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格子玻尔兹曼方法概述:详尽的历史性文献及待探讨的理论问题

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摘要： 本文给出了详尽的格子玻尔兹曼方法的概述：包含其理论基础、起源、基本思想及主要特征，历史进展、重要的综述、著名书刊、应用及可用计算机代码，从而为从事有关研究的学生与研究人员提供了丰富的参考文献．通过文献检索阅读，揭示了以下有待探讨的理论问题：(a) 麦克斯韦-玻尔兹曼分布(Maxwell-Boltzmann distribution)的建立只涉及稀薄气体的压力内能，但未考虑粘性应力的内能；(b) 三个守恒律无法从玻尔兹曼方程直接导出，必须借助外加的小参数展开完成，同时在守恒方程中无法引入外力及能源的贡献；(c) Lattice Boltzmann Method (LBM)执行中，只更新流体的物质密度和平均速度，不更新其内能参数．由于在复杂流动中，流体的内能是时间及空间的函数，因此其理论是不完整的．以上揭示的理论问题是现有LBM方法不能有效地求解涉及高速及大压缩性引起内能剧烈变化的复杂流场的原因．作者给出一篇理论研究文章以回答揭示的理论问题．

关键词： LBM概述；LBM理论；麦克斯韦-玻尔兹曼分布；宏观内能参数；守恒律；LBM历史文献

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A Short Review on Lattice Boltzmann Method: Comprehensive Historic Resources and Theoretical Problems to be Addressed

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Abstract: This short review presents a detailed introduction to lattice Boltzmann method (LBM) involving its theoretical background, originality, fundamental ideas with main characteristics, historic developments, important review papers, recognized books, applications, and available computer codes, which provides comprehensive reference resources for students and researchers intending to engage the related research. Through reading the publications, it is revealed that the following theoretical problems need to be addressed. (a) Maxwell-Boltzmann distribution developed from dilute gases concerns only the pressure-internal energy, but does not reflect the one produced by viscous stresses. (b) Three conservation laws cannot be directly derived by the lattice Boltzmann transport equation, but need a multi-scaling expansion, and the energy conservation equation does not include the external energy generation source. (c) LBM has an implementation process that only updates the two macroscopic parameters: the mass density and the mean velocity, without updating the internal energy, and therefore is not a complete theory, since the internal energy in complex flows is a function of time and space points. These revealed issues could be the reasons causing current LBM

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schemes failed to simulate the flows with high speeds or high compressibility concerning obvious change of internal energy in flow fields. Finally a paper of theoretical investigations on LBM is given as an effort to address these revealed problems.

Key words: short review on LBM; LBM theory; maxwell-boltzmann distribution; macroscopic internal energy parameter; conservation laws; LBM historic references

1 Short introduction review

1.1 Theoretical background

Lattice Boltzmann method (LBM) is based on the Boltzmann's contribution in microscopic molecule dynamics[1-5], of which the system under consideration in the classical kinetic theory of gases is a dilute gas of N molecules enclosed in a box of volume V with a sufficiently high temperature, and the density is sufficiently low with large average intermolecular distance. It is not interested in the motion of each molecule in details, but in its distribution, defined as the number of molecules at a time and at a position of the phase space.

As discussed by [6], the Boltzmann transport equation (BTE), created by Boltzmann in 1872[7-9], governs this distribution function, and the moment equations of the distribution functions yield the conservation laws for macroscopic systems. Furthermore, the Boltzmann H theorem confirms that the equilibrium distribution function (EDF) satisfying BTE makes the time derivative of H-functional $\leqslant 0$, and the theoretical EDF satisfying the conservation laws is the Maxwell-Boltzmann distribution (MBD) [7]. These theoretical results opened the door to an understanding of the macroscopic world based on molecular dynamics, which builds a solid theoretical foundation for LBM, as a mesoscopic method, to deal with macroscopic motions in continuum mechanics, and to solve partial differential equations[10-12].

The Boltzmann equation is a differential-integral equation, of which the differential cross-section area involves complex different types of collisions, so that the solution is very difficult, and attempts have been made to "model" and simplify the collision term. The best-known model equation is constructed by [13] based on which LBM to be implemented for simulations of fluid flows.

1.2 Originality

Originally, LBM was developed from the lattice gas automata (LGA) [14-15], a discrete particle kinetics utilizing a discrete lattice and discrete time, which is constructed as a simplified, fictitious molecular dynamics with all discrete space, time, and particle velocities. In LGA method, at a lattice node the particle occupation is identified by a virtual Boolean variable with only values 0 or 1. McNamara and Zanetti[16] contributed a historic development to replace the Boolean variable in LGA by a real variable, single particle distribution function f_I, and neglecting individual particle motion with particle-particle correlations in the kinetic equations, which eliminates statistical noise in LGA, so that LBM was originally created.

1.3 Fundamental ideas with main characteristics

The fundamental idea in LBM is that gases/fluids are imagined as consisting of a finite number of small particles moving with random motions. The exchange of momentum and energy is achieved through particle streaming and billiard-like particle collision modelled by BTE. The main contribution of LBM is to simplify it by reducing the number of particles and confining them onto the several lattice nodes. Such particles, with their sizes in a mesoscopic scale between the microscopic and macroscopic ones, perform consecutive propagation and collision processes over a discrete lattice mesh. The main characteristics of LBM to solve partial differential equations governing fluid flows are as follows.

(a) LBM is a new approach for fluid dynamics, which is quite different from the classical CFD techniques. The solution equation of LBM is the lattice Boltzmann equation (LBE), and the solution variable is the distribution function, a mesoscopic variable describing the probability of particle distribution, which provides the potential to model nonequilibrium flows not-governed by Navier-Stokes equations (NSE). However, the macroscopic variables satisfying NSE can be derived from the distribution function based on its moment equations governing the macroscopic conservation laws.

(b) The kinetic nature of LBE makes LBM suitable to model the internal micro-interactions among the fluid particles as well as the fluid interactions with external environments, giving a means to deal with complex geometric boundary conditions and to simulate complex flows, such as multi-components/phases, flows in porous media, fluid-solid interactions, etc.

(c) As same as LGA, LBM is a mesoscopic numerical model based on the facts that the behaviours of physical phenomena are their statistical average of microscale motions, so that different phenomena may have same microscale behaviours. Therefore, LBM is a very attractive numerical tool to simulate quite wide physical problems.

(d) The implementation of LBM consists of two steps: collision and streaming, of which the collision update of the state at each node is completely local, and the streaming process can be done by simple index shift operation, so that the algorithm exhibits natural parallelism and thus is easily to be run with parallel computations.

It has been found that the current available schemes of LBM are difficult to simulate flows with high-Mach number in aerodynamics, and there is not a good consistent thermo-hydrodynamic scheme to be developed. There have been some publications to try using Galilean transformation to address the simulation approach for high-Mach number flows, which might be a further research direction on LBM.

1.4 Historic developments

The following key publications in LBM developing history should be highlighted, from which LBM started into a new stage.

(1) The idea of using the simplified kinetic equation with a single-particle speed to simulate fluid flows was employed by Broadwell[17] for studying shock structures, which is a simple one-dimensional LBE.

(2) McNamara & Zanetti[16] established the main feature of LBM by replacing the particle occupation Boolean variables in LGA[18-19] by single-distribution functions

(3) An important simplification of LBE was made by Higuera and Jimenez[20] which linearized the collision operator by assuming that the distribution is close to the local equilibrium state. Higuera et al.[21] proposed an enhanced collision operator approach that is linearly stable, which makes use of a relaxation time towards the local equilibrium using single time relaxation.

(4) The commonly used relaxation term in LBM is known as the Bhatnagar-Gross-Krook (BGK) collision operator[13], and it has been independently suggested by several authors[22-23]. In BGK model, the local EDF is chosen to recover the NSE by Chen et al.[24], which gave a general form of EDF with three lattice constants up to the second order of macroscopic velocity, and Qian and colleagues[22,25-26] analytically obtained the three lattice constants and developed the famous DnQm models. The BGK model has been widely used in LBM, see for examples, [27-28].

(5) Several groups[29-33] have shown that LBM can be obtained from the continuum BTE for discrete velocities by using a small Mach number expansion / Hermite polynomial expansion, of which the starting point in the derivations is BGK equation[13, 34-35].

(6) The wall boundary conditions in LBM were originally taken from LGA, in which a particle distribution function bounce-back scheme, such as by Wolfram[36] and Lavallee et al.[37], was used to obtain non-slip velocity condition, which have been discussed, modified, and improved by many authors, see for example, Chen et al. [38] and the references listed in the review paper[39]. For this condition, the two types of implementations: the on-grid and the mid-grid ones[40-41] are widely adopted. On physical flow boundaries, it is very often to require the fluid flows with the prescribed velocity or pressure. Zou and He[42] developed a velocity/ pressure boundary conditions, and [43] adopted a non-equilibrium extraction approach to build the velocity/ pressure boundary conditions. The curved boundaries normally can be approximated by many connected planes, so that the bounce-back methods and the kinetic boundary conditions can be adopted, see for example, He and Doolen[44] adopted the bounce-back method to solve the flows around a circular cylinder. Furthermore, Filippova and Hanel[45] and Mei and Shyy[46] proposed an interpolation method to build 2-D boundary conditions for curved boundaries, which was further extended to 3-D case by Mei et al.[47].

(7) For external forces in the simulated physical problems, He et al. [48] proposed a force term using the macroscopic acceleration of the particle. Lee and Lin[49] in a research paper on simulation of incompressible two-phase flows at high density ratio, proposed a force model, based on the physical force component in the node velocity direction, which is constructed by using the form of discrete distribution function.

(8) The convergence, consistency, stability, and numerical efficiency were investigated by many authors, for examples[24, 50-54]. To increase numerical efficiency and accuracy, some techniques in the traditional CFD have been adopted in LBM, such as nonuniform grid[55], the finite volume method[56-57], the nonuniform finite difference[54] and the time-dependent interpolation scheme[58], etc.

(9) For the contributions to deal with various types of problems, there have been a lot of particular approaches and models with numerical techniques discussed in the historic review papers in the subsection 1.5, among which the review papers by [39,59-63] before 2 000, when the LBM was faster developed, provide more very important historic information.

1.5 Important review papers

With the very fast developments of LBM and its widely applications in simulating many complex problems in engineering, there have been many review papers published, so that it is very difficult to list all publications herein, and only some of them are introduced as follows.

Before the year 2 000, the following six review papers should provide the fundamental theory and applications involving LBE and LBM. The two papers by Succi and colleagues[59-60] presented the most advances at until that time and the basic elements of theory of the topic and special lattice kinetic model for fluid dynamics problems, such turbulent flows, and low-Reynolds flows in porous media. Rothman and Zaleski[61] contributed a review paper, which describes the derivation of macroscopic constitutive equations from microscopic dynamics, emphasizing Lattice-gas models of phase separations to simulate certain complex-fluid problems, such as multiphase flow through porous media and the interaction of phase transitions with hydrodynamics. In the review paper by Chen et al.[62] mainly concerns lattice methods and their applications to reacting systems, which presents the development of LGA method and its extension LBM, new computational schemes for solving a variety of partial differential equations and modelling chemically reacting systems. The basic principles of LGA and LBM, their numerical implementations, and applications to chemically reacting systems are introduced. Comparisons of LBM with LGA technique and other traditional numerical schemes, including the finite difference (FD) scheme and the pseudo-spectral method, for solving the NSE are discussed. The article by Qian et al.[63], in the title: recent advances in LB computing, is a comprehensive document on the developments in the theory of LBE, particularly, lattice BGK models with various applications. Chen and Doolen[39] presented an overview of LBM, considered as a parallel and efficient algorithm for simulating single-phase and multiphase fluid flows and for incorporating additional physical complexities with modelling complicated boundary conditions and multiphase interfaces of the related problems, such as fluid turbulences, suspension flows, and reaction diffusions.

From 2001 to 2010, three review papers on LBM were searched. The first one by Premnath et al.[64] in the title: a review of LBM for multiphase flows relevant to engine sprays, gave applications of LBM to compute multiphase flows. The method is based on the solution of a kinetic equation describing the evolution of the distribution of the population of particles of which the collective behaviour reproduces fluid behavior. The distribution is modified by particle streaming and collisions on a lattice in a mesoscopic level, which naturally incorporates physical properties needed to compute complex flows, the surface tension and phase segregation in multiphase interactions by considering intermolecular attraction forces. It was presented as an example of the model, resulting of drop-drop collisions, drop deformation and liquid jet break-up phenomenon. Challenges in employing LBM were highlighted. The rest two papers were published in 2010[65-66]. The former by Aidum and Clausen[65] concerns LBM for complex flows and gives many significant developments over the past decade with specific examples. Some of the most active developments include the entropic LBM and the application to turbulent flows, multiphase flows, and deformable particle and fiber suspensions. Hybrid methods based on the combination of the Eulerian lattice with a Lagrangian grid system for the simulation of moving deformable boundaries show promise for more efficient applications to a broader class of problems. It also discussed higher-order boundary conditions and the simulation of microchannel flow with finite Knudsen number. Additionally, the remarkable scalability of the LBM for parallel processing was shown with examples. The later titled progress in LBM in a Japanese journal of multiphase flow, reviews the progress and successful applications of LBM to CFD. The author clarified the important issue in the LBM simulation, showing the progress, and summarizing both the advantages and disadvantages of LBM as well as discussing the immersed boundary-lattice Boltzmann method (IB-LBM). Due to the common feature of using the Cartesian mesh, the IB-LBM successfully calculates the rigid particle motions in a viscous fluid. It presents one of key issues in the IB-LBM and examines the applicability of the Immersed Boundary Method to the lattice kinetic scheme (LKS) for particulate flow.

According to an insufficient search, there have been more review papers published after the year 2010. In 2012, Yin et al.[67] presented a paper on mass and momentum transfer across solid-fluid boundaries (SFB) in LBM, that has been one of active topics through the development of LBM. This paper reviews typical treatments to prevent net mass transfer across SFB in LBM and argue that such efforts are in general not necessary and could lead to incorrect results. The designed simulations are conducted to examine the effects of normal boundary movement, tangential density gradient, and lattice grid resolution, of which the results show that the global mass conservation can be well satisfied even with local unbalanced mass transfer at boundary nodes, while a local mass conservation constraint can produce incorrect flow and pressure fields. Therefore it is suggested that (1) local mass conservation, at either a fluid or solid boundary node, is not only an unnecessary consequence to maintain the global mass conservation, but also harmful for meaningful simulation results; (2) the concern on the momentum addition and reduction associated with status-changing nodes is also not technically necessary; (3) including the momentum addition or reduction has no direct influence on flow and pressure fields, the incorrect fluid-particle interaction may affect simulation results of particulate suspensions.

Jahanshaloo et al.[68] is a review on the application of LBM for turbulent flow simulation, which discusses the previous studies on turbulence in the frame of LBM before its publication year and categories the related extensions of LBM as to three main groups of turbulence simulation: DNS, LES and RANS methods. For the problem of turbulence, Djenidi[69] reported a brief review of numerical simulations of homogeneous isotopic turbulence (HIT) using LBM, which shows that the details of HIT are well captured and in agreement with existing data, indicating that LBM is as good as NSE solvers and is very much adequate for turbulence investigations.

The two papers contributed by Che Sidik and Aisyah Razali[70-71] reviewed LBM for numerical prediction of nanofluid flow concerning the heat transfer enhancement using LBM. The paper provides a brief review of applications of LBM on the prediction of nanofluid and identifies opportunities for future research. Meanwhile, Perumal and Dass[72] presented the development of lattice Boltzmann computation of macro fluid flows and heat transfer, which reviews the philosophy and the formal concepts behind LBM and gives progress in the areas of incompressible fluid flows, compressible fluid flows and free surface flows.

A review paper on LB modeling of water-like fluids was contributed by Succi et al.[73], which reviews the advances on the mesoscopic modeling of water-like fluids, based on the LB methodology before 2014. The paper’s main aim is to enrich the basic LB (hydro)-dynamics with angular degrees of freedom responding to suitable directional potentials between water-like molecules. The model is shown to reproduce some microscopic features of liquid water, such as an average number of hydrogen bonds per molecules (HBs) between 3 and 4, as well as a qualitatively correct statistics of the hydrogen bond angle as a function of the temperature. The advanced future developments, based on the coupling the present water-like LB model with the dynamics of suspended bodies, such as biopolymers, may open new angles of attack to the simulation of complex biofluidic problems, such as protein folding and aggregation, and the motion of large biomolecules in complex cellular environments. For gaseous flows, Wang et al.[74] presented a paper discussing LBM for isothermal micro-gaseous flow and its application in shale gas flow. It is mentioned that the gas flow in shale matrix is mostly in the slip flow and transition flow regimes, given the difficulties of experimental techniques to determine extremely low permeability, therefore the computational methods especially LBM can be an attractive choice for simulation of these micro-gaseous flows. The paper gives an extensive overview on several relaxation time and boundary conditions used in LBM models for micro-gaseous flow, their advantages and disadvantages. Furthermore, potential application of LBM in flow simulation in shale gas reservoirs on pore scale and representative elementary volume scale is evaluated and summarized. The review indicates that LBM can capture gas flow in continuum to slip flow regimes which cover significant proportion of the pores in shale gas reservoirs and identifies opportunities for future research.

Yoon et al.[75] gave a review paper on LB-based approaches for pore-scale reactive transport involving reactive flows and multicomponent transport in the subsurface environment. It is mentioned that reactive transport processes can change the pore morphology at the pore scale, thereby leading to nonlinear interactions with advective and diffusive transport, which can strongly influence larger-scale properties such as permeability and dispersion. Therefore, one of the greatest research challenges is to improve our ability to predict these processes across scales. The development of pore-scale modelling methods to study reactive processes involving mineral precipitation and dissolution, and biofilm dynamics allows more fundamental investigation of physical behaviour so that more accurate and robust upscaled constitutive models can be developed for the continuum scale. A pore-scale model provides fundamental mechanistic explanations of how biogeochemical processes and pore-scale interfacial reactions alter flow paths by pore plugging (and dissolving) under different geochemical compositions and pore configurations. Recent advances in multiscale imaging techniques for the analysis of complex pore structures and mineralogy have revolutionized our ability to characterize geomaterials quantitatively at the pore scale. Concerning the multiphase LBM simulations for porous media applications, a review paper by Liu et al.[76] provides more useful information, which gives an extensive overview on several the diffuse interface models, and discusses their advantages and disadvantages, and shortly reports multiphase flows containing solid particles, as well as implementation details and optimization issues.

Review paper by Sharma et al. [77] mainly concerns LBM for industrial applications giving recent advancements and potentialities of LBMs. Various processes and phenomena with industrial importance such as flow in microchannels, dissolution and precipitation of solids, bubble dynamics, droplet formation and breakage, chemical reactions and reactors, mass transfer and optimization in fuel cells, flow in stirred tanks, multicomponent-multiphase flow, flow in porous media, and natural and convective heat transfer have been covered. LBM implementation for such applications is presented, and the results are analyzed. Various LBM collision schemes and their impact on the numerical stability and accuracy in the above-mentioned processes are also discussed. The applications of LBM to computational aeroacoustics (CAA) can be read in the review paper by Shao and Li[78], which presents the research studies on this topic. It is mentioned that (1) NSE-based solver faces the difficulty of computational efficiency when it has to satisfy the high-order of accuracy and spectral resolution, and LBM shows its capabilities in direct and indirect noise computations with superior space-time resolution; (2) The combination of LBM with turbulence models work very well for practical engineering machinery noise; (3) The hybrid LBM decouples the discretization of physical space from the discretization of moment space, resulting in flexible mesh and adjustable time-marching; (4) New solving strategies and acoustic models are developed to further promote the application of LBM to CAA.

Recently, Carenza et al.[79] presented a review on LBM and active fluids, which emphases that active fluids are living matter or biologically inspired systems, consisting of self-propelled units that burn stored or ambient energy and turn it into work, eventually giving rise to systematic movement. It reviews the state of the art of active fluids with particular attention to hydrodynamic continuous models and to the use of LBM in this field, and presents the thermodynamics of active fluids, in terms of liquid crystals modelling adapted to describe large-scale organization of active systems, as well as other effective phenomenological models. The paper discusses how LBM can be implemented to solve the hydrodynamics of active matter, starting from the case of a simple fluid, for which it explicitly recovers the continuous equations by means of Chapman-Enskog expansion (CEE). Going beyond this simple case, the paper summarizes how LBM can be used to treat complex and active fluids, and then reviews recent developments concerning some relevant topics in active matter that have been studied by LBM: spontaneous flow, self-propelled droplets, active emulsions, rheology, active turbulence, and active colloids. In the same year 2019, Wang et al.[80] gave a brief review of the phase-field-based LBM for multiphase flows, which first introduces the mathematical theory of phase-field models for multiphase flows, and then present some recent progress on LBM for the phase-field models composed of the classic NSE and the Cahn-Hilliard or Allen-Cahn equation. Finally, some applications of the phase-field-based LBM are discussed.

In the year 2020, ten authors[81] contributed a review paper in the title of LBM for fluid-thermal systems: status, hotspots, trends, and outlook. This paper presents a systematic overview of LBM from 1990 to 2018, based on bibliometric analysis and the Science Citation Index Expanded (SCI-E) database. The results showed that China took the leading position in this field, followed by USA and UK. The Chinese Academy of Sciences had the most publications, while the Los Alamos National Laboratory was the first as far as highest average citation per paper and h-index were concerned. Physical Review E was the most productive journal and "Mechanics" was the most frequently used subject category. Keyword analysis indicated that recent research has focused on the natural convection and heat transfer of nanofluid or multiphase flow in complex porous media. Hydrothermal treatment of nanofluid with shape factor on the conditions, such as variable magnetic fields, thermal radiation and slipping boundary, were the research hotspots. Further research perspectives mainly explore the multiscale models for coupling multiple transport phenomena, morphology optimization of porous parameters, new nanoparticles with shape factor, multicomponent LBM considering Knudsen diffusion effect, LB-based hybrid methods, radiation performance or boiling-heat transfer of nanofluid, and the active control of droplets, may continue to attract more attention. Moreover, some new applications, such as phase change of metal foam, erosion induced by nano-fluid, anode circulating, 3D modelling in thermal systems with vibration, and magnetohydrodynamics microfluid devices, could be of interest going forward.

1.6 Recognized books

There have been several books on LBM published, of which some of them are introduced as follows.

The important proceedings of a workshop sponsored by the Centre for Nonlinear Studies, Los Alamos National Laboratory (CNLS) was edited by Gutowitz[82], in which many authors provided the contributions in theory and experiment on cellular automata.

It seems that the first book on LBM by Wolf-Gladrow[83] provides an introduction for graduate students and researchers. Working knowledge of calculus is required and experience in PDEs and fluid dynamics is recommended. Some peculiarities of cellular automata, the properties of various LGCA and special coding techniques are outlined and discussed. Concepts from statistical mechanics provide the necessary theoretical background for LGCA and LBM. The properties of LBM models and a method for their construction are presented.

Succi[84] contributed a book as one of the series publications of numerical mathematics and scientific computation by Oxford University Press. The author claimed that this book provided the first detailed survey of LBE theory and its major applications to 2001. Accessible to a broad audience of scientists dealing with complex system dynamics, the book also portrays future developments in allied areas of science (material science, biology etc.) where fluid motion plays a distinguished role. The book consists of 16 chapters covering kinetic theory and LG, LBM models and wide applications. In 2018, the author further contributed on this topic giving a unique description of a major technique, which is based on LBM to simulate complex flows around us, from daily-life vital process concerning breathing and blood circulations to industrial, environmental, biological, and medical sciences. The book presents the recent developments of LBM for non-ideal fluids, micro-and nanofluidic flows with suspended bodies of assorted nature and extensions to strong non-equilibrium flows beyond the realm of continuum fluid mechanics. In the final part of the book, it presents the extension of LBM to quantum and relativistic matter, in attempt to match the major surge of interest spurred by recent developments in the area of strongly interacting holographic fluids, such as electron flows in graphene.

The book by Sukop & Thorne[85] provides a basic introduction that emphasizes intuition and simplistic conceptualization of processes. It avoids the more difficult mathematics that underlies LBM models. The model is viewed from a particle perspective where collisions, streaming, and particle-particle/particle-surface interactions constitute the entire conceptual framework. Beginners and those with more interest in model application than detailed mathematical foundations will find this a powerful "quick start" guide. Example simulations, exercises, and computer codes are included. Working code is provided on the Internet.

For molecular simulations, the book by Satoh[5] presents the most important and main concepts of the molecular and microsimulation techniques, in which the theoretical background of LBM and its practice are discussed in two chapters.

The second edition of the book by Mohamad[86] continues its first edition published in 2011 with its Chinese version translated by Yang[87] to introduce readers to LBM for solving transport phenomena-flow, heat, and mass transfer-in a systematic way. Providing explanatory computer codes throughout the book, the author guides readers through many practical examples, such as: flow in isothermal and non-isothermal lid-driven cavities; flow over obstacles; forced flow through a heated channel; conjugate forced convection; and natural convection. The codes are written in MATLAB in a way to be easily converted to other languages, and to be extended with little effort to multi-phase and multi-physics problems. The second edition of the book adds new chapters and includes new theory and applications. It discusses more practical examples, and explains in connection with various engineering topics, especially the transport of mass, momentum, energy and molecular species.

The book by Guo and Shu[88], as one of series publications in Advances in CFD by World Scientific Publishing Company, covers the fundamental and practical application of LBM by two parts, of which the first one consists of three chapters presenting the theory, basic models, initial and boundary conditions, and theoretical analysis to improved models[89]. The second part includes six chapters, addressing applications of LBM in various aspects of CFD, such as thermo-hydrodynamics, compressible flows, multicomponent/ multiphase flows, microscale flows, flows in porous media, turbulent flows, and suspensions.

The book by Huang et al.[90] presents a comprehensive review of popular multiphase LBM developed thus far and is aimed at researchers and practitioners within relevant Earth Science disciplines as well as Petroleum, Chemical, Mechanical and Geological Engineering, which is a valuable reference on the current state of multiphase LBMs. The advantages and disadvantages of each model are presented to enable the reader to choose the model most suitable for their problems. The book is targeted at graduate students and researchers who plan to investigate multiphase flows using LBMs. The authors present the detailed mathematical derivations of models than the ones in the existing literatures. The approach to understanding and classifying the various models is based on simulations compared with analytical/observational results and discovery of undesirable terms in the macroscopic equations with their correction. A repository of FORTRAN codes for multiphase LBM models is also provided.

The book by Krüger et al.[91] is an introduction to the theory, practice, and implementation of LBM that is steadily gaining attention due to its simplicity, scalability, extensibility, and simple handling of complex geometries. The authors claimed that the book was strong on basics but also included in-depth descriptions of the latest applications of LBM. Chapter summaries, example codes, and frequently asked questions made the book suitable as both textbook and handbook for practitioners. The book webpage gives the full code corresponding to the examples presented in the text.

The book by Montessori and Falcucci[92] concerns LBM modelling of complex and multiscale phenomena involving the presence of one or more fluids flowing, merging, and evolving around us, especially in the fields connected with the simulation of complex and soft matter flows from nano-active materials, free surface, and multiphase and reactive flows to the ones inside engines and fluid machinery. The author claimed that the book presented the most recent advances of the application of LBM to complex flow phenomena of scientific and technical interest with focus on the multiscale modelling of heterogeneous catalysis within nano-porous media and multiphase, multicomponent flows.

The book edited by Akker[93] was published as Volume 55 in the *Advances in Chemical Engineering* series, which highlighted new advances in the field, and it presents interesting chapters on simulations of homogeneous and heterogeneous chemical reactions, LBM for 3D chemical reactors, simulations of PEM fuel cells, and for separation processes, two-phase flow bioreactors, and more. Bolton et al.[94] presented a webpage to give some detailed information on LBM.

There are three books published in Chinese: He et al.[95], Guo and Zheng[96] and Wang and Li[97], which present the theory and applications of LBM. The authors of the first one claimed that they were based on their research practices presenting the fundamental concepts of LBM, including models, boundary conditions, grid generation, numerical implementation and development state at that time, as well as the computer code and numerical examples developed by them. The third one shows a mathematical book style concerning the LBM solutions of PDEs of soliton waves, such as: Kdv equation with its coupled and modified forms, nonlinear Schrodinger equations etc.

1.7 Applications and available computer source codes

LBM with its kinetic nature is a mesoscopic and dynamic description of the flow physics, which can be considered as an effective numerical method to model both macroscopic and microscopic statistical problems, especially some new phenomena that are not yet easily described by macroscopic equations. Therefore, this method has been widely used to simulate various engineering problems, such as flows in complex geometries, nonhomogeneous turbulent flows, multiphase and multicomponent flows with their interactions, heat transfer and reaction-diffusion problems involving phase changes, electroosmotic flows, flows in porous media, etc, see for examples[98]. To list but too many, the readers may refer the review papers and the books mentioned in the above subsections 1.5~1.6.

There have been many computer codes for LBM implementation to solve various physical problems. The many books listed in section 1.6 present their computer codes at the end of the book with examples to illustrate how to use it. For examples, the book by Sukop and Thorne[85], Mohamad[86] and its Chinese version translated by Yang[87]. On some open webpages, such as the book webpage by Krüger et al.[91], it gives the full code corresponding to the examples presented in the book. Wagner[99] lists the source codes, provided under the GNU copyright, which can be downloaded at the given webpage of the document. Chen[100] gives a review paper in the title: LB for flow and transport phenomena on the webpage with a computer code.

2 Revealed problems on LBM theory to be addressed

Following reading the searched publications reviewed above, we have revealed the following problems of the current LBM theory, which need to be addressed. As we have learnt that the theoretical background of the LBM is the kinetic theory and BTE developed by studying the distribution of molecules of ideal dilute gases. The theoretical EDF obtained is the famous MBD, in which three macroscopic variables, the mass density, the velocity and the temperature T in association of the Boltzmann constant K are included as the parameters. In this theoretical EDF, the parameter KT reflecting the bulk energy was derived only by the equation of state of the gas[6], but not concerning any other types of energy, such as the work done by viscous stress in viscous flows and the one caused by the gradient of the mass density. Therefore, the momentum and energy conservation equations, based on small parameter expansions derived from MBD function, do not include the contribution from the full stress tensor in continuum mechanics, and there is not a term in the energy conservation equation concerning the contribution of possible external energy generation source. In practical simulations, it has been realized that this type of distribution function and the corresponding LBM models are probably most suitable for isothermal flows with low speeds. To solve this problem, many publications proposed some technical modification, but no theoretical check on the current LBM theory. For simulating multicomponent flows, Swift et al.[101-102] added an additional term of the free energy in EDF, so that the conservation of the total energy, including the surface energy, kinetic energy and internal energy can be properly satisfied[103]. Meanwhile, for studying thermodynamics in incompressible limit, He et al.[104] proposed a novel LB thermal model, in which an internal energy density distribution function, defined by a multiplication of MBD function and the kinetic energy function, so that the evolution equation of this introduced energy distribution function together with the original Boltzmann equation were solved to simulate the temperature field. However, the introduced internal energy function and the man-added additional term do not match the structure of MBD function, so that it may not be logically considered as a parameter to reveal the inherent mechanism of the physical phenomena. We have clearly known that the physical flows in the continuum mechanics are governed by three conservation laws, of which the three variables, the mass density, the velocity, and the internal energy are key parameters included in the equations of conservation laws. When we study the macroscopic flows from a viewpoint in the statistical mechanics, it should have a corresponding inherent theoretical EDF including these three key parameters to allow the three conservation laws to be satisfied. Corresponding this new theoretical EDF, an improved LBM can be developed to simulate complex problems, of which the characteristics is dominated by changes of internal energy. These revealed theoretical problems could be the reasons causing current LBM schemes failing to simulate flows with high speeds or high compressibility concerning changes of mass density in flow fields. The above-mentioned problems are some essential research directions to improve LBM to a new stage.

Trying to address them, using the knowledges on statistical mechanics, H theorem with variational analysis [6], continuum mechanics[105-106], energy flow equilibrium and energy flow density[107-110], author has completed a theoretical investigation paper accepted in press recently[111], in which a modified MBD and an improved LBM are developed allowing the three conservation laws directly derived from a modified Boltzmann transportation equation without extra small parameter expansions, as well as external forces and energy generation sources as generalised forces introduced into LBM process. The internal energy parameter like mass density and mean velocity to be updated during simulations to deal with complex flows concerning high speed/compressibility and obvious large heat energy exchanges, etc. However, only hand-workable examples are given to illustrate and validate the developed theory and method. We have expected that interested readers may follow the theoretical results to do more numerical investigations revealing some numerical techniques together to develop a theoretical-completed LBM benefiting to advances of sciences and engineering.

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