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A Quadrature-Based Kinetic Model for Dilute Non-Isothermal Granular Flows

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Abstract. A moment method with closures based on Gaussian quadrature formulas is proposed to solve the Boltzmann kinetic equation with a hard-sphere collision kernel for mono-dispersed particles. Different orders of accuracy in terms of the moments of the velocity distribution function are considered, accounting for moments up to seventh order. Quadrature-based closures for four different models for inelastic collision-the Bhatnagar-Gross-Krook, ES-BGK, the Maxwell model for hard-sphere collisions, and the full Boltzmann hard-sphere collision integral-are derived and compared. The approach is validated studying a dilute non-isothermal granular flow of inelastic particles between two stationary Maxwellian walls. Results obtained from the kinetic models are compared with the predictions of molecular dynamics (MD) simulations of a nearly equivalent system with *finite-size* particles. The influence of the number of quadrature nodes used to approximate the velocity distribution function on the accuracy of the predictions is assessed. Results for constitutive quantities such as the stress tensor and the heat flux are provided, and show the capability of the quadrature-based approach to predict them in agreement with the MD simulations under dilute conditions.

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1 Introduction

The behavior of a granular flow can be described by the Boltzmann-Enskog kinetic equation [4, 14, 35], in terms of the velocity distribution function. Depending on the value of the Knudsen number of the flow, defined as the ratio between the molecular mean free path and a characteristic length scale of the system under consideration, it is often possible to find a simplified set of equations to describe the flow [4, 12, 13, 35]. In particular, when the Knudsen number is zero, a granular flow of elastic particles behaves as an inviscid flow and can be described by the Euler equation. When the Knudsen number is between zero and 0.01, the Navier-Stokes-Fourier (NSF) equations, computed with no-slip boundary condition, represent a simplified set of equations, derived considering the lower-order moments of the kinetic equation. When the Knudsen number is between 0.01 and 0.1, the NSF equations require the introduction of partial-slip boundary conditions to account for rarefaction effects due to the presence of a significant Knudsen layer near the walls. For even larger Knudsen numbers, higher-order solutions of the Boltzmann-Enskog kinetic equation are required to obtain satisfactory results, since the rarefaction effects extend from the walls to the bulk of the fluid, and cannot be treated with the simple modification of the boundary conditions.

Different strategies have been developed to find solutions of the kinetic equation. A possible strategy is to directly discretize the seven-dimensional phase space [2, 11], in order to reconstruct the velocity distribution function. However, the high dimensionality of the equation often makes the direct approach impractical due to its high computational cost. An alternative approach to solve the kinetic equation is given by discrete methods, where the trajectory of the particles and their interactions are tracked. In particular, the Direct Simulation Monte Carlo (DSMC) method [4], which relies on notional particles and a statistical description of their interaction, has been widely applied in rarefied gas dynamics to obtain solutions of the kinetic equation for point particles (Boltzmann equation). Molecular dynamics (MD) has been used to compute granular flows of finite-size[†] particles [23], providing solutions of the complete Boltzmann-Enskog kinetic equation. These approaches are efficient for systems with a relatively low number of particles (order of millions), but become intractable for systems of larger scale, related to industrial applications of granular flows and fluid-particle flows.

An interesting and more computationally efficient approach for complex flows is represented by the method of moments, where the idea of reconstructing the velocity distribution is usually abandoned in favor of tracking the spatial and temporal evolution of a finite set of its moments. Moment methods have been widely studied in the literature and a good summary can be found in [35]. The main difficulties in moment methods are

[†]With *finite-size particles* we indicate particles that are *not* assumed to be points. Finite-size particles cannot overlap, as it happens with point particles. In the framework of kinetic theory, *point particles* are described by the Boltzmann collision integral, while finite-size particles are described by the Boltzmann-Enskog collision integral. In terms of the moment equations, the point-particle approximation neglects the contribution due to the collisional fluxes.