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Discrete Boltzmann equation model for nonideal gases

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A discrete model based on the Boltzmann equation with a body force and a single relaxation time collision model is derived for simulations of nonideal-gas flow. The interparticle interaction is treated using a mean-field approximation. The Boltzmann equation is discretized in a way that preserves the derivation of the hydrodynamic equations from the Boltzmann equation, using either the Chapman-Enskog method or the Grad 13-moment method. The previously proposed nonideal-gas lattice Boltzmann equation model can be analyzed with rigor. [S1063-651X(98)50401-1]

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Computer simulations of fluid dynamical problems involving fluid interfaces and phase transitions are of both fundamental and practical importance. Traditional computational fluid dynamics (CFD) methods for solving macroscopic hydrodynamic equations have many difficulties in this area. For instance, fluid interfaces often undergo topological change due to both coalescence and phase transitions. In problems where the capillary effect is important, high resolution is required for accurate computation of interface curvature. The treatment of these problems using a Navier-Stokes solver is cumbersome, if not impossible, in many situations. The macroscopic motion of a fluid can also be solved by computing motions of its constituent particles. Since the complexity of the nonideal-gas fluid systems is essentially due to the microscopic interparticle interaction, particle methods such as molecular dynamics can simulate complex fluid phenomena naturally by implementing the correct interparticle potential. However, these methods are very inefficient for fluid simulations.

At the mesoscopic level, the lattice-Boltzmann-equation (LBE) method simulates the motion of fluids by following the evolution of a lattice Boltzmann equation that governs the behavior of the single-particle distribution function. It was found that solving the LBE directly is an efficient and accurate method for simulating fluid motion [1]. More importantly, the interparticle interaction can be easily incorporated into the LBE method to form a model that can simulate macroscopic complex fluid phenomena at least as efficiently as the conventional CFD methods solve the hydrodynamic equations for simple fluids [2].

Although the LBE method has shown its ability to simulate complex fluids, a recent study [3] shows that this method can be greatly improved if one can establish the relationship between the LBE and the continuous Boltzmann equation [3]. Historically, the continuous Boltzmann equation has mainly been used to solve supersonic flows [4]. This is partially due to both the extreme complexity of the collision kernel when dealing with dense, interacting particles and the tremendous computer resources required to resolve the six-dimensional distribution function. In this paper, we propose a computational scheme for the simulation of nonideal gases based on the continuous Boltzmann equation using a single-relaxation-time approximation, also known as the Bhatnagar-Gross-Krook (BGK) collision model [5]. The interparticle attraction is treated using a mean-field approximation in the same way that the Coulomb interaction among the charged particles of a plasma is treated in the Vlasov equation [5]. Following the work of Enskog, the effect of the exclusion volume is taken into account by an additional term in the collision operator. The final Boltzmann equation is then discretized in the velocity space in a way that guarantees that the Navier-Stokes equation is obtained at the macroscopic level. This discretization is similar to the truncation made in the well-known 13-moment method of Grad [6]. The previously proposed nonideal LBE model [2] can be obtained with only minor differences. The present derivation allows the LBE model to be implemented on nonuniform grids. The ''interaction potential'' introduced previously now has a clear connection with the interparticle pairwise potential in real fluids. Analysis of some other schemes [7,8] for incorporating interparticle forces into LBE models in the framework of the present derivation shows that anisotropy is a consequence of an inappropriate intermolecular interaction.

We start from the following Boltzmann equation in which the collision term is replaced by the BGK collision model,

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f+\mathbf{F}\cdot\nabla_{\xi}f=-\frac{f-f^{\mathrm{eq}}}{\lambda},\tag{1}$$

where $f\equiv f(\mathbf{x},\boldsymbol{\xi},t)$ is the single-particle distribution function in the phase space $(\mathbf{x},\boldsymbol{\xi})$, $\boldsymbol{\xi}$ is the microscopic velocity, $\mathbf{F}$ is an external body force which can depend on both space and time, λ is the relaxation time due to collision, and f^{eq} is the Maxwell-Boltzmann distribution function:

$$f^{\mathrm{eq}}\equiv\frac{\rho}{(2\pi RT)^{D/2}}\exp\left[-\frac{(\boldsymbol{\xi}-\mathbf{u})^{2}}{2RT}\right],\tag{2}$$

with R and D being the gas constant and dimension of the space, respectively. The macroscopic density ρ, velocity $\mathbf{u}$, and temperature T are calculated as the moments of the distribution function:

$$\rho = \int f d\boldsymbol{\xi}, \tag{3}$$

$$\rho\mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \tag{4}$$

$$\frac{D}{2}\rho RT = \int (\boldsymbol{\xi}-\mathbf{u})^2 f d\boldsymbol{\xi}. \tag{5}$$

These macroscopic fluid variables can be shown to obey the familiar Navier-Stokes equations.

The derivative $\nabla_\xi f$ cannot be calculated directly because the dependence of the distribution function on the microscopic velocity is unknown. Considering that f^{eq} is the leading part of the distribution f and the gradient of f^{eq} has the most important contribution to the gradient of f, we assume

$$\nabla_\xi f \approx \nabla_\xi f^{\mathrm{eq}} = -\frac{\boldsymbol{\xi}-\mathbf{u}}{RT} f^{\mathrm{eq}}. \tag{6}$$

Consequently, we obtain

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\nabla f = -\frac{f-f^{\mathrm{eq}}}{\lambda} + \frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{RT} f^{\mathrm{eq}}. \tag{7}$$

In the simplified Boltzmann equation above, **F** is the external force experienced by each particle. In this paper, we will use the same term to account for the particle interaction, similarly to the Vlasov approximation in which each particle experiences an averaged electric field arising from the Coulomb interaction from the other particles [5]. To simulate a nonideal gas, two important factors have to be taken into consideration: the intermolecular attraction and the exclusion volume of molecules.

The intermolecular attraction is treated using the same mean-field approximation, i.e., a particle can be considered to move in the following averaged force potential due to intermolecular attraction [9]:

$$V(\mathbf{r}_1) = \int_{r_{12}>\sigma} u_{\mathrm{attr}}(r_{12})\rho(\mathbf{r}_2) d\mathbf{r}_2, \tag{8}$$

where, $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, $u_{\mathrm{attr}}(r_{12})$ is the attractive component of the intermolecular pairwise potential, and σ is the diameter of the molecules. Expanding $\rho(\mathbf{r}_2)$ in Eq. (8) about $\mathbf{r}_1$ and assuming that the gradient of ρ is small, the leading two terms are

$$V = -2a\rho - \kappa\nabla^2\rho, \tag{9}$$

where a and κ are constants given by

$$a = -\frac{1}{2}\int_{r>\sigma} u_{\mathrm{attr}}(r) d\mathbf{r},$$

$$\kappa = -\frac{1}{6}\int_{r>\sigma} r^2 u_{\mathrm{attr}}(r) d\mathbf{r}.$$

According to the analysis of Enskog (c.f. Chap. 16 of Ref. [10]), when the temperature is a constant, the effects of the exclusion volume of the molecules on the equilibrium properties of a dense gas can be approximated by the following addition to the collision term:

$$-f^{\mathrm{eq}} b\rho\chi(\boldsymbol{\xi}-\mathbf{u})\cdot\nabla \ln(\rho^2\chi), \tag{10}$$

where $b=2\pi\sigma^3/3m$, m is the mass of a single molecule, and χ is the increase in collision probability due to the increase in fluid density, which has the following asymptotic form:

$$\chi = 1 + \frac{5}{8}b\rho + 0.2869(b\rho)^2 + 0.1103(b\rho)^3 + \cdots . \tag{11}$$

The form of Eq. (10) allows it to be combined with the corrections due to intermolecular attraction, yielding a single equivalent force field in Eq. (7):

$$\mathbf{F} = -\nabla V - b\rho RT\chi\nabla \ln(\rho^2\chi). \tag{12}$$

It should be noted that in the derivation above a few crude approximations have been employed. The correspondence with the details of the molecular properties should only be taken as heuristic when the equations above are applied to real systems to obtain quantitative results.

To solve Eq. (7) numerically, we first discretized it in time. The equation can be integrated over a time step of δt to become

$$\begin{aligned} &f(\mathbf{x}+\boldsymbol{\xi}\delta t,\boldsymbol{\xi},t+\delta t) - f(\mathbf{x},\boldsymbol{\xi},t) \\ &\quad = -\int_t^{t+\delta t} \frac{f-f^{\mathrm{eq}}}{\lambda} dt + \int_t^{t+\delta t} \frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{RT} f^{\mathrm{eq}} dt. \end{aligned} \tag{13}$$

Following previous lattice Boltzmann models for an ideal gas, the integrand of the first term on the right-hand side of Eq. (13) is assumed to be constant over one time step. This assumption yields an artificial viscosity that can be absorbed into the real viscosity of fluids. However, a trapezoidal rule is necessary for the second integration as discussed later. With these considerations, Eq. (13) becomes

$$\begin{aligned} &f(\mathbf{x}+\boldsymbol{\xi}\delta t,\boldsymbol{\xi},t+\delta t) - f(\mathbf{x},\boldsymbol{\xi},t) \\ &\quad = -\frac{f-f^{\mathrm{eq}}}{\tau}\bigg|_t + \frac{\delta t}{2}\left[\frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{RT} f^{\mathrm{eq}}\bigg|_{t+\delta t} \right. \\ &\qquad \left. + \frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{RT} f^{\mathrm{eq}}\bigg|_t\right], \end{aligned} \tag{14}$$

where $\tau=\lambda/\delta t$ is the nondimensional relaxation time. The right-hand side involves quantities evaluated at $t+\delta t$. To eliminate this implicity, we introduce the following new variable:

$$h = f - \frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{2RT} f^{\mathrm{eq}}\delta t, \tag{15}$$

in terms of which, Eq. (14) becomes

$$\begin{aligned} &h(\mathbf{x}+\boldsymbol{\xi}\delta t,\boldsymbol{\xi},t+\delta t) - h(\mathbf{x},\boldsymbol{\xi},t) \\ &\quad = -\frac{h(\mathbf{x},\boldsymbol{\xi},t) - h^{\mathrm{eq}}(\mathbf{x},\boldsymbol{\xi},t)}{\tau} + \frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{RT} f^{\mathrm{eq}}\delta t, \end{aligned} \tag{16}$$

where

$$h^{\mathrm{eq}}=\left[1-\frac{\mathbf{F}\cdot(\boldsymbol{\xi}-\mathbf{u})}{2RT}\,\delta t\right]f^{\mathrm{eq}}. \tag{17}$$

Here we restrict our interest to the recovery of mass and momentum equations only and will defer the discussion of the temperature equation to future publications. The macroscopic density and momentum are now related to h by

$$\int h\,d\boldsymbol{\xi}=\rho, \tag{18}$$

$$\int h\boldsymbol{\xi}\,d\boldsymbol{\xi}=\rho\mathbf{u}-\tfrac{1}{2}\rho\mathbf{F}\delta t. \tag{19}$$

To solve the time-discretized system given by Eqs. (16), (18), and (19) numerically, the velocity space, denoted by $\boldsymbol{\xi}$, must be discretized. It is well known that the form of the distribution in the velocity space affects the macroscopic fluid equations through its first few moments. When deriving the Navier-Stokes equations from the the Boltzmann equation with the BGK collision model using the Chapman-Enskog expansion, only velocity moments of the Maxwellian distribution up to third order are used. Alternatively, Grad [6] was able to obtain the hydrodynamic equations from the Boltzmann equation by expanding the distribution function in the velocity space in terms of Hermite polynomials, and keeping only the first three terms in the expansion. For any function that can be represented by a finite number of Hermite polynomials, the moments, or, equivalently, the expansion coefficients, can be *exactly* computed by Gaussian integration using the function values at a set of discrete points [11]. Truncating the higher-order Hermite polynomials in the functional space is equivalent to truncating the continuous velocity space into a finite set of discrete points. After this truncation, the moment integrals in Eqs. (18) and (19) are replaced by summations of the function values using a Gaussian quadrature of the following form:

$$\int \psi(\boldsymbol{\xi})h(\mathbf{x},\boldsymbol{\xi},t)\,d\boldsymbol{\xi}=\sum_a w_a\psi(\mathbf{e}_a)h(\mathbf{x},\mathbf{e}_a,t), \tag{20}$$

where $\{\mathbf{e}_a\}$ is the set of collocation points in velocity space, w_a are the corresponding weight coefficients, and $\psi(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$. In order for the velocity moments to have the correct hydrodynamic behavior, it is sufficient to have only information of the distribution function at the points in the velocity space given by the Gaussian quadrature formula. As long as the integration scheme is accurate for polynomials $\psi(\boldsymbol{\xi})$ of up to third order, the summation in velocity space yields the correct moments, and the derivation of the Navier-Stokes equation from the Boltzmann equation survives the discretization of the velocity space. For more details, readers are referred to [3]. Here we only focus on the two-dimensional, isothermal, low-Mach-number flow, (i.e., $T=$const and $\mathbf{u}^2\ll RT$). Under these assumptions, the f^{eq} can be expanded as

$$f^{\mathrm{eq}}=\frac{\rho}{2\pi RT}\exp\left(-\frac{\xi^2}{2RT}\right)\times\left[1+\frac{\boldsymbol{\xi}\cdot\mathbf{u}}{RT}+\frac{(\boldsymbol{\xi}\cdot\mathbf{u})^2}{2(RT)^2}-\frac{\mathbf{u}^2}{2RT}\right]+O(\mathbf{u}^3). \tag{21}$$

With $\exp(-\xi^2/2RT)$ being the weight function, the integration scheme has to be a Gauss-Hermite quadrature of at least fifth order. On a hexagonal lattice, for example, it has been shown [3] that these restrictions yield the following collocation points:

$$\mathbf{e}_a=\begin{cases}\mathbf{0} & a=0,\\ c\left(\cos\frac{a-1}{3}\pi,\sin\frac{a-1}{3}\pi\right) & a=1,\ldots,6,\end{cases} \tag{22}$$

where $c=2\sqrt{RT}$, and the corresponding weight coefficients of $w_0=\pi RT$, and $w_a=\pi e^2RT/6$ for $a=1,\ldots,6$. By introducing

$$h_a=w_ah(\mathbf{x},\mathbf{e}_a,t), \tag{23}$$

and the similar definitions for f_a and f_a^{eq}, Eq. (16) can be written as

$$h_a(\mathbf{x}+\mathbf{e}_a\delta t,t+\delta t)-h_a(\mathbf{x},t)=-\frac{1}{\tau}[h_a(\mathbf{x},t)-h_a^{\mathrm{eq}}]+4\frac{\mathbf{F}\cdot(\mathbf{e}_a-\mathbf{u})}{c^2}f_a^{\mathrm{eq}}\delta t, \tag{24}$$

where,

$$f_a^{\mathrm{eq}}=t_a\rho\left[\frac{1}{2}+2\frac{\mathbf{e}_a\cdot\mathbf{u}}{c^2}+\frac{4(\mathbf{e}_a\cdot\mathbf{u})^2}{c^4}-\frac{\mathbf{u}^2}{c^2}\right], \tag{25}$$

with $t_0=1$ and $t_a=1/6$ for $a=1,\ldots,6$. The corresponding equilibrium distribution for h can be calculated using

$$h_a^{\mathrm{eq}}=\left[1-2\frac{\mathbf{F}\cdot(\mathbf{e}_a-\mathbf{u})}{c^2}\,\delta t\right]f_a^{\mathrm{eq}}, \tag{26}$$

and the macroscopic density and velocity given by Eqs. (18) become

$$\sum h_a=\rho, \tag{27}$$

$$\sum h_a\mathbf{e}_a=\rho\mathbf{u}-\tfrac{1}{2}\rho\mathbf{F}\delta t. \tag{28}$$

The discretized equations have the same form as LBE models if the space $\mathbf{x}$ is discretized so that $\mathbf{e}_a\delta t$ is the distance between two neighboring grid points.

It is interesting at this point to use our results to analyze the previous lattice Boltzmann models with interparticle interactions. A direct comparison can be made with the nonlocal model proposed by Shan and Chen [2]. By realizing that the distribution function in Refs. [2] corresponds to the function h in the present model, and replacing $\mathbf{F}$ with $\rho\mathbf{F}\delta t$, the previous model is equivalent to the present model except for a minor difference on the right-hand side of the evolution equation. This difference, which can be written as

$$w_a\rho\left\{\tau\left(\tau-\frac{1}{2}\right)^2\left[\frac{\mathbf{F}^2}{c^2}-\frac{4(\mathbf{e}_a\cdot\mathbf{F})^2}{c^4}\right]+\left(1-\frac{1}{2\tau}\right)\times\left[\frac{8(\mathbf{F}\cdot\mathbf{u})(\mathbf{e}_a\cdot\mathbf{u})}{c^4}-\frac{4\mathbf{F}\cdot(\mathbf{e}_a-\mathbf{u})\mathbf{u}^2}{c^4}+\frac{16\mathbf{F}\cdot(\mathbf{e}_a-\mathbf{u})(\mathbf{e}_a\cdot\mathbf{u})^2}{c^6}\right]\right\}, \tag{29}$$

is of second order in $\mathbf{u}^2/c^2$ and $\mathbf{F}^2/c^2$. As long as the velocity and interparticle force are small, this difference is negligible.

Attention needs to be drawn here to the choice of $\mathbf{F}$. Previously [2], it was defined as

$$\mathbf{F}=-\mathcal{G}\psi(\mathbf{x})\sum_a \psi(\mathbf{x}+\mathbf{e}_a\delta_t)\mathbf{e}_a, \tag{30}$$

where ψ is the ''effective mass'' which is a function of density. By expanding $\psi(\mathbf{x}+\mathbf{e}_a)$ about $\mathbf{x}$, we have

$$\mathbf{F}=-\nabla\left(\frac{3\mathcal{G}c^2\delta_t\psi^2}{2}\right)-\frac{3\mathcal{G}c^4\delta_t^3}{8}\psi\nabla\nabla^2\psi, \tag{31}$$

whereas in the present results, from Eq. (12), we have

$$\rho\mathbf{F}\delta_t=\nabla(a\rho^2-b\rho^2RT\chi)\delta_t+\kappa\rho\delta_t\nabla\nabla^2\rho. \tag{32}$$

By matching the first-order derivative term of Eqs. (31) and (32), the following relation between the previously unspecified ''effective mass'' and the molecular properties can be identified:

$$\psi=\frac{\rho}{c}\left(\frac{2bRT\chi-2a}{3\mathcal{G}}\right)^{1/2}. \tag{33}$$

Another class of LBE models [7,8,12] implements momentum conservation at each collision. Since only local information is used at each collision, the integrand of the second term in Eq. (13) must be treated as a constant during one time step if these models are to be derived with the present method. This leads to the following evolution equation of f:

$$\begin{aligned} f_a(\mathbf{x}+\mathbf{e}_a\delta t,t+\delta t)-f_a(\mathbf{x},t) \\ =-\frac{1}{\tau}[f_a(\mathbf{x},t)-f_a^{\mathrm{eq}}]+4\frac{\mathbf{F}\cdot(\mathbf{e}_a-\mathbf{u})}{c^2}f_a^{\mathrm{eq}}\delta t. \end{aligned} \tag{34}$$

It can be shown that the local-interaction-based LBE models can be obtained from Eq. (34) if the fluid velocity $\mathbf{u}$ is neglected in the second term on the right-hand side of Eq. (34). In the model proposed by Gunstensen *et al.* [7] and Grunau, Chen, and Eggert [12], the difference between two components [13] satisfies an evolution equation similar to Eq. (34) but with the second interaction term on the right-hand side replaced by

$$\frac{A}{2|\nabla\rho|}\mathbf{e}_a\cdot\mathbf{\Pi}\cdot\mathbf{e}_a, \tag{35}$$

where $\mathbf{\Pi}=\nabla\rho\nabla\rho-\frac{1}{2}|\nabla\rho|\mathbf{I}$ is the stress tensor due to interparticle interaction and ρ is the difference of the densities of the two components (the so-called color field). Similar results have been found for the model proposed by Swift, Osborn, and Yeomans [8]. By regrouping the equilibrium distributions in [8], the interaction term can be identified as $\mathbf{e}_a\cdot\mathbf{\Pi}\cdot\mathbf{e}_a$, with $\mathbf{\Pi}=\frac{2}{3}\kappa(\nabla\rho\nabla\rho-\frac{1}{2}|\nabla\rho|\mathbf{I})$.

The neglect of the velocity in the second collision term in this class of models is not a coincidence because the interaction in these models was constructed based on equilibrium information only. The consequence, however, leads to the following two unsatisfactory results. First, after neglecting the velocity dependence, the interparticle force, which can be found as proportional to $\mathbf{e}_a\cdot\mathbf{\Pi}$, has a dependence on the lattice structure, which we believe is responsible for the anisotropic features in these models. Second, the interaction term in Eq. (34) does not depend on fluid velocity. Microscopically, the velocity distribution in the laboratory reference frame, instead of that in the reference frame moving with the fluid, was used in computing the interaction term. This might result in the lack of Galilean invariance in these models. The shortcomings of the local-interaction-based models have been shown in a recent numerical study [14].

In summary, we have proposed a discrete model for computer simulation of nonideal gases based on the Boltzmann equation with the BGK collision model. A mean-field approximation is used for the interparticle interaction. The discretization of the velocity space ensures that the Navier-Stokes equation can be obtained at a macroscopic level. This discretization effectively provides a numerical scheme for the solution of the Grad 13-moment system. A previously proposed LBE model is found to be consistent with the present analysis. It is also found that anisotropy might be inevitable in this type of model if a nonlocal interaction is not included in momentum space.

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