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Evaluation of the external force term in the discrete Boltzmann equation

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A representation of the forcing term in the Boltzmann equation based on a Hermite expansion of the Boltzmann distribution function in velocity phase space is derived. Based on this description of the forcing term, a systematic comparison of previous lattice Boltzmann models describing a nonideal gas behavior is given. [S1063-651X(98)12010-X]

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It has recently been shown that a class of discrete-velocity models (e.g. lattice Boltzmann) correspond to the truncation of the Boltzmann equation in an Hermite velocity spectrum space [1]. In this paper, we extend the above mentioned work to include an external force term in the Boltzmann equation. We then examine two previous lattice Boltzmann models, describing nonideal gas behavior, which relied on assumptions for the functional form of forcing without rigorous proof.

We start by briefly reviewing the basic equations in Ref. [1] with the inclusion of a linear forcing term. The dimensionless Boltzmann-BGK equation in an external acceleration field $\mathbf{F}$ can be written as

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

where f is the velocity distribution, $\boldsymbol{\xi}$ is the microscopic velocity, τ is a relaxation parameter, and $f^{(0)}$ is the following Maxwellian distribution

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

where D is the dimension of the space, ρ is the mass density, $\mathbf{u}$ the fluid velocity, and θ is a normalized temperature. The velocities, $\boldsymbol{\xi}$ and $\mathbf{u}$ are in units of $c_0=\sqrt{k_BT_0/m_0}$, where k_B is the Boltzmann constant, and T_0 and m_0 are units of the temperature and the molecular mass, respectively. The characteristic length L and time t_0 are free to choose, provided they satisfy the relation $L/t_0=c_0$. The relaxation time τ and the externally maintained acceleration $\mathbf{F}$ are therefore in units of t_0 and c_0/t_0, respectively. The constant c_0 is the sound speed in a gas consisting of particles of mass m_0 and at temperature T_0. The dimensionless temperature θ is defined as $\theta=Tm_0/T_0m$. Readers are referred to Ref. [1] for more background and detail.

The distribution function f can be expanded in terms of Hermite polynomials $\mathcal{H}$ [2] in the following way:

$$f(\mathbf{x},\boldsymbol{\xi},t)=\omega(\boldsymbol{\xi})\sum_{n=0}^{\infty}\frac{1}{n!}\mathbf{a}^{(n)}(\mathbf{x},t)\mathcal{H}^{(n)}(\boldsymbol{\xi}), \tag{3}$$

where ω is the weight function defined as follows:

$$\omega(\boldsymbol{\xi})=\frac{1}{(2\pi)^{D/2}}e^{-\xi^2/2}, \tag{4}$$

and $\mathbf{a}^{(n)}$ is an nth-rank tensor obtained from the following equation:

$$\mathbf{a}^{(n)}=\int f\mathcal{H}^{(n)}(\boldsymbol{\xi})d\boldsymbol{\xi}. \tag{5}$$

Note that the product $\mathbf{a}^{(n)}\mathcal{H}^{(n)}$ denotes contraction on all the n subscripts. As argued by Grad [2], expansion (3) is valid in the sense of mean convergence provided that $\omega^{-1/2}f$ is square integrable. The distribution in Eq. (2) satisfies this condition when $\theta<2$. It was previously shown [1] that the approximation made in the discrete velocity method corresponds to the truncation of the Hermite expansion of the distribution function when the discrete velocities chosen are the notes of a Hermite quadrature. Further, this truncation preserves the macroscopic hydrodynamics such as that described by the Navier-Stokes equations.

Evaluating the term $\mathbf{F}\cdot\nabla_{\xi}f$ in the Hermite series representation is straightforward [2]. Using the relation

$$\omega\mathcal{H}^{(n)}=(-1)^n\nabla_{\xi}^n\omega, \tag{6}$$

the Hermite expansion of the distribution function can be written as

$$f(\mathbf{x},\boldsymbol{\xi},t)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\mathbf{a}^{(n)}\nabla_{\xi}^n\omega, \tag{7}$$

and its gradient in velocity space is

$$\nabla_{\xi}f=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\mathbf{a}^{(n)}\nabla_{\xi}^{n+1}\omega=-\omega\sum_{n=1}^{\infty}\frac{1}{n!}n\mathbf{a}^{(n-1)}\mathcal{H}^{(n)}. \tag{8}$$

The nth Hermite coefficient of the force term, $\mathbf{F}\cdot\nabla_{\xi}f$, is simply $n\mathbf{F}\mathbf{a}^{(n-1)}$, where the product is a tensor product. Explicitly, the external forcing term in Eq. (1) can be written by noting that due to the conservation of the mass and momentum, the first two Hermite coefficients of f are always $\mathbf{a}^{(0)}=\rho$ and $\mathbf{a}_i^{(1)}=\rho u_i$. Also the components of the first and second Hermite polynomials are $\mathcal{H}_i^{(1)}=\xi_i$ and $\mathcal{H}_{ij}^{(2)}=\xi_i\xi_j-\delta_{ij}$ [2] so that we may write

$$\mathbf{F}\cdot\nabla_\xi f=-\rho\omega[\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})+(\mathbf{F}\cdot\boldsymbol{\xi})(\mathbf{u}\cdot\boldsymbol{\xi})+\cdots], \tag{9}$$

where we have kept terms explicitly up to second order.

Note, the Hermite representation preserves the correct moments associated with the forcing term:

$$\int \mathbf{F}\cdot\nabla_\xi f d\boldsymbol{\xi}=0, \tag{10a}$$

$$\int \boldsymbol{\xi}\mathbf{F}\cdot\nabla_\xi f d\boldsymbol{\xi}=-\rho\mathbf{F}, \tag{10b}$$

$$\int \boldsymbol{\xi}\boldsymbol{\xi}\mathbf{F}\cdot\nabla_\xi f d\boldsymbol{\xi}=-\rho(\mathbf{Fu}+\mathbf{uF}). \tag{10c}$$

In fact, the correct coefficients for the Hermite expansion of the forcing term can also be determined, without explicit calculation of the velocity gradient, by taking proper moments of the forcing term and using the orthogonality properties of the Hermite functions.

To make a connection with discrete lattice Boltzmann models [1] note that the lattice Boltzmann distribution function f_i is represented as $f_i\equiv\omega_i/\omega(\xi)\bar{f}(\boldsymbol{\xi}_i)$, where ω_i are weights associated with the Gaussian quadrature, $\bar{f}$ is the distribution function truncated to a specified order in the Hermite spectrum space, and $\boldsymbol{\xi}_i$ are discrete velocities associated with the Hermite quadrature. We may then immediately write down the discrete Boltzmann representation of the forcing term in Eq. (9) by replacing $\omega(\xi)$ with ω_i and $\boldsymbol{\xi}$ with $\boldsymbol{\xi}_i$.

We now compare this model to two previous proposed lattice Boltzmann models that incorporate forcing. One model due to Shan and Chen [3], describing a nonideal gas, incorporated interparticle forces by adding an extra momentum in the equilibrium distribution function [i.e., $f^{(0)}(\rho,\mathbf{u},\theta)\rightarrow f^{(0)}(\rho,\mathbf{u}+\tau\mathbf{F},\theta)$]. To make a connection with this model we first note that Eq. (1) can be written in the following form, in which the effect of the external force is formally absorbed into the equilibrium distribution:

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=-\frac{1}{\tau}(f-f^{\mathrm{eq}}), \tag{11}$$

where

$$f^{\mathrm{eq}}=f^{(0)}+\tau\omega\sum_{n=1}^{\infty}\frac{1}{n!}n\mathbf{F}\mathbf{a}^{(n-1)}\mathcal{H}^{(n)}. \tag{12}$$

When solving the Boltzmann-BGK equation at discrete velocities we effectively restrict the distribution function in a subspace spanned by the leading Hermite polynomials so that the equilibrium distribution function, f^{eq}, has to be truncated in the Hermite spectrum space accordingly. We notice that the Maxwellian distribution can be expanded in the form of Eq. (3), with the first three coefficients being ρ, $\rho\mathbf{u}$, and $\rho\mathbf{uu}+(\theta-1)\rho\boldsymbol{\delta}$. Therefore to second order, we have

$$\begin{aligned}f^{\mathrm{eq}}&=\omega\rho\{1+(\mathbf{u}+\tau\mathbf{F})\mathcal{H}^{(1)}\\&\quad+\tfrac{1}{2}[\mathbf{uu}+\tau\mathbf{uF}+\tau\mathbf{Fu}+(\theta-1)\boldsymbol{\delta}]\mathcal{H}^{(2)}\}\\&=\bar{f}^{(0)}(\rho,\mathbf{u}+\tau\mathbf{F},\theta)-\frac{\omega\rho\tau^2}{2}[(\mathbf{F}\cdot\boldsymbol{\xi})^2-F^2],\end{aligned} \tag{13}$$

where $\bar{f}^{(0)}$ is the Maxwellian distribution truncated to second order and the last term would serve as a correction to the model of Shan and Chen.

A more recent model of He *et al.* [4] proposed that the interaction between fluid particles could be modeled as an external force in the Boltzmann equation using a mean-field approximation [4]. This approach involved the approximation, without proof, of substituting the distribution function in the force term [Eq. (1)] with its equilibrium value, e.g., the local Maxwellian distribution. We find that $\mathbf{F}\cdot\nabla_\xi f$ is identical to $\mathbf{F}\cdot\nabla_\xi f^{(0)}$ up to second order because the first two Hermite coefficients of the distribution function are always the same as those in the local Maxwellian distribution.

It is interesting that an earlier approach to solve the Vlasov equation with forcing adopted a Fourier-Hermite expansion of the distribution function [5]. Utilizing the recursion properties of Hermite polynomials an infinite set of first order nonlinear difference equations for the Fourier expansion coefficients is obtained. Truncating high order terms, a finite system of equations is integrated forward in time to obtain the Fourier coefficients of the distribution function.

The approach described in this paper may also have application in problems describing strong interactions where higher powers of the forcing appear. Recall that the linear forcing in Eq. (1) results from the first order expansion of the distribution function. A higher order expansion gives

$$f(\boldsymbol{\xi}+\mathbf{F})=f(\boldsymbol{\xi})+F_i\nabla_{\xi_i}f(\boldsymbol{\xi})+\tfrac{1}{2}F_iF_j\nabla_{\xi_i}\nabla_{\xi_j}f(\boldsymbol{\xi})+\cdots. \tag{14}$$

Clearly the higher order velocity derivatives are readily evaluated in terms of Hermite polynomials although care should be taken to maintain the same order of approximation in Hermite spectrum space. We note that Chapman and Cowling [6] describe a similar form of the forcing term for the case of electrons in a strong electric field, however, a clear connection between the velocity gradient terms and the coefficients of expansion found in Ref. [6] was not established.

In summary, starting from the continuum Boltzmann-BGK equation we have obtained a representation for the velocity gradient term based on a Hermite polynomial expansion of the velocity distribution function. As a result, we can easily derive the forcing term in a self-consistent fashion to any order in Hermite polynomials for use in discrete Boltzmann models. This systematic procedure should be of benefit to computer modelers of complex fluids.

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