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NOTE

Derivation of the Lattice Boltzmann Method by Means of the Discrete Ordinate Method for the Boltzmann Equation

Recently the lattice Boltzmann equation method has been extensively studied in a view point of its applicability and has been applied to various problems [1–5]. The lattice Boltzmann method proposed by Chen *et al.* [6, 7] and Qian *et al.* [8] which ensures isotropy, Galilean invariance, and possesses a velocity-independent pressure, is called the lattice Boltzmann BGK method, since it employs the single relaxation time approximation first introduced by Bhatnagar, Gross, and Krook [9] in 1954 to greatly simplify the collision operator of the Boltzmann equation. The lattice Boltzmann method was proposed as an extension of lattice gas automata [10–14] which was found to include various drawbacks according to the extensive study [4]. Like the derivation of the lattice gas automata [10–14], the derivation of the lattice Boltzmann method is also based on a requirement that it gives a Navier–Stokes equation at a limit of small ''Knudsen number.'' In fact, the lattice Boltzmann method in standard use was designed to give an incompressible Navier–Stokes equation [4]. The derivation of it is complicated and, therefore, it is not clear enough how to extend the lattice Boltzmann method so that, for example, it reduces to the Navier–Stokes equation for compressible gas flow, multicomponent mixture gas flow, and so on.

In this note, we show that the lattice Boltzmann BGK method in common use [4] can be derived from the Boltzmann equation itself. According to the present derivation, it is apparent that the equation thus derived can be reduced to the Navier–Stokes equation at a limit of small Knudsen number since the equation thus derived is the Boltzmann equation itself. Hence the present derivation method gives us a simple and flexible recipe to construct the lattice Boltzmann method, and makes it easy to construct an extended lattice Boltzmann method in various ways.

Let us consider the Boltzmann equation for a single molecule with BGK type collision operator,

$$\frac{\partial f}{\partial t} + \mathbf{c}\frac{\partial f}{\partial \mathbf{x}} = \nu(f_M - f), \tag{1}$$

where f is a distribution function, $\mathbf{c}$ is a molecular velocity, and ν is a collision frequency [9]. Here we consider the 2 dimensional fluid motion. Hence only the reduced distribution function,

$$\int_{-\infty}^{\infty} f\, dc_z, \tag{2}$$

is considered hereafter and is redefined as f. The redefined distribution function is governed by an equation similar to Eq. (1) and an equilibrium distribution function f_M is defined as

$$f_M = \frac{\rho}{2\pi RT}\exp\left(-\frac{1}{2RT}(\mathbf{c}-\mathbf{u})^2\right), \tag{3}$$

where ρ is a density, $\mathbf{u}$ a fluid velocity, T a temperature, and R is the gas constant. The macroscopic values such as the density and the velocity of the fluid are defined as

$$\begin{aligned}\rho &= \iint_{-\infty}^{\infty} f\, d\mathbf{c},\\ \rho\mathbf{u} &= \iint_{-\infty}^{\infty} \mathbf{c} f\, d\mathbf{c}.\end{aligned} \tag{4}$$

Hereafter we assume that the molecular velocity and fluid velocity are normalized by a quantity of $\sqrt{3RT}$ after the definition in the paper by Hou *et al.* [4]. Under this assumption, the equilibrium distribution function is

$$f_M = \frac{\rho}{2\pi/3}\exp\left(-\frac{3}{2}(\mathbf{c}-\mathbf{u})^2\right), \tag{5}$$

and the acoustic velocity defined by $c_s = \sqrt{RT}$ becomes $1/\sqrt{3}$.

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First we briefly describe the discrete ordinate method to solve the integro-differential equation defined by Eqs. (1), (3), and (4), which has been utilized for a rarefied gas flow analysis as a standard technique [15]. To solve the above equation by means of the discrete ordinate method, a set of discrete molecular velocity must be defined, on which the distribution function is evaluated. Hence the Boltzmann equation, which is an integro-differential equation in nature, reduces to the system of differential equations

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \frac{\partial f_i}{\partial \mathbf{x}} = \frac{\nu}{\delta}(f_{M,i} - f_i), \tag{6}$$

where f_i is the distribution function evaluated at the ith discrete velocity point of the set of discrete velocities. In the equation, since, as a goal of the present paper, we derive a lattice Boltzmann method in which the time and the physical space is discretized, it was assumed that the time and space coordinate is normalized by means of the time step Δt and $c_s \Delta t$, respectively. The nondimensional parameter $\delta = 1/(\nu_0 \Delta t)$ plays a roll of Knudsen number. Here ν_0 is a reference value for the collision frequency. To solve the discretized Boltzmann equation (6) with respect to t and $\mathbf{x}$, the equilibrium distribution function f_M in the right hand side of the equation must be evaluated. This evaluation can be carried out, once the macroscopic values (ρ and $\rho\mathbf{u}$) are evaluated in advance. The macroscopic values ρ and $\rho\mathbf{u}$ are evaluated by Eq. (4). Since only the distribution functions at discrete velocity points are defined, after an approximate function for the distribution function is chosen Eq. (4) reduces to a weighted summation of the distribution function defined on the discrete velocity points,

$$\begin{aligned} \rho &= \sum_i W_i f_i, \\ \rho\mathbf{u} &= \sum_i W_i' f_i, \end{aligned} \tag{7}$$

where W_i and W_i' are the coefficients for the quadrature. The system of Eq. (6) and the definition of macroscopic values (7) give a basic system of equations in the discrete coordinate method to solve the Boltzmann equation.

Now we consider the low speed fluid motion. Under this condition, the equilibrium distribution function can be linearized around the state at rest; for example, the equilibrium distribution function is linearized as

$$f_M = \frac{\rho}{2\pi/3}\left(1 + 3(\mathbf{c}\cdot\mathbf{u}) + \frac{9}{2}(\mathbf{c}\cdot\mathbf{u})^2 - \frac{3}{2}u^2\right) \exp\left(-\frac{3}{2}c^2\right). \tag{8}$$

Here we assume that a deviation of temperature from the state at rest can be neglected. Since the deviation of the distribution function from the one at rest is also small, it is assumed that the distribution function is approximated as

$$f = \frac{\varphi(\mathbf{c})}{2\pi/3} \exp\left(-\frac{3}{2}c^2\right). \tag{9}$$

The perturbed distribution function φ also satisfies the system of equations similar to the one for the original distribution function (6),

$$\frac{\partial \varphi_i}{\partial t} + \mathbf{c}_i \frac{\partial \varphi_i}{\partial \mathbf{x}} = \frac{\nu}{\delta}(\varphi_{M,i} - \varphi_i), \tag{10}$$

where the perturbed equilibrium distribution function φ_M becomes

$$\varphi_M = \rho\left(1 + 3(\mathbf{c}\cdot\mathbf{u}) + \frac{9}{2}(\mathbf{c}\cdot\mathbf{u})^2 - \frac{3}{2}u^2\right), \tag{11}$$

and the macroscopic values are defined as,

$$\begin{aligned} \rho &= \int_{-\infty}^{\infty}\!\!\int f\, d\mathbf{c} = \sum_i w_i \varphi_i, \\ \rho\mathbf{u} &= \int_{-\infty}^{\infty}\!\!\int \mathbf{c} f\, d\mathbf{c} = \sum_i w_i' \varphi_i, \end{aligned} \tag{12}$$

where w_i and w_i' are coefficients for a quadrature.

To obtain coefficients of the quadrature for calculating the macroscopic values, the perturbed distribution function is approximated by using an appropriate function of $\mathbf{c}$. The approximated distribution function must satisfy the restrictions

$$\tilde{\varphi}(\boldsymbol{c}_i) = \varphi_i. \tag{13}$$

That is, the approximate distribution function must have a specified value at each discrete velocity point. As for an appropriate approximate function, we employ the function

$$\tilde{\varphi}(\mathbf{c}; \varphi_i) = a_0 + (\mathbf{c}\cdot\mathbf{a}_1) + (\mathbf{c}\cdot\mathbf{a}_2)^2. \tag{14}$$

This function includes 5 unknown parameters (a_0, $\mathbf{a}_1$, and $\mathbf{a}_2$) which can be determined by using the values of the

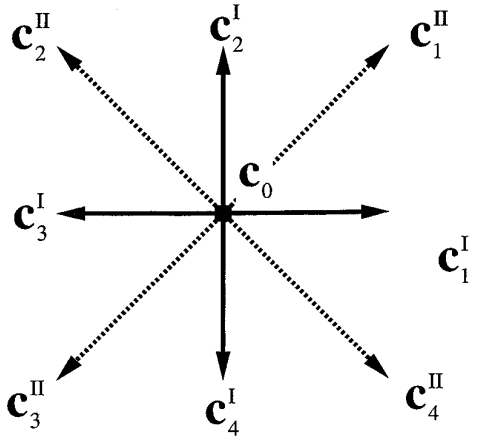

FIG. 1. Sketch for the discrete velocity points.

distribution function at 5 discrete velocity points. As for the discrete points on which the distribution function is defined, we consider the following set of discrete points,

$$\begin{aligned}
&\mathbf{c}_0 = (0,0),\\
&\mathbf{c}_i^I = \left(\cos\frac{i-1}{2}\pi, \sin\frac{i-1}{2}\pi\right) \quad (i=1,...,4)\\
&\mathbf{c}_i^{II} = \left(\cos\left(\frac{i-1}{2}\pi+\frac{\pi}{4}\right), \sin\left(\frac{i-1}{2}\pi+\frac{\pi}{4}\right)\right) \quad (i=1,...,4),
\end{aligned} \tag{15}$$

which corresponds to the 9 velocity model of the lattice Boltzmann method (see Fig. 1). Since we need 5 values of the distribution function to determine the unknown parameters included in the approximate function (14), the 5 discrete velocity points must be selected from the 9 discrete points. Even though several possibilities for the selection exists, we select the following two sets of 5 velocity points. One is

$$\begin{aligned}
&\mathbf{c}_0 = (0,0)\\
&\mathbf{c}_i^I = \left(\cos\frac{i-1}{2}\pi, \sin\frac{i-1}{2}\pi\right) \qquad (i=1,...,4)
\end{aligned} \tag{16}$$

and another is

$$\begin{aligned}
&\mathbf{c}_0 = (0,0),\\
&\mathbf{c}_i^{II} = \left(\cos\left(\frac{i-1}{2}\pi+\frac{\pi}{4}\right), \sin\left(\frac{i-1}{2}\pi+\frac{\pi}{4}\right)\right) \quad (i=1,...,4).
\end{aligned} \tag{17}$$

From a requirement defined by Eq. (13), the relation between the unknown parameters included in the approximate function (14) and the distribution functions at discrete velocity points can be obtained as

$$\begin{aligned}
a_0 &= \varphi_0,\\
a_{1,x} &= \frac{1}{2}[(\varphi_1^I - \varphi_0) - (\varphi_3^I - \varphi_0)],\\
a_{1,y} &= \frac{1}{2}[(\varphi_2^I - \varphi_0) - (\varphi_4^I - \varphi_0)],\\
(a_{2,x})^2 + (a_{2,y})^2 &= \frac{1}{2}[\varphi_1^I + \varphi_2^I + \varphi_3^I + \varphi_4^I - 4\varphi_0],
\end{aligned} \tag{18}$$

for the first set of discrete velocity points, and

$$\begin{aligned}
a_0 &= \varphi_0,\\
a_{1,x} &= \frac{1}{4}[(\varphi_1^{II} - \varphi_3^{II}) + (\varphi_4^{II} - \varphi_2^{II})],\\
a_{1,y} &= \frac{1}{4}[(\varphi_1^{II} - \varphi_3^{II}) - (\varphi_4^{II} - \varphi_2^{II})],\\
(a_{2,x})^2 + (a_{2,y})^2 &= \frac{1}{4}[\varphi_1^{II} + \varphi_2^{II} + \varphi_3^{II} + \varphi_4^{II}],
\end{aligned} \tag{19}$$

for the second set of discrete velocity points. On the other hand, the relations between the macroscopic values (ρ and $\rho\mathbf{u}$) and the unknown parameters are obtained as

$$\begin{aligned}
\rho &= \left(a_0 + \frac{1}{3}|\mathbf{a}_2|^2\right),\\
\rho\mathbf{u} &= \frac{1}{3}\mathbf{a}_1,
\end{aligned} \tag{20}$$

by substituting the approximated distribution function to the definition (12). Finally, by combining the relation (20) and Eq. (18) (or (19)), the relations between the macroscopic values (ρ, $\rho\mathbf{u}$) and the distribution function are obtained as

$$\begin{aligned}
\rho^I &= \frac{1}{3}\varphi_0 + \frac{1}{6}\sum_i \varphi_i^I,\\
(\rho\mathbf{u})^I &= \frac{1}{6}\sum_i \varphi_i^I \mathbf{c}_i^I,
\end{aligned} \tag{21}$$

for the discrete distribution function defined on the first set of discrete velocity points and

$$\begin{aligned}\rho^{II} &= \frac{2}{3}\varphi_0 + \frac{1}{12}\sum_i \varphi_i^{II},\\ (\rho\mathbf{u})^{II} &= \frac{1}{12}\sum_i \varphi_i^{II}\mathbf{c}_i^{II},\end{aligned} \tag{22}$$

for the one defined on the second set of discrete velocity points.

There are a variety of choices for an approximation function besides the present selection of Eq. (14). However, the advantage of this approximate function is that it can be reduced exactly to the equilibrium distribution function when the distribution function approaches an equilibrium state; i.e., for an equilibirum state, the coefficients in it are reduced to

$$\begin{aligned}a_0 &= \rho\left(1 - \frac{3}{2}u^2\right),\\ \mathbf{a}_1 &= 3\rho\mathbf{u},\\ \mathbf{a}_2 &= \mathbf{u}\sqrt{\frac{9}{2}\rho}.\end{aligned} \tag{23}$$

Let us see what kind of equation is obtained for the macroscopic values at small Knudsen number limit, from the discretized Boltzmann equation. By employing the Chapman–Enskog expansion method, we can obtain the equation accurate to the first order of Knudsen number,

$$\begin{aligned}\frac{\partial\rho}{\partial t} + \nabla\rho\mathbf{u} &= 0,\\ \frac{\partial\rho\mathbf{u}}{\partial t} + \nabla\mathbf{\Pi}^0 &= 0,\end{aligned} \tag{24}$$

where the momentum transfer tensor $\mathbf{\Pi}^0$ is defined as

$$\Pi^0_{\alpha\beta} = \left[\frac{\rho}{3} - \frac{1}{2}\rho u^2\right]\delta_{\alpha\beta} + \frac{3}{2}\rho u_\alpha u_\beta\delta_{\alpha\beta}, \tag{25}$$

for the discretized Boltzmann equation defined on the first set of the discrete velocity points (i.e., a set of Eqs. (10) and (21)), and

$$\Pi^0_{\alpha\beta} = \left[\frac{\rho}{3} + \rho u^2\right]\delta_{\alpha\beta} + 3\rho u_\alpha u_\beta - 3\rho u_\alpha u_\beta\delta_{\alpha\beta}, \tag{26}$$

for the equation defined on the first set of the discrete velocity points (i.e., a set of Eqs. (10) and (22)). The equations thus obtained are expected to be the so-called Euler equations. Unfortunately both of them are slightly deviated from the Euler equation, although we can expect that from the discretized Boltzmann equation at a limit of infinite discrete velocity points, the Euler equation is obtained at an accuracy up to the first order of Knudsen number. Hence the present deviation from the Euler equation is attributed to the limitation in the number of discrete velocity points. Fortunately, by combining the contributions from the first and second set of the discrete velocity points, we can show that this drawback can be overcome. To combine the contributions from both of the sets, we assume the linear combination. That is, the definition of macroscopic values is assumed to be

$$\begin{aligned}\rho &= (1-\alpha)\rho^I + \alpha\rho^{II},\\ &= \frac{1}{3}(1+\alpha)\varphi_0 + (1-\alpha)\frac{1}{6}\sum_i \varphi_i^I + \alpha\frac{1}{12}\sum_i \varphi_i^{II},\end{aligned} \tag{27}$$

$$\begin{aligned}\rho\mathbf{u} &= (1-\alpha)(\rho\mathbf{u})^I + \alpha(\rho\mathbf{u})^{II},\\ &= (1-\alpha)\frac{1}{6}\sum_i \varphi_i^I\mathbf{c}_i^I + \alpha\frac{1}{12}\sum_i \varphi_i^{II}\mathbf{c}_i^{II}.\end{aligned} \tag{28}$$

It should be noted that, in a view point of recovering the macroscopic values, any number of α is acceptable. However, to recover the Euler equation, it is easily shown that the free parameter α must be set as $\alpha = 1/3$. Hence the definition of the macroscopic values reduces to

$$\begin{aligned}\rho &= \frac{4}{9}\varphi_0 + \frac{1}{9}\sum_i \varphi_i^I + \frac{1}{36}\sum_i \varphi_i^{II},\\ \rho\mathbf{u} &= \frac{1}{9}\sum_i \varphi_i^I\mathbf{c}_i^I + \frac{1}{36}\sum_i \varphi_i^{II}\mathbf{c}_i^{II}.\end{aligned} \tag{29}$$

In fact, by applying the Chapman–Enskog expansion to the discretized Boltzmann equation defined on the 9 discrete velocity points (i.e., a set of Eqs. (10) and (29)) up to an accuracy of second order of Knudsen number, we can get the equations

$$\begin{aligned}\frac{\partial\rho}{\partial t} + \nabla\rho\mathbf{u} &= 0,\\ \frac{\partial\rho\mathbf{u}}{\partial t} + \nabla(\mathbf{\Pi}^0 + \mathbf{\Pi}^1) &= 0,\end{aligned} \tag{30}$$

where

$$\begin{aligned}\Pi^0_{\alpha\beta} &= \frac{\rho}{3}\delta_{\alpha\beta} + \rho u_\alpha u_\beta,\\ \Pi^1_{\alpha\beta} &= \frac{\delta\rho}{3\nu}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right),\end{aligned} \tag{31}$$

and the subscripts α, β represent the components for the x, y coordinates. Here, in the derivation procedure, the terms including the third power of the velocity were neglected. This equation is exactly the same as the incompressible Navier–Stokes equation if we define a pressure as $p = c_s^2\rho = \rho/3$ and a viscosity as $\mu = \delta\rho/3\nu$ and consider a flow in which the density variation is neglected.

To show the relation between the present method and the lattice Boltzmann method in common use, we redefine the distribution function as

$$\bar{\varphi}_i = \begin{cases} \dfrac{4}{9}\varphi_0 \\ \dfrac{1}{9}\varphi_i^I \\ \dfrac{1}{36}\varphi_i^{II} \end{cases} . \tag{32}$$

Then the ρ and $\rho\mathbf{u}$ can be rewritten by using the redefined distribution function,

$$\begin{aligned} \rho &= \sum_i \bar{\varphi}_i, \\ \rho\mathbf{u} &= \sum_i \bar{\varphi}_i \mathbf{c}_i. \end{aligned} \tag{33}$$

The equation for the redefined perturbed distribution function $\bar{\varphi}_i$ becomes

$$\frac{\partial\bar{\varphi}_i}{\partial t} + \mathbf{c}_i\frac{\partial\bar{\varphi}_i}{\partial\mathbf{x}} = \frac{\nu}{\delta}(\bar{\varphi}_{M,i} - \bar{\varphi}_i), \tag{34}$$

which is similar to Eq. (10). Once in a physical space, we set a rectangular mesh with a size of Δx $(= \Delta y)$, replace the spatial derivative with a first order upwind difference, and replace the temporal derivative with a first order explicit difference with a time step Δt $(= \Delta x = 1)$; this equation then reduces to

$$\bar{\varphi}_i(\mathbf{x} + \Delta t\mathbf{c}_i, t + \Delta t) - \bar{\varphi}_i(\mathbf{x}, t) = \frac{\nu}{\delta}(\bar{\varphi}_{M,i}(\mathbf{x}, t) - \bar{\varphi}_i(\mathbf{x}, t)) \tag{35}$$

and, with the definitions (33), gives exactly the same equation for the lattice Boltzmann BGK method [4]. That is, the lattice Boltzmann BGK method is exactly equivalent to the BGK Boltzmann equation defined on an appropriate set of discrete velocity points with some approximations.

As demonstrated above, the lattice Boltzmann BGK method in common use [4] can be derived from the Boltzmann equation defined on an appropriate set of discrete velocity points with some approximations. Hence, by using the present derivation procedure, it may be possible to produce a variety of the lattice Boltzmann method by changing various assumptions included, such as an assumption of linearized equation and selection of the approximate distribution function and the set of discrete velocity points. Also it may be possible to construct a lattice Boltzmann method applicable to a mixture gas flow, being based on an appropriate Boltzmann equation.

In the present note, we have shown that the lattice Boltzmann BGK method can be derived from the Boltzmann equation by means of the discrete ordinate method which is a standard technique for analyzing the Boltzmann equation. Apparently, the thus derived Boltzmann equation with the BGK type collision operator reduces to the Navier–Stokes equation at a limit of small Knudsen number, which is a primary application regime for the lattice Boltzmann method. With respect to the derivation procedure, the present method shows a clear contrast with the original lattice Boltzmann BGK method which was constructed from the requirement that it is reducible to the Navier–Stokes equation. In the present derivation, however, the reducibility to the Navier–Stokes equation is ensured if we select a proper set of discrete velocity points. Since the present derivation method is simple and flexible enough, it enables us to extend the lattice Boltzmann method in various ways.

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