Connection Between the Lattice Boltzmann Equation and the Beam Scheme

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Abstract. In this paper we analyze and compare the lattice Boltzmann equation with the beam scheme in details. We notice the similarity and differences between the lattice Boltzmann equation and the beam scheme. We show that the accuracy of the lattice Boltzmann equation is indeed second order in space. We discuss the advantages and limitations of lattice Boltzmann equation and the beam scheme. Based on our analysis, we propose an improved multi-dimensional beam scheme.

Key words. kinetic theory, hydrodynamics, lattice Boltzmann method, beam scheme, Euler and Navier-Stokes equations.

Subject classification. Fluid Mechanics

1. Introduction. The method of lattice Boltzmann equation (LBE) [1, 2, 3, 4, 5] is a gas kinetics based method invented to solve mainly hydrodynamic systems described by the Navier-Stokes equations. The lattice Boltzmann equation is fully discrete in time and phase space. It is a drastically simplified version of the continuous Boltzmann equation [6, 7]. The lattice Boltzmann method has a number of computational advantages: simplicity of programming, intrinsic parallelism of the algorithm and data structure, and consistency of thermodynamics. These advantages of the lattice Boltzmann method are due to the following facts: first of all, the Boltzmann equation has a linear convective term; second, the velocity space is reduced to a set of very small number of discrete velocities in the lattice Boltzmann formalism; third, model potential or interaction, and free energies can be directly implemented into the lattice Boltzmann models [8]. It can be shown that the lattice Boltzmann equation recovers the near incompressible Navier-Stokes equations [9]. There is numerical evidence that the lattice Boltzmann method can indeed faithfully simulate the incompressible Navier-Stokes equations with high accuracy [10, 11, 12, 13].

Historically, the lattice Boltzmann equation evolves from its predecessor, the lattice gas automata [14, 15]. Recently it has been shown that the lattice Boltzmann equation is a special finite difference form of the continuous Boltzmann equation [6, 7]. This result has set the mathematical foundation of the lattice Boltzmann equation in a rigorous footing [6, 7]. It also provides insights to relate the lattice Boltzmann equation to other existing gas kinetics based schemes [16, 17, 18]. In this paper, we discuss the mathematical connections between the lattice Boltzmann equation and the beam scheme [16].

This paper is organized as follows. In Sec. 2 we briefly discuss the BGK Boltzmann equation and its hydrodynamics. In Sec. 3, we describe the derivation of the lattice Boltzmann equation by discretizing the continuous BGK Boltzmann equation, and the derivation of hydrodynamic equations from the lattice Boltzmann equation via Chapman-Enskog procedure. We also analyze the validity and accuracy of lattice Boltzmann method. In Sec. 4 we describe the beam scheme and connect the beam scheme with the lattice Boltzmann equation.
Boltzmann method. In Sec. 5 we compare the beam scheme and the lattice Boltzmann method. In Section 6, we propose an improved beam scheme and conclude the paper.

2. BGK Boltzmann Equation and its hydrodynamics. We begin with the Bhatnagar-Gross-Krook (BGK) [19] Boltzmann equation, which is a model kinetic equation widely studied [20, 21]:

\[
\partial_t f + \xi \nabla f = -\frac{1}{\tau} (f - g),
\]

where the single particle (mass) distribution function \( f \equiv f(x, \xi, t) \) is a time-dependent function of particle coordinate \( x \) and velocity \( \xi \), \( \tau \) is the relaxation time which characterizes typical collision processes, and \( g \) is the local Maxwellian equilibrium distribution function defined by

\[
g(\rho, u, \theta) = \rho (2\pi \theta)^{-D/2} \exp \left[ -\frac{1}{2} \frac{(\xi - u)^2}{\theta} \right],
\]

where \( D \) is the dimension of the velocity space \( \xi \); \( \rho, u, \) and \( \theta = k_B T/m \) are the mass density, macroscopic velocity, and normalized temperature per unit mass, respectively; \( k_B, T, \) and \( m \) are the Boltzmann constant, temperature, and particle mass, respectively. The mass density \( \rho \), velocity \( u \), and the temperature \( \theta \) (or internal energy density) are the hydrodynamic moments of \( f \) or \( g \):

\[
\begin{align*}
\rho &= \int d\xi f = \int d\xi g, \\
\rho u &= \int d\xi \xi f = \int d\xi \xi g, \\
\frac{D}{2} \rho \theta &= \int d\xi \frac{1}{2} (\xi - u)^2 f = \int d\xi \frac{1}{2} (\xi - u)^2 g.
\end{align*}
\]

At equilibrium \( f = g \), the Boltzmann equation (2.1) becomes

\[
D_t g = 0,
\]

where

\[
D_t \equiv \partial_t + \xi \nabla.
\]

The Euler equations can be easily derived from the above equation by evaluating its hydrodynamic moments:

\[
\begin{align*}
\partial_t \rho + \nabla (\rho u) &= 0, \\
\partial_t (\rho u) + \nabla (\rho uu + \rho \theta) &= 0, \\
\partial_t \left( \frac{D}{2} \rho \theta + \frac{1}{2} \rho u^2 \right) + \nabla \left( \gamma \rho \theta u + \frac{1}{2} \rho u^2 u \right) &= 0,
\end{align*}
\]

where \( \gamma = (D + 2)/2 \) is the ratio of specific heats of an ideal gas, \( uu \) denotes a second rank tensor \( u_i u_j \), and \( u^2 = u \cdot u \). It should be noted that \( \gamma \) is related to the number of the degree of freedom of a particle, which is \( D \) in the case of mono-atomic ideal gases. The momentum equation (2.6b) can also be rewritten as the following

\[
\rho \partial_t u + \rho u \nabla u = -\nabla P,
\]

where

\[
P = \rho \theta
\]
is the equation of state for ideal gas.

The Chapman-Enskog analysis [20, 21] gives the first order solution

\[
(2.9) \quad f^{(1)} = -\tau D_t g.
\]

Therefore,

\[
(2.10) \quad f = f^{(0)} + f^{(1)} = g - \tau D_t g.
\]

With the above solution of \( f \), the BGK equation, Eq. (2.1), becomes

\[
(2.11) \quad D_t g - \tau D_t^2 g = -\frac{1}{\tau} f^{(1)}.
\]

The moments of the above equation leads to the Navier-Stokes equations

\[
(2.12a) \quad \partial_t \rho + \nabla \cdot (\rho u) = 0,
\]

\[
(2.12b) \quad \partial_t (\rho u) + \nabla (\rho u u + \phi) = -\nabla \Pi^{(1)},
\]

where \( \Pi^{(1)} \) is the first order shear-stress tensor

\[
(2.13) \quad \Pi^{(1)}_{ij} = \int d\xi \xi_i \xi_j f^{(1)} = -\tau \phi (\partial_i u_j + \partial_j u_i).
\]

It is obvious that the kinematic viscosity in Eq. (2.12b) is

\[
(2.14) \quad \nu = \tau \phi.
\]

3. Lattice Boltzmann equation and its hydrodynamics.

3.1. Lattice Boltzmann equation. The continuous BGK equation, Eq. (2.1), admits a formal integral solution given by [20]:

\[
(3.1) \quad f(x + \xi \delta_t, \xi, t + \delta_t) = e^{-\delta_t/\lambda} f(x, \xi, t) + \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^t' g(x + \xi t', \xi, t + t') dt'.
\]

The lattice (BGK) Boltzmann equation can be derived by discretizing the above integral solution in both time and phase space [6, 7]. The obtained lattice Boltzmann equation is

\[
(3.2) \quad f_\alpha(x + e_\alpha \delta_t, t + \delta_t) - f_\alpha(x, t) = -\frac{1}{\tau} [f_\alpha(x, t) - f^{(eq)}_\alpha(x, t)],
\]

where \( \tau = \lambda/\delta_t, f_\alpha(x, t) = W_\alpha f(x, e_\alpha, t), f^{(eq)}_\alpha \) is the discretized equilibrium distribution function, and \( \{e_\alpha\} \) and \( \{W_\alpha\} \) are the discrete velocity set and associated weight coefficients, respectively. The discretized equilibrium distribution function \( f^{(eq)}_\alpha \), and both the discrete velocities \( \{e_\alpha\} \) and their corresponding weight coefficients \( \{W_\alpha\} \) depend upon the particular lattice space chosen. For the sake of explicitness, we use the nine-bit lattice Boltzmann equation in two-dimensional space in the following discussion. In this case, we have \( W_\alpha = 2\pi \phi \exp(e^2_\alpha/2\phi)w_\alpha \), where

\[
(3.3) \quad w_\alpha = \begin{cases} 
4/9, & \alpha = 0 \\
1/9, & \alpha = 1, 2, 3, 4 \\
1/36, & \alpha = 5, 6, 7, 8 
\end{cases}
\]
\[ e_\alpha = \begin{cases} (0, 0), & \alpha = 0 \\ (\cos \phi_\alpha, \sin \phi_\alpha), & \alpha \neq 0, \end{cases} \]

and \( \phi_\alpha = (\alpha - 1)\pi/2 \) for \( \alpha = 1-4 \), and \( (\alpha - 5)\pi/2 + \pi/4 \) for \( \alpha = 5-8 \), and \( c = \delta_x/\delta_t \). (Here \( \theta = c^2/3 \) for the nine-bit model has been substituted to obtain a uniform lattice structure \([6, 7]\)). Then, the equilibrium distribution function of the 9-bit model is:

\[ f_{\alpha}^{(eq)} = w_\alpha \rho \left[ 1 + \frac{3(e_\alpha \cdot u)}{c^2} + \frac{9(e_\alpha \cdot u)^2}{2c^4} - \frac{3u^2}{2c^2} \right]. \]

The hydrodynamic moments of the lattice Boltzmann equation are given by

\[ \rho = \sum_\alpha f_\alpha = \sum_\alpha f_{\alpha}^{(eq)} \]

\[ \rho u = \sum_\alpha e_\alpha f_\alpha = \sum_\alpha e_\alpha f_{\alpha}^{(eq)} \]

\[ \frac{D}{2} \rho \theta = \sum_\alpha \frac{1}{2} (e_\alpha - u)^2 f_\alpha = \sum_\alpha \frac{1}{2} (e_\alpha - u)^2 f_{\alpha}^{(eq)}. \]

Note that the quadrature used in the above equations must be exact for these hydrodynamic moments in order to preserve the conservation laws \([6, 7]\).

The algorithm for the lattice Boltzmann equation consists of two steps: collision and advection on a lattice space as prescribed by Eq. (3.2). The collision is accomplished as follows: first of all the hydrodynamic moments are computed at each lattice site \( \{x\} \) according to Eqs. (3.6), the equilibrium \( f_{\alpha}^{(eq)} \) can be calculated then according to Eq. (3.5). The distribution \( f_\alpha \) is updated on each site by using the relaxation scheme: \( f_\alpha(x, t + \delta_t) = f_\alpha(x, t) - [f_\alpha(x, t) - f_{\alpha}^{(eq)}(x, t)]/\tau. \) After collision, \( f_\alpha \) advects to the next site \( (x + e_\alpha \delta_t) \) according to the velocity \( e_\alpha \), i.e., \( f_\alpha(x + e_\alpha \delta_t, t + \delta_t) = f_\alpha(x, t + \delta_t). \) It is obvious that the algorithm is simple, explicit, and intrinsically parallel. All the calculations are local and data communications are uniform to the nearest neighboring sites.

### 3.2. Chapman-Enskog analysis

The hydrodynamics of the lattice Boltzmann equation can be derived via Chapman-Enskog analysis \([20, 21]\) with the following expansion \([9, 22]\):

\[ f_\alpha(x + e_\alpha \delta_t, t + \delta_t) = \sum_{n=0}^{\infty} \frac{\delta_t^n}{n!} D_t^n f_\alpha(x, t), \]

\[ f_\alpha = \sum_{n=0}^{\infty} \epsilon^n f_{\alpha}^{(n)}, \]

where

\[ D_t' \equiv (\partial_t + e_\alpha \nabla), \]

and \( \epsilon = \delta_t \). The normal solution of the lattice Boltzmann equation, up to the first order in expansion parameter \( \epsilon \) (which is the Knudsen number), from Chapman-Enskog analysis is

\[ f_{\alpha}^{(0)} = f_{\alpha}^{(eq)}, \]

\[ f_{\alpha}^{(1)} = -\tau D_t' f_{\alpha}^{(0)}. \]

With the above solution, we can, accordingly, derive the following governing equations for the lattice Boltzmann equation through Chapman-Enskog procedure:

\[ D_t' f_{\alpha}^{(eq)} = 0, \]

\[ D_t' f_{\alpha}^{(0)} = -\frac{1}{2} (2\tau - 1) \delta_t D_t^2 f_{\alpha}^{(eq)} = -\frac{1}{\tau} f_{\alpha}^{(1)}. \]
The hydrodynamic equations, the Euler and the Navier-Stokes equations, can be obtained by taking the moments of the above governing equations.

3.3. Hydrodynamics of lattice Boltzmann equation. The moments of the zeroth order equation, Eq. (3.10a), in the discrete momentum space [defined by Eqs. (3.6)] lead to the Euler equations

\begin{align}
(3.11a) & \quad \partial_t \rho + \nabla \cdot (\rho u) = 0, \\
(3.11b) & \quad \partial_t (\rho u) + \nabla (\rho u + \rho u u) = 0, \\
(3.11c) & \quad \partial_t \left( \frac{D}{2} \rho \theta + \frac{1}{2} \rho u^2 \right) + \nabla \cdot (\gamma \theta u) = 0,
\end{align}

Note that Eq. (3.11c) differs from its counterpart, Eq. (2.6c), derived from the continuous BCK Boltzmann equation, Eq. (2.1). The energy flux $\frac{1}{2} \rho u^2 u$ due to the advection of fluid is missing. The omission of the energy flux term $\frac{1}{2} \rho u^2 u$ can only be justified if

$$
\frac{1}{2} \rho u^3 \ll \gamma \rho \theta u,
$$

where $u \equiv ||u||$. Because $\theta = c_s^2 = c^2/3$ in the case of the nine-bit model, where $c_s$ is the sound speed, therefore

$$
M \ll \sqrt{2 \gamma} = \sqrt{(D + 2)},
$$

where $M \equiv u/c_s$ is the Mach number. From above analysis, it becomes clear that the lattice Boltzmann equation is only valid for low Mach number flow, or in the incompressible limit. This is consistent with the low velocity expansion made to obtain the equilibrium distribution function $f_{\text{eq}}$.

The moments of the first order equation, Eq. (3.10b), give the Navier-Stokes equations similar to Eqs. (2.12) with the viscosity given by

\begin{equation}
\nu = \frac{1}{2} (2\tau - 1) \delta_t \theta = \frac{1}{6} (2\tau - 1) \frac{\delta \theta^2}{\delta_t},
\end{equation}

where $\theta = c^2/3$ and $c = \delta_x / \delta_t$. The Navier-Stokes equation from lattice BGK Boltzmann equation can be easily derived by noticing the similarity of Eq. (3.10b) and Eq. (2.11), provided that the quadrature to evaluate the moments

\begin{equation}
\int d\zeta \zeta^m e^{-\zeta^2} = \sum_\alpha w_\alpha \zeta_\alpha^m
\end{equation}

is exact for $m \leq 5$, because $m = 1$ from the first order moment, $m = 2$ from $f_{\text{eq}}$, and $m = 2$ from the term $(e_\alpha \cdot \nabla)^2 f_{\text{eq}}$ in Eq. (3.10b). To obtain the two-dimensional nine-bit lattice Boltzmann equation, the third order Gaussian quadrature is the optimal choice to the aforementioned goal of evaluating the necessary hydrodynamic moments exactly [6, 7].

In the above derivation of the Navier-Stokes equation, and the governing equation Eq. (3.10b) in particular, one can immediately realize that the accuracy of the LBE method is of second order, as previously speculated [23], because all the second order terms in the Taylor expansion are included in Eq. (3.10b), and the truncation error is of third order. The term $-\delta_t \theta/2$ in the viscosity is the manifest of the inclusion of second order terms (in space). The simplicity of this proof for the second order accuracy of the lattice BGK Boltzmann method is due the simplicity of the collision operator in LBE method.
4. Beam Scheme. The beam scheme [16] is a finite volume, gas-kinetic based scheme to solve hydrodynamic equations. In the beam scheme, hydrodynamic variables (mass density $\rho$, momentum $\rho u$, and temperature $\theta$) are given at a particular time in each volume cell. The equilibrium distribution function constructed from the hydrodynamic variables can be approximated by a finite number of “beams,” or a distribution of finite number of discrete velocities. Consider in an one dimensional case in which we want to use three discrete velocities in the velocity space, then the equilibrium distribution $g$ is approximated in $\xi_x$ coordinate with three Kornick delta functions:

$$g_x = \rho (2\pi \theta)^{-1/2} \exp\{-\left(\xi_x - u_x\right)^2/2\theta\}$$

(4.1)

$$\approx \rho [a_0 \delta(\xi_x - u_x) + a_1 \delta(\xi_x - u_x + \Delta u_x) + a_2 \delta(\xi_x - u_x - \Delta u_x)].$$

We can calculate the unknowns ($a_0$, $a_1$, $a_2$, and $\Delta u_x$) from the following moment constraints:

(4.2a) $$\rho = \int d\xi_x g_x$$

(4.2b) $$\rho u_x = \int d\xi_x \xi_x g_x$$

(4.2c) $$\rho \theta = \int d\xi_x (\xi_x - u_x)^2 g_x$$

(4.2d) $$3 \rho \theta^2 = \int d\xi_x (\xi_x - u_x)^4 g_x.$$

The equations for the unknowns are:

$$a_0 + a_1 + a_2 = 1,$$

$$a_1 - a_2 = 0,$$

$$a_1 + a_2 \Delta u_x^2 = \theta,$$

$$a_1 + a_2 \Delta u_x^4 = 3 \theta^2.$$

And the results are

(4.3a) $$a_0 = \frac{2}{3},$$

(4.3b) $$a_1 = a_2 = \frac{1}{6},$$

(4.3c) $$\Delta u_x = \sqrt{3 \theta}.$$

Therefore, there are three “beams” or “particles” in the beam scheme with the velocity $u_x - \sqrt{3\theta}$, $u_x$, and $u_x + \sqrt{3\theta}$. Note that the weight coefficients of these three particles, $a_0$, $a_1$ and $a_2$, are identical to those derived in the lattice Boltzmann equation by using Gaussian quadrature. Thus, in the situation of $u_x = 0$, the beam scheme is similar to the lattice Boltzmann equation with the three discrete velocity of $-c$, 0, and $c$ in one-dimensional case, where we have substitute $3 \theta = c^2$ for isothermal fluids.

However, the difference between the lattice Boltzmann equation and the beam scheme outweighs the similarity between the two, for the reason that the lattice Boltzmann equation is a finite difference scheme, while the beam scheme is a finite volume one. In the beam scheme, the “particles” move in and out each cell according to the velocity of these “particles.” After this advection process, the hydrodynamic quantities ($\rho$, $u$, and $\theta$) are obtained through an averaging process in each volume cell. The “particles” with different velocity are mixed first to compute the averaged hydrodynamic quantities in the cell, and redistributed.
through the calculation illustrated previously. This mixing (or averaging) process inevitably introduces artificial dissipation. And this dissipation is implicit, just as for any other upwind finite volume scheme. Therefore, the transport coefficients, such as viscosity, cannot be explicitly derived in the beam scheme, and thus the beam scheme cannot solve the Navier-Stokes equations quantitatively.

5. Lattice Boltzmann Method and Beam Scheme. We now compare the pros and cons of the lattice Boltzmann equation and the beam scheme. Theoretically, the lattice Boltzmann equation accurately approximates the incompressible Navier-Stokes equations [9]. The method is simple, explicit, and intrinsically parallel. The transport coefficients can be obtained explicitly, and therefore there is no numerical dissipation in the simulations by using the lattice Boltzmann method. In addition, the lattice Boltzmann method is an intrinsically multidimensional scheme. The disadvantages of the lattice Boltzmann method are the obvious consequences of the low Mach number expansion and the regular lattice structure. Because of the low Mach number expansion, the lattice Boltzmann method is limited to incompressible flows and therefore is not applicable to compressible flows and shocks. In addition, the regular lattice structure of the lattice Boltzmann method is a direct consequence of constant temperature, i.e., \( \theta = c^2/3 = \text{constant} \) in the case of the nine-bit lattice Boltzmann model. This, we suspect, is partly the reason for the failures of the thermal lattice Boltzmann models. Furthermore, because the equilibrium distribution function is not a Maxwellian, the \( H \)-theorem for the continuous Boltzmann equation no longer holds for the lattice Boltzmann equation. That is to say, the \( f^{(eq)} \) is an attractor of the lattice Boltzmann equation, but it may not be the equilibrium in the sense of the \( H \)-theorem.

In contrast to the low Mach number expansion used in the lattice Boltzmann equation, the Maxwellian equilibrium distribution is expanded around the averaged macroscopic velocity in each volume cell. The discrete velocity set depends on the averaged velocity and temperature within each cell, and therefore it varies from cell to cell. The beam scheme leads to correct hydrodynamic equations, including the energy equation. Consequently, the beam scheme can well capture thermal and compressible effects in flows. Thus it is suitable for simulations of high-speed (hypersonic) flows, and it is also more stable for high Reynolds number flows. The beam scheme is a finite volume, upwind shock capturing scheme. Its natural shortcomings, like any other such schemes, are that it has intrinsic and implicit numerical dissipations due to the mixing of particles in each volume cell, and the transport coefficients cannot be obtained explicitly. Therefore it cannot solve the Navier-Stokes equations quantitatively.

6. Conclusion. As we have shown in this paper, while the lattice Boltzmann equation and the beam scheme share the same philosophy in the discretization of velocity space (in one dimensional space) – all the conserved quantities are preserved exactly in the process of discretization, their distinctive difference lies in their equilibrium distribution function. The lattice Boltzmann equation expands the equilibrium at \( u = 0 \) and uses a polynomial (of \( u \)) to approximate the Maxwellian, therefore the method is limited to apply only to the near incompressible Navier-Stokes equations. The beam scheme obtains particle beams around the average velocity of the Maxwellian distribution, thus avoiding the low Mach number expansion in the lattice Boltzmann method. Naturally, the beam scheme is suitable for shock capturing in the compressible flows. Moreover, the lattice Boltzmann equation evolves on a lattice structure, information advects exactly from one node to another thus there is no mixing process involved. In contrast, the particle beams in the beam scheme move from one volume cell to another, and the mixing among the beams occurs in the construction of local Maxwellian equilibrium. Because of the uncontrollable numerical dissipation in the beam scheme caused by the mixing, it is difficult to use the scheme to simulate hydrodynamics quantitatively.

It is interesting to compare the lattice Boltzmann method and the beam scheme in multi-dimensional
space. In two-dimensional space, the beam scheme only uses five velocities [16], i.e., one central beam with the bulk velocity \((u_x, u_y)\), and two side beams each in \(x\)- and \(y\)-directions, \((u_x \pm \sqrt{3} \theta, u_y)\) and \((u_x, u_y \pm \sqrt{3} \theta)\).

Based on the analysis of the lattice Boltzmann equation [9, 14, 15, 22], it is well understood that such a discrete velocity set inevitably introduces anisotropy into the hydrodynamic equations resulted from the scheme. To removed the anisotropy, one can use the nine velocity set derived in the lattice Boltzmann equation. That is, the diagonal velocities, \((u_x \pm \sqrt{3} \theta, u_y \pm \sqrt{3} \theta)\), must be included in the two-dimensional beam scheme. With this modification, the volume cell in two-dimensional space become an octagon, instead of a square. This is equivalent to use the product of two one-dimensional Maxwellian, each approximated by three “beams.” This is feasible because Maxwellian is factorizable in the Cartesian, or other, coordinate system.

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