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A direct method for the Boltzmann equation based on a pseudo-spectral velocity space discretization

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ABSTRACT

A deterministic method is proposed for solving the Boltzmann equation. The method employs a Galerkin discretization of the velocity space and adopts, as trial and test functions, the collocation basis functions based on weights and roots of a Gauss–Hermite quadrature. This is defined by means of half- and/or full-range Hermite polynomials depending whether or not the distribution function presents a discontinuity in the velocity space. The resulting semi-discrete Boltzmann equation is in the form of a system of hyperbolic partial differential equations whose solution can be obtained by standard numerical approaches. The spectral rate of convergence of the results in the velocity space is shown by solving the spatially uniform homogeneous relaxation to equilibrium of Maxwell molecules. As an application, the two-dimensional cavity flow of a gas composed of hard-sphere molecules is studied for different Knudsen and Mach numbers. Although computationally demanding, the proposed method turns out to be an effective tool for studying subsonic slightly rarefied gas flows.

1. Introduction

The conventional continuum approach to gas dynamics, namely the Navier–Stokes equations with no-slip boundary conditions, is justified when the average distance traveled by molecules between two successive collisions, λ, is much smaller than a characteristic length, L, associated with the flow geometry. This condition breaks down in several physical situations ranging from the re-entry of spacecraft in upper planetary atmospheres, characterized by large λ, to fluid–structure interaction in small-scale micro-electro-mechanical systems, characterized by small L. In such situations, a microscopic description of the gas based on the Boltzmann equation is required [1,2]. In the absence of external forces, the Boltzmann equation for a gas composed of a single monatomic species takes the form

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \mathcal{C}(f, f), \tag{1}$$

where

$$\mathcal{C}(f, f) = \int_{\mathbb{R}^3} \int_{\mathcal{S}^2} \left[f^* f_1^* - f f_1 \right] \sigma\left(\|\boldsymbol{v}_r\|, \hat{\boldsymbol{k}} \cdot \boldsymbol{v}_r \right) \|\boldsymbol{v}_r\| \, d\boldsymbol{v}_1 \, d^2\hat{\boldsymbol{k}}. \tag{2}$$

In Eqs. (1) and (2), $f(\boldsymbol{x}, \boldsymbol{v}, t)$ denotes the distribution function of atomic velocities $\boldsymbol{v}$ at spatial location $\boldsymbol{x}$ and time t, whereas $\mathcal{C}(f, f)$ gives the collisional rate of change of f at the phase space point $(\boldsymbol{x}, \boldsymbol{v})$ at time t and we have used the shorthand

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$f^* = f(\boldsymbol{x}, \boldsymbol{v}^*, t)$, $f_1^* = f(\boldsymbol{x}, \boldsymbol{v}_1^*, t)$ and $f_1 = f(\boldsymbol{x}, \boldsymbol{v}_1, t)$. As is clear from Eq. (2), $\mathcal{C}(f, f)$ is a non-linear operator of f, whose precise structure depends on the differential cross section $\sigma(\|\boldsymbol{v}_r\|, \hat{\boldsymbol{k}} \cdot \boldsymbol{v}_r)$ calculated from the interatomic potential for the system studied. The dynamics of binary encounters determines the differential cross section as a function of the modulus $\|\boldsymbol{v}_r\|$ of the relative velocity $\boldsymbol{v}_r = \boldsymbol{v}_1 - \boldsymbol{v}$ of two colliding atoms and of the orientation of the unit impact vector $\hat{\boldsymbol{k}}$ with respect to $\boldsymbol{v}_r$. The collisional dynamics also gives the relationship between the pre-collisional velocities, $\boldsymbol{v}^*$ and $\boldsymbol{v}_1^*$, and the post-collisional velocities, $\boldsymbol{v}$ and $\boldsymbol{v}_1$, in a binary collision

$$\boldsymbol{v}^* = \boldsymbol{v} + (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}}, \tag{3}$$

$$\boldsymbol{v}_1^* = \boldsymbol{v}_1 - (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}}. \tag{4}$$

The prevalent approach for numerically solving Eq. (1) is a stochastic-based method called the Direct Simulation Monte Carlo (DMSC) [3]. The distribution function is represented by a number of particles which move in the computational domain and collide according to stochastic rules derived from Eqs. (1) and (2). Macroscopic flow properties are obtained by time averaging particle properties. If the averaging time is long enough, then accurate flow simulations can be obtained by a relatively small number of particles. Variants of the DSMC have been proposed over the years to improve solution accuracy in the presence of high density gradients [4] and for low Mach number flows [5]. Although particle-based methods are by far the most effective tools in describing non-equilibrium gas flows, they are not well suited to simulate unsteady gas flows. Indeed, in this case the possibility of time averaging is lost or reduced. Acceptable accuracy can only be achieved by increasing the number of simulation particles or superposing several flow snapshots obtained from statistically independent simulations of the same flow but, in both cases, the computing effort is considerably increased. The simulation of steady gas flows in the near-continuum limit represents an additional challenge since the time scale on which the particle-based methods are forced to operate is much shorter than the characteristic macroscopic time and therefore explicit integration to steady-state is computationally demanding. Approaches based on a direct discretization of the Boltzmann equation in the phase space are believed to be a feasible alternative in these cases since they provide solutions with high accuracy even in unsteady conditions and offer the possibility of a direct steady-state formulation [6,7]. As such, they have been applied to study several problems of both theoretical interest and practical importance, including the viscous gas damping in microfluidic devices [8,9], the onset of instability in a rarefied gas environment [10] and the investigation of ghost effects [2,11]. Deterministic methods of solution present some further assets compared to particle-based methods. Firstly, they are more suited to be adopted within a domain decomposition approach since the need to exchange information between kinetic and macroscopic equations requires smooth numerical solutions [12,13]. Secondly, unlike particle-based methods their implementation on massively parallel computers with Single Instruction Multiple Data (SIMD) architecture, such as multi-cores and Graphic Processing Units (GPUs), can easily realize the full potential of these processors [14–16]. These aspects also prompted the development of deterministic methods of solution.

Considerable progress has been accomplished in developing deterministic method for kinetic model equations [17,18]. By contrast, an accurate and efficient direct solution of the Boltzmann equation itself remains a challenging problem. A common strategy adopted for solving Eq. (1) consists in decoupling the transport and the collision terms by time-splitting the evolution operator into a transport step and a collisional step. The transport step requires to solve a system of hyperbolic conservation laws coupled at the boundaries. Their discretization can be performed in a variety of ways, including finite-difference, finite-volume, finite-element or spectral methods [19]. The collision step consists of solving a spatially homogeneous relaxation equation. This is the more computationally demanding part since it involves the computation of the bilinear five-fold integral defining the collision operator, Eq. (2). The numerical approaches to evaluate the collision step may be grouped into two broad categories. To the first category belong methods referred to as discrete velocity models (DVM). They make use of a Cartesian grid in velocity space and construct a discrete collision mechanics on the points of the grid that preserve the main physical properties of the collision integral, namely equilibrium states, collision invariants and entropy inequality [20]. DVM methods have high computational cost and low order of accuracy although fast algorithms have been recently developed for a restricted set of collision kernels [21]. To the second category belong methods which adopt a Galerkin discretization of the velocity space. They are based on expanding the velocity dependence of the distribution function in a set of trial functions with expansion coefficients that depend on position and time. The Galerkin ansatz is substituted in the space homogeneous relaxation equation which is subsequently multiplied by test functions and integrated in the velocity space. According to the Galerkin approach, test and trial functions are assumed to be the same. The above procedure yields a system of hyperbolic partial differential equations for the expansion coefficients. Galerkin methods can be further distinguished depending on the basis functions which they employ. In Fourier–Galerkin approach, the distribution function is expanded in trigonometric polynomials and the fast Fourier Transform is used to accelerate the computation of the collision integral in the velocity space. Several different methods have been developed starting from different representation of the collision integral [22–25]. These methods are generally very efficient and spectrally accurate for smooth solutions. Their major shortcoming is the loss of some of the properties of the solution such as positivity and conservation of momentum and energy. Preservation of collision invariants can be enforced but the use of correction procedures may limit the accuracy of the solutions. Discontinuous Galerkin methods adopt discontinuous piecewise polynomials as test and trial functions [26–29]. Although computationally demanding, these methods have the remarkable feature to provide spectral accuracy in the velocity space even for discontinuous solutions which typically occur in the presence of solid surfaces. A hybrid approach is adopted in Refs. [30,31] where the distribution function is expanded in Laguerre polynomials with