Discretization of the Velocity Space in the Solution of the Boltzmann Equation

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We point out an equivalence between the discrete velocity method of solving the Boltzmann equation, of which the lattice Boltzmann equation method is a special example, and the approximations to the Boltzmann equation by a Hermite polynomial expansion. Discretizing the Boltzmann equation with a Bhatnagar-Gross-Krook collision term at the velocities that correspond to the nodes of a Hermite quadrature is shown to be equivalent to truncating the Hermite expansion of the distribution function to the corresponding order. The truncated part of the distribution has no contribution to the moments of low orders and is negligible at small Mach numbers. [S0031-9007(97)04950-8]

The Boltzmann equation is a well accepted mathematical model of a fluid at the microscopic level. It describes the evolution of the single particle distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ in the phase space $(\mathbf{x}, \boldsymbol{\xi})$, where $\mathbf{x}$ and $\boldsymbol{\xi}$ are the position and velocity vectors, respectively. This description of a fluid is more fundamental than the Navier-Stokes (NS) equations. It has a broader range of application and provides more detailed microscopic information which is critical for the modeling of the underlying physics behind complex fluid behavior. However, direct solution of the full Boltzmann equation is a formidable task due to the high dimensions of the distribution and the complexity in the collision integral. Among the various techniques developed [1], the discrete velocity method was introduced [2] based on the intuitive assumption that the gas particles can be restricted to have only a small number of velocities. The lattice Boltzmann equation (LBE) method formally falls into this category.

The development of the LBE method for simulation of fluid dynamics was independent of the continuum Boltzmann equation. The discrete LBE was first written to describe the dynamics of the distribution function in the lattice gas automaton (LGA) [3,4], in which the fluid physics is simulated at the microscopic level by "Boolean" particles moving with discrete velocities on a regular lattice, mimicking the motion of the constituent particles of a fluid. A Bhatnagar-Gross-Krook (BGK) collision model [5] was later adopted in the LBE in place of the complicated collision term [6,7]. In this lattice Boltzmann BGK model, the equilibrium distribution is chosen *a posteriori* by matching the coefficients in a small velocity (Mach number) expansion so that the correct hydrodynamic equations can be derived using the Chapman-Enskog method.

Recently it has been argued [8,9] that the LBE method can be derived from the continuum Boltzmann equation with a BGK collision model. In the new derivations, the Maxwellian distribution is Taylor expanded to second order in the fluid velocity scaled with the sound speed. Abe [9] employed a special functional form for the dis-

tribution function so that the macroscopic fluid variables are completely determined by the values of the distribution function at a set of discrete velocities. By noticing that in the Chapman-Enskog calculation, the functional form of the equilibrium distribution function in velocity space is only relevant in the calculation of the low-order moments, and for the Taylor expanded Maxwellian, those moments can be calculated exactly using a Gaussian quadrature, it is concluded that the NS equations can be derived from the Boltzmann equation evaluated on the nodes of the quadrature [8]. On substituting the weights of the corresponding quadrature into the expansion of the Maxwellian, the coefficients of the LBE equilibrium distribution function are recovered. The Boltzmann equation evaluated at the discrete velocities can then be further discretized in $\mathbf{x}$ and t in various ways for numerical integration [8]. The LBE models are shown to correspond to solving the discrete Boltzmann equations with a particular finite difference scheme [10].

The recovery of the NS equations from the Boltzmann equation by using a small number of collocation points in velocity space is not accidental. Almost a half century ago, Grad [11] introduced a sequence of approximations to the Boltzmann equation by expanding the distribution function in terms of Hermite polynomials in velocity space. The Hermite coefficients are directly related to the macroscopic fluid variables such as density, velocity, internal energy, stress, and so on. By keeping Hermite polynomials of up to third order, Grad obtained a system of equations for thirteen moments of the distribution function. This system of equations, known as the 13 moment approximation, was argued to be a better approximation than the Chapman-Enskog calculation [12,13]. By noticing that the Hermite coefficients for a given function can be estimated using a Hermite quadrature formula, and that this estimation is exact when the function satisfies certain conditions, an important correspondence between the LBE method and the approximation by Hermite polynomial expansion can be immediately identified. In this Letter, we show that by

discretizing the Boltzmann-BGK equation at a set of velocities that correspond to the nodes of a Gauss-Hermite quadrature in velocity space, we effectively project and solve the Boltzmann equation in a subspace spanned by the leading Hermite polynomials. The truncated part of the distribution has no contribution to the low-order moments that appear explicitly in the conservation equations.

We start from the following Boltzmann-BGK equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = -\frac{1}{\tau}(f - f^{(0)}), \qquad (1)$$

where τ is a relaxation time, $f^{(0)}$ is the Maxwellian

$$f^{(0)} = \rho\left(\frac{m}{2\pi k_B T}\right)^{D/2} e^{-m/2k_B T|\boldsymbol{\xi}-\mathbf{u}|^2}, \qquad (2)$$

where D is the dimension of the space, k_B is the Boltzmann constant, and m is the mass of the molecule. The mass density ρ, macroscopic fluid velocity $\mathbf{u}$, and the temperature T, are all functions of $\mathbf{x}$ and t. We introduce the dimensionless quantity $\theta = Tm_0/T_0 m$, where T_0 is a characteristic temperature and m_0 is a unit of the molecular mass. After rescaling the velocities $\boldsymbol{\xi}$ and $\mathbf{u}$ in units of the constant $c_0 = \sqrt{k_B T_0/m_0}$, which is the sound speed in a gas consisting of molecules of mass m_0 and at temperature T_0, the Maxwellian takes the following simple form:

$$f^{(0)} = \frac{\rho}{(2\pi\theta)^{D/2}} e^{-(1/2\theta)|\boldsymbol{\xi}-\mathbf{u}|^2}. \qquad (3)$$

For a single component system we can chose $m = m_0$ and have $\theta = T/T_0$. If the time and length scales t_0 and L are chosen so that $L/t_0 = c_0$, the dimensionless Boltzmann-BGK equation will have the same form as Eq. (1) with τ being the dimensionless relaxation time. The mass density ρ, the dimensionless fluid velocity $\mathbf{u}$, and the dimensionless internal energy density $\epsilon = D\theta/2$, are expressed as the *velocity moments* of the form $\int f\varphi(\boldsymbol{\xi})\,d\boldsymbol{\xi}$, with $\varphi = 1$, $\boldsymbol{\xi}$, and ξ^2, respectively:

$$\rho = \int f\,d\boldsymbol{\xi}, \quad \rho\mathbf{u} = \int f\,d\boldsymbol{\xi},$$

$$2\rho\epsilon + \rho u^2 = \int f\xi^2\,d\boldsymbol{\xi}. \qquad (4)$$

In discussions hereafter, the dimensionless variables are used unless otherwise specified.

Grad introduced the approximations by Hermite expansion in his 13 moment system [11]. Defining the following weight function

$$\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} e^{-(1/2\xi^2)}, \qquad (5)$$

where $\xi^2 = \boldsymbol{\xi}\cdot\boldsymbol{\xi}$, as argued by Grad, if $\omega^{-1/2}f$ is square integrable, i.e., if f approaches zero faster than $e^{-\xi^2/4}$ as $\boldsymbol{\xi}\to\infty$, the following Hermite expansion is valid in the sense of mean convergence:

$$f(\mathbf{x},\boldsymbol{\xi},t) = \omega(\boldsymbol{\xi})\sum_{n=0}^{\infty}\frac{1}{n!}a_i^{(n)}(\mathbf{x},t)\mathcal{H}_i^{(n)}(\boldsymbol{\xi}), \qquad (6)$$

where $\mathcal{H}^{(n)}$ is the nth order Hermite polynomial [14]. This expansion, also known as the Gram-Charlier series,

was also used in the solution of the Vlasov equation [15]. Clearly, the Maxwellian in Eq. (3) has such an expansion if the choice of T_0 and m_0 ensures that $\theta < 2$. On the right-hand side of Eq. (6), both $a^{(n)}$ and $\mathcal{H}^{(n)}$ are symmetric tensors of order n. The subscript i is an abbreviation for the multiple indices $\{i_1,\ldots,i_n\}$. The products denote contraction on all the n indices. The Hermite polynomials are a set of complete orthonormal basis of the Hilbert space with the inner product $\langle f, g\rangle = \int \omega f g\,d\boldsymbol{\xi}$. They satisfy the orthonormal relation

$$\int \omega\,\mathcal{H}_i^{(m)}\mathcal{H}_j^{(n)}\,d\mathbf{x} = \delta_{mn}\boldsymbol{\delta}_{ij}, \qquad (7)$$

where $\boldsymbol{\delta}_{ij} = 1$ if $i = \{i_1,\ldots,i_m\}$ is a permutation of $j = \{j_1,\ldots,j_n\}$, and $\boldsymbol{\delta}_{ij} = 0$ otherwise. For any function f, the nth Hermite coefficient can be obtained by the following equation:

$$a^{(n)} = \int f\mathcal{H}^{(n)}(\boldsymbol{\xi})\,d\boldsymbol{\xi}. \qquad (8)$$

The function f is completely determined by all of its Hermite coefficients.

The moments given in Eqs. (4) are invariants of both the original Boltzmann collision term and the BGK collision model. The hydrodynamic equations are simply the corresponding conservation equations

$$\frac{\partial}{\partial t}\int f\varphi\,d\boldsymbol{\xi} + \nabla\cdot\int f\boldsymbol{\xi}\varphi\,d\boldsymbol{\xi} = 0. \qquad (9)$$

The lowest order moments have the most significant contribution to the macroscopic hydrodynamics. Since the Hermite expansion has the feature that a velocity moment of a given order is solely determined by the Hermite coefficients up to that order and are not changed by the truncation of the higher-order terms, a sequence of approximations to Eq. (1) can be made by seeking the approximate solution of the following form:

$$\tilde{f}(\mathbf{x},\boldsymbol{\xi},t) = \omega(\boldsymbol{\xi})\sum_{n=0}^{N}\frac{1}{n!}a_i^{(n)}(\mathbf{x},t)\mathcal{H}_i^{(n)}(\boldsymbol{\xi}). \qquad (10)$$

The momentum and energy conservation equations explicitly involve moments of up to the second and the third order, respectively. It is necessary to require $N \geq 2$ if the momentum equation is to be obtained and $N \geq 3$ if the energy conservation equation is needed.

By the approximation above, we have assumed that the distribution function lies entirely in the subspace spanned by Hermite polynomials up to order N. For higher orders,

$$a^{(n)} \equiv \mathbf{0} \quad \text{if} \quad n > N. \qquad (11)$$

Although the terms that are truncated do not appear explicitly in the conservation equations, they affect the fluid variables through their contributions to the dynamic equations of the lower order moments. We will return to the validity of the assumption Eq. (11) later.

Let $\boldsymbol{\xi}_i$ and w_i, $i = 1, \ldots, d$, be the nodes and weights of a quadrature of degree $2N$, i.e., if $p(\boldsymbol{\xi})$ is a polynomial with a degree not greater than $2N$, we have

$$\int \omega(\boldsymbol{\xi}) p(\boldsymbol{\xi}) \, d\boldsymbol{\xi} = \sum_{i=1}^{d} w_i p(\boldsymbol{\xi}_i). \qquad (12)$$

Because $\tilde{f} \mathcal{H}^{(n)} / \omega$ is such a polynomial if $n \leq N$, the Hermite coefficients of $\tilde{f}$ can be calculated using the values of $\tilde{f}$ at the nodes $\boldsymbol{\xi}_i$ as the following:

$$a^{(n)} = \int \omega \frac{\tilde{f}}{\omega} \mathcal{H}^{(n)} \, d\boldsymbol{\xi} = \sum_{i=1}^{d} \frac{w_i f_i \mathcal{H}^{(n)}(\boldsymbol{\xi}_i)}{\omega(\boldsymbol{\xi}_i)}, \quad (13)$$

where $f_i = \tilde{f}(\mathbf{x}, \boldsymbol{\xi}_i, t)$. The knowledge of f_i as functions of position and time is equivalent to that of the truncated distribution function itself and therefore, that of the fluid variables calculated from the truncated distribution. These variables are

$$\rho = \sum_{i=1}^{d} \frac{w_i f_i}{\omega(\boldsymbol{\xi}_i)}, \qquad \rho \mathbf{u} = \sum_{i=1}^{d} \frac{w_i f_i \boldsymbol{\xi}_i}{\omega(\boldsymbol{\xi}_i)},$$

$$2\rho\epsilon + \rho u^2 = \sum_{i=1}^{d} \frac{w_i f_i \xi_i^2}{\omega(\boldsymbol{\xi}_i)}. \qquad (14)$$

By defining the auxiliary variables $g_i = w_i f_i / \omega(\boldsymbol{\xi}_i)$, Eqs. (14) can be put into a more efficient form for computation:

$$\rho = \sum_{i=1}^{d} g_i, \quad \rho \mathbf{u} = \sum_{i=1}^{d} g_i \boldsymbol{\xi}_i, \quad 2\rho\epsilon + \rho u^2 = \sum_{i=1}^{d} g_i \xi_i^2. \qquad (15)$$

This has the same form as how the fluid variables are calculated in the LBE method, where the distribution function is defined from the beginning as the populations of particles moving at discrete velocities.

We now turn to the discussion of the equations that the functions f_i satisfy. By directly evaluating Eq. (1) at the nodes $\boldsymbol{\xi}_i$, we have

$$\frac{\partial f_i}{\partial t} + \boldsymbol{\xi}_i \cdot \nabla f_i = -\frac{1}{\tau} [f_i - f^{(0)}(\boldsymbol{\xi}_i)]. \qquad (16)$$

Because $f^{(0)}$ has nonzero Hermite coefficients at all orders, on substituting $f^{(0)}(\boldsymbol{\xi}_i)$ into the right-hand side of Eqs. (14), the equalities hold only approximately. For the conservation laws to hold exactly, $f^{(0)}$ has to be projected into the subspace in which $\tilde{f}$ lies. Namely, in Eq. (16), the Maxwellian has to be replaced by its Nth order Hermite expansion. Denoting the values of the auxiliary variables g_i corresponding to the truncated Maxwellian by $\tilde{g}_i^{(N)}$, Eq. (16) can be written as

$$\frac{\partial g_i}{\partial t} + \boldsymbol{\xi}_i \cdot \nabla g_i = -\frac{1}{\tau} (g_i - \tilde{g}_i^{(N)}), \qquad i = 1, \ldots, d. \qquad (17)$$

It is to be noted that the positivity of the distribution function is lost in this truncation.

The first few Hermite coefficients of the Maxwellian can be obtained using Eq. (8). They are $a^{(0)} = \rho$, $a_i^{(1)} =$

ρu_i, $a_{ij}^{(2)} = \rho u_i u_j + (\theta - 1)\rho \delta_{ij}$, and $a_{ijk}^{(3)} = \rho u_i u_j \times u_k + (\theta - 1)\rho(u_i \delta_{jk} + u_j \delta_{ik} + u_k \delta_{ij})$. Using the explicit form of the Hermite polynomials, at the second and third orders, we have

$$\tilde{g}_i^{(2)} = w_i \rho \left[1 + \gamma_i + \boldsymbol{\xi}_i \cdot \mathbf{u} + \frac{1}{2}(\boldsymbol{\xi}_i \cdot \mathbf{u})^2 - \frac{u^2}{2} \right], \qquad (18)$$

$$\tilde{g}_i^{(3)} = w_i \rho \left[1 + \gamma_i + (1 + \zeta_i)\boldsymbol{\xi}_i \cdot \mathbf{u} + \frac{1}{2}(\boldsymbol{\xi}_i \cdot \mathbf{u})^2 \right.$$
$$\left. - \frac{u^2}{2} + \frac{1}{6}(\boldsymbol{\xi}_i \cdot \mathbf{u})^3 - \frac{1}{2}(\boldsymbol{\xi}_i \cdot \mathbf{u})u^2 \right], \qquad (19)$$

where $\gamma_i = (\xi_i^2 - D)(\theta - 1)/2$, $\zeta_i = (\xi_i^2 - D - 2) \times (\theta - 1)/2$. Equations (17)–(19) are the projection of the Boltzmann-BGK equation in the subspace spanned by the leading Hermite polynomials. They are in the configuration space $(t, \mathbf{x})$ and have a linear differential operator on the left-hand side. The fluid variables defined by Eqs. (15) obey the NS hydrodynamics. As previously shown [8,9], the LBE equilibrium distributions of Refs. [6,7] are obtained when the proper nodes and weights are substituted into Eq. (18), and the lattice Boltzmann equations are particular finite difference discretizations of Eq. (17).

It can be easily verified that moments of up to second and third orders calculated from Eqs. (18) and (19), respectively, are those of the Maxwellian. In particular, the tensor $p_{ij} \equiv \int f^{(0)} \xi_i \xi_j \, d\boldsymbol{\xi} = \rho u_i u_j + \rho\theta\delta_{ij}$ survives the truncation. The hydrostatic pressure is given by the equation of state $p = \rho\theta$, which translates to $p = \frac{\rho}{m} k_B T$ in laboratory units. When measured in the magnitude of one of the nodes of the quadrature, e.g., ξ_i, as in the LBE models, the sound speed is $\sqrt{\theta}/\xi_i$. In a single component isothermal system, θ becomes a free parameter which can be used to adjust the nominal sound speed with respect to the nodes of the quadrature. When $\theta = 1$, the Maxwellian has a very simple expansion:

$$f^{(0)} = \omega \rho \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{u}^{(n)} \mathcal{H}^{(n)}, \qquad (20)$$

and the truncated part of the distribution function is proportional to the power of the Mach number. Equations (18) and (19) are also simplified since $\gamma_i = \zeta_i = 0$. For a multiple component system, a different $\theta \sim 1/m$ has to be chosen for each component if all the components are at thermal equilibrium. This requirement was found necessary to obtain a correct equation of state in a previous multiple component LBE model [16].

The truncation made in Eq. (11) is similar to, but not exactly the same as the third order approximation in the Grad 13 moment system. In the latter the distribution function is expanded around the local fluid velocity before it is truncated. This is certainly a better approximation than expanding around the absolute equilibrium. However, it is not possible to use such an expansion in

the method discussed above because it would yield a set of nodes that depend on the local velocity.

The difference between the two expansions can be estimated by expanding the following approximated distribution function of the 13 moment system [11] around the absolute equilibrium

$$f^{(0)} \sum_{i=0}^{3} \frac{b^{(i)}}{i!} \mathcal{H}^{(i)}(\boldsymbol{\xi} - \mathbf{u}), \tag{21}$$

where $b^{(0)} = 1$, $b^{(1)} = 0$, and $b_{ii}^{(2)} = 0$. The Hermite coefficients in the expansion around the absolute equilibrium $a^{(n)}$ can be calculated as the following:

$$a^{(n)} = \int f^{(0)} \sum_{i=0}^{3} \frac{b^{(i)}}{i!} \mathcal{H}^{(i)}(\boldsymbol{\xi} - \mathbf{u}) \mathcal{H}^{(n)}(\boldsymbol{\xi}) \, d\boldsymbol{\xi} \tag{22}$$

$$= \rho \sum_{i=0}^{3} \frac{b^{(i)}}{i!} \int \omega(\boldsymbol{\xi}) \mathcal{H}^{(i)}(\boldsymbol{\xi}) \mathcal{H}^{(n)}(\boldsymbol{\xi} + \mathbf{u}) \, d\boldsymbol{\xi}. \tag{23}$$

Noticing that $\mathcal{H}^{(n)}(\boldsymbol{\xi} + \mathbf{u}) = \sum_{i=0}^{n} \mathbf{u}^{(n-i)} \mathcal{H}^{(i)}(\boldsymbol{\xi})$, we find that $a^{(0)} = \rho$, $a^{(1)} = \rho \mathbf{u}$, $a^{(2)} = \rho(\mathbf{u}^{(2)} + b^{(2)})$, and for $n \geq 3$,

$$a^{(n)} = \rho(\mathbf{u}^{(n)} + \mathbf{u}^{(n-2)} b^{(2)} + \mathbf{u}^{(n-3)} b^{(3)}). \tag{24}$$

With nonzero Hermite coefficients at all orders, the distribution function in the 13 moment system does not meet the assumption in Eq. (11). Since these coefficients are proportional to the power of the Mach number, Eqs. (19) approximate the 13 moment system only at the small Mach number limit.

Finding the quadrature formula with a minimum number of nodes for given geometry, weight function, and degree of accuracy is generally an unsolved problem. For the weight function in Eq. (5), quadrature formulas of different degrees are listed in Ref. [17]. Some of those are believed to be minimum without proof. In two dimensions, the minimum formula seems to be the 4th degree, 6-point formula (origin and the vertices of a pentagon) for isothermal models and the 7th degree, 12-point formula for thermodynamics models. In three dimensions, the minimum formulas are those of 5th degree, 13 point (origin and the vertices of a regular icosahedron) and 7th degree, 27 point for isothermal and thermodynamic systems, respectively. The nodes of these formulas usually do not coincide with those of a regular lattice. Equations (17) have to be solved using schemes such as the finite difference method [8,10].

The methodology of the discrete Boltzmann equation can be summarized as the following: The discretization of the continuum distribution function into values at the nodes of a quadrature formula is equivalent to the truncation of the high-order terms in the Hermite spectral space. The information that is lost in this procedure is represented by the high-order Hermite polynomials which do not explicitly appear in the conservation equations. This error is negligible at small Mach numbers and can always be made smaller by using a quadrature of a higher degree. With such a discretization, the Boltzmann equation becomes a homogeneous set of linear equations in the configuration space. Comparing with the nonlinear NS equations, these equations are easier to solve, have a broader range of application, and more importantly, allow the underlying fluid physics to be simulated directly at the cost of a macroscopic simulation. In addition, higher order approximations to the Boltzmann equation can be easily achieved by adding more points to the system.

Some of the limitations that LBE methods inherited from the Boolean LGA models can be removed with the present formulation. The equilibrium distribution is now obtained through a systematic orthogonal expansion of the Maxwellian, eliminating the tedious parameter-matching procedure which usually produces results that are not unique and contain erroneous terms at higher orders. The inflexible lattice structure and time stepping scheme of the LBE method are inconvenient for practical applications and often result in poor stability. By realizing that the LBE models are merely simple and rather primitive finite difference representations of the discrete Boltzmann-BGK equation, we can employ more sophisticated numerical techniques in solving these equations with better efficiency, stability, and flexibility.

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