Lattice Boltzmann Method – Current Status and Prospects for Computing Compressible Flows at Moderate Knudsen Numbers

Ramesh K. Agarwal

Department of Mechanical and Aerospace Engineering
Washington University in St. Louis, MO 63130, USA, rka@me.wustl.edu

Abstract. During the past two decades the Lattice Boltzmann Method (LBM) has developed into a very promising numerical approach for simulating fluid flows. The LBM has been successfully applied to compute flows modeled by the incompressible Navier-Stokes equations including reactive and multiphase flows. Attempts have also been made to include the turbulence models in LBM. However, the LBM has been restricted to small Mach numbers, because in the standard LBM the particle velocities belong to a finite set, and the resulting macroscopic velocity is always much smaller than the speed of sound calculated from the macroscopic diffusion velocity. In addition, several fundamental difficulties remain in extending the LBM to flows in continuum-transition regime at moderate Knudsen numbers by including the general temperature-jump and slip velocity boundary conditions. Both the specular bounce back and extrapolation boundary conditions remain far from satisfactory for transitional flows at moderate Knudsen numbers. These issues are manifested in computing flows past space vehicles or in micro-fluidic devices. This paper describes the current status of the LBM in addressing these issues and its prospects/limitations in computing compressible flows with shocks at moderate Knudsen numbers.

Keywords: Lattice Boltzmann Method, Compressible Flows, Transitional Flows, Slip Boundary Conditions
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INTRODUCTION

Historically originating from the seminal work of Frisch, Hasslacher, and Pomeau [1] in 1986 on lattice gas automata (LGA), the lattice Boltzmann method (LBM) has recently developed into an alternative and very promising numerical scheme for simulating fluid flows [2]. The lattice Boltzmann algorithms are simple, fast and very suitable for parallel computing. It is also easy to incorporate complicated boundary conditions for computing flows in complex geometries. The algorithms have been successfully applied to compute flows modeled by the incompressible Navier–Stokes equations including reactive and multiphase flows. Attempts have also been made to include the turbulence models in LBM. Unlike the conventional numerical methods which directly discretize the continuum equations of fluid dynamics on a finite-difference, finite-volume or finite-element mesh, the LBM derives its basis from the kinetic theory which models the microscopic behavior of gases. The fundamental idea behind LBM is to construct the simplified kinetic models that capture the essential physics of microscopic behavior so that the macroscopic flow properties (calculated from the microscopic quantities) obey the desired continuum equations of fluid dynamics. Thus LBM is based on the particle dynamics governed by a simplified model of the Boltzmann equation, the simplification is usually to the nonlinear collision integral. In 1992, a major simplification to the original LBM was achieved by Chen et al. [3] and Qian et al. [4] by employing a single relaxation time approximation due to Bhatnagar, Gross and Krook (BGK) to the collision operator in the lattice Boltzmann equation. In this lattice BGK (LBGK) model, one solves the evolution equations of the distribution functions of fictitious fluid particles colliding and moving synchronously on a symmetric lattice. The symmetric lattice space is a result of the discretization of the particle velocity space and the condition for synchronous motions. That is, the discretizations of time and particle phase space are coherently coupled together. This makes the evolution of lattice Boltzmann equation very simple; it consists of only two steps: collision and advection. Furthermore, the advection operator in phase space (velocity space) is linear in contrast to the nonlinear convection terms in the macroscopic continuum equations of fluid dynamics. Thus, this simple linear advection operator in LBM combined with the simplified BGK collision operator results in the recovery of nonlinear macroscopic convection. It has been shown by Qian et al. [4] among others, using multiple scale expansion that the local equilibrium particle distribution function obtained from the BGK-Boltzmann equation can recover the Navier-Stokes equations and the incompressible Navier-Stokes equations can be obtained in the nearly incompressible limit of LBGK method.

Thus, there are three essential ingredients in the development of a lattice Boltzmann method for a single physics or multi-physics fluid flow problem which are needed to be completely specified: (1) a discrete lattice on which the fluid particles reside, (2) a set of discrete velocities $\mathbf{e}_i$ to represent particle advection from one node of the lattice to its nearest neighbor, and (3) a set of rules for the redistribution of particles on a node to mimic collision processes in the fluid, which are provided by the distribution functions f_i of these particles; the evolution of distribution functions in time (for a discrete time step Δt) is obtained by solving the LBGK equation. The LBGK equation for f_i requires the knowledge of the equilibrium distribution function $f_i^{(0)}$. The discrete velocities $\mathbf{e}_i$ are determined so that the macroscopic density and momentum satisfy the constraints $\rho = \sum_i f_i$ and $\rho\mathbf{u} = \sum_i f_i \mathbf{e}_i$ respectively, where $\mathbf{u}$ is the macroscopic-averaged fluid velocity. Therefore, the determination of appropriate equilibrium particle distribution function for a given fluid flow problem is essential for solving the problem by LBM.

However, several fundamental difficulties remain in extending the LBM to computing compressible flows with shocks at high Mach numbers and in computing flows in continuum-transition regime at moderate Knudsen numbers by including general temperature-jump and slip velocity boundary conditions associated with these flows. These issues are manifested for example in computing flows past space vehicles or in micro-fluidic devices. The LBM has been restricted to small Mach numbers, because in the standard LBM the particle velocities belong to a finite set, and the resulting macroscopic velocity is always much smaller than the speed of sound calculated from the macroscopic diffusion velocity. Efforts have been made by many investigators to increase the allowable Mach number [5] and to include the effects of temperature in LBM [6]. However, all the proposed approaches to date lack generality and are restrictive. As early as 1992, Alexander et al. [7] proposed an approach to control the sound speed by means of a modified equilibrium distribution function, however the energy equation was not recovered by the modified distribution function. Yu and Zhao [8] included an attractive force in the Lattice Boltzmann formulation to reduce the sound speed, again the energy equation was not recovered. Ansumali and Karlin [9] have recently proposed the entropy function approach based on H-theorem. The method shows promise in a simple application; however their approach needs further investigation for computing flows with shocks. Dellar [10] has proposed a thermal BGK method with a unique set of equilibria for Navier-Stokes and energy equations for computing the flow in a shock tube. The results are not very promising compared to the finite-difference/finite-volume method applied to the discrete BGK equation. Tsutahara et al. [11, 12] have proposed a multi-speed model which has been successfully employed for computing flows with shocks in both monoatomic and diatomic gases. The method is however very complicated. In this author's view, the most promising approach for computing compressible flows appears to be a locally adaptive LB model that allows large variations in the mean velocity by introducing a large particle velocity set [13]. On a 2D square lattice, the support set of equilibrium distribution requires only four directions and three particle velocity levels (the third level is introduced to improve the stability of the model) [14]. The model recovers both the Navier-Stokes equations and the energy equation. Such a multi-level lattice Boltzmann method has been successfully applied by Sun and Hsu [14] to compute 2D shock waves and compressible boundary layer flows at very high Mach numbers (as high as Mach 10).

The domain of validity of the continuum equations can be extended to higher Knudsen numbers in the range corresponding to the slip regime, for example in moderately rarefied gas flows and in microflows, if accurate slip velocity and temperature jump relations are used as boundary conditions. In this regard, it is necessary to model the physical phenomenon at the free mean path scale to obtain accurate slip velocity and temperature jump conditions at the wall. Traditionally the temperature jump relations are derived using either a complete diffuse scattering kernel [15] or at best using only one accommodation coefficient in surface modeling [16]. A very similar approach is used to obtain the slip velocity [17]. However it is well known that the complete diffuse scattering kernel is not a good surface description [18]. Furthermore the single accommodation coefficient process is a rough qualitative description of the particle reflection at the wall related to Maxwell boundary condition formulation. Maxwell boundary condition exhibits only one accommodation coefficient for accommodation of any kinetic property. However it is possible to calculate different accommodation coefficient for each kinetic property (i.e. the three components of momentum and energy) by using an anisotropic scattering kernel [19], which describes the non-specular reflection law governing reflection of the distribution function at the boundary. Thus, contrary to the standard formulation [18], the temperature jump problem is connected to the gas macroscopic motion at the wall and thus the slip velocity problem is completely coupled with the temperature jump problem. This approach has been able to resolve such anomalous phenomenon as "inverted velocity profile in cylindrical Couette flow of a rarefied gas" [20].

In LBM, the standard treatment of "no-slip" boundary condition at a solid wall is "bounce back" boundary condition which is second-order accurate on a flat wall. On a curved wall, the "bounce back" B.C. becomes first-order accurate and most B.C. treatments proposed in the literature for increasing the accuracy to second-order require that the particle distribution function be handled with given macroscopic quantities. For flows in continuum-transition regime at moderate Knudsen numbers, the treatment of temperature-jump and slip-velocity boundary conditions becomes even more important for accurate calculation of the flow field. Both the specular bounce back and extrapolation boundary conditions have been investigated but they remain far from satisfactory. Recently a new slip velocity boundary condition has been derived by Toschi and Succi [21], called the virtual wall condition (VWC) which takes into account the diffuse scattering from the wall. This B.C. has been successful in predicting the fully-developed plane channel flow ranging from hydrodynamic regime to quasi-free flow regime at moderate Knudsen numbers [21]. In this paper, we will briefly describe the various formulations/extensions of LBM for computing compressible flows and various treatments of slip flow boundary conditions for computing flows at moderate Knudsen numbers. The reader should refer to appropriate references for details.

Brief Review of Basic Theory of Lattice Boltzmann Method

We briefly describe here the basic equations for the simplest and most widely used form of LBM, known as the Lattice-BGK (LBGK) method. For simplicity, we consider a square lattice in 2D, as shown in Figure 1, with unit spacing on which each node has eight nearest neighbors connected by eight links. Particles can only reside on the nodes and move to their nearest neighbors along the links in unit time. There are two types of moving particles: the particles that move along the axis with speed $|\mathbf{e}_i| = 1$, i = 1, 2, 3, 4 and the particles that move along the diagonals with speed $|\mathbf{e}_i| = \sqrt{2}$, i = 5, 6, 7, 8. Also, there are rest particles with speed zero at each node. The occupation of these three types of particles is described by the single particle distribution function f_i where the subscript i indicates the velocity direction. The distribution function f_i is the probability of finding a particle i at node $\mathbf{x}$ at time t with velocity $\mathbf{e}_i$. We assume that the particle distribution function f_i evolves in time according to the LBGK equation:

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i \Delta t \qquad \text{where} \qquad \Omega_i = -\frac{1}{\tau}\left[f_i(\mathbf{x}, t) - f_i^{(0)}(\mathbf{x}, t)\right], \tag{1}$$

which is a discretized form of the discrete BGK equation

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right). \tag{2}$$

In equations (1) and (2), $f_i^{(0)}$ is the equilibrium particle distribution function and τ is the single relaxation time which controls the rate of approach to equilibrium. The hydrodynamic equilibrium particle distribution function (derived from the Maxwellian) is given by:

$$f_i^{(0)} = \rho w_i \left[1 + \frac{\mathbf{u} \cdot \mathbf{e}_i}{c_s^2} + \frac{\mathbf{uu} \cdot \left(\mathbf{e}_i \cdot \mathbf{e}_i - c_s^2 I\right)}{2 c_s^4}\right] \tag{3}$$

where ρ is the fluid density, $\mathbf{u}$ is the flow speed, I is the identity tensor, and c_s is the lattice sound speed defined by the condition:

$$c_s^2 I = \sum_i w_i \mathbf{e}_i \mathbf{e}_i \; . \tag{4}$$

In equation (4), w_i are a set of directional weights normalized to unity. These weights are given as $w_0 = 4/9$, $w_1 = w_2 = w_3 = w_4 = 1/9$, and $w_5 = w_6 = w_7 = w_8 = 1/36$. The local equilibria obey the following conservation relations:

$$\rho = \sum_i f_i \quad , \qquad \rho\mathbf{u} = \sum_i f_i \mathbf{e}_i \qquad \text{and} \qquad \sum_i f_i \mathbf{e}_i \mathbf{e}_i = \rho\left[\mathbf{uu} + c_s^2 I\right] \tag{5}$$

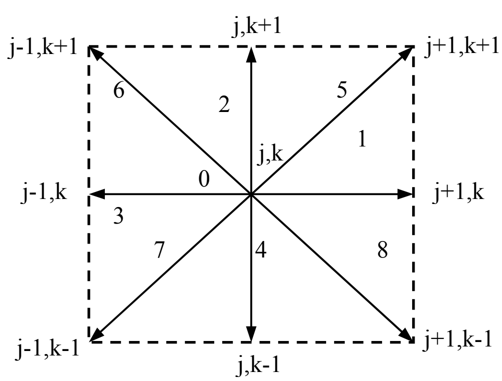


FIGURE 1. Nine-Speed Square Lattice

In the limit of long wavelengths, where a particle's mean free-path sets the scale, the fluid density and velocity satisfy the Navier-Stokes equations for a quasi-incompressible fluid. The macroscopic fluids equations can be derived using the Chapman-Enskog expansion as:

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0 \tag{6}$$

$$\frac{\partial\rho\mathbf{u}}{\partial t}+\nabla\cdot\rho\mathbf{uu}=-\nabla P+\nabla\cdot\left[\mu(\nabla\mathbf{u})_S+\lambda(\nabla\cdot\mathbf{u})I\right] \tag{7}$$

where P is the fluid pressure, $(\nabla\mathbf{u})_S$ is the symmeterized strain tensor, μ is the dynamic viscosity, and λ is the bulk viscosity. According to the definition of the pressure P, the LBGK fluid obeys an ideal equation of state. Using the standard linear transport theory, with careful handling of the artifacts the lattice introduces, the dynamic and bulk viscosity coefficients become

$$\mu=c_s^2\left(\tau-\frac{\Delta t}{2}\right)\rho \qquad \text{and} \qquad \lambda=\left(1-2c_s^2\right)\rho\left[1-\frac{\Delta t}{2}\right]. \tag{8}$$

In equation (7), $P=\rho\cdot c_s^2$. The derivation of LBGK equation (1) assumes that the particles velocities are much smaller than the sound speed and the flow is isothermal, thus the flow field is quasi-incompressible. For computing the LBGK solution, a uniform lattice with equally spaced points is created with square cells. The relaxation time τ is calculated from equation (8). The flow field is initialized by assuming a distribution of density and velocity field. The initial values of the distribution function (as equilibrium distribution function $f_i^{(o)}$ at t = 0) is then determined on the lattice from equations (5). The updating of the particle distribution functions f_i at subsequent time steps is done as described in equation (1). The procedure is repeated until the convergence of the distribution function is obtained. The macroscopic variables are then calculated from equations (5).
In equations (1) – (5), i represents summation over all lattice points.

Extension to Compressible Flow

As indicated in the previous section, the standard LBM is applicable to quasi-incompressible flows. Since early nineties, many attempts have been made to extend the method to compressible flows with shocks. However the success has been limited and the LBM has found little enthusiasm among researchers interested in computation of compressible flows at supersonic/hypersonic Mach numbers. Nevertheless, here we review some of the attempts towards this direction. It should be noted this review is not inclusive of all the approaches reported in literature. One of the earlier extensions of LBM to compressible flows is due to Alexander et al. [7], who tried to control the sound speed by means of a modified equilibrium distribution function with the following form:

$$f_i^{(0)}=\rho w_i\left[1+\frac{\mathbf{u}\cdot\mathbf{e}_i}{c_s^2}+\frac{\rho\mathbf{uu}\cdot\left(\mathbf{e}_i\cdot\mathbf{e}_i-c_s^2 I\right)}{2c_s^4}\right]+\delta\rho c_s^2 \tag{9}$$

In equation (9), δ was fixed by the Chapman-Enskog expansion. By properly choosing δ, Alexander et al. [7] were able to obtain accurate solutions of the Burger's equation. It should be noted that the energy equation is not recovered by equation (9). Yu and Zhao [8] employed an attractive force in the distribution function to reduce the sound speed:

$$f_i^*(\mathrm{x},t)=f_i(\mathrm{x},t)+\Phi_i\ , \tag{10}$$

where Φ_i is an attractive force given by

$$\Phi_i=\frac{4}{9}gc_s^2\left\{\rho(\mathbf{x}+\mathbf{e}_i)-\rho(\mathbf{x}-\mathbf{e}_i)-\frac{1}{8}[\rho(\mathbf{x}+2\mathbf{e}_i)-\rho(\mathbf{x}-2\mathbf{e}_i)]\right\}\approx\frac{1}{3}gc_s^2\mathbf{e}_i\cdot\nabla\rho \tag{11}$$

By a suitable choice of g, Yu and Zhao were able to calculate flows at both high subsonic as well as supersonic Mach numbers by substantially reducing the effective sound speed. The altered sound speed becomes

$$c_s^*=\sqrt{1-g}\,c_s\ . \tag{12}$$

Thus a value of g close to unity reduces the effective sound speed significantly. With the new distribution function f_i^*, the hydrodynamic equations (6) and (7) are recovered with f_i replaced by f_i^*. However, the energy equation is not recovered which is important in accurate calculation of heat transfer in high speed flows. Ansumali and Karlin [9] have recently proposed a new construction of the LBM based on H-theorem. They employ the entropy functions whose local equilibria are suitable to recover the Navier-Stokes equations in the framework of LBM. The entropy functions are used to construct a single relaxation time model of the collision integral instead of BGK which requires polynomial ansatz for local equilibrium. They derive a collision integral which enables simple identification of transport coefficients and which circumvents the construction of the equilibrium. They have applied the Entropy Function LBM (ELBM) to compute the flow in a shock tube. Some of their results for the evolution of density and velocity field are shown in Figure 2. The ELBM results show a better agreement with the exact analytical results compared to those obtained by LBGK and LBM. ELBM appears to be promising but needs further investigation for computing compressible flow. Additionally the implementation of ELBM in 2D and 3D is quite complex compared to LBGK.

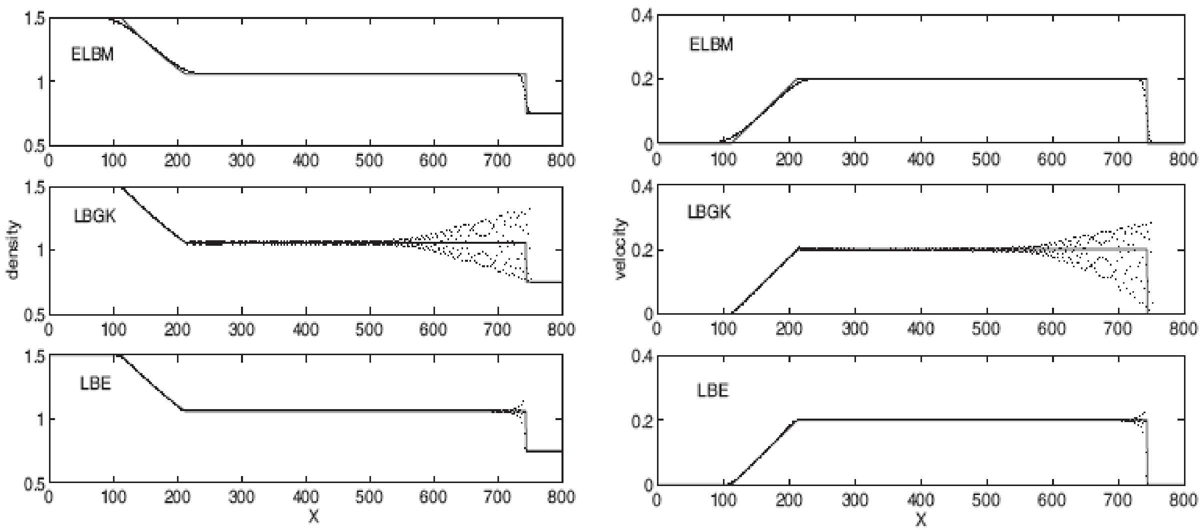


FIGURE 2. Density and velocity profiles for 1-D shock tube simulation at t = 500 for kinematic viscosity $\nu = 3.3333\times10^{-2}$. At t = 0, $\rho_- = 1.5$ for $0 \le x \le 400$ and $\rho_+ = 0.75$ for $400 \le x \le 800$. Thin line: exact solution. Symbol: simulation [9]

Dellar [10] has also formulated the LBGK method with a unique set of equilibria which recover both the Navier-Stokes and energy equations for a compressible thermal flow. However, he has shown that his D1Q5 LBGK formulation applied to the calculation of Sod's shock tube problem exhibits instability, a fact also demonstrated in Figures 2 and 3 with LBGK. He recommends the solution of discrete BGK equation by finite-volume method for obtaining stable solutions for compressible flows with shocks. Tsutahara and colleagues, in a series of papers [11, 12], have proposed thermally correct multispeed LBGK models that recover both the Navier-Stokes and energy equations. They have also extended their models to diatomic gases. They have successfully demonstrated the accuracy of their multi-speed thermal LBGK formulation by computing the flow in a shock tube. The formulation and its implementation are quite complex. This method again seems to have great potential but needs further investigation and demonstration by computing supersonic blunt body flow for example. In view of the author of this paper, the LBM that appears to have the most promise for computing high speed compressible flows is due to Sun and Hsu [13, 14]. Sun and Hsu formulate a multi-level lattice Boltzmann model which allows large variations in the mean velocity by introducing a large particle velocity set. The support set of equilibrium distribution is chosen to have only four directions and three levels of particle velocities; the third level is introduced to improve the stability of the model. A velocity in the velocity set consists of three parts: (1) the macroscopic velocity which is explicitly included in the microscopic velocity; (2) there is a set of diffusion velocity which has three levels. The diffusion velocities are determined by the macroscopic quantities; and (3) the third set of velocities is introduced to carry the particles to nearest vertex nodes. The relatively simple structure of the equilibrium distribution makes the model efficient for the simulation of flows over a wide range of Mach numbers and gives it the capability of capturing shock jumps. In contrast to standard lattice Boltzmann model, Sun and Hsu's formulation eliminates the fourth-order velocity tensors which have been the source of concern over the homogeneity of square lattices. A modified collision invariant eliminates the second-order discretization error of the fluctuation velocity in the macroscopic conservation equation from which the Navier-Stokes and energy equations are recovered. Some impressive results have been obtained. Figure 3 shows the simulation of a square shock on a 400x400 lattice using the three level model after 80 and 150 iterations. Figure 4 shows the computed density, pressure, internal energy and velocity profiles at y = 0.5 at 80th iteration and their comparison with the exact analytical solution. The agreement is excellent. Figure 5 shows the pressure, density, and entropy contours for a double Mach reflection on a 30 degree wedge in Mach 10 flow. These results are similar to those obtained by other investigators using the finite-volume method [22]. Finally, Figure 6 shows the velocity profiles for boundary layer over a flat plate and their comparisons with the exact Blasius solution. The agreement is excellent.

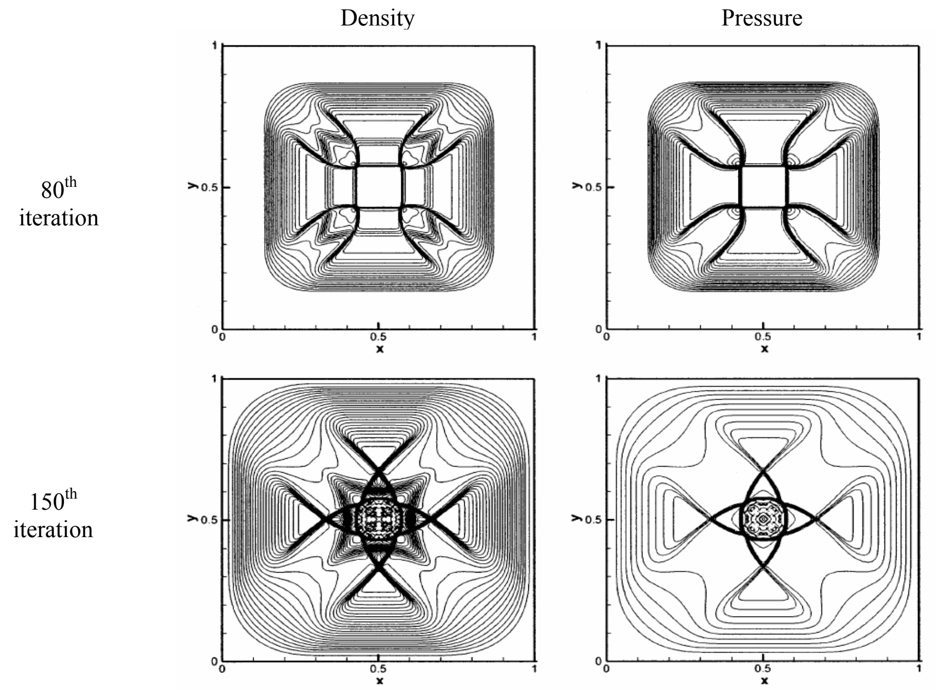


FIGURE 3. Simulation of a square shock in a (1×1) domain with 400×400 nodes. At t = 0, $(\rho, p, u) = (0.125, 0.025, 0)$ for $0.25 \le x \le 0.75$ and $0.25 \le y \le 0.75$; $(\rho, p, u) = (1, 0.25, 0)$ for the rest of the domain [14].

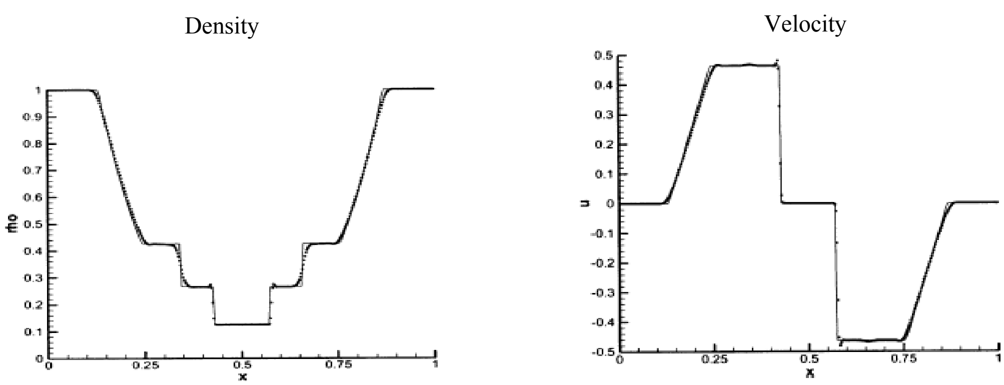


FIGURE 4. Simulation of a square shock of Figure 3: Density and Velocity distribution at $y = 0.5$ at the 80th iteration. Solid lines are the exact solutions [14].

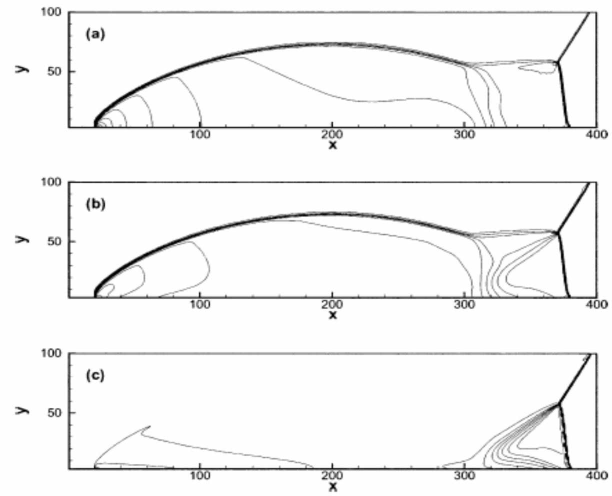


FIGURE 5. Double Mach reflection over a 30° wedge in Mach 10 flow: (a) pressure, (b) density, (c) entropy [14].

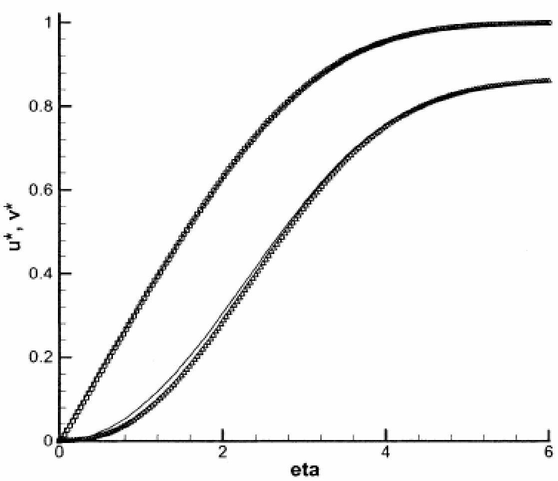
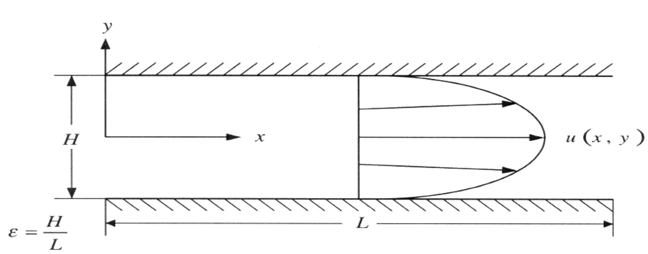


FIGURE 6. Boundary layer simulation on a flat plate. Dimensionless velocities $u^* = u/U$ and $v^* = (v/U)\sqrt{Ux/\nu}$ versus $\eta = y\sqrt{U/\nu x}$ on a lattice of 400x200 at Re = 1000. Solid lines are Blasius solution [14].

Based on the review of the key developments towards the formulation of LBM for compressible flows with shocks, it appears that the method of Sun and Hsu [14] demonstrably holds most promise. ELBM [9] and multi-speed model of Tsutahara et al. [11, 12] also appears to have potential. However, all the three approaches need further investigation and benchmark demonstrations for them to become competitive with the finite-difference/finite-volume/finite-element methods. These three methods have not been further investigated or applied by the researchers in the LBM community and have been primarily employed by the developers themselves. Thus the prospects for wide use of LBM for computing compressible flows with shocks appear to be limited, unless an unforeseen major breakthrough takes place in the near future.

Extension to Low Speed Flows at Moderate Knudsen Numbers

Another challenging area of research in LBM has been its extension to compute flows at moderate Knudsen numbers beyond the continuum regime. Such flow regimes are encountered on space vehicles flying in low earth orbit at an altitude of 150-250K feet as well as in micro-fluidic devices. The problem of computing hypersonic flows about space vehicles in transition regime (Kn > 0.01) by LBM becomes twice complicated because it requires extension of LBM to compressible flows with shocks as well as to higher Knudsen numbers. In a previous section, we have focused on the difficulties involved and the current state of the art in computing compressible flows in continuum regime only. In this section, we will focus on computing low speed flows at moderate Knudsen numbers and consider the difficulties involved and the current state of the art by considering flow in microdevices. Figure 7 shows the geometry of a 2D microchannel and the non-dimensional parameters involved.



Mach number: $M = \bar{u}/c$

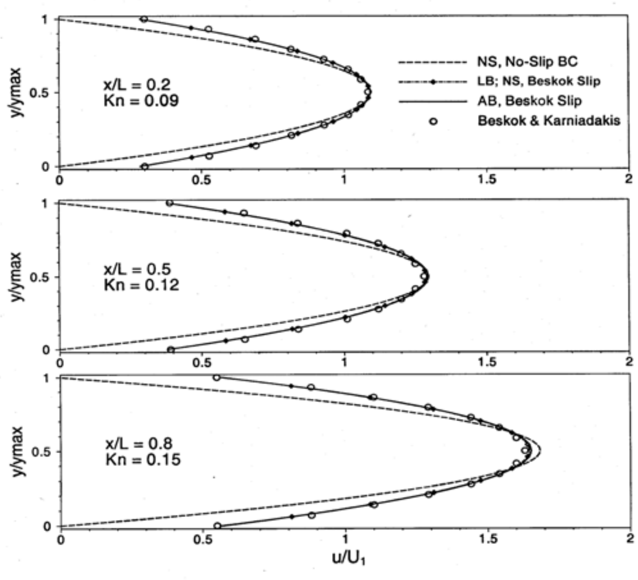
Reynolds number: $\mathrm{Re} = \bar{\rho}\bar{u}H/\mu$

Knudsen number: $Kn = (\pi\gamma/2)^{0.5}\, M/\mathrm{Re}$

"–" denotes the average outlet conditions

FIGURE 7. Schematic of slip flow in a microchannel [27]

In computing the flow in the microchannel, there are two issues involved: (1) the relaxation time τ is no longer constant. It is a function of the Knudsen number which varies along the channel from the inlet to outlet. Over the years, a number of proposal have been made [23–25] to quantify the variation of τ with Kn. In all the formulations τ varies linearly with Kn, (a* Kn +b); the only difference is in the value of the coefficients "a" and "b", (2) the flow slips along the boundaries of the channel. The correct formulation of slip boundary conditions is important for obtaining accurate results with both the conventional finite-volume continuum solvers and the LBGK solvers. The correct formulation of slip boundary conditions remains a major research issue in all flow solvers. Beginning with the formulation of Maxwell and Smoulchowski [17], significant advances have been made in recent years to improve on their seminal work. For isothermal LBGK solvers, the earliest paper of Niu, Doolan and Chen [23] employed the modified bounce-back type boundary condition by assuming slip velocity known from the data. Lim et al. [25] successfully employed the specular B.C. at low Knudsen numbers. Tang, Tao and He [26] have recommended the combined bounce-back and specular B.C. Several researchers have proposed kinetic B.C. to account for the particles and solid surface interactions in a more realistic manner to include diffuse-scattering [21]. Agarwal [28] employed the specular B.C. like Lim et al. [25] in the LBGK simulation of microchannel flow and obtained good agreement with the calculations using both the Navier-Stokes and Burnett equations in conjunction with second-order Beskok slip B.C. [28] as shown in Figure 8 for velocity profiles at various streamwise locations along the channel. However, all the calculations reported in the literature are for Kn < 1 with the exception of those of Ansumali et al. [29] and Toschi and Succi [21]. Figure 9 shows the variation of mass flow with Knudsen number for fully developed plane channel flow using the newly developed virtual wall kinetic boundary condition (VWC) by Toschi and Succi [21] that takes into account the diffuse scattering from the wall. The graph shows that for Kn >1, VWC has much better agreement with the analytical solution of Boltzmann equation by Cercignani [15] compared to the LBGK calculation using bounce-back (No VWC) B.C. The calculations of Ansumali et al. [29] and Toschi and Succi [21] show the importance of slip B.C. in extending the LBM to moderate Knudsen numbers. In this regard, the kinetic boundary conditions that account for diffuse scattering at the wall seem to hold promise. However, a great deal of further research is needed in this area. It is again the general feeling among researchers that the alternative methods based on the solution of Boltzmann equation using DSMC or finite-volume method hold more promise for computing flows from moderate to high Knudsen numbers than the LBM.



Comparison of velocity profiles at various streamwise locations of the microchannel: $Kn_{in} = 0.088$, $Kn_{out} = 0.2$, and $P_{in}/P_{out} = 2.28$.

FIGURE 8. Comparison of velocity profiles at various streamwise locations of the micro-channel [27]

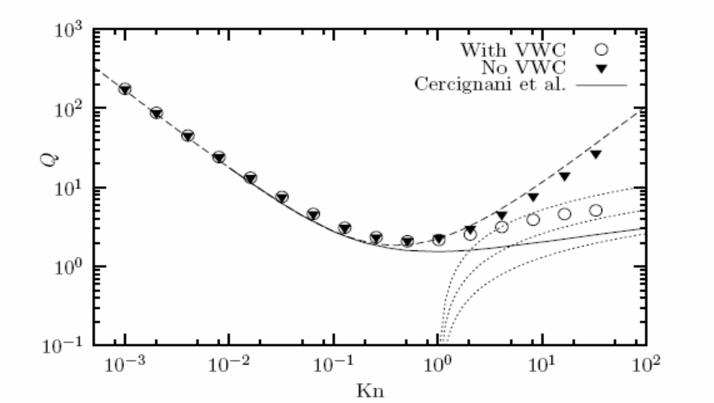


FIGURE 9. Normalized mass flux as a function of Knudsen number for a fully developed channel flow. VWC denotes Virtual Wall Condition. Cercignani's analytical solution of from Ref. [15]. The dotted lines can be ignored [21].

CONCLUSIONS

Although there have been several attempts to extend the Lattice Boltzmann Method (LBM) to compute the compressible flows with shocks, the success has been limited. The existing formulations that have shown some promise need extensive further investigation to acquire the current status of LBM for incompressible or low Mach number flows where it is increasingly being employed in lieu of the conventional finite-difference/finite-volume methods. Unless there is a major breakthrough, the current prospects of the LBM for computing compressible flows are not very encouraging. Same is the situation for computing flows in continuum-transition regime at moderate Knudsen numbers; LBM is not a preferred method even with the inclusion of higher-order terms beyond quadratic. Based on the discussions with several leading researchers working with LBM method, the author believes that the finite-difference/finite-volume/finite-element methods applied to compressible Navier-Stokes equations will remain the mainstream approaches for computing compressible flows with shocks in continuum regime. In moderately rarefied regimes, alternatively approaches based on the numerical solution of BGK equation and Boltzmann equation will continue to be employed and explored. The solution of the Boltzmann equation can be obtained either by DSMC or the finite-difference method; one method over the other may be preferred depending upon the Knudsen number.

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