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A fast spectral method for the Boltzmann equation for monatomic gas mixtures

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ABSTRACT

Although the fast spectral method has been established for solving the Boltzmann equation for single-species monatomic gases, its extension to gas mixtures is not easy because of the non-unitary mass ratio between the different molecular species. The conventional spectral method can solve the Boltzmann collision operator for binary gas mixtures but with a computational cost of the order $m_r^3 N^6$, where m_r is the mass ratio of the heavier to the lighter species, and N is the number of frequency nodes in each frequency direction. In this paper, we propose a fast spectral method for binary mixtures of monatomic gases that has a computational cost $O(\sqrt{m_r} M^2 N^4 \log N)$, where M^2 is the number of discrete solid angles. The algorithm is validated by comparing numerical results with analytical Bobylev–Krook–Wu solutions for the spatially-homogeneous relaxation problem, for m_r up to 36. In spatially-inhomogeneous problems, such as normal shock waves and planar Fourier/Couette flows, our results compare well with those of both the numerical kernel and the direct simulation Monte Carlo methods. As an application, a two-dimensional temperature-driven flow is investigated, for which other numerical methods find it difficult to resolve the flow field at large Knudsen numbers. The fast spectral method is accurate and effective in simulating highly rarefied gas flows, i.e. it captures the discontinuities and fine structures in the velocity distribution functions.

1. Introduction

There are a large number of applications for the Boltzmann equation (BE) in modeling rarefied gas flows frequently encountered in high-altitude aerodynamics, vacuum technologies, and microelectromechanical systems. While there is a great need for efficient and accurate methods for solving the BE, this is a challenge because the BE employs a molecular velocity distribution function (VDF) defined in a six-dimensional phase space to describe the system state, and the Boltzmann collision operator is highly complicated.

In 1912, Hilbert proposed obtaining approximate solutions to the BE by a series expansion in Knudsen number (*Kn*, defined as the ratio of the molecular mean free path to the characteristic flow length). The Hilbert expansion inspired Sone to develop an asymptotic analysis of the BE at small *Kn*, which helped reveal many interesting phenomena including the 'ghost effect' [1,2]. In 1917, Chapman and Enskog (CE) obtained approximate solutions to the BE and calculated transport coefficients from first principles [3]. The first-order CE expansion recovers the Navier–Stokes equations, while the second-

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and third-order expansions lead to the Burnett and super-Burnett equations, respectively. Although the Burnett equations can be more accurate than the Navier–Stokes equations in some cases [4], they are rarely used nowadays due to their intrinsic instability to small-wavelength perturbations [5]. In 1949, by expanding the VDF into Gauss–Hermite polynomials, Grad proposed the moment method [6]. This has led to the development of regularized 13-moment [7] and 26-moment [8] equations, which have been successfully applied to rarefied gas flows up to $Kn \sim 1$ in some circumstances. For large Kn, a great number of moments are necessary but the convergence rate with increasing moment number is rather slow [9]. Moreover, multiple new boundary conditions are needed, so this approach it is not suitable to simulate highly rarefied gas flows.

For moderate and highly rarefied gas flows it is necessary to directly solve the BE. The direct simulation Monte Carlo (DSMC) method is the prevailing numerical technique for this [10]. In DSMC, the VDF is represented by a number of simulated particles that move in the computational domain and collide according to stochastic rules. The simulated particles automatically concentrate in regions where the VDF has large values, and discontinuities/fine structures in VDFs can be captured without difficulty. This method is efficient for hypersonic flows, however, its stochastic nature makes it not well suited for unsteady and low-speed flows. For instance, for a gas flow with a Mach number 0.001 (typically in micro-devices), about 10^8 independent samples are needed to reduce the error to 1% when there are 100 simulated particles in a cell [11]. Also, DSMC is an inefficient method for near-continuum flows, since the spatial and temporal steps must be smaller than the molecular mean free path and collision time, respectively. Progress has been made to ease these difficulties: to resolve small macroscopic quantities, the information preserving [12] and low variance [13,14] DSMC methods have been proposed; to simulate near-continuum flows, hybrid continuum-particle approaches [15–21], time relaxed Monte Carlo method [22,23], and particle–particle hybrid methods [24,25] have been proposed. Recently, a new multiscale method has also been developed to simulate flows in geometries with high aspect ratio [26–28].

Deterministic numerical methods [29–40], based on the direct discretization of the BE in phase space, have distinct advantages in resolving small signals and low-speed flows as they are free of noise. Also, implicit time-marching can be employed to enlarge the time step [29,30,41–43]. Furthermore, compared to continuum/particle coupling, deterministic methods can be coupled more efficiently to macroscopic equations [44] such as the Navier–Stokes/moment equations and equations from the asymptotic kinetic analysis [2]. Among these deterministic solvers, however, only a few have been applied to spatially-inhomogeneous problems. The numerical kernel method [29,30], in which the VDF is expanded into Laguerre polynomials for velocity components parallel to solid surfaces and quadratic finite-element functions for normal velocity component, provides accurate numerical results for many one-dimensional problems. As it allows non-uniform discretization of the normal velocity component, VDF discontinuities at large Kn are captured: for linearized Poiseuille and thermal transpiration flows, accurate results are produced up to $Kn \sim 20$ for hard-sphere molecules [45]. The conservative projection-interpolation method, in which uniform Cartesian velocity discretization is usually employed, and post-collision velocities are interpolated to closest neighbors, has been proposed to solve the BE with realistic intermolecular potentials in three-dimensional space [32], with a numerical error of the order $\Delta v|f - f_M|$ (Δv is the velocity grid step, f is the VDF, and f_M is the equilibrium VDF) [44]. Since VDFs at post-collision velocities are obtained by polynomial interpolation, this method is accurate at small Kn where the VDF is usually smooth (in a recent paper [46] an accuracy of $(\Delta v)^2$ has been demonstrated), but loses accuracy at large Kn where VDFs have discontinuities or steep variations. Discontinuous Galerkin methods, although able to capture VDF discontinuities, turn out to be feasible only for slightly rarefied subsonic gas flows [40] because of the high computational cost.

Recently, the fast spectral method (FSM) has been developed to numerically solve the BE for single-species monatomic gases [35,47,41–43]. It employs a Fourier–Galerkin discretization in velocity space, and handles binary collisions in the corresponding frequency space. The method is of spectral accuracy, and has a computational cost of $O(M^2N^3 \log N)$, where N is the number of frequency nodes in each frequency direction and M^2 is the number of discrete solid angles. Since it allows non-uniform velocity discretizations, and the number of frequency nodes can be far smaller than the number of velocity nodes [42,43], the FSM is good at dealing with highly rarefied gas flows, where large numbers of velocity nodes are used to capture discontinuities/fine structures in the VDF: for linearized Poiseuille and thermal transpiration flows, accurate numerical results have been obtained even for $Kn \sim 10^6$ (note that even at such high Knudsen numbers, collision cannot be ignored). The FSM can be 50 times faster than the low variance DSMC method [42], and it is very efficient in dealing with linearized oscillatory flows [43] and Rayleigh–Brillouin scattering of light by rarefied gases [48,49].

Deterministic numerical methods for the BE for mixtures of monatomic gases are even more scarce. Compared to the single-species BE, the non-unitary mass ratio between different molecular species poses an additional difficulty. Accurate numerical results have previously only been reported for hard-sphere molecules in some simple spatial configurations [50–55]. For general cases, a multipoint conservative projection-interpolation method has been developed for an arbitrary ratio of molecular masses [56], but its accuracy is not known, especially at large Knudsen numbers. Recently, a spectral-Lagrangian method with a computational cost of $O(m_r^3 N^6)$ has been proposed (where m_r is the mass ratio of the heavier to the lighter species), and a normal shock wave in a binary mixture with a mass ratio of about 2 has been simulated [57]. As this method uses the same velocity discretization for each component, it cannot be applied to mixtures with large mass ratios, since the computational cost and storage are m_r^3 and $m_r^{3/2}$ times larger than that for the single-species BE, respectively. As an example, calculation of an argon–helium mixture with the mass ratio $m_r \approx 10$ requires a 30-times increase in velocity grid points, and a 1000-times increase in computational time.