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Fast spectral solution of the generalized Enskog equation for dense gases

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ABSTRACT

We propose a fast spectral method for solving the generalized Enskog equation for dense gases. For elastic collisions, the method solves the Enskog collision operator with a computational cost of $O(M^{d-1}N^d \log N)$, where d is the dimension of the velocity space, and M^{d-1} and N^d are the number of solid angle and velocity space discretizations, respectively. For inelastic collisions, the cost is N times higher. The accuracy of this fast spectral method is assessed by comparing our numerical results with analytical solutions of the spatially-homogeneous relaxation of heated granular gases. We also compare our results for force-driven Poiseuille flow and Fourier flow with those from molecular dynamics and Monte Carlo simulations. Although it is phenomenological, the generalized Enskog equation is capable of capturing the flow dynamics of dense granular gases, and the fast spectral method is accurate and efficient. As example applications, Fourier and Couette flows of a dense granular gas are investigated. In addition to the temperature profile, both the density and the high-energy tails in the velocity distribution functions are found to be strongly influenced by the restitution coefficient.

1. Introduction

When the gas molecular mean free path (MFP) is comparable to the characteristic flow length, the Navier–Stokes equations based on the continuum-fluid assumption fail, and the Boltzmann equation is needed to study the rarefied gas dynamics [1]. Since in most situations the MFP is much larger than the molecular dimension, the binary collision modeled by the Boltzmann collision operator is localized in space. However, the collision is delocalized when the gas is compressed to such a density that the ratio of the molecular dimension to the MFP becomes appreciable; yet the continuum-fluid assumption is still inappropriate because of the small characteristic flow system size. This situation occurs, for instance, in gas flow in ultra-tight shale strata. For these dense gases, the Boltzmann equation is extended to the Enskog equation for hard-sphere molecules:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + a\frac{\partial f}{\partial v} = \sigma^{d-1}\int\int k\cdot u\left[g(x,k,v'_*)f(x,v') - g(x,-k,v_*)f(x,v)\right]dv_*dk, \tag{1}$$

where $f(t,x,v)$ is the velocity distribution function (VDF) of molecular velocity v at spatial location x and time t, and a is the external acceleration. The right-hand side of Eq. (1) is the Enskog collision operator (ECO), where σ is the molecular

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diameter, d is the dimension of the velocity space, k is a unit vector associated with the relative position of two molecules at the time of their impact, and $u = v - v_*$ is the relative pre-collision velocity of two colliding molecules. The post-collision velocities v' and v'_* are related to the pre-collision molecular velocities v and v_* through $v' = v - (u \cdot k)k$ and $v'_* = v_* + (u \cdot k)k$. Finally, the nonlocal collision is characterized by the product of the VDF and a pair correlation function at different locations:

$$g(x, k, v) = \chi\left(x + \frac{\sigma k}{2}\right) f(x + \sigma k, v). \tag{2}$$

The velocity-independent pair correlation function χ is a given function of gas density. In the standard Enskog theory, χ coincides with the pair correction function in a state of uniform equilibrium evaluated at the contact point, while in the revised Enskog theory it is evaluated as the local equilibrium value in a nonuniform state [2]. In this paper, the former is adopted and the detailed expressions for the pair correlation function will be given below.

The ECO has been extended to dense granular gases (i.e. materials composed of many small discrete grains), where the kinetic energy is not conserved during collisions [3–5]. A restitution coefficient $0 \le \alpha \le 1$, which is a function of the normal relative pre-collision velocity $|u \cdot k|$, is introduced to characterize the loss of kinetic energy. Neglecting rotational degrees of freedom, the generalized Enskog collision operator (GECO) becomes:

$$\mathcal{Q} = \sigma^{d-1} \int\int k \cdot u \left[\frac{J}{\alpha} g(x, k, \tilde{v}_*) f(x, \tilde{v}) - g(x, -k, v_*) f(x, v)\right] dv_* dk, \tag{3}$$

where $\tilde{v}$ and $\tilde{v}_*$ are the pre-collision velocities producing post-collision ones v and v_* after collision, and J is the Jacobian of the transformation from $(\tilde{v}, \tilde{v}_*)$ into (v, v_*).

The generalized Enskog equation has applications ranging from astrophysics (e.g. stellar cloud formation) to industrial processes (e.g. fluidized beds and transport lines, handling of pharmaceuticals, and shale gas exploitation). The Enskog–Vlasov equation with the mean-field potential is even able to describe both liquid and vapor phases, and automatically capture liquid–vapor and fluid–solid interfaces [6,7], which has potential applications to multiphase flows in micro/nano-electromechanical systems.

While various numerical methods have been proposed for the Boltzmann equation, there are only a few for the Enskog equation, let alone for the generalized equation. The most difficult part is the numerical solution of the collision operator. For elastic collisions, the ECO was first solved using a Monte Carlo quadrature method [8], and the study of shock propagation in a dense hard-sphere gas indicated that the Enskog equation can produce exact solutions comparable to molecular dynamics (MD) simulations [9]. Later, inspired by direct simulation Monte Carlo (DSMC) methods for the Boltzmann equation [10,11], several particle schemes were proposed for the simulation of dense gases [12–15], as well as the MD-DSMC hybrid method [16]. For inelastic collisions, the GECO has been solved by the DSMC [17,18] and spectral [19] methods for spatially-homogeneous relaxation problems.

As is well-known, the DSMC method has a computational cost proportional to the number of simulated particles (which may be far fewer than the actual number of molecules). However, particle-based methods are vulnerable to noise when macroscopic flow quantities are much smaller than the corresponding characteristic values (for example, when the flow velocity is much smaller than the sound speed). On the other hand, the spectral method is a deterministic numerical approach which solves the GECO with a computational cost $O(N^{2d})$, where N is the number of discretized velocities in each direction [19]. It is good at resolving small flow signals (e.g. it can easily capture the high-energy tail of the VDF in a heated granular gas [19]) but has greater computational complexity than the DSMC method. A deterministic numerical method with high accuracy but small computational cost would be in strong demand.

Recently, a fast spectral method (FSM) with a computational cost of $O(N^d \log N)$ has been proposed for solving the Boltzmann equation with spectral accuracy [20–22]. It has been successfully applied to many challenging cases for which the DSMC method is extremely time-consuming [23–25]. In this paper, we investigate the applicability of the FSM for solving the generalized Enskog equation.

This paper is organized as follows. The weak form of the GECO is expressed in the Carleman representation in Section 2, and is approximated by the FSM in Section 3. In Section 4, the accuracy of the FSM is assessed in several numerical tests. In Section 5, Fourier and Couette flows of a dense granular gas are investigated. Finally, concluding remarks are made in Section 6.

2. Weak form of the GECO in the Carleman representation

When the restitution coefficient α is a constant, we have $\tilde{v} = v - (1+\alpha)/(2\alpha)(u \cdot k)k$, $\tilde{v}_* = v_* + (1+\alpha)/(2\alpha)(u \cdot k)k$, and the Jacobian is $J = 1/\alpha$. When α is a function of $|u \cdot k|$, it is hard to express $\tilde{v}$ and $\tilde{v}_*$ as functions of v and v_*, and the Jacobian is very complicated. Therefore, it is convenient to write the GECO (3) in its weak form which does not involve the Jacobian and the pre-collision velocities $\tilde{v}$ and $\tilde{v}_*$.

For all smooth functions $\Psi(v)$, the following equation holds for the GECO (we omit the location variable in what follows)

$$\int \mathcal{Q}\Psi(v) dv = \sigma^{d-1} \int\int\int k \cdot u g(-k, v_*) f(v) \left[\Psi(v') - \Psi(v)\right] dv_* dk dv. \tag{4}$$