Toward efficient numerical methods for solving the Boltzmann equation for low-speed flows

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Summary

When the Knudsen number, typically defined as the ratio of the molecular mean free path to the characteristic length scale of a dilute gas flow, is larger than approximately 0.1, the Navier-Stokes equations cease to provide an accurate description of the flow. In this case, which is frequently encountered in small-scale flows, one must solve the more general Boltzmann equation. The objective of this work is to develop a method which requires a lower computational cost than existing methods for low speed flows. To this end, we have focused on direct numerical methods rather than the more prevalent stochastic molecular simulation approach known as the Direct Simulation Monte Carlo (DSMC) method. In this work, the evaluation of the collision integral of the Boltzmann equation is performed using a quasi-random Monte Carlo integration approach. In addition, interpolation is used to reduce the effect of discretization errors. We find that this method leads to accurate solutions which exhibit excellent conservation properties. Solutions of the Boltzmann equation using this method are shown to agree well with analytical solutions and the results of molecular simulation.

Introduction

Efficient numerical techniques for modeling small-scale and low-speed dilute gas flows are expected to be of increasing importance as micro- and nano-scale engineering becomes more prevalent. At present, the most widely used method for modeling these flows is a stochastic molecular simulation method known as the Direct Simulation Monte Carlo (DSMC) method. (See [3] for an extensive discussion.) Our motivation to seek an alternative approach stems from the fact that the computational cost associated with DSMC scales poorly as the mean flow speed decreases or as the desired accuracy increases. For example, to estimate the local fluid velocity using DSMC, the computational cost for low Mach numbers (Ma) scales as Ma^{-2} [4].

In this paper, we discuss an alternative approach based on a direct numerical solution of the governing Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}} = \int_{\mathbf{v_1}}\int_{\Omega}\left(f' f_1' - f f_1\right) V\sigma d^2\Omega d^3\mathbf{v_1} \tag{1}$$

Here, $\mathbf{x}$ is the coordinate in physical space and $\mathbf{v}$ is the coordinate in velocity space. The distribution function $f = f(\mathbf{x},\mathbf{v},t)$ is defined such that $f\,d^3\mathbf{x}\,d^3\mathbf{v}$ is the expected number of molecules in the range $d^3\mathbf{x}\,d^3\mathbf{v}$ of physical and velocity space and $f_1 \equiv f(\mathbf{x},\mathbf{v_1},t)$, $f' \equiv f(\mathbf{x},\mathbf{v}',t)$, $f_1' \equiv f\left(\mathbf{x},\mathbf{v_1'},t\right)$, where a prime indicates post-collision velocities[2]. Additionally, V is the relative pre-collision speed, Ω is the scattering solid angle, σ is the collision cross section, $\mathbf{F}$ is the force acting on a molecule and m is the mass of a molecule.

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[2]Post-collision velocities depend on the pre-collision velocities and the scattering angle.

The right side of the Boltzmann equation is typically referred to as the collision integral, and is, perhaps, the most challenging aspect of solving the Boltzmann equation. For this reason, much of this paper focuses on methods for evaluating the collision integral.

Method for evaluating the collision integral

The collision integral in the form presented in equation (1) can be evaluated with Monte Carlo or quasi-random Monte Carlo methods [1], [7]. A more efficient method can be devised by considering the following alternative form of the collision integral [11], [12]

$$\left[\frac{df^*}{dt^*}\right]_{\text{coll}} = \frac{\sqrt{\pi}}{4}\int\int\int \left(\delta' + \delta_1' - \delta - \delta_1\right) f^* f_1^* V^* \sigma^* d^2\Omega d^3\mathbf{v}_1^* d^3\mathbf{v} \tag{2}$$

where $\delta' \equiv \delta\left(\mathbf{v}^{*\prime} - \mathbf{u}^*\right)$, $\delta_1' \equiv \delta\left(\mathbf{v}_1^{*\prime} - \mathbf{u}^*\right)$, $\delta \equiv \delta(\mathbf{v}^* - \mathbf{u}^*)$, and $\delta_1 \equiv \delta\left(\mathbf{v}_1^* - \mathbf{u}^*\right)$. Here, and in the remainder of the paper, we denote non-dimensional quantities with stars. These quantities are non-dimensionalized by using $\bar{v}$, the most probable thermal speed, as a velocity scale, λ, the mean free path, as a characteristic length scale and $t_c = (\sqrt{\pi}/2)(\lambda/\bar{v})$, the collision time, as a characteristic time scale. As shown in [11], the above formulation of the collision integral can be used to derive efficient numerical methods. Their efficiency arises from performing a type of importance sampling, namely choosing pre-collision velocities with a probability proportional to the value of the distribution function at those velocities; compared to Monte Carlo integration of the collision integral in the standard form (1), this has the effect of reducing the amount of computational effort expended on less probable collisions. This focus on collisions involving velocities for which the value of the distribution function is relatively large is shared with DSMC; in fact the resulting method used to evaluate the collision integral is analogous to DSMC.

By assuming a discrete distribution function, and performing Monte Carlo summation, this sum can be reduced to the expression [11]

$$\left[\frac{df^*}{dt^*}\right]_{\text{coll}} \approx \mathcal{N}^{*2}\frac{\pi^{3/2}}{L}\sum_{r=1}^{L}\left(\delta'_{\alpha,r} + \delta'_{\beta,r} - \delta_{i,r} - \delta_{j,r}\right) V_r^* \sigma_r^* \tag{3}$$

where $\mathcal{N}^{*2}$ is the local (non-dimensional) number density, and $\delta_{\gamma,r}$ denotes a discrete set of delta functions centered on the velocity node $\mathbf{v}_\gamma$. The index r runs over all collisions sampled to evaluate the sum (3), in which $\mathbf{v}_i$ and $\mathbf{v}_j$ are the pre-collision velocities and $\mathbf{v}'_\alpha$ and $\mathbf{v}'_\beta$ are the post-collision velocities. Though not explicitly indicated in (3), $\mathbf{v}_i$ and $\mathbf{v}_j$ are chosen with a probability proportional to the distribution function at these nodes[3]. The present work extends this method by adding interpolation to reduce the errors due to discretization and by using a more efficient quasi-random sampling method to accelerate convergence [9].

The motivation for interpolation arises from the following considerations. In [11], only collisions for which both the pre- and post-collision velocities lie precisely on a discretization node are considered. To reduce the effects of discretization errors, we have

[3] Assuming uniform node spacing, see [11] for more details.

relaxed the restriction that all post-collision velocities lie on nodes; instead we estimate the collision integral at a node as a weighted sum of the number of collisions that terminate near the node (see [2] for details). At present, we have taken the weights to correspond to polynomial interpolation coefficients, although other methods are being evaluated.

Spatially homogeneous relaxation

An analytical solution to the Boltzmann equation for spatially homogeneous relaxation for Maxwellian molecules from an initial distribution shown in figure 1 is given in [5]. Figure 1 shows the analytic and calculated solution for this problem at various times. The solutions are calculated using 21^3 nodes in velocity space, and the timestep, number of samples, and velocity space volume are chosen so as to contribute a negligible amount of error. The calculated solution provides a very good approximation to the analytical solution when using cubic interpolation coefficients; the results with closest point interpolation yield poor results, illustrating the error resulting from discretization effects.

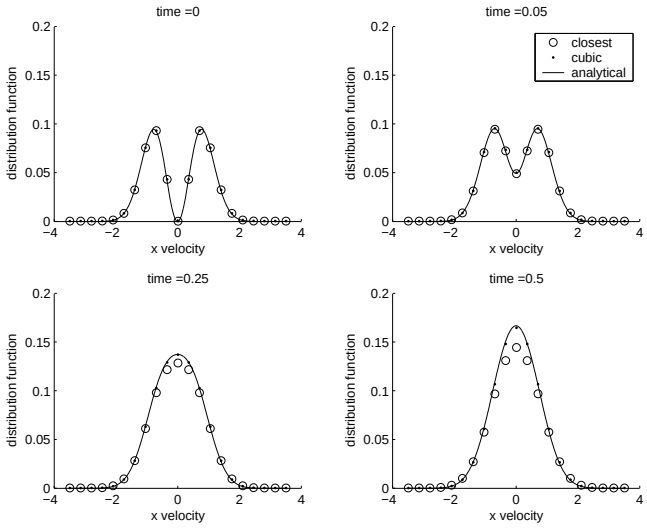

Figure 1: Evolution of the distribution function with 21^3 nodes in velocity space

Figure 2 shows a plot of the mean error in the collision integral at time $t^* = 0$ versus the number of samples. The error initially decreases at a rate of about $N^{-1/2}$, as expected for Monte Carlo methods. Quasi-random sequences exhibit a convergence rate that is somewhat better, although it does not approach the expected asymptotic value of $\log^d N/N$, where d is the dimensionality of the integral [9]. This is because the error saturates at a constant value due to the discretization effects[4]. For calculations with higher accuracy (i.e. finer discretization), quasi-random integration shows a more significant benefit; in other

[4]When the convergence to the asymptotic rather than the exact value is considered, convergence with quasi-random integration exhibits a convergence trend that is closer to the expected one.

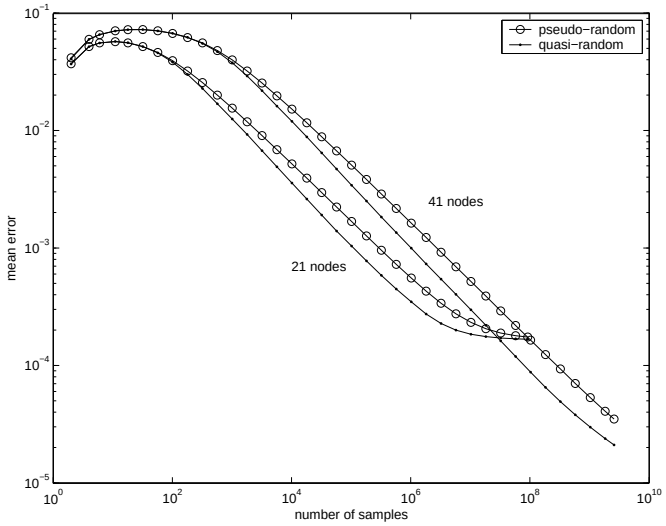

Figure 2: Convergence of the mean error in the collision integral with 21^3 and 41^3 nodes in velocity space using cubic interpolation

words, the relative performance advantage due to quasi-random integration is larger for the cases that are more computationally expensive. To ensure conservation of mass, momentum and energy, past direct methods for evaluating the collision integral have often relied on correcting the collision integral or strongly restricting the set of collisions considered. We have found that cubic interpolation very closely conserves mass, momentum and energy, thus making artificial methods to ensure conservation unnecessary.

Couette flow

The method used above to calculate the collision integral can be easily adapted to problems with a spatial dependence. As an example, we consider Couette flow with diffuse walls [3]. We use an iterative method (as opposed to the more costly explicit time integration) for obtaining steady-state solutions, as discussed in [13]: At each iteration, we update the value of the distribution function using an explicit upwind finite difference approach to discretize the spatial derivative. The boundary conditions require that the net mass flux be zero at the boundary, and that the distribution function for particles moving away from the wall be an equilibrium distribution at the wall conditions.

Figure 3 shows a comparison of a Couette flow problem with $\mathrm{Kn} \equiv \lambda/L = 0.1$, with L the channel width, and non-dimensional wall velocities of ± 0.1. This illustrates that the results of the present method closely match those of DSMC; the small discrepancy is expected to diminish with finer discretization. The distribution function is expected to be discontinuous near the wall for Couette flow problems [13]; at present it is unknown whether the interpolation method used has an adverse effect upon the accuracy of the so-

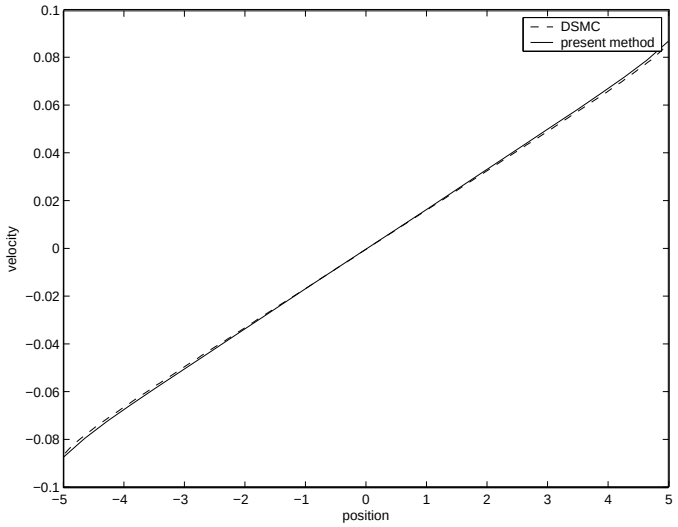

Figure 3: Comparison with DSMC results for Couette flow for Kn $= 0.1$

lution in this region; this will be further investigated in the future. In addition, the effects of density variations in (3) are neglected; density variations are expected to be small, and future work will take these into account.

Conclusion

We have presented an initial investigation of a class of direct numerical methods for solving the Boltzmann equation with the goal of obtaining efficient solution methods for low-speed flows. We used the discrete velocity method for evaluating the collision integral of [11], which provides a good compromise between speed and accuracy. To this, we have added the use of quasi-random sequences to accelerate convergence and a weighting method to reduce the degree of discretization error. This appears to have been reduced to the extent that our solution exhibits excellent conservation properties. Preliminary work suggests that this method will perform well when used for low-speed flows, although more investigation is needed to quantify this. Future work will focus on the development of more sophisticated methods for treating the differential part of (1) (with the collision integral viewed as a source term), as well as further refinements in evaluating the collision integral.

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