mathbf{e}_i\cdot\mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}\cdot\mathbf{u}}{2c^2}\}. \tag{4}$$

3. Compressible Lattice Boltzmann Method

This study simulates the compressible flow using the new LBM model[11].The equilibrium density distribution is expressed as:

$$\begin{aligned} f_i^{eq} &= \omega_i\rho\{1 + \mathbf{e}_i\cdot\mathbf{u} + \frac{1}{2}((\mathbf{e}_i\cdot\mathbf{u})^2 - \mathbf{u}\cdot\mathbf{u} + (\theta-1)(\mathbf{e}_i\cdot\mathbf{e}_i - D)); \\ &\quad + \frac{\mathbf{e}_i\cdot\mathbf{u}}{6}[(\mathbf{e}_i\cdot\mathbf{u})^2 - 3(\mathbf{u}\cdot\mathbf{u}) + 3(\theta-1)(\mathbf{e}_i\cdot\mathbf{e}_i - D - 2)]\}, \end{aligned} \tag{5}$$

where θ is dimensionless temperature, D is spatial dimension. The macroscopic density, temperature and velocity are calculated from:

$$\rho = \sum_{i=0}^{n} f_i; \tag{6}$$

$$\rho\mathbf{u} = \sum_{i=0}^{n} f_i\mathbf{e}_i; \tag{7}$$

$$\rho(D\theta + \mathbf{u}\cdot\mathbf{u}) = \sum_{i=0}^{n} f_i\mathbf{e}_i\cdot\mathbf{e}_i. \tag{8}$$

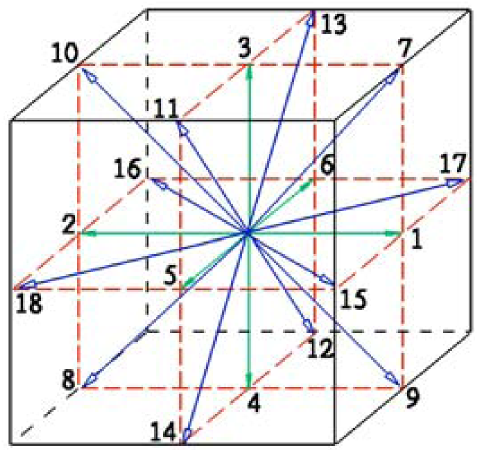

FIGURE 1. Qian's D3Q19 model

4. The Complex Boundary Conditions Handling

In the compressible lattice Boltzmann method, the boundary conditions handling approach plays an important effect on the accuracy and stability of the Boltzmann model. Macroscopic hydrodynamic equations, such as the Navier-Stokes equations, by the fluid velocity, pressure and so on the actual situation, is more convenient and directly given boundary conditions. But the compressible lattice Boltzmann method, through the dynamic equations of a particle distribution function of micro-state to describe fluid movement, the distribution function is not known on the boundary, and therefore need to construct a definite pattern, from the microscopic point of view the distribution function is given boundary conditions, so a lot of the boundary conditions handling approach are designed to appease the macro-flow boundary conditions. In the computing fluid problem, the no-slip boundary condition is a very important type of boundary condition. In the lattice Boltzmann method, the bounce back reflection is most common as the no-slip boundary condition. This method is relatively simple and handle easily, but this format is only a first-order accuracy, while the formula (2) is the second-order accuracy at the internal nodes, thereby reducing the overall accuracy of lattice Boltzmann method, and can only be used for no-slip boundary and not for movement boundary and Neumann boundary conditions and other complex boundary conditions.

In this paper, we use a non-equilibrium extrapolation method to handle boundary conditions. The non-equilibrium extrapolation boundary handling method draw the basic idea of extrapolation method in the design of numerical algorithm, it divide the distribution function f_i at the boundary nodes $\mathbf{x}_b$ into equilibrium and non-equilibrium two parts as follow:

$$f_i(\mathbf{x}_b, t) = f_i^{(0)}(\mathbf{x}_b, t) + f_i^{(1)}(\mathbf{x}_b, t), \tag{9}$$

the non-equilibrium part $f_i^{(1)}(\mathbf{x}_b, t)$ is the error of the equilibrium part $f_i^{(0)}(\mathbf{x}_b, t)$, satisfy $\left|f_i^{(1)}(\mathbf{x}_b, t)\right| << \left|f_i^{(0)}(\mathbf{x}_b, t)\right|$. So depending on the boundary conditions define a new equilibrium distribution to approximate equilibrium part, the non-equilibrium part obtained by the non-equilibrium extrapolation (a first-order format), the overall approximation accuracy of the attaining distribution function possess second order accuracy.

In this paper, this method is improved so that it applies more broadly, in particular the transition at the boundary corner points in the following ways will be more smooth, and the error smaller. Specific treatment methods are as follows. For velocity boundary condition, $u(x_b, t)$ is known, but the pressure $p(x_b, t)$is unknown, at this time the distribution function at boundary is determined by the following formula:

$$f_i(x_b, t) = \bar{f}_i^{(0)}(x_b, t) + (f_i(x_f, t) - f_i^{(0)}(x_f, t)), \tag{10}$$

Where $x_f$is the nearest fluid grid point withx_b , $\bar{f}_i^{(0)}(x_b, t)$ is a approximation of $f_i^{(0)}(x_b, t)$, it is computed by the following formula:

$$\bar{f}_i^{(0)}(x_b, t) = \begin{cases} \frac{w_0 - 1}{c_s^2} p(x_f, t) + s_0(u(x_b, t)) & i = 0, \\ \frac{w_i}{c_s^2} p(x_f, t) + s_i(u(x_b, t)) & i \neq 0, \end{cases} \tag{11}$$

5. The Advantages of LBM Method

With the traditional finite element and finite volume methods, LBM method has the following advantages:

(1) The natural parallel performance. LBM method only requires each node to independently calculate the collision and moving process, so the parallel performance of LBM method is very good, according to tests was almost linear speedup, see fig.2.

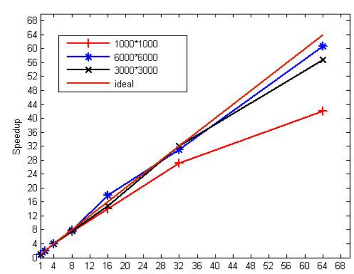

FIGURE 2. The speedup of cavity flow in different computing scales

(2) Simple boundary conditions handling. Just at the boundary can be a simple reflection.

(3) Simple mesh generation. In the usual entire aircraft CFD calculation, the mesh generation is generally the total workload of 60-70%, This is because the entire aircraft has very complex geometry, to obtain high-quality three dimensional structural or non-structural mesh, need to do a lot of meticulous work. However, The LBM method needs only the geometric shape of the entire aircraft to make a three dimensional surface mesh, and then can generate three dimensional Cartesian meshes. At the same time, we can see from their generation process, in the traditional method, the total number of body mesh and the number of the surface mesh are related, such as generating 10,000,000 body meshes, its surface meshes only 500,000-600,000(for

example, the boundary layer is generated 10 layer). In the LBM method, the total number of body mesh and the number of the surface mesh are irrespective, in order to characterize the complex geometric structure of the entire aircraft, resulting in 10,000,000 body meshes, see fig.3, we can use 1,000,000 or more surface meshes, which can be more subtle describe the complex geometry of the entire aircraft, in order to obtain accurate results lay the foundation.

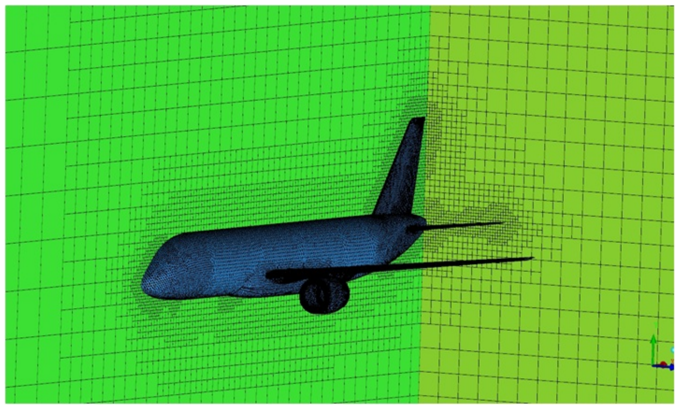

FIGURE 3. Mesh profile diagram of an aircraft model

6. Numerical Experiments

6.1. One-Dimensional Shock Tube. Sod shock tube problem is a classic problem, it can be verified that the algorithm is reasonable. Initial conditions: At $t = 0$,

$$p_l = 10, \rho_l = 8, v_l = 0, x < 250,$$
$$p_r = 1, \rho_r = 1, v_r = 0, x > 250,$$

For the ideal gas, gas constant $\gamma = 1.40$, in Calculation, taking quality points to 500. Fig.4 shows the calculation results, we can see that these new LBM method can be well simulated shock interruption to verify our algorithm.

6.2. Two-Dimensional NACA0012 Transonic Airfoil. Transonic flow region, including the flow Mach number is greater than 1.0, less than 1.0, equal to 1.0 situation, the flow phenomenon more complicated, more difficult to solve, the next figure shows the calculation results of new LBM methods.

6.2.1. Three-Dimensional Cavity Flows. In this calculation of three-dimensional lid-driven cavity flow problem, the area size is the length width height each for 100 meshes, a total of 1,000,000 meshes. Lid-driven flow Mach number is 0.7, the dimensionless pressure 1.0, the density 1.0, the result as shown below.

6.2.2. High-Speed Train. This Calculation takes into account three trains models (including the locomotive, the middle compartment, and tail each one). The space mesh is Cartesian orthogonal mesh, a total number of space mesh is about 40 million. Speed is 250 km/h.

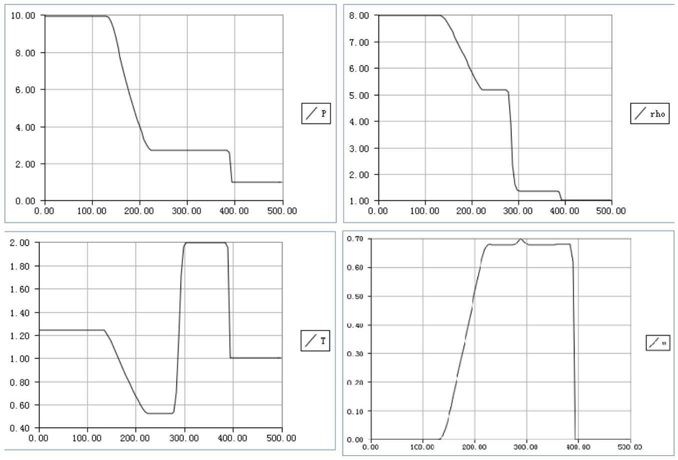

FIGURE 4. The calculation results of Sod shock tube

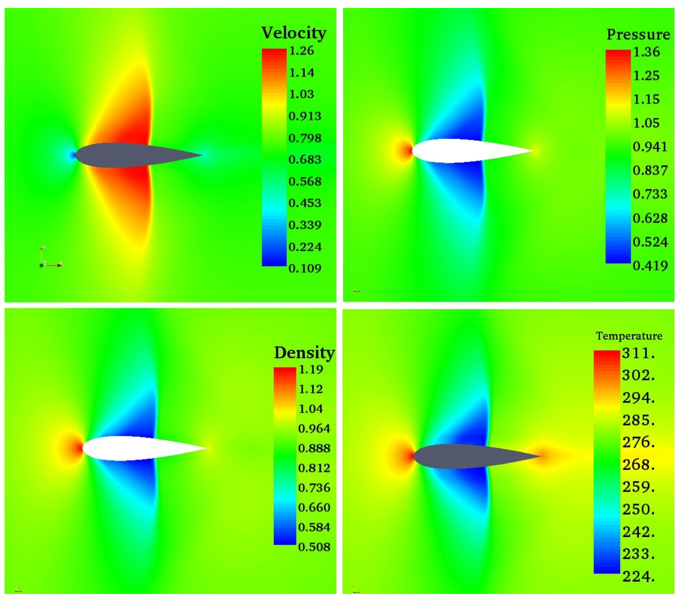

FIGURE 5. The calculation results of NACA0012 transonic airfoil

7. Conclusion

Compressible LBM are studied and the applications to 2-D and 3-D flows are fulfilled. Large-scale 3-D transient Lattice Boltzmann code with the capabilities of handling multi-component flow, complex geometry and turbulence modeling will be studied in the future.

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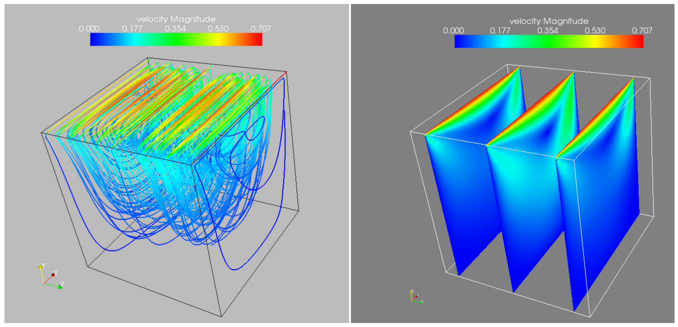

FIGURE 6. The calculation results of three-dimensional cavity flow

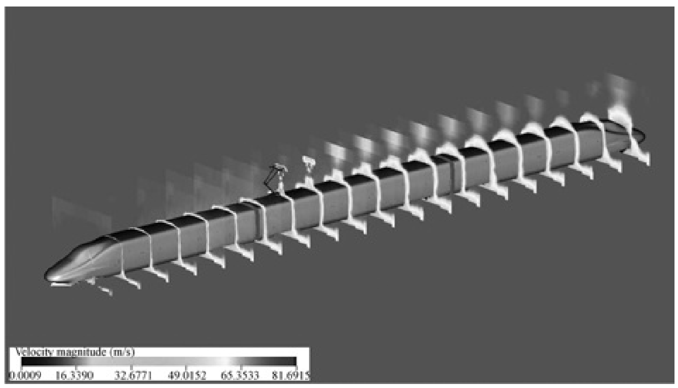

FIGURE 7. The calculation results of high-speed train

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