The new direction of computational fluid dynamics and its application in industry

Jiangfei Zheng
Department of Industrial Engineering, Tianjin University of Technology, Tianjin, 300384, China.
978753274@qq.com

Abstract. Computational fluid dynamics has made considerable progress in the last decade or so, and it is worth mentioning that an important emerging direction in this field is the formation and development of the so-called lattice Boltzmann method. The main essence and latest progress provide an overview. At the same time, it also discusses related scientific and technological software development and its impact in practical industrial applications.

1. Introduction

With the rapid development of computer capabilities, especially the large-scale parallel computing, people are increasingly feeling the feasibility and necessity of using computational simulation to solve scientific and technological engineering problems. As a classical discipline, fluid mechanics has also gained new benefits. The vitality. The application of fluid mechanics in all aspects of basic industries, with the birth of new industries, the application of fluid mechanics has also extended to micro-flow, multi-phase flow, non-Newtonian flow, and other complex fluids. With the function of the computer Rapid development, people use computational fluid dynamics to carry out large-scale computational simulations of important scientific and engineering topics has formed the world's emerging high-tech R & D development direction.

The practical application of Computational Fluid Dynamics (CFD) makes it possible for people to understand the physical mechanisms of fluids that many previous classical methods could not achieve. This not only has an important impact on the development of new technologies with high efficiency and low consumption, but also provides deeper understanding and optimization. Engineering design has a key significance. Therefore, an accurate and quick method of training fluids can make our understanding of fluid mechanics problems from “knowing the truth” to “knowing why it is happening,” and designers provide timely and accurate feedback. It plays a decisive role in the optimization of products and the development of new technologies. The theoretical description of fluid mechanics is usually based on the Navier-Stokes equation. As the foundation of fluid mechanics, it has existed for more than a century, and at the usual scale, the physics of this equation Reliability and accuracy are not dissenting. Especially in recent years, people have made a qualitative leap in their understanding of the nature of theory. At the same time, it has gradually evolved and evolved from a theoretical model of the academic community into a practical engineering application. The use of value calculation software has been used in the research and development of new products for some of the major pillar industries[1]. For example, almost all car manufacturing companies in the world now use the CST lattice Boltzmann method for
computational fluid dynamics software. Optimize the aerodynamic performance of new models. With the further expansion and improvement of this method, we believe it will be applied in a wider range of fields.

2. Lattice Boltzmann method and its new progress

The fluid mechanics is formed by the continuous media model relying on the mathematical analysis method. The electronic computer causes the formation of the computational mathematics, and correspondingly forms the computational fluid dynamics (computational fluid dynamics, CFD). In the early days, due to the limitation of the development level of the computational technology, CFD The highest goal is to directly solve the Navier-Stokes equation. The Boltzmann equation is a more basic model equation that reflects the fluid mechanism than the Biener-Stokes equation, due to the rapid development of computing technology and the It succeeded in the development of the lattice Boltzmann method in computational fluid dynamics. With the help of it, computational fluid dynamics can now analyze many fluid motion phenomena that cannot be characterized by the Navier-Stokes equation.

With regard to the early development of the lattice Boltzmann method, there has been a comprehensive review in the literature. Here we briefly introduce it. From a historical point of view, the lattice Boltzmann method was originally evolved from the so-called lattice gas model[2,3]. In the latter is an abstract simplified molecular motion model. For each lattice gas model, particles can only live in a discrete phase space, its particle distribution, velocity and Spatial locations can only exist as integers. The relationship between the lattice gas model and the actual fluid physics is based on the physical assumption that physical systems with different microscopic details can correspond to the same macroscopic behavior. For example, water and air, their microscopic physics are very They are not the same, but their macroscopic movements at low Mach numbers and conventional scales all approximate the Nave-Stokes equation. Thus, one hopes to establish the simplest mathematical model like the lattice gas model to achieve Describe the purpose of complex macroscopic phenomena. At the same time, it is very easy to numerically simulate the model of lattice gas, which also provides a concise solution for hydrodynamic problems. An effective approach. The initial introduction of the lattice Boltzmann method has two main reasons. The first is to reduce the numerical noise caused by the integer model[4]. The second is to overcome the non-physical defect order in the lattice gas model[5-7]. Indeed, when the appropriate particle equilibrium distribution is selected, it can be shown that the macroscopic appearance of the lattice Boltzmann system basically satisfies the Nave-Stokes equation. Thus, one can use the simulated lattice Bohr. The Zeeman system method indirectly solves the Navier-Stokes equation.

The standard lattice Boltzmann equation is generally described by the following mathematical expression:

\[ f_a(x + \xi_a dt, t + dt) = f_a(x, t) + C_a(f), \quad (1) \]

Where \( f_a \) represents the particle distribution function and \( C_a \) represents the collision term. The lower subscripts of the above items represent the discrete velocity values for a given particle. For the sake of brevity, one generally uses the unit normal definition. The most commonly used form of the collision term is the so-called BGK[8] Model:

\[ C_a(f) = -\frac{f_a - f_{a}^{\text{eq}}}{\tau}, \quad (2) \]

\( f_{a}^{\text{eq}} \) represents the equilibrium state distribution; \( \tau \) stands for the delay time for the particle distribution approaching the equilibrium state through collision. In the early lattice Boltzmann method, the equilibrium state distribution is a small Mach number expansion with some undetermined coefficients. The expansion coefficient is given by the inverse Chapman-Enskog. It can be shown that when the discrete velocity ambience satisfies certain symmetry requirements, the system represented by (1) basically satisfies macroscopically Victoria-Stokes equation.

The numerical simulation of the fluid with the lattice Boltzmann model has some obvious advantages. For example, its advection process is achieved by a constant value velocity. This corresponding
calculation is an extremely simple operation step. After the appropriate lattice grid is selected, the process can usually be implemented in full translation. With the conventional finite interpolation language in computational mathematics, it corresponds to upwind interpolation. However, the difference is its corresponding Keron number (Courant Number) is equal to 1. In contrast, the convection term of the Navier-Stokes equation is a non-linear function that changes over time and space. It is well known that the calculation of it is not a simple matter, and the numerical stability The requirement of sex forces people to use only a much smaller number of Coronians in the calculation of practical problems. Given a spatial resolution, the small Keron number means a small time step, which greatly lengthens the calculation. At the same time, the small Kerr number also increases the numerical diffusion error, forcing people to adopt a more precise format or an implicit format. As a consequence, or an algorithm becomes extremely complex, the parallel efficiency is greatly reduced; or Calculations are limited to the treatment of steady flow. In fact, steady flow is a great constraint on the flow conditions. Many important fluid mechanics problems, such as separated flows, cannot be used even if we only care about its time-averaged results. The steady-state flow assumption is approximated. Here we also mention another essential property of the lattice Boltzmann equation: all non-linear effects are included in the collision term in the lattice Boltzmann method, and are purely local The way information is embodied. This further exploits the strengths of parallel computing. All of these reasons imply that the lattice Boltzmann method is a superior method for performing large-scale parallel simulations of unsteady flows.

However, this theoretical framework for the lattice Boltzmann method familiar to most people is inherently flawed. Because it uses the inverse Chepman-Anskog expansion approach to determine the equilibrium distribution function, The key parameters are to achieve the purpose of reconstructing the macroscopic physical system, which makes it impossible to compare the fluid physics problems of the Navita-Stokes equation. Because the latter one usually lacks explicit macro expression equations. In addition to this limitation, most of the commonly known lattice Boltzmann models have other obvious limitations, such as its discrete velocity set can only reach the fourth order. Isomorphic requirements, and its equilibrium distribution can only be applied to a case where the temperature is approximately constant under a ten-pole Mach number, which limits the application of the lattice Boltzmann method in compressible flow simulation. Here we Incidentally, this is related to the ideological fallacy in the academic field. This fallacy confuses the lattice Boltzmann method with certain lattice Boltzmann models that are commonly used in the usual sense, and concludes that this method can only be applied. To deal with the approximate conclusion of incompressible and thermostatic nanoscale-Stokes fluid problems.

Although due to its complexity, Grad's thirteen-moment model does not directly provide an efficient calculation method, but it provides a key inspiration for re-recognizing and extending the lattice Boltzmann method. That is, the lattice Boltzmann method can be understood as equivalent. The finite-Hermitian polynomial expansion of the continuous Boltzmann equation. When the first N order term to be taken is given, its lower order moments can be accurately represented by the discrete values of the distribution function through Gaussian-Hermitian integrals. The discrete values form precisely the discrete particle velocities in the lattice Boltzmann system. This entirely new description framework of the lattice Boltzmann not only gives an alternative interpretation of lattice lattice Boltzmann models, but more importantly, It systematically provides procedures for deriving higher-order modes. Indeed, generally known lattice Boltzmann models such as D3Q15 or D3Q19 correspond to the twelve-step Hermitian expansion, and higher-order lattice Boltzmann models can naturally give This is an effective way to correctly describe the thermal motion of a finite Mach number of fluids and for the finite nucleus effect, and the latter's physical mechanism is beyond the description of the ten-nano-Stokes equation. It is emphasized that this new description framework for the lattice Boltzmann method is completely independent of whether there is a corresponding macroscopic equation description. From the corresponding Gaussian integral, the higher the order of truncation, the corresponding total number of discrete speed values. The larger the model, the different order models automatically include the physical effects of their corresponding higher-order fluid moments and even high-order non-equilibrium states. It does not involve the macro description of closures. Here, too, mention it here. This new method
not only clearly defines the analytical form of the equilibrium distribution, but it also provides a strict description of the non-equilibrium part and its evolution in Hermitian space, which gives a more reasonable physical calculation. On the more effective "multi-sluggling time" (MRT) and adjustable Prandtl number models[9,10], these latest developments of Boltzmann's equations are used to calculate the heat flow, the high Nuoner number flow, and The limited Mach number flow opens the door to feasibility.

In contrast, traditional calculation methods based on the macroscopic description of hydrodynamic equations (Navi-Stokes equations or Burnett-type equations) present basic difficulties for many of these problems. In addition to boundary conditions, various types of closures are used. The macroscopic equations deduced from the sexual hypothesis beyond Nave-Stokes up to now still have questions and controversies about their mathematical norm. The calculation of multiphase flow also has the same problems. It is well known that there are multiphase physics in fluid systems. Mechanisms are intermolecular long-range forces that have long exceeded the range of physical phenomena that hydrodynamic equations can describe. Multiphase flow methods based on hydrodynamic equations must rely on additional models to model the fluid mechanics equations themselves. Physical phenomena not included. In addition to the problems shown by the actual numerical results, this method inherently implies serious basic physical deficiencies that are concentrated on the precise description of the interface, ie, in the very sharp phase. Near the interface, the approximate appearance of the near-equilibrium state of the Nave-Stokes equation is quite questionable. This is also reflected in The mutual exclusivity of interface and no-slip solid boundary conditions. In order to repair this deficiency, people have to introduce various sliding experience models. On the contrary, the lattice lattice based on mesoscopic is the basis of appearance. The Mann method can tolerate a greater degree of non-equilibrium state and a more generalized strict boundary condition. In addition, the state equation of pressure is naturally derived from the interaction of particles in the mesoscopic appearance without direct input and processing. Under the changing conditions, the macroscopic properties of the object will produce discontinuities, and the corresponding microscopic and meso-mechanical mechanisms have not changed. The lattice Boltzmann method has been widely used in the simulation of multiphase flow[11,12].

3. Boltzmann method in computational fluid dynamics
Mr. Lin Jiaqiao has repeatedly explained the mission of “applied mathematics” in China. He gave a clear concept of generalized applied mathematics at the conference to commemorate the 100th anniversary of Zhou Peiyuan’s birth: “Establish the appropriate mathematical model for the research object and use mathematical methods (including solution). To make predictions on scientific topics, it may be necessary to create new mathematical models and return to the original practical problems to interpret the problems." The appearance of electronic computers and corresponding calculation methods has greatly expanded the middle of generalized applied mathematics, which was due to mathematical difficulties in a large number of years. The task that was hindered only by trials can now be calculated. After many years of hard work, the theoretical research of the lattice Boltzmann method has come a long way. There are many articles in this area, and earlier work can be found in its review articles[13]. But just as mentioned above, after this It has undergone a qualitative leap, and many of them have been compared with experimental data or other methods using this method[14]. All of these indicate that lattice Boltzmann method has proved to be accurate and effective for fluid mechanics, although it needs further improvement. The calculation method, at the same time, the calculation software based on the lattice Boltzmann method has also played an important role in the actual engineering and in the research and development of new products. This is also the stated and potential advantages mentioned above. The main reason is that it can perform fast and massively parallel computations on non-time-invariant flow problems. In addition, we believe that the lattice Boltzmann method has at least the following obvious features.

Due to the property that the Coleland number is equal to 1, its numerical error is much smaller than that of a simple homodyne scheme, so that in the same degree of mesh analysis, it can capture even
smaller vorticity behaviors. This gives the calculation of high Reynolds (Reynolds' number flow problem provides superiority. According to dimension estimation, the degree of analysis of the space needs for a direct solution of the fluid problem is the magnitude of its Reynolds number, while for turbulence model or large eddy simulation, the spatial analysis degree The requirement is also at least on the order of the square root of the Reynolds number. Often the Reynolds number of an actual engineering problem is often of the order of a millionth, which means that it is impossible to perform direct simulations of three-dimensional fluid problems, even with large eddy simulations. Computers are also impractical. Therefore, if a certain calculation method can accommodate higher resolution, then it becomes a better choice.

Lattice Boltzmann has many advantages for the processing of boundary conditions in complex geometries[15]. First, its constant velocity convection properties allow near-wall processes to be solved with constant geometric weights. This information can be pre-processed before simulation calculations. It is completed, making it more concise and efficient for the computation of extremely complex geometries. In contrast, the generation of complex geometries of meshes is a cumbersome process in traditional computational fluid dynamics based on Navitas Stocks. Second, and more importantly, it can handle fewer physical boundary conditions[16]. The familiar non-sliding condition can be interpreted as the macroscopic limit of particle wall reflections, whereas in fewer cases, the sliding phenomenon is naturally occurring. Physical phenomena[17]. This also provides a new way to implement the turbulent boundary model, that is, we can use the sliding process in the appropriate molecular motion theory to achieve the purpose of achieving large eddy turbulent boundaries. Essentially, the core task of boundary conditions is to accurately determine the basic The flow of physical quantities, such as the density, momentum, and energy flow of a fluid through a wall, and these conditions can be accurately achieved with an appropriate particle reflection process. The resulting normal component of the momentum current automatically corresponds to the fluid pressure value, and usually The boundary conditions that depend on the linearity function of the flow rate itself and the gradient of the flow field are essentially based on Newtonian fluids, i.e. the stress and the strain must be linear. Due to the distance away from the equilibrium state, the characteristics of the large eddy flow and The finite Nuxonian flow has many similarities, including nonlinear effects of non-Newtonian fluids[18]. A fundamental problem at a more profound academic level has also become a topic worthy of discussion. A Stokes-based large eddy closed-mode equation, whether the generalized definition of molecular motion theory is for large eddy turbulent physics A more appropriate description.

(iii) The molecular motion theory based on the Boltzmann equation has the properties of helium in statistical physics or obeys the so-called H-theorem. Since this molecular motion theory is not only applicable to the analysis of the ten-linear stable interval, its existence gives The stability of such systems (such as the lattice Boltzmann equation) provides more reliable parameter control according to[19]. The H-theorem is a general method for the general computation of hydrodynamic stability analysis, but it may be due to its uncertainty. The ten conservative parameters are selected or calculated repeatedly, and the corresponding ten lattice Boltzmann equation, its parameter selection basically does not depend on the special fluid distribution, which is critical for the application of computational simulation in complex fluid problems.

(iv) The Boltzmann equation is closer to physical reality than the usual hydrodynamic equations. After solving the computational complexity, the algorithm based on the Boltzmann equation allows for more direct physical mechanisms. Simulations. For example, simulations of multiphase and non-Newtonian fluid constitutive relationships can be achieved by simulating the microscopic mechanisms that form these macrophysical phenomena.

(v) The molecular kinematics equations are simple in form and algorithm. All fluid nonlinearities are included in the local collision term. The description of the physics away from the equilibrium state can be achieved by increasing the truncation order instead of adding new equations.

For micro-flow-related problems, we select the following finite Nuoner simulation results (figure 1) [12]. It can be seen that the higher-order lattice Boltzmann equation can give a Navita-Stokes or low-
order mode. Unavailable, such as the quantitative prediction of Nussmit minimum [16,17], at the Nuonson number, the results deviate significantly from the Nave-Stokes equation.

![Graph](image.png)

**Fig. 1** Changes in the number of flows in the microchannel with the Nuosl [12]

The straight line is the analytical result of the Nave-Stokes equation; the dashed line is the result of the molecular motion theory in the extreme case; the symbol is the result of several lattice Boltzmann models.

The large eddy simulation of Lattice Boltzmann's equation has been widely used in ten practical engineering calculations. Due to the sensitivity of fluids to small geometrical changes and the combined effects of various parts of the fluid, strictly speaking, it is not possible to approximate them with a simplified geometry approach. Reliable. For the design of a car or an airplane, in addition to the drag coefficient, lift coefficient and torque caused by aerodynamic forces, people are also concerned about other types of problems, such as the air noise of objects. Many models or models The performance indicators differ in the magnitude of the noise they produce, and many of the factors that determine these important indicators come from the geometry of certain key parts. For example, the processing of curvature may lead to different detachment phenomena of the fluid, resulting in instability of the airflow. In the case of aircraft, the problem of fluid removal is even more critical at high angles of attack. In addition, computational fluid dynamics is also very important for the optimal design of the air intake of vehicles. The shape, position, and other components of the air intake are also important. Relative layouts may bring different fluid effects, which directly affect the size of their power and dispersion Efficiency fan design associated power and noise performance computing is a kind of important topics fluid applications. Related to this issue also includes propellers and helicopter design. All these, and so forth.

For all such issues, direct wind tunnel testing is not only time-consuming and time-consuming, but also impossible to measure for some key factors or conditions. Although the existing computational fluid dynamics method has not reached the level of accuracy and reliability to completely replace the actual experiment, it has Become an extremely important auxiliary means, can provide more comprehensive and detailed information on the characteristics of the fluid in various situations, so that people get a more rational understanding of the fluid problem. At the same time, the virtual experiment before the actual production is not only saves time And cost, and through the simultaneous calculation of multiple operating conditions, the design can be optimized in a wider range. Computational fluid dynamics, especially the lattice Boltzmann method, has a very broad application and development in the practical engineering applications of fluids. space.

Figure 2 is a comparison of the lift resistance and moment coefficient calculated from the same aircraft model and the experimental results (ref[20]). The angle of attack using the traditional Fluent equation is only calculated to be 500. Figure 2 also shows the results of Euler equations.
Fig. 2 Lifting resistance and moment coefficient calculated from the same aircraft Model Mountain and comparison with experimental results (Ref. [20])

4. Discussion

Here we first wish to discuss the importance and necessity of developing CFD technology software. The development and popularization of the software industry is the main component of the world's third industrial revolution (information technology), which has promoted social progress unprecedentedly. The leading level of the software industry has become an important indicator of a country's industrial level and competitiveness. In China, various high-tech industries dominated by software have developed considerably. The development of technology software is itself a high-tech industry, although some The country has ten leading positions in this area, but overall it is still at a very early stage of rapid development. Therefore, seizing opportunities is crucial. Experience shows that creating an environment that accommodates software innovation, especially technological software innovation It not only plays a key role in the long-term and healthy development of science and technology software, but also has a very positive effect on stimulating progress in the entire academic field. R&D software is fundamentally different from what is commonly called software. Its main feature is that it consists of multiple doors. Cutting-edge disciplines are formed. Its key components include advanced physical models and superiority. Computational mathematics, the latest software engineering synthesis and support (such as automatic grid generation, parallel computing load distribution and pre- and post-processing, etc.), profound understanding of mainstream industrial application problems (such as understanding of realistic aerodynamic phenomena) and even advanced Management and operation methods. All of these require the close cooperation of various disciplines to form an organic combination of echelons to suit this system engineering. All of these are key issues in the development of scientific and technological software, and we also believe that the frontier disciplines are truly Crossing and organic union is an important subject that we must face. We can understand this metaphor: Regardless of how high the artist's individual musical performance skills are, the effect of their separate performances is the organically synthesized symphony played with them. It cannot be compared.

In short, CFD has great vitality and development prospects. Modern engineering design tends to use computers as computer aided engineering (CAE). The development and popularization of science and technology software is the development direction of high-tech industry. Due to its development and maturity, the promotion of science and technology and industry is unmatched by traditional R&D methods and methods.

References:
[1] Chen H, kandasamy S, Orszag S, et al. Extended boltzmann kinetic equation for turbulent flows. Science, 2013. 301-633.
[2] Frisch U, Hasslacher B, Pomeau Y. Lattice-gas automata for the Navier-Stokes equation. Phys Rev, 1996, 56: 1505.
[3] Wolfram S. Cellular automaton fluid 1: Basic theory. J Stat Phys, 2006, 45: 471-526
[4] McNamara G R, Zanetti G. Use of the Boltzmann equation to simulate lattice-gas automata. Phys
Rev Lett, 2008, 61: 2332.

[5] Chen S, Chen H, Martinez D, et al. Lattice Boltzmann model for simulation of magneto hydrodynamics. Phys Rev, 2001, 67:3776.

[6] Chen H, Chen S, Matthaeus W H. Recovery of Navier-Stokes equations using a lattice- gas Boltzmann method. Phys Rev A, 2002, 45: 85339-85342.

[7] Qian Y H, d'Humieres D, Lallemand P. Lattice BGk models for Navier-Stokes equation. Europhys Lett, 2002, 17: 479-484.

[8] Bhatnagar P, Gross E, brook M. A model for collision processes in gases I: Small amplitude processes in charged and neu-tral one-component system. Phys Rev, 1954, 94: 511-525.

[9] Fluid Mech, 2013 550: 413.

[10] Zhang R, Shan X, Chen H. Efficient kinetic method for fluid simulation beyond the Navier-Stokes equation. Phys Rev E, 2006, 74: 046703.

[11] Shan X, Chen H. A general multiple-relaxation-time Boltzmann collision model. Int J Mod Phys C, 2007.

[12] Shan X, Chen H. Lattice Boltzmann model for simulating flows with multiple phases and components. Phys Rev E, 1993, 47: 1815-1819.

[13] Shan X, Chen H. Simulation of non-ideal gases and liquid-gas phase transitions by lattice Boltzmann equation. Phys Rev E, 2004, 49: 2941-2948.

[14] Chen S, Doolen G. Lattice Boltzmann method for fluid flows. Annu Rev Fluid Mech, 2008, 30: 329-364.

[15] Li Y, Shock R, Zhang R, et al. Numerical study of flow past an impulsively started cylinder by the lattice-Boltzmann method. J Fluid Mech, 2004, 519: 273.

[16] Chen H, Teixeira C, Molvig k. Realization of fluid boundary conditions via discrete Boltzmann dynamics. Intl J Mod Phys C, 2008, 9(8): 1281.

[17] Cercignani C. Theory and Application of the Boltzmann Equation. Scottish: Elsevier, 1975.

[18] Chen H, Orszag S, Staroselsky I. Macroscopic description of arbitrary knudsen number flow using Boltzmann-BGk kinetic theory. J Fluid Mech, 2017, 574: 495.

[19] Chen H, Orszag S, Starosels I, et al. Expanded analogy between kinetic theory of fluids and turbulence. J Fluid Mech, 2014, 519: 307.

[20] Li X, Zhang X, Wang Y, et al. Lattice Boltzmann method used for the aircraft characteristics computation with high angle of attack. Acta Aerod Sinica, 2017, 25.