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Deterministic numerical solutions of the Boltzmann equation using the fast spectral method

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ABSTRACT

The Boltzmann equation describes the dynamics of rarefied gas flows, but the multidimensional nature of its collision operator poses a real challenge for its numerical solution. In this paper, the fast spectral method [36], originally developed by Mouhot and Pareschi for the numerical approximation of the collision operator, is extended to deal with other collision kernels, such as those corresponding to the soft, Lennard–Jones, and rigid attracting potentials. The accuracy of the fast spectral method is checked by comparing our numerical solutions of the space-homogeneous Boltzmann equation with the exact Bobylev–Krook–Wu solutions for a gas of Maxwell molecules. It is found that the accuracy is improved by replacing the trapezoidal rule with Gauss–Legendre quadrature in the calculation of the kernel mode, and the conservation of momentum and energy are ensured by the Lagrangian multiplier method without loss of spectral accuracy. The relax-to-equilibrium processes of different collision kernels with the same value of shear viscosity are then compared; the numerical results indicate that different forms of the collision kernels can be used as long as the shear viscosity (not only the value, but also its temperature dependence) is recovered. An iteration scheme is employed to obtain stationary solutions of the space-inhomogeneous Boltzmann equation, where the numerical errors decay exponentially. Four classical benchmarking problems are investigated: the normal shock wave, and the planar Fourier/Couette/force-driven Poiseuille flows. For normal shock waves, our numerical results are compared with a finite difference solution of the Boltzmann equation for hard sphere molecules, experimental data, and molecular dynamics simulation of argon using the realistic Lennard–Jones potential. For planar Fourier/Couette/force-driven Poiseuille flows, our results are compared with the direct simulation Monte Carlo method. Excellent agreements are observed in all test cases, demonstrating the merit of the fast spectral method as a computationally efficient method for rarefied gas dynamics.

1. Introduction

The fundamental task in the study of gas dynamics is to obtain the evolution of macroscopic quantities such as density, bulk velocity, temperature, pressure tensor, and heat flux. Only when the Knudsen number (the ratio of the molecular mean free path to a characteristic flow length, or characteristic flow frequency to mean collision frequency) is small, can the evolution of macroscopic quantities be governed by partial differential equations such as the Navier–Stokes–Fourier equations, Burnett equations, or the Grad-13 moment equations [1]. As the Knudsen number becomes appreciable, it is necessary to adopt microscopic descriptions. Since the gas consists of a large number of molecules, the Newtonian

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description is computationally unrealistic. So we turn to the Boltzmann equation under the assumptions of molecular chaos and binary collisions. This uses the one-particle distribution function to describe the system state, and macroscopic quantities are derived from the velocity moments of the distribution function. In Boltzmann's description, all molecules move in straight lines with fixed velocities until they encounter elastic collisions with other molecules. The collision is modelled by a nonlinear collision operator, where the intermolecular potential is incorporated into the collision kernel. The structure of the collision operator is rather complicated: it is a fivefold integral with three dimensions in velocity space and two dimensions in a unit sphere.

The multidimensional structure of the collision operator poses a real challenge to the numerical solution of the Boltzmann equation. From a historical point of view, realistic numerical computations of the Boltzmann equation are based on probabilistic methods. Well-known examples are the direct simulation Monte Carlo (DSMC) methods developed by Bird and Nanbu [2,3]. Despite their stochastic nature, DSMC solutions converge to those of the Boltzmann equation for a monatomic gas in the limit of vanishing discretization and stochastic errors [4]. The main advantages of the DSMC method are: (i) the simulated particles in DSMC represent a large number of real molecules so that the number of operations is greatly reduced; (ii) it does not need artificial boundaries in velocity space; (iii) particles concentrate in regions where the distribution function is not small so that computer memory is not wasted; (iv) it is very efficient for high-speed rarefied gas flows. However, DSMC becomes time-consuming if the flow is in the continuum-fluid regime, especially when the Mach number is small. Note that recently developed information preserving DSMC method [5,6], hybrid continuum/particle approaches [7–10], and the variance reduced DSMC method [11,12] have partly eased these difficulties.

Contrasting with the particle methods, there are numerical methods that solve the Boltzmann equation deterministically, including the discrete velocity model (DVM), the finite-difference method, and the Fourier spectral method. A brief introduction to these methods is given below.

In 1989, Goldstein, Sturtevant, and Broadwell developed the first version of DVM [13]. They used a fixed set of discrete velocities to approximate the continuous velocity space, and constructed a discrete collision mechanics on the velocity nodes in order to preserve the main physical properties of the collision operator. However, a large amount of computational resources are wasted since the post-collision velocities must lie on the velocity nodes. Bobylev, Palczewski, and Schneider considered the direct approximation of the collision operator and demonstrated that the computational cost is of the order $O(N^7)$, while the formal accuracy is less than first order in velocity, where N is the number of grid points in each velocity direction [14]. The high computational cost drove researchers to consider mixed deterministic and stochastic methods [15–18]. Recently, Morris, Varghese, and Goldstein used an interpolation scheme to map the post-collision velocities back onto the velocity nodes and found that the performance of DVM is comparable to (or even faster than) DSMC in normal shock wave simulations [19,20]. Also note that Mouhot, Pareschi, and Rey constructed a DVM for hard sphere molecules with computational cost $O(\overline{N}^3 N^3 \log N), \overline{N} \ll N$ [21].

The kinetic theory group in Kyoto has developed a family of finite difference methods for the Boltzmann equation. In 1989, Sone, Ohwada, and Aoki proposed an accurate numerical kernel method for computing the linearized collision operator for hard sphere molecules [22]. Four years later, Ohwada extended the finite-difference method to calculate the full nonlinear collision operator for hard sphere molecules [23,24]. This method seems to be restricted to one-dimensional problems such as normal shock flow and Fourier heat flow between two parallel plates where the velocity distribution function has a cylindrical symmetry, i.e., it is a function of the longitudinal and transversal velocities. In this way, the number of velocity nodes and the computational cost are dramatically reduced. In 2001, the finite difference method was applied by Kosuge, Aoki, and Takata to the Boltzmann equation for a binary gas mixture of hard sphere molecules [25].

In 1996, inspired by the pioneering work of Bobylev using Fourier transform techniques in the analysis of the Boltzmann equation for Maxwell molecules [26], Pareschi and Perthame proposed a spectral method to approximate the collision operator for a class of collision kernels, where the computational cost is of the order $O(N^6)$ [27]. One year later, Bobylev and Rjasanow developed a numerical method to solve the collision operator for Maxwell molecules with computational cost of the order $O(N^4)$ [28]. This is in general the fastest algorithm to date. However, its formal accuracy is only of the order $O(N^{-1/2})$. For one-dimensional problems such as Fourier heat flow and normal shock flow, Watchararuangwita, Grigoriev, and Meleshko observed that cylindrical symmetry allows a reduction of the computational cost to the order $O(N^2 \log N)$ by employing the fast Fourier transform (FFT) in the longitudinal velocity direction and Hankel transform in the transverse direction [29]. In 1999, based on the Carleman representation, Bobylev and Rjasanow were able to solve the collision operator for hard sphere molecules with a computational cost $O(N^6 \log N)$ and formal accuracy $O(N^{-2})$, using generalized Radon and X-ray transforms [30]. A faster numerical method with a computational cost $O(N^6)$ and formal accuracy $O(N^{-2})$ has also been proposed for the variable hard sphere (VHS) model by Ibragimov and Rjasanow [31]. Based on these Fourier spectral methods, Gamba and Tharkabhushanam developed a spectral-Lagrangian method both for elastic and inelastic collision operators and investigated space-inhomogeneous problems, i.e., one-dimensional Fourier heat flow and shock flow [32,33].

In 2000, Pareschi and Russo developed an algorithm to solve the collision operator for the VHS model with a computational cost of $O(N^6)$ [34]. The approximation of the collision operator is spectrally accurate for smooth velocity distribution functions, where the decay rate of the error is faster than any polynomial, i.e., faster than O (N^{-r}) for any $r > 0$. The method has been successfully applied to space-inhomogeneous problems in two-dimensional velocity space [35]. Six years later, by means of the Carleman-like representation, Mouhot and Pareschi developed a faster spectral algorithm with a computational cost $O(M^2 N^3 \log N)$ and spectral accuracy, where M is the number of grid points in the discretizations of polar and azimuthal