Computer Physics Communications 129 (2000) 63–74

Computer Physics Communications

www.elsevier.nl/locate/cpc

Some recent results on discrete velocity models and ramifications for lattice Boltzmann equation ☆

Li-Shi Luo [1]

Institute for Computer Applications in Science and Engineering (ICASE), MS 132C, NASA Langley Research Center, 3 West Reid Street, Building 1152, Hampton, VA 23681-2199, USA

Abstract

Some rigorous results on discrete velocity models are briefly reviewed and their ramifications for the lattice Boltzmann equation (LBE) are discussed. In particular, issues related to thermodynamics and H-theorem of the lattice Boltzmann equation are addressed. It is argued that for the lattice Boltzmann equation satisfying the correct hydrodynamic equations, there cannot exist an H-theorem. Nevertheless, the equilibrium distribution function of the lattice Boltzmann equation can closely approximate the genuine equilibrium which minimizes the H-function of the corresponding continuous Boltzmann equation. It is also pointed out that the "equilibrium" in the LBE models is an attractor rather than a true equilibrium in the rigorous sense of H-theorem. Since there is no H-theorem to guarantee the stability of the LBE models at the attractor, the stability of the attractor can only be studied by means other than proving an H-function.

Keywords: Discrete velocity model; Boltzmann equation; Lattice Boltzmann equation; Thermodynamic consistency; H-theorem

1. Introduction

Although the method of the lattice Boltzmann equation (LBE) was developed only a decade ago [1–3], it has attracted significant attention recently [4,5]. There has been a substantial body of evidence accumulated validating the LBE method as a viable alternative to simulate hydrodynamics of simple fluids [6–8], and complex fluids such as multi-phase fluids [9,10], suspensions in fluids [11], and visco-elastic fluids [12]. The lattice Boltzmann equation was introduced to overcome some serious deficiencies of its historic predecessor: the lattice gas automata (LGA) [13–15]. The lattice Boltzmann equation circumvents two major shortcomings of the lattice gas automata: intrinsic noise and very limited range of transport coefficients, both due to the Boolean nature of the LGA method. However, despite the notable success of the LBE method in many computational applications, a thorough theoretical understanding of the LBE method within the framework of kinetic theory has been neglected by and large in the LGA and LBE research community. One reason is that many people in the community hold the viewpoint that the lattice Boltzmann equation is a derivative of the lattice gas automata, and they also ignore

☆ This work is based on a contributed talk given by the author at International Symposium on the Discrete Simulation of Fluid Dynamics/LGA'99 held in University of Tokyo, Tokyo, Japan, July 28–30, 1999.

[1] E-mail: luo@icase.edu.

0010-4655/00/$ – see front matter
PII: S0010-4655(00)00093-X

the theoretical connection between the lattice gas automata and the kinetic theory of the discrete velocity models (DVM). This narrow viewpoint isolates the lattice Boltzmann method from other kinetic models and classical theory, and is still predominant among researchers in the LBE and LGA methods (see, for instance, Refs. [16,17]). It was only very recently that the formal connections between the lattice Boltzmann equation and the continuous Boltzmann equation [18–20] and other kinetic schemes [21,22] were established.

It is interesting and important to note that there was indeed an interplay between the lattice-gas automata and lattice Boltzmann equation [15,23] and kinetic theory of the discrete velocity models in the beginning of the LGA/LBE methods [24,25]. From the very beginning the LGA and LBE methods put the emphasis on hydrodynamic simulations [13,15]. Therefore, isotropy, Galilean invariance, dissipation and dispersion, and consistent thermodynamics were the central concerns to the founders of the lattice gas automata [15,23], nevertheless they were not the focus of those interested on kinetic theory of the discrete velocity models. The early work of the lattice gas automata in fact inspired some work related to these issues in the field of DVM [24, 25]. However, the question related to the thermodynamic consistency of the LGA and LBE methods remains unanswered. In particular, there is a large gap between the theory and the application of the methods: there is not much rigorous mathematical work in kinetic theory directly related to the lattice gas automata or the lattice Boltzmann equation, and yet, many practitioners who use the LGA and LBE methods in various applications either simply believe in the methods and ignore the issues, or make claims on the basis of “better physics”. One purpose of this review is to re-emphasize the importance of theoretical issues concerning the thermodynamic consistency of the LGA and LBE methods, in particular, the H-theorem of the lattice Boltzmann models.

Recently it has been explicitly shown that the LBE method is a special finite difference form of the Boltzmann equation [18,19]. The lattice Boltzmann equation is obtained by discretizing the velocity space into a small set of fixed discrete velocities, and then by discretizing space and time according to the discrete velocity set to form a lattice structure. The lattice Boltzmann equation is related to the discrete velocity model of the Boltzmann equation in the sense that the LBE is, first, DVM with finite discrete velocities, and second, with fully discretized space and time tied to the discrete velocity set. Therefore, LBE is a discrete approximation of DVM. It should be stressed that the discrete velocity set in the lattice Boltzmann equation is obtained by enforcing the conservation laws of the system through quadrature in velocity space such that the discrete velocity set is sufficient to preserve the conservation laws exactly [18,19]. Because of the close connection between DVM and the LBE method, the results on DVM should have significant relevance to the LBE method in theory.

One early discrete velocity model was due to Broadwell [26,27]. There is a vast literature on the subject of the Broadwell model (see, e.g., [28]). The Broadwell model has only a very small set of discrete velocities and yet it can produce shocks and acoustic waves. It serves as an interesting mathematical model in statistical mechanics. Previous research on DVM has mostly dealt with models similar to the Broadwell model but with more and more complicated collision terms involving more and more particles. This type of DVM departs from the field of the Boltzmann equation significantly, and has developed into an interesting subject by itself. Only about a decade ago, DVM with a large number of discrete velocities and only two-body collisions started to attract some attention [29, 30]. With a large number of discrete velocities ($>10^3$), DVM becomes an accurate approximation of the Boltzmann equation [29,30].

In recent years there has been some rigorous work on DVM to prove the convergence of DVM to the Boltzmann equation [31]. We believe these rigorous results on DVM have important implications for the LBE method. In the next section, recent results of research on DVM are briefly reviewed. There is a vast literature on the subject of DVM, and the review presented here is not intended to be thorough or exhaustive. We only summarize the important results which we believe to be relevant to the lattice Boltzmann method. In Section 3 the ramifications for the lattice Boltzmann equation, especially for the thermodynamics and H-theorem of the LBE, are discussed. Section 4 concludes this paper with some comments and discussion.

2. Some recent results on discrete velocity models

In this section, the DVM with an infinite number of discrete velocities on $\mathbb{Z}_h^D$ (with lattice spacing h) is described. The theoretical results concerning the consistency of the DVM on $\mathbb{Z}_h^D$ is reviewed. The DVM with a finite number of discrete velocities is also discussed. Finally the thermodynamics of DVMs is briefly presented.

2.1. Discrete velocity models on $\mathbb{Z}_h^D$

We start with the Boltzmann equation:

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = Q(f, f), \tag{1}$$

where $f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the single particle distribution function, $\boldsymbol{x}, \boldsymbol{\xi} \in \mathbb{R}^D$, D is the dimension of the space, and $Q(f, f)$ is the bilinear collision integral:

$$Q(f, f) = \int_{\mathbb{R}^D} \mathrm{d}\boldsymbol{\xi}_1 \int_{S^{D-1}} \mathrm{d}\boldsymbol{\zeta}\, \eta\sigma(\eta, \boldsymbol{\zeta}) \left[f(\boldsymbol{\xi}') f(\boldsymbol{\xi}_1') - f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_1) \right], \tag{2}$$

where $\sigma(\eta, \boldsymbol{\zeta})$ is the differential collision cross-section, $\eta = |\boldsymbol{\eta}|$; $\boldsymbol{\xi}$, $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}'$, $\boldsymbol{\xi}_1'$ are pre-collision and post-collision velocities, respectively:

$$\boldsymbol{\xi}' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} + \boldsymbol{\zeta} \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}_1|}{2}, \tag{3a}$$

$$\boldsymbol{\xi}_1' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} - \boldsymbol{\zeta} \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}_1|}{2}, \tag{3b}$$

$$\boldsymbol{\eta} = \boldsymbol{\xi} - \boldsymbol{\xi}_1. \tag{3c}$$

The conservation laws of momentum and energy impose further constraints on velocities $\boldsymbol{\xi}$, $\boldsymbol{\xi}_1$, $\boldsymbol{\xi}'$, $\boldsymbol{\xi}_1'$, $\boldsymbol{\eta}$, and $\boldsymbol{\zeta}$.

The velocity space $\boldsymbol{\xi}$ can be discretized into a regular cubic lattice with lattice constant h such that the Boltzmann equation becomes:

$$\partial_t f_\alpha(\boldsymbol{x}, t) + \boldsymbol{\xi}_\alpha \cdot \nabla f_\alpha(\boldsymbol{x}, t) = Q_\alpha^{(h)}\left(\{f_\beta\}\right), \tag{4}$$

where $f_\alpha(\boldsymbol{x}, t) \equiv f(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$ is the distribution function in the discretized velocity space $\{\boldsymbol{\xi}_\alpha\}$, and

$$\boldsymbol{\xi}_\alpha \in \mathbb{Z}_h^D \equiv h\mathbb{Z}^D = \left\{ h(i, j, k) \mid i, j, k = 0, \pm 1, \pm 2, \pm 3, \ldots \right\}.$$

The collision integral in velocity space reduces to a quadrature on $\mathbb{Z}_h^D$:

$$Q_\alpha^{(h)} = \sum_{\{\beta, \gamma, \mu\}}^{N} \Gamma_{\alpha\beta}^{\gamma\mu} \left[f_\gamma f_\mu - f_\alpha f_\beta \right], \tag{5}$$

where the summation is over a subset of discrete velocities which satisfy the following conservation conditions:

$$\boldsymbol{\xi}_\alpha + \boldsymbol{\xi}_\beta = \boldsymbol{\xi}_\gamma + \boldsymbol{\xi}_\mu, \tag{6a}$$

$$\boldsymbol{\xi}_\alpha^2 + \boldsymbol{\xi}_\beta^2 = \boldsymbol{\xi}_\gamma^2 + \boldsymbol{\xi}_\mu^2, \tag{6b}$$

and the collision probability possesses the following symmetry:

$$\Gamma_{\alpha\beta}^{\gamma\mu} = \Gamma_{\gamma\mu}^{\alpha\beta} = \Gamma_{\beta\alpha}^{\mu\gamma} \geqslant 0. \tag{7}$$

With the assumption that there exit no spurious conserved quantities, it can be shown that the DVM of Eq. (4) possesses many properties of the Boltzmann equation, such as conservation laws, an H-theorem with a Maxwellian equilibrium, and so on [28].

2.2. Consistency of DVM

The DVM with a countable discrete velocities on a regular lattice space $\mathbb{Z}_h^D$ is considered as an approximation to the Boltzmann equation. Consistency of the DVM with the Boltzmann equation means that the DVM collision operator $Q_\alpha^{(h)}$ on $\mathbb{Z}_h^D$ converges to the Boltzmann collision integral $Q(f,f)$ on $\mathbb{R}^D$ as $h \to 0$, for any reasonable function f.

If the following properties of the DVM collision operator are postulated:

(1) Bilinearity (only binary collisions are considered);
(2) Translational invariance on the lattice space $\mathbb{Z}_h^D$;
(3) Invariance under reflection $\boldsymbol{\xi}_\alpha \to -\boldsymbol{\xi}_\alpha$;
(4) Local conservation laws of mass, momentum, and energy;
(5) Microscopic reversibility: the transition probability between two states satisfies

$$P\big((\boldsymbol{\xi}_\alpha, \boldsymbol{\xi}_\beta) \to \big(\boldsymbol{\xi}'_\alpha, \boldsymbol{\xi}'_\beta\big)\big) = P\big(\big(-\boldsymbol{\xi}'_\alpha, -\boldsymbol{\xi}'_\beta\big) \to (-\boldsymbol{\xi}_\alpha, -\boldsymbol{\xi}_\beta)\big); \tag{8}$$

(6) $Q_\alpha = Q_\alpha^+ - Q_\alpha^-$, $Q_\alpha^\pm \geqslant 0$, $Q_\alpha^- = 0$ iff $f_\alpha = 0$;

then the following lemma for the uniqueness of $Q_\alpha^{(h)}$ can be proved [32,31].

Lemma 1. *The above specified properties uniquely define the discrete collision operator $Q_\alpha^{(h)}$, of $\{\boldsymbol{\xi}_\alpha\} \in \mathbb{Z}_h^3$, with an accuracy up to a function $A(\boldsymbol{\zeta}, \boldsymbol{\eta})$ $[= A(-\boldsymbol{\zeta}, \boldsymbol{\eta}) = A(\boldsymbol{\zeta}, -\boldsymbol{\eta})]$, where $\boldsymbol{\zeta}$ and $\boldsymbol{\eta}$ are two orthogonal vectors in $\mathbb{Z}_h^3$. Specifically*:

$$\begin{aligned} Q(f,f)|_{\boldsymbol{\xi}=\boldsymbol{\xi}_\alpha} \approx Q_\alpha^{(h)} &= h^3 \sum_{\{\beta,\gamma\}} A(\boldsymbol{\xi}_\beta, \boldsymbol{\xi}_\gamma)[f_{\alpha+\beta} f_{\alpha+\gamma} - f_\alpha f_{\alpha+\beta+\gamma}] \\ &= \sum_{\{\beta,\gamma,\mu\}} \Gamma_{\alpha\beta}^{\gamma\mu}[f_\gamma f_\mu - f_\alpha f_\beta], \end{aligned} \tag{9}$$

where $\boldsymbol{\xi}_\beta \cdot \boldsymbol{\xi}_\gamma = 0$, and $\Gamma_{\alpha\beta}^{\gamma\mu} = \Gamma_{\alpha\beta}^{\gamma\mu}(A)$.

The convergence of $Q_\alpha^{(h)}$ to $Q(f,f)$ in three-dimensional space is proved in the following theorem [32].

Theorem 2. *Let $\sigma(\eta, \boldsymbol{\zeta})$ be such that $\tilde{\sigma} \equiv \sigma(\eta, \boldsymbol{\zeta}/\eta)/\eta^2 \in C^k$, and $f \in C_0^k(\mathbb{R}^3)$ with $\operatorname{supp}(f) \subset B(0, R/2)$ for some $R > 0$, for $k \leqslant 6$. Then for every point in the three-dimensional discrete velocity space $\boldsymbol{\xi}_\alpha \in \mathbb{Z}_h^3$, we have*:

$$\big|Q(f,f) - Q_\alpha^{(h)}\big| \leqslant c(\epsilon, k)\|f\|_k^2 R^5 h^{\frac{2}{175}-\epsilon}, \tag{10}$$

where

$$\|f\|_k = \sum_{i=0}^{k} \sum_{|\alpha|=i} \sup_{\boldsymbol{x}} \big|D^\alpha f(\boldsymbol{x})\big|.$$

For sufficiently smooth functions σ and f, the exponent $\frac{2}{175}$ can be improved to $\frac{1}{14}$. The exponent can be further improved to $\frac{1}{2}$ by Ramanujan's conjecture.

Similar results can also be obtained in two-dimensional space [33].

The key to prove the above theorem relies on the proof that the solutions of Diophantine equation,

$$\xi_1^2 + \xi_2^2 + \cdots + \xi_D^2 = m^2, \quad \xi_i,\ m \in \mathbb{Z},$$

are uniformly dense on the sphere of radius $|m|$, as $|m| \to \infty$. It is interesting to note that this number theoretical result was only obtained as recently as 1987 [34].

2.3. BGK DVM with a finite number of discrete velocities

The DVM of the BGK Boltzmann equation is given by:

$$\partial_t f_\alpha + \boldsymbol{\xi}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\lambda}\big[f_\alpha - f_\alpha^{(0)}\big], \tag{11}$$

where the collision integral is approximated by a single relaxation parameter λ. The BGK model equation is widely used in the LBE method [2,3]. The following theorem is for the DVM of the BGK Boltzmann equation with a finite number of discrete velocities [35].

Theorem 3. *Let the total number of $\boldsymbol{\xi}_\alpha$ be $N \geqslant (D+2)$, and $N_i \geqslant 1$ $\forall i = 1, 2, \ldots, D$, and $\exists\, i$ such that $N_i > 2$, and if Eq.* (11) *with strictly positive initial values has a solution $\boldsymbol{f} \equiv (f_1, \ldots, f_\alpha, \ldots, f_N)^{\mathrm{T}}$, then it can be formally proved that*:

$$f_\alpha > 0, \quad \forall \alpha,\ \boldsymbol{x},\ t, \tag{12a}$$

$$f_\alpha^{(0)} = \exp(\boldsymbol{a} \cdot \boldsymbol{h}_\alpha), \quad \forall \alpha, \tag{12b}$$

$$\partial_t \langle \boldsymbol{h} f_\alpha \rangle + \nabla \langle \boldsymbol{\xi}_\alpha \boldsymbol{h} f_\alpha \rangle = 0, \tag{12c}$$

$$\partial_t \langle f_\alpha \log f_\alpha \rangle + \nabla \langle \boldsymbol{\xi}_\alpha f_\alpha \log f_\alpha \rangle \leqslant 0, \tag{12d}$$

where $\langle \cdot \rangle \equiv \sum_\alpha$, $\boldsymbol{h}_\alpha \equiv (1, \xi_{\alpha,1}, \ldots, \xi_{\alpha,D}, \xi_\alpha^2)^{\mathrm{T}}$, and the vector $\boldsymbol{a} \in \mathbb{R}^{D+2}$ can be uniquely determined.

The above theorem states that, for a discrete velocity set of a minimum number of discrete velocities equal to $(D+2)$, which is also equal to the number of conserved hydrodynamic moments in $\boldsymbol{\xi}$-space of f_α in D-dimensional space, satisfying certain symmetry criteria, then the DVM has unique positive solution such that the equilibrium is a Maxwellian, the hydrodynamic moments form a hyperbolic system, and there exists an H-theorem, provided that the initial data for f_α are strictly positive.

It is interesting to note that the DVM with a finite number of discrete velocities and the LBE models share a common feature that they all have a small number of discrete velocities. However, the DVM evolves on a continuous space and time whereas the LBE evolves on a highly symmetric discrete space and time. This difference has some significant consequences.

2.4. Thermodynamics of DVM

In general, one can prove that, for the DVM satisfying certain conditions mentioned previously, there exists an H-theorem, with a Maxwellian equilibrium:

$$f_\alpha^{(0)} = \varrho \exp\left[-\frac{1}{2}\frac{(\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2}{RT}\right]. \tag{13}$$

The parameters ϱ, $\boldsymbol{u}$, and T in $f_\alpha^{(0)}$ are related to, but are not equal to, the hydrodynamic moments of f_α:

$$\rho = \sum_\alpha h f_\alpha = \sum_\alpha h f_\alpha^{(0)}, \tag{14a}$$

$$\rho \boldsymbol{v} = \sum_\alpha h \boldsymbol{\xi}_\alpha f_\alpha = \sum_\alpha h \boldsymbol{\xi}_\alpha f_\alpha^{(0)}, \tag{14b}$$

$$\rho e = \frac{1}{2}\sum_\alpha h |\boldsymbol{\xi}_\alpha - \boldsymbol{v}|^2 f_\alpha = \frac{1}{2}\sum_\alpha h |\boldsymbol{\xi}_\alpha - \boldsymbol{v}|^2 f_\alpha^{(0)}. \tag{14c}$$

The relationships between the parameters ϱ, $\boldsymbol{u}$, and T and the hydrodynamic moments ρ (density), $\boldsymbol{v}$ (flow velocity), and e (specific internal energy) are one-to-one in general. Moreover, in the limit of $h \to 0$, it can be shown that (see details in Appendix A):

(1) For the density, $\varrho \to \rho(2\pi RT)^{-D/2} + \mathrm{O}(e^{-\pi^2/h^2})$, as $h \to 0$.

(2) For the velocity: $\rho\boldsymbol{v} \equiv \langle \boldsymbol{\xi}_\alpha \rangle = \rho\boldsymbol{u}$ iff $\boldsymbol{u} \in \mathbb{Z}_h^D$, otherwise

$$\boldsymbol{v} = \boldsymbol{u} + \mathrm{O}(h^{-1} e^{-\pi^2/h^2});$$

(3) For the temperature:

$$e = \frac{D}{2} RT \psi(z), \tag{15}$$

where $z = h/\sqrt{2RT}$, and

$$\psi(z) = 2 \frac{\sum_{n=-\infty}^{+\infty} (nz)^2 e^{-(nz)^2}}{\sum_{n=-\infty}^{+\infty} e^{-(nz)^2}}. \tag{16}$$

The function $\psi(z)$ has the following property:

$$\lim_{z\to 0} \psi(z) = \lim_{h\to 0} \psi(z) = \lim_{T\to\infty} \psi(z) \approx 1 + \mathrm{O}(h^{-2} e^{-\pi^2/h^2}). \tag{17}$$

Therefore, with a fixed h, the thermodynamics of DVM differs from the continuous thermodynamics of the Boltzmann equation at low temperature limit $z = h/\sqrt{2RT} \to \infty$. The coincidence of the thermodynamic properties between DVM and the Boltzmann equation only occurs at the high temperature limit $z = h/\sqrt{2RT} \to 0$. Furthermore, the discrete thermodynamics of DVM has a smooth transition to the continuous thermodynamics of the Boltzmann equation as $h \to 0$ [31], with an exponential speed of convergence (see Appendix A).

The above results imply that the collisions in DVM lead to the equilibrium of the parameters $\boldsymbol{u}$ and T in the Maxwellian, but not the hydrodynamic moments $\boldsymbol{v}$ and e. In addition, DVM is only partially Galilean invariant (only on $\mathbb{Z}_h^D$), as expected for a lattice velocity space. Moreover, it can be shown that for any DVM (independent of specific collision operator) with a finite number of velocities, the macroscopic velocity $\boldsymbol{v}$ in the system is bounded by the discrete velocity set:

$$\min_\alpha \xi_{\alpha,i} \leqslant v_i \leqslant \max_\alpha \xi_{\alpha,i}. \tag{18}$$

Similarly, the "temperature" T is also bounded in a range determined by the discrete velocity set:

$$\frac{1}{DR} \min_\alpha |\boldsymbol{\xi}_\alpha - \boldsymbol{v}|^2 \leqslant T \leqslant \frac{1}{DR} \max_\alpha |\boldsymbol{\xi}_\alpha - \boldsymbol{v}|^2. \tag{19}$$

The upper and lower bound of T are determined by the maximum speed and the resolution of the discrete velocity space of the system, respectively:

$$T_{\max} \sim \frac{1}{DR} \max_\alpha |\boldsymbol{\xi}_\alpha|^2, \qquad T_{\min} \sim \frac{1}{DR} \min_{\alpha,\beta} |\boldsymbol{\xi}_\alpha - \boldsymbol{\xi}_\beta|^2 = \frac{1}{DR} h^2. \tag{20}$$

It is very apparent that the thermodynamic properties of the DVM with a small number of discrete velocities are significantly different from that of the Boltzmann equation.

3. Consequences for the lattice Boltzmann equation

The LBE method is mainly applied to simulate hydrodynamic systems. So far the LBE method is only successful in simulations of athermal fluid flows. In order to construct viable LBE models for thermal fluids, it is essential to understand the thermodynamics of the LBE models. Furthermore, the existence of an H-theorem for the lattice Boltzmann equation still remains an open question. The issues of the thermodynamics and H-theorem for the lattice Boltzmann equation are next addressed and discussed in light of the above results on DVM.

3.1. Thermodynamics

The above results on DVM have several immediate ramifications for the lattice Boltzmann equation. First, because the LBE method uses a lattice in physical space which is coupled to the discrete velocity set, the system evolves on a lattice in discrete time. The LBE dynamics which is dictated by the symmetry of the underlying lattice inherently possesses some spurious conservation laws. Obviously, in order to eliminate spurious conserved quantities due to the lattice symmetry, the minimum number of the discrete velocities, $(D+2)$, must be increased.

Second, in the LBE method, the equilibrium distribution function $f_\alpha^{(\mathrm{eq})}$ is a second order Taylor expansion of the Maxwellian [18,19], such that $\boldsymbol{v} = \boldsymbol{u}$, the equations of state are $P = \rho RT$ and $e = \frac{D}{2}RT$. Consequently, the thermodynamic consistency of the system is sacrificed. Specifically, the lattice Boltzmann equation does not satisfy Eqs. (12) – there is no positivity of the solution, nor the hyperbolic system of equations for the hydrodynamic moments, nor an H-theorem.

Third, since there are only very few discrete velocities in LBE models and the resolution in velocity space is rather coarse, the temperature range becomes very narrow. For example, for the 9-velocity LBE model on a two-dimensional square lattice,

$$\frac{1}{2} \leqslant T(\boldsymbol{x}, t) \leqslant 1,$$

where we set $R = 1$ and assume $\boldsymbol{u} = 0$. This severely limits the possibility of applying the LBE model to simulate thermo-hydrodynamics. It may also explain the numerical instability observed in many LBE thermal models.

3.2. H-theorem

Recently, there have been several attempts to prove an H-theorem for the lattice Boltzmann equation [36–39]. So far, no one has proven the H-theorem for the LBE systems which have the correct hydrodynamics. This is consistent with the above rigorous results on DVM, because, by using a second order Taylor expansion of the Maxwellian as the equilibrium, the positivity criterion of the system is no longer strictly satisfied. Consequently one cannot obtain an H-theorem. This conclusion also emerges from an analysis of recent work attempting to prove an H-theorem for the lattice Boltzmann equation.

First, in Ref. [36], it is shown that the equilibrium distribution given by quadratic form:

$$f_\alpha^{(\mathrm{eq})} = \frac{\rho}{b}\frac{1}{R}\left(R + \frac{\boldsymbol{e}_\alpha \cdot \boldsymbol{u}}{2c_s^2}\right)^2, \qquad R = \frac{1}{2}\left(1 + \sqrt{1 - \mathrm{M}^2}\right), \tag{21}$$

where $\mathrm{M} = u/c_s$ is the Mach number, and b is the number of discrete velocities, minimizes the following entropy function:

$$S = -\sum_\alpha f_\alpha^{3/2}. \tag{22}$$

An H-theorem was proved for the under-relaxed lattice BGK Boltzmann equation when the system is spatially homogeneous. It should be noted that the equilibrium given by Eq. (21) cannot lead to the correct Navier–Stokes equations, because Galilean invariance is lost. Furthermore, the H-theorem for spatially homogeneous lattice BGK system can be easily obtained without using the elaborate method employed in Ref. [36].

Subsequently, in Ref. [37] it was shown that an auxiliary equilibrium which is linear in $(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})$ can be used to minimize an entropy function $S = -\sum_\alpha f_\alpha^2$. The (linear) auxiliary equilibrium is then extended (extrapolated) to a “target equilibrium” which includes higher order velocity-moments (fluxes) such that the hydrodynamic constraints are satisfied. Then for the distribution function f_α of which the velocity moments are equal to that of the "target equilibrium" up to a given order, a *global* H-theorem can be obtained for a system with proper boundary conditions, such as periodic one. We note that one does not have a *local* H-theorem in this case.

In Ref. [38], it was shown that, assuming there exists a convex function h_α such that

$$f_\alpha^{(\mathrm{eq})} = h_\alpha'^{-1}(a + \boldsymbol{b} \cdot \boldsymbol{e}_\alpha + c\boldsymbol{e}_\alpha^2), \tag{23}$$

where a, $\boldsymbol{b}$, and c are Lagrange multipliers, then for the under-relaxed BGK LBE model, a global H-theorem can be proved. As for the usual lattice Boltzmann equation, it is shown that for the same h_α the local equilibrium distribution function $f_\alpha^{(\mathrm{eq})}$ has to be a quadratic polynomial, similar to the result of reference [36]. Furthermore, there exists no H-theorem for the equilibrium distribution function (a second order polynomial in $\boldsymbol{u}$) commonly used in the BGK LBE model, whereas for a Maxwellian type equilibrium distribution similar to the one for DVM, there is an H-theorem. However, such an equilibrium cannot lead to desirable hydrodynamic equations exactly.

In a most recent work concerning the H-theorem for the LBE models [39], it is shown that an exponential type (Maxwellian) equilibrium of the Lagrange multipliers due to the conservation constraints can minimize a Boltzmann type entropy function

$$H = \sum_\alpha f_\alpha \big[\ln(w_\alpha f_\alpha) - C_\alpha\big], \tag{24}$$

where w_α and C_α are constants. In the low Mach number limit up to second order in $\boldsymbol{u}$, the expansion of the Maxwellian-type equilibrium coincides with the equilibrium of polynomial type which leads to correct hydrodynamic equations. Incidentally, this result is similar to the result for DVMs, as discussed in the previous section. We also note that the equilibrium obtained in [39] can be obtained by discretization of the continuous Boltzmann equation by the procedure described in [18,19].

In summary, the results in Refs. [36–38] clearly lead to the same conclusion that an H-theorem does not exist for the BGK LBE models with the equilibrium distribution function taken as the second order polynomial in $\boldsymbol{u}$ which yields the hydrodynamic equation only up to the second order in $\boldsymbol{u}$ in the low Mach number limit. Furthermore, the choice of an entropy function, if exists, is certainly not unique for the lattice Boltzmann equation. Also, we cannot help but to note the fact that the aforementioned work on proving H-theorem for the lattice Boltzmann equation has no practical impact to the application of the LBE method.

It is worth noting that there are two salient features of the LBE models which distinguish the LBE models from DVMs:

(1) The discrete space and time of the LBE models may lead to spurious conservation laws;
(2) The equilibrium distribution function used in the LBE models is a low order Taylor expansion of the Maxwellian distribution function. This compromises the positivity condition which is necessary for the proof of an H-theorem.

Therefore, in light of the above rigorous results on DVM and the relevant results on the LBE method, it can be concluded that there exists no H-theorem for the LBE models of which the equilibrium is a polynomial in $\boldsymbol{u}$. Although Eq. (11) clearly implies that $f_\alpha^{(\mathrm{eq})}$ is an attractor for the LBE system, it is definitively not an equilibrium in the sense of an H-theorem. It is important to recognize the distinction between an attractor and an equilibrium that an attractor only possesses local stability under certain conditions, whereas an equilibrium has local as well as global stability guaranteed by H-theorems. Nevertheless, since $f_\alpha^{(\mathrm{eq})}$ is obtained through the Taylor expansion of the true equilibrium – the Maxwellian [18,19], $f_\alpha^{(\mathrm{eq})}$ may remain close to the genuine equilibrium if the expansion parameter (usually the Mach number) remains small. Since one cannot rely on an H-theorem to guarantee the stability of the LBE method, one must use other means such as linear analysis of the evolution operator of the LBE models to study the stability of the LBE method [40].

4. Conclusion

The discrete velocity models of the Boltzmann equation with continuous space and time lead to a hyperbolic system of equations for the hydrodynamic moments, a unique Maxwellian equilibrium distribution function, an H-theorem, and positivity of the solution of the initial value problem. The collisions in DVM lead to the relaxation of the parameters in the Maxwellian equilibrium, but not the hydrodynamic moments. This implies that the equations of state in DVMs are different from the equations of state in the Boltzmann equation. Nevertheless, when the lattice constant of the discrete velocity space $h \to 0$, solutions of DVM in $\mathbb{Z}_h^D$ converge to solutions of the Boltzmann equation: DVM in $\mathbb{Z}_h^D$ is consistent with the Boltzmann equation.

In contrast with DVM, the dynamics of the lattice Boltzmann equation with a small set of discrete velocities evolves on a highly symmetric lattice space with discrete time. In addition, the so-called equilibrium distribution function used in the LBE method is usually a low order Taylor expansion of the Maxwellian, if one wants to accurately simulate hydrodynamics. These features of the LBE models prevent them from possessing an H-theorem or a consistent thermodynamics in a rigorous and theoretical sense. This is also confirmed by recent work attempting to prove an H-theorem for LBE models [36–39]. Since there is no H-theorem (or consistent thermodynamics) for the LBE models leading to the correct hydrodynamic equations, the best one can do is construct a "*faithful*" local attractor in the LBE models to approximate the genuine equilibrium as accurately as possible [18,19]. Therefore, it is more appropriate to view the "equilibrium" in the LBE models as an attractor. The stability of the attractor defined by $f_\alpha^{(\mathrm{eq})}$ can be determined only by other means than proving an H-theorem [40].

In light of the rigorous results on DVM, it is also evident that the LBE models for thermo-hydrodynamics generally have a very narrow range of *temperature* owing to the small set of discrete velocities. This may also be a possible source of instability in thermo-LBE models.

The discrete velocity models of the Boltzmann equation are fully compressible, although their thermodynamics may be significantly different from that of ideal gases (described by the continuous Boltzmann equation), depending on the discrete velocity set. Nevertheless, DVM is a self-consistent system possessing an H-theorem. In contrast, the LBE method does not have these self-consistent properties. One difficulty encountered in the LBE model for compressible thermal fluids is that the equilibrium distribution function $f_\alpha^{(\mathrm{eq})}$ which is a Taylor expansion in $\boldsymbol{u}$ has an incorrect asymptotic behavior. The insights gained from the rigorous results on DVM should help us to construct better LBE models for compressible thermo-hydrodynamics.

Acknowledgements

The author is grateful to Prof. J. Nuttall of the University of Western Ontario and Prof. A. Magnus of the Catholic University of Louvain for the useful information regarding the Poisson sum formula; to Prof. P. Charrier and Dr. L. Mieussens of Université Bordeaux 1 for providing the preprints of Refs. [31,35]; and to Dr. R. Rubinstein of ICASE for helpful discussions on the Poisson sum formula and for his careful reading of the manuscript. Critical comments from Prof. D. d'Humières and Dr. S. Succi, and helpful discussions with Dr. A. Wagner and Dr. I. Karlin are also gratefully acknowledged. This work is partially support by NASA Langley Research Center under the program of Innovative Algorithms for Aerospace Engineering Analysis and Optimization.

Appendix A. Thermodynamics of DVM and Poisson sum

For any non-negative, continuous, decreasing, and Riemann integrable function $f(x)$ on $\mathbb{R}$, the Fourier transform of $f(x)$ is defined as follows:

$$F(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) e^{ikx}. \tag{A.1}$$

The Poisson sum formula relates $f(x)$ and $F(k)$ as follows [41]:

$$\sum_{n=-\infty}^{\infty} f(\alpha n) = \frac{\sqrt{2\pi}}{\alpha} \sum_{m=-\infty}^{\infty} F\left(\frac{2m\pi}{\alpha}\right). \tag{A.2}$$

The Poisson sum formula is applied to evaluate the hydrodynamic moment of DVM.

For the sake of simplicity, the one-dimensional case is studied first. The following function and its Fourier transform,

$$f(x) = e^{-(x-x_0)^2}, \qquad F(k) = \frac{1}{\sqrt{2}} e^{ikx_0} e^{-k^2/4}, \tag{A.3}$$

lead to the following equality according to the Poisson sum formula:

$$\alpha \sum_{n=-\infty}^{\infty} e^{-\alpha^2(n-\epsilon)^2} = \sqrt{\pi} \sum_{n=-\infty}^{\infty} e^{i2\pi n\epsilon} e^{-n^2\pi^2/\alpha^2},$$

where the substitution $x_0 = \alpha\epsilon$ has been made. By setting $\alpha = h$, the above equality becomes:

$$\sum_{n=-\infty}^{\infty} h e^{-(n-\epsilon)^2 h^2} = \sqrt{\pi} \sum_{n=-\infty}^{\infty} e^{i2\pi n\epsilon} e^{-n^2\pi^2/h^2}.$$

In the limit of $h \to 0$, besides the constant term, the leading terms in the right hand side of the above equality are those of $|n| = 1$. Therefore,

$$\begin{aligned}\sum_{n=-\infty}^{\infty} h e^{-(n-\epsilon)^2 h^2} &\approx \sqrt{\pi}\left[1 + 2\cos(2\pi\epsilon) e^{-\pi^2/h^2}\right] \\ &= \left[1 + 2\cos(2\pi\epsilon) e^{-\pi^2/h^2}\right] \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-(x-x_0)^2}.\end{aligned} \tag{A.4}$$

That is, the sum in the right hand side of the above equation is accurately approximated by the integral, with an exponentially small error.

Similarly, for the following function and its Fourier transform,

$$f(x) = x e^{-(x-x_0)^2}, \qquad F(k) = \frac{1}{\sqrt{2}}\left(\epsilon + i\frac{k}{4}\right) e^{ikx_0} e^{-k^2/4}, \tag{A.5}$$

the corresponding Poisson sum formula in the limit of $h \to 0$ leads to:

$$\begin{aligned}\sum_{n=-\infty}^{\infty} hn e^{-(n-\epsilon)^2 h^2} &\approx \epsilon\sqrt{\pi}\left[1 - \frac{2\pi}{h}\sin(2\pi\epsilon) e^{-\pi^2/h^2}\right] \\ &= \left[1 - \frac{2\pi}{h}\sin(2\pi\epsilon) e^{-\pi^2/h^2}\right] \int_{-\infty}^{\infty} \mathrm{d}x\, x e^{-(x-x_0)^2}.\end{aligned} \tag{A.6}$$

It should be noted that, due to the periodicity in the sum $\sum_{n=-\infty}^{\infty} f(n+1) = \sum_{n=-\infty}^{\infty} f(n)$,

$$\sum_{n=-\infty}^{\infty} hn e^{-(n-\epsilon)^2 h^2} = \epsilon \sum_{n=-\infty}^{\infty} h e^{-n^2 h^2}, \tag{A.7}$$

for $\epsilon \in \mathbb{Z}$.

Finally, for the following function $f(x)$ and its Fourier transform:

$$f(x) = (x - x_0)^2 e^{-(x-x_0)^2}, \qquad F(k) = \frac{1}{\sqrt{2}}\left(\frac{1}{2} - \frac{k^2}{4}\right) e^{ikx_0} e^{-k^2/4}, \tag{A.8}$$

the corresponding Poisson sum formula in the limit of $h \to 0$ gives:

$$\begin{aligned} \sum_{n=-\infty}^{\infty} h(n-\epsilon)^2 e^{-(n-\epsilon)^2 h^2} &= \sqrt{\pi} \sum_{n=-\infty}^{\infty} \left(\frac{1}{2} - \frac{\pi^2 n^2}{h^2}\right) e^{i2\pi n\epsilon} e^{-n^2\pi^2/h^2} \\ &\approx \left[1 - \frac{4\pi^2}{h^2}\cos(2\pi\epsilon) e^{-\pi^2/h^2}\right] \int_{-\infty}^{\infty} \mathrm{d}x\,(x-x_0)^2 e^{-(x-x_0)^2}. \end{aligned} \tag{A.9}$$

By straightforward generalization to D-dimensional space, the following results can be obtained:

$$\rho = \sum_{\boldsymbol{\xi}_\alpha \in \mathbb{Z}_h^D} h f_\alpha^{(0)} = \varrho(2\pi RT)^{D/2} + \mathrm{O}(e^{-\pi^2/h^2}), \tag{A.10a}$$

$$\rho \boldsymbol{v} = \sum_{\boldsymbol{\xi}_\alpha \in \mathbb{Z}_h^D} h \boldsymbol{\xi}_\alpha f_\alpha^{(0)} = \rho \boldsymbol{u} + \mathrm{O}\big(h^{-1} e^{-\pi^2/h^2}\big), \quad \boldsymbol{u} \notin \mathbb{Z}_h^D, \tag{A.10b}$$

$$\rho e = \sum_{\boldsymbol{\xi}_\alpha \in \mathbb{Z}_h^D} h \frac{1}{2}(\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2 f_\alpha^{(0)} = \frac{D}{2}\rho RT + \mathrm{O}(h^{-2} e^{-\pi^2/h^2}), \tag{A.10c}$$

where

$$f_\alpha^{(0)} = \varrho\, e^{-(\boldsymbol{\xi}-\boldsymbol{u})^2/(2RT)}.$$

It is easy to show that, because of the periodicity of the Poisson sum formula, $\boldsymbol{v} = \boldsymbol{u}$, $\forall \boldsymbol{u} \in \mathbb{Z}_h^D$. It should be noted that the convergence of the sums to the integrals is exponentially fast. It is also interesting to note that the error due to the discretization is independent of the space dimension D.

References

[1] G. McNamara, G. Zanetti, Phys. Rev. Lett. 61 (1988) 2332–2335.
[2] H. Chen, S. Chen, W.H. Matthaeus, Phys. Rev. A 45 (1991) R5339–R5342.
[3] Y.H. Qian, D. d'Humières, P. Lallemand, Europhys. Lett. 17 (1992) 479–484.
[4] R. Benzi, S. Succi, M. Vergassola, Phys. Rep. 222 (1992) 145–197.
[5] S. Chen, G.D. Doolen, Annu. Rev. Fluid Mech. 30 (1998) 329–364.
[6] L.-S. Luo, Int. J. Mod. Phys. C 8 (1997) 859–867.
[7] X. He, G.D. Doolen, J. Comput. Phys. 134 (1997) 306–315.
[8] F. Toschi, G. Amati, S. Succi, R. Benzi, R. Piva, Phys. Rev. Lett. 82 (1999) 5044–5047.
[9] L.-S. Luo, Phys. Rev. Lett. 81 (1998) 1618–1621.
[10] X. He, S. Chen, R. Zhang, J. Comput. Phys. 152 (1999) 642–663.
[11] D. Qi, J. Fluid Mech. 385 (1999) 41–62.
[12] L. Giraud, D. d'Humières, P. Lallemand, Europhys. Lett. 42 (1998) 625–630.
[13] U. Frisch, B. Hasslacher, Y. Pomeau, Phys. Rev. Lett. 56 (1986) 1505–1508.
[14] S. Wolfram, J. Stat. Phys. 45 (1986) 471–526.
[15] U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, J.-P. Rivet, Complex Systems 1 (1987) 649–707.
[16] D.H. Rothman, S. Zaleski, Lattice-Gas Cellular Automata: Simple Models of Complex Hydrodynamics (Cambridge Univ. Press, Cambridge, 1997).
[17] B. Chopard, M. Droz, Cellular Automata Modeling of Physical Systems (Cambridge Univ. Press, Cambridge, 1998).
[18] X. He, L.-S. Luo, Phys. Rev. E 55 (1997) R6333–R6336.
[19] X. He, L.-S. Luo, Phys. Rev. E 56 (1997) 6811–6817.

[20] T. Abe, J. Comput. Phys. 131 (1997) 241–246.
[21] K. Xu, L.-S. Luo, Int. J. Mod. Phys. C 9 (1998) 1177–1187.
[22] M. Junk, J. Comput. Phys. 151 (1999) 947–968.
[23] D. d'Humières, in: Rarefied Gas Dynamics: Theory and Simulations, B.D. Shizgal, D.P. Weaver (Eds.), Progress in Astronautics and Aeronautics 159 (1992) 450–458.
[24] C. Cercignani, Transp. Theoret. Stat. Phys. 23 (1994) 1–8.
[25] C. Cercignani, J. Stat. Phys. 87 (1997) 1097–1109.
[26] J.E. Broadwell, J. Fluid Mech. 19 (1964) 401–414.
[27] J.E. Broadwell, Phys. Fluids 7 (1964) 1243–1247.
[28] R. Gatignol, Théorie Cinétique des Gaz à Répartition Discrète des Vitesses, Lecture Notes in Physics 36 (Springer, Berlin, 1975).
[29] D. Goldstein, B. Sturtevant, J. Broadwell, in: Rarefied Gas Dynamics: Theoretical and Computational Techniques, E.P. Muntz, D.P. Weaver, D.H. Campbell (Eds.), Progress in Astronautics and Aeronautics 118 (1989) 100–117.
[30] T. Inamuro, B. Sturtevant, Phys. Fluids A 2 (1990) 2196–2203.
[31] A.V. Bobylev, 21st International Symposium on Rarefied Gas Dynamics, Marseille, France, Preprint (July 1998).
[32] A. Palczewski, J. Schneider, A.V. Bobylev, SIAM J. Numer. Anal. 34 (1997) 1865–1883.
[33] J. Schneider, P. Michel, Preprint (1997).
[34] H. Iwaniec, Invent. Math. 87 (1987) 385–401.
[35] L. Mieussens, Math. Models Mathods Appl. Sci. (1998) to appear.
[36] I.V. Karlin, A.N. Gorban, S. Succi, V. Boffi, Phys. Rev. Lett. 81 (1998) 6–9.
[37] I.V. Karlin, S. Succi, Phys. Rev. E 58 (1998) R4053–R4056.
[38] A.J. Wagner, Europhys. Lett. 44 (1998) 144–149.
[39] I.V. Karlin, A. Ferrante, H.C. Öttinger, Europhys. Lett. 47 (1999) 182–188.
[40] P. Lallemand, L.-S. Luo, Phys. Rev. E (1999), to appear.
[41] P.M. Morse, H. Feshbach, Methods of Theoretical Physics, Part I (McGraw-Hill, New York, 1953).