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Improvement of a Discrete Velocity Boltzmann Equation Solver With Arbitrary Post-Collision Velocities

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Abstract. We present a discrete velocity scheme which solves the Boltzmann equation and show numerical results for homogeneous relaxation problems. Although direct simulation of the Boltzmann equation can be efficient for transient problems, computational costs have restricted its use. A velocity interpolation algorithm enables us to select post-collision velocity pairs not restricted to those that lie precisely on the grid. This allows efficient evaluation of the replenishing part of the collision integral with reasonable accuracy. In previous work [1] the scheme was demonstrated with the depleting terms evaluated exactly, which made the method of $O(N^2)$ where N is the number of grid points in the velocity space. In order to reduce the computational cost, we have developed an acceptance-rejection scheme to enable more efficient evaluation of the depleting term. We show that the total collision integral can be evaluated accurately in combination with the mapping scheme for the replenishing term. To improve our scheme, we study the error and computational time associated with the number of depleting and replenishing points. We predict the correct relaxation rate for the Bobylev-Krook-Wu distribution and obtain exact conservation of mass, momentum, and energy. Comparisons between computed and reference solutions are shown as well, demonstrating the correct relaxation rate and dependence of error on parameters in the computational scheme.

Keywords: Boltzmann equation, collision integral, discrete velocity scheme, Monte Carlo method
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INTRODUCTION

Direct numerical simulation of the Boltzmann equation via a discrete velocity model can be used to describe a non-equilibrium gas flow, but computational costs limit its use. Since there is little statistical noise associated with the macroscopic flow variables, a discrete velocity model may be more efficient than the Direct Simulation Monte Carlo method for transient problems. We have developed a discrete velocity scheme for a monatomic gas and an interpolation algorithm that projects points that lie off the grid onto the grid while conserving mass, momentum, and energy. In order to be computationally efficient, discretization of velocity space must be relatively coarse. Traditionally, problems arise when evaluating the replenishing integral because post collision velocities are limited to points that lie on the grid [2]. For collision pairs with small relative velocities, there exist few post-collision velocities that lie on the grid. To overcome this problem, we pick an arbitrary orientation of the post-collision velocity vector and use the interpolation scheme to map those points back onto the grid. The described mapping can introduce small negative changes of mass and portions of the distribution function can become very slightly negative, particularly near the fringes of the domain. When developing a scheme we look to understand where the negative mass comes from and how to remove it. The interpolation scheme gives us the ability to consider many replenishing pairs, regardless of the relative velocity. In previous work [1], we have shown that accurate evaluation of the replenishing integral can be obtained using a very coarse approximation, only replenishing to several pairs. Originally, the depleting integral was evaluated by considering collisions between every grid point with every other point in velocity space. Since accurate results were obtained using a coarse description of the replenishing integral, a coarser description of the depleting integral was also developed. One way to coarsen evaluation of the depleting integral is to collide every grid point with only a handful of partners, where unique collision partners are selected via an acceptance rejection algorithm. Instead of colliding with a fixed number of points, a more general method that collides with a certain mass fraction is used. We will show that by depleting from a fraction of the distribution function, computational time can be substantially reduced.

BACKGROUND

For simplicity this work is restricted to single species monatomic gas flows with no body forces. Further, the differential cross section is assumed to be isotropic, so integration over all scattering angles yields the total cross section, σ_T. Under these simplifications, the Boltzmann equation for homogeneous relaxation problems reduces to

$$\frac{\partial \varphi}{\partial t} \Delta t = \frac{1}{Kn} \left[\Delta \varphi_{repl} - \Delta \varphi_{depl} \right]$$

$$\Delta \varphi_{depl} = \Delta t \int_{\zeta_i} \varphi(\zeta_i) \varphi(\eta_i) g \sigma_T d\zeta_i = \Delta t \varphi(\eta_i) \int_{\zeta_i} \varphi(\zeta_i) g \sigma_T d\zeta_i \qquad (1)$$

$$\Delta \varphi_{repl} = \Delta t \int_{\zeta_i} \varphi(\zeta_i') \varphi(\eta_i') g \sigma_T d\zeta_i$$

where the Knudsen number, Kn, is the ratio between the mean free path and a characteristic length scale and φ is the distribution function normalized by the number density. The velocities are denoted by η and ζ, where the primes indicate post-collision velocities, and g is the relative velocity. To evaluate the collision integral, we move to a finite velocity space which is large enough that the distribution function becomes vanishingly small near the boundary [3]. In this framework, the depleting integral is approximated by

$$\left(\Delta \varphi_{IJK} \right)_{depl} = \Delta t \beta^3 \varphi_{IJK} \sum_{I_1 J_1 K_1} \varphi_{I_1 J_1 K_1} g \sigma_T, \qquad (2)$$

where β is the velocity space scaled discretization parameter and I, J, and K are indices that denote position on the grid. The depleting integral can generally be evaluated for any known cross section but variable hard sphere molecules (VHS) are commonly used for many practical engineering problems. VHS molecules relate the cross section to the relative velocity by $\sigma_T = g^{-\kappa}$, where κ is typically fractional. Maxwell molecules correspond to the special case where $\kappa = 1$. In this work Maxwell molecules are used to further simplify the depleting integral because $\sigma_T g$ is constant in this case and can be factored out of the summation. For Maxwell molecules, the depleting integral becomes

$$\left(\Delta \varphi_{IJK} \right)_{depl} = \Delta t \varphi_{IJK} n_r, \qquad (3)$$

where n_r is the reference number density.

The depleting integral can be evaluated by the above equation, but the replenishing integral is more difficult and is determined statistically. For elastic collisions mass, momentum, and energy are conserved and in a discrete velocity framework, all possible collision outcomes lie on the sphere of diameter g centered about the center of mass velocity. (Fig. 1a) In principle the replenishing integral is evaluated by considering all possible post-collision velocities. We approximate this integral by sampling several post-collision velocities by arbitrarily rotating the relative velocity vector about the center of mass velocity. The resulting floating velocities must be projected onto the discrete grid in a way that preserves mass, momentum, and energy. Other conservative schemes that do not require interpolation have been developed in [2, 4,5].
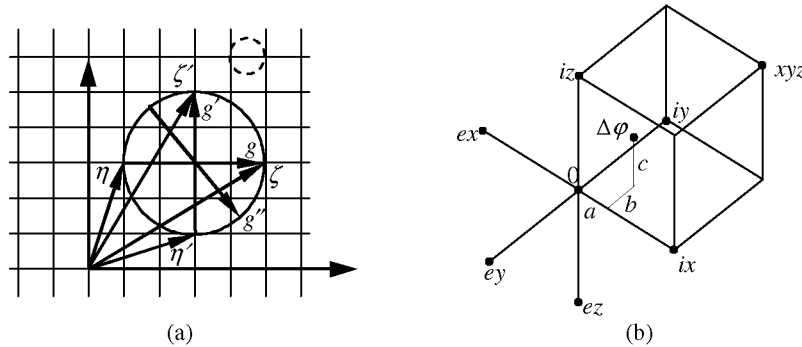

(a)   (b)

FIGURE 1. (a) 2-D representation of collisions on a discrete velocity grid. (b) 3-D interpolation stencil with points ex, ey, and ez being the points external to the unit cell surrounding point $\Delta\varphi$.

INTERPOLATION SCHEME

While projecting points off the grid onto the grid, the 5 conservation equations must be satisfied. It is possible to obtain a unique interpolation onto the grid by using 4 'internal' points that lie on the cube surrounding the interpolating point and a 5th 'external' point that is outside of the box. (Fig. 1b) The stencil used here is the 3-D analog of the stencils used in the 2-D scheme of Honma, *et al.* [6].

The conservation equations for a symmetric 7-point stencil with three external points and the resulting interpolating equations are

$$
\begin{matrix} mass \\ x-mom \\ y-mom \\ z-mom \\ energy \end{matrix}
\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & 1 & 1 & 3 \end{pmatrix}
\begin{pmatrix} f_o \\ f_{ix} \\ f_{iy} \\ f_{iz} \\ f_e \end{pmatrix}
=
\begin{pmatrix} 1 \\ a \\ b \\ c \\ a^2+b^2+c^2 \end{pmatrix},
\quad
\begin{aligned}
f_o &= 1-a^2-b^2-c^2 \geq 0 \\
f_{ext} &= -\left(|a|+|b|+|c|-a^2-b^2-c^2\right)/6 \leq 0 \\
f_{ix} &= \left(|a|+f_{ext}\right) \\
f_{iy} &= \left(|b|+f_{ext}\right) \\
f_{iz} &= \left(|c|+f_{ext}\right)
\end{aligned}
\tag{4}
$$

The interpolation equations result in negative changes at the three external points of the stencil. As noted in [1] the negative mass change is necessary to satisfy the energy constraint because the only way to cancel the relative kinetic energy introduced by distributing the mass to different velocities is to introduce a negative change of mass.

The interpolation equations were derived for the common case where the point to be interpolated lies within the chosen velocity space domain. Occasionally collisions yield velocities that are outside the domain. Using a similar procedure, it is also possible to map these points to the nearest stencil on the grid. When capturing post-collision velocities that extend off the grid, a penalty is paid by the creation of negative mass. In particular, one can map any point to the above 7-point stencil and conserve mass, momentum, and energy regardless of the orientation of the interpolating point. As the distance from the interpolating point to the stencil origin (point O) increases, more negative mass must be created to satisfy the conservation equations. Therefore, for the case where an interpolating point is far from an origin, i.e. for points outside the domain, additional negative mass must be created. In general this is not a serious problem because collisions that result in velocities that lie outside of the grid boundaries are infrequent and the fractional masses that are moved outside are very small, of the order 10^{-6}.

The negative mass generated is typically very small, but it is still not physical and can make evaluation of the entropy impossible. The scaled entropy of the distribution function is defined by

$$
S \equiv -\beta^3 \sum_{IJK} \varphi_{IJK} \ln \varphi_{IJK}. \tag{5}
$$

In the limit $\varphi \to 0$ the contribution to the entropy also goes to zero, but small negative values of φ that occasionally occur leave entropy undefined. To solve this problem, the negative mass must be removed and we do this by rescaling the distribution function. All points in the distribution with negative mass are set to zero and the entire distribution is then rescaled to ensure mass conservation. This operation results in small errors in the momentum and energy, so corrections are added near the origin to preserve the momentum and energy balance. This step is only required to determine the entropy, not to evaluate the collision integral.

DEPLETING INTEGRAL

In previous work [1], the collision integral was evaluated by considering all possible collision partners. Although this results in correct evaluation of the depleting integral, it is computationally expensive and of order N^2, where N is the number of points in velocity space. Throughout the remainder of this report, this method of evaluating the collision integral will be referred to as the N^2 method. The replenishing integral is evaluated statistically by considering post-collision pairs chosen at random.

The major difference between the N^2 method and our new method is that only a relatively few (N_c) of collision partners are considered for each grid point. A similar optimization approach was implemented in [7]. This reduces the order of the scheme from N^2 to NN_c. One simple approach is to randomly choose a set of collision partners without bias. Since many points of the velocity space have relatively low mass, much effort is wasted performing collisions that do not contribute much to the depleting collision integral. For Maxwell molecules, $\sigma_T g$ is constant and we use an acceptance-rejection scheme that weights accepted points by the mass. This scheme is used because points with more mass contribute more to the collision integral than points with little mass. Collision partners can be selected more than once and we continue to pick points until a certain mass fraction of the distribution function is

selected. In this paper, the cutoff fraction is referred to as the depleting fraction. Once all partners are selected, the total amount depleted is equally shared among all collision partners. This is different than the N^2 method, where the amount depleted from each partner is weighted by the mass of the collision partner.

NUMERICAL RESULTS

Five different parameters, N, β, Δt, depleting fraction and number of replenishing pairs can be varied. However, our results focus on using different depleting fractions and number of replenishing pairs while keeping all other parameters fixed. An 11^3 grid with a scaled velocity spacing of 0.5 and time step of 0.2 are used in all of the following test cases.

Relaxation of the Bobylev-Krook-Wu (BKW) distribution [8,9] using different depleting fractions is studied and these results are compared to the N^2 method using 20 replenishing pairs per collision. In previous work [1] it was found that 2 replenishing pairs are sufficient for a smooth solution, but 10 pairs are used to ensure that this solution best approximates the exact solution. This solution is referred to as the "gold standard" (GS) for BKW relaxation. Analytic results can be obtained by projecting a continuous distribution function onto a discrete grid, but these results are not used because a continuous distribution function relaxes slightly differently than a discrete distribution function.

Figure 2 shows slices of the distribution function plotted at different times for depleting fractions of 5%, 40%, and 80%. A cubic spline is passed through the discrete data to guide the eye. Depleting fractions of 80% and 40% yield results that very closely match the gold standard, but as the depleting fraction decreases the statistical noise increases. This occurs because at lower depleting fractions larger amounts of mass are distributed among fewer points. Despite the increased noise for the 5% case, the computational time associated with this method is nearly two orders of magnitude quicker than the N^2 method. To reduce the noise, the 5% run was ensemble averaged 10, 100, and 1000 times, and the resulting smooth distribution is compared to the GS results in Fig. 3.
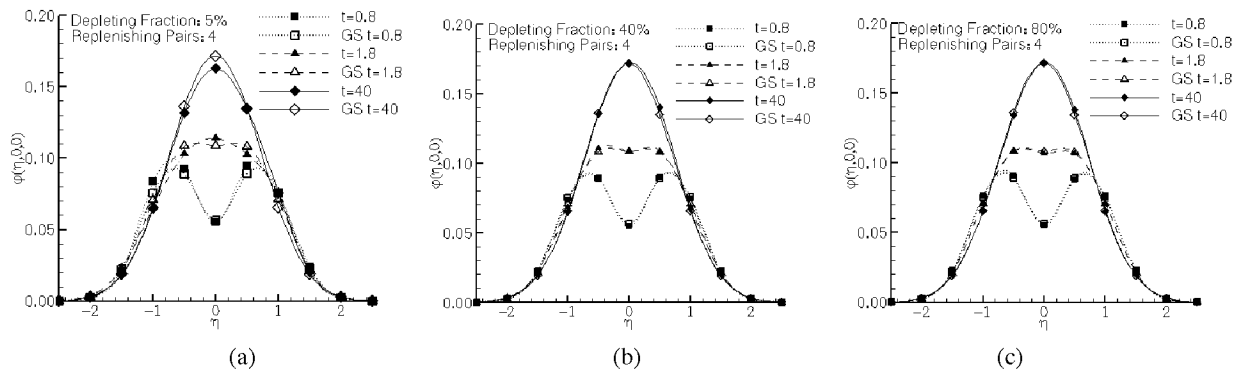

(a)   (b)   (c)

FIGURE 2. Homogeneous relaxation of the BKW distribution using the proposed scheme for evaluating the depleting integral compared to the GS solution. (a) Instantaneous sections of the distribution obtained by a 5% depleting fraction and 4 replenishing pairs. (b) 40% depleting fraction and 4 replenishing pairs. (c) 80% depleting fraction and 4 replenishing pairs.
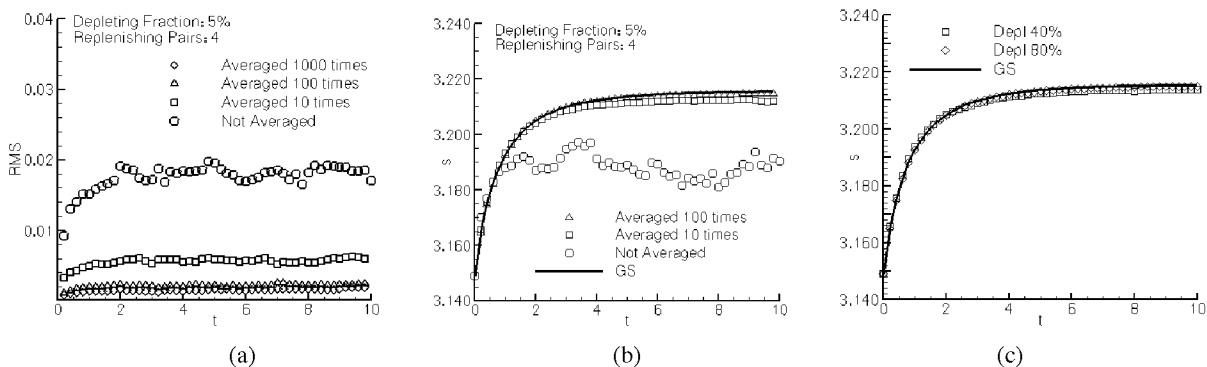

(a)   (b)   (c)

FIGURE 3. Computed RMS and entropy of the homogeneous BKW relaxation using different depleting fractions compared to the GS solution. (a) RMS of the 5% depleting fraction case ensemble averaged 10,100, and 1000 times. (b) Entropy of the 5% depleting fraction case ensemble averaged 10,100, and 1000 times. (c) Entropy of the 40% and 80% cases without averaging.

After ensemble averaging the 5% scheme over as few as 10 independent relaxations, the entropy converges to within 2% of the GS (Fig. 3b). When ensemble averaged for longer, the RMS decreases and the distribution converges to the GS (Fig. 3a). The entropy variation for this case is shown in Fig. 3b. It tends to follow the GS curve for the first several time steps because the relaxation starts with a smooth distribution and the statistical fluctuations take several steps to grow. Averaging non-equilibrium distributions obtained from independent relaxations gives rapid convergence to the GS. For transient problems ensemble averaging can become expensive, but for steady problems one can obtain acceptable results using very small depleting fractions. On Fig. 3c the entropy variation is plotted for the 80% and 40% cases to show that accurate transient solutions can be obtained without averaging. The slight difference between the gold standard entropy and the 80% entropy can be accounted for by statistical noise in the depleting as well as replenishing steps. In addition to modifying the depleting fraction to reduce the noise, one can also change how many replenishing pairs are used: four were used here. The noise associated with the replenishing integral is highly dependent on the depleting fraction because the depleting fraction determines how much mass must be depleted and consequently replenished with each collision partner. As the depleting fraction decreases, the number of replenishing pairs becomes increasingly important.

We now consider time evolution of a Maxwellian distribution with a fixed depleting fraction of 40% and 1, 4, and 8 replenishing pairs. A Maxwellian should remain Maxwellian, but statistical fluctuations are introduced by the evaluation of the collision integral. The gold standard for this set of plots was generated by using the N^2 method with 10 replenishing pairs and then ensemble averaged 200 times. Although small, the N^2 method still has statistical noise due to the replenishing integral and this noise is also plotted as a reference.

(a)   (b)   (c)
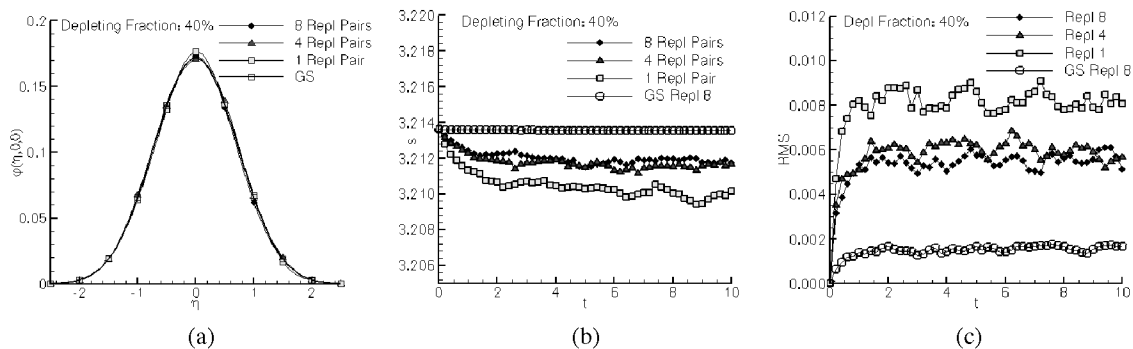
FIGURE 4. Time evolution of a Maxwellian using different numbers of replenishing pairs and a fixed depleting fraction of 40%. (a) Slice of the distribution after 50 time steps. (b) Instantaneous entropy versus time for various replenishing pairs. (c) RMS versus time compared to the RMS of the N^2 method.

Increasing the number of replenishing pairs from 1 to 4 reduces noise and improves accuracy of the entropy, but accuracy is not greatly improved by replenishing to 8 pairs instead of 4. The decrease of error resulting from replenishing to 4 pairs instead of 1 pair occurs because the replenished mass can be distributed over more points. However, after a certain point, further refinement of the replenishing integral does not help much because the error mostly stems from the depleting integral. To optimize the scheme, it is important to match the errors associated with the replenishing and depleting steps.

To characterize the performance of the scheme, we relax a Maxwellian distribution for many different depleting and replenishing configurations and look at the computational time and RMS. The RMS is normalized by the peak value of the distribution function.

Figure 5 shows the mean error plotted against computational time for both methods. Replenishing pairs ranging from 1 to 10 were used with the N^2 method. Depleting fractions between 1% and 90% and replenishing pairs between 1 and 10 were used with the new scheme. When plotted on a logarithmic scale, both schemes show the same rate of convergence. To reduce the error by an order of magnitude, computational time must increase by two orders of magnitude. The vertical thickness represents the range of errors that can be obtained by varying the depleting fraction and replenishing terms. Typically the band is relatively thin, however small improvements can be obtained by choosing a depleting fraction and number of replenishing pairs that yield comparable errors to the depleting and replenishing integrals. Additionally, it is impossible to reduce the computational time of the N^2 method below the time for computing with one replenishing pair. If a problem does not have strict limitations on the noise, one can reduce the computational cost by using the new method where it may be impossible to do so with the N^2 method.
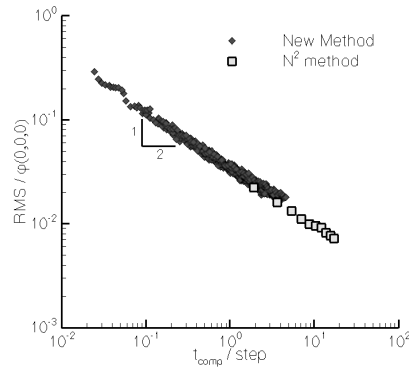
Figure 5. Normalized RMS and computational times generated by multiple depleting fractions and replenishing pairs compared to the N^2 solution.

CONCLUSIONS

We have shown that efficient evaluation of the depleting integral can be achieved by considering a set of random collision partners that are chosen based on mass. Using a depleting fraction of 5% noisy results were generated, but it was possible to converge on the analytic solution by ensemble averaging. In general, increasing the number of replenishing pairs reduces the noise, but after a certain threshold the error associated with a coarse depletion dominates and improvements to the replenishing integral do not improve the overall accuracy. If the depleting errors and the replenishing errors are closely matched, accurate solutions can be generated efficiently.

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