Arbitrary Post-Collision Velocities In A Discrete Velocity Scheme For The Boltzmann Equation

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Abstract. I present a numerical strategy for evaluation of the non-linear Boltzmann collision integral in a discrete velocity framework and show preliminary numerical results. Direct numerical solution of the Boltzmann equation can be more efficient than the Direct Simulation Monte Carlo method for transient problems. Additionally, such a numerical scheme is better adapted to conventional flow solvers in hybrid schemes for continuum-rarefied flow calculations. In a typical discrete velocity scheme the velocity discretization has to be relatively coarse so that the computational scheme can be efficient. This creates problems in the computation of the collision integral because points close to each other in velocity space have very few post-collision velocities available other than the original velocity points. I present a scheme for projecting arbitrary post-collision velocities back onto the velocity grid while conserving mass, momentum, and kinetic energy and demonstrate it on some homogeneous test problems.

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

It is well known that the Boltzmann equation can be used to describe a non-equilibrium gas flow but the computational cost and difficulties associated with the solution of the equation have restricted its use. Direct numerical solution of the Boltzmann equation via a discrete velocity model could be more efficient than the Direct Simulation Monte Carlo method for transient problems. Additionally, there is little statistical noise in the macroscopic variables with this solution method, so it could be readily used in hybrid computational schemes for flows that span the continuum-rarefied regime, or for simulation of flows in nanostructures. We have developed such a discrete velocity scheme for a monatomic gas [1,2] and shown how it can be extended to a polyatomic gas with internal energy [3]. The scheme described in [2] is one of a class of discrete schemes for the Boltzmann equation [e.g. 4-10] where the nominally infinite velocity space is discretized and truncated for purposes of calculation, but velocity moduli are not restricted to a very small number of values. In [2] the collision integral is computed by moving segments of the distribution function (that can be regarded as quasi-particles) to new positions on the velocity grid while conserving mass, momentum, and energy. In order for the computational scheme to be efficient the velocity discretization has to be relatively coarse. This creates some problems in the computation of the collision integral because adjacent samples of the distribution function, i.e., quasi-particles with small relative velocities, have very few post-collision velocities available other than the original points on the velocity grid. Adjacent grid points in velocity space can only be mapped back on themselves. One solution to this problem is to permit an arbitrary re-orientation of the relative velocity vector of the quasi-particles, and then to map the particles back onto the discrete velocity grid while conserving mass, momentum, and energy. In the following section we show that this decomposition is singular and cannot be performed if one attempts to project to the corners of the velocity-space cell containing the arbitrarily rotated quasi-particle. However, it is possible to perform a unique decomposition that properly preserves the collision invariants if one extends the stencil of points in velocity-space onto which one is projecting. We present one such scheme and demonstrate its use by computing some test problems on a uniform velocity grid. A projection scheme of this type is needed to extend the discrete velocity method for the Boltzmann equation to gas mixtures. It could also be used for computations with non-uniform velocity space grids that enable more efficient representation of the distribution function.

BACKGROUND

For simplicity this work is restricted to flows of a single species monatomic gas with no body forces. We choose reference number density n_r, temperature T_r, and molecular velocity $\eta_r \equiv (2kT_r/m)^{1/2}$ where m is the molecular mass. We also define a reference mean free path $\lambda_r \equiv 1/(n_r\sigma_r)$ based on a reference total collision cross-section σ_r. The mean time between collisions is the characteristic time for the variation of the distribution function so the reference time is $\tau_r \equiv \lambda_r/\eta_r = (n_r\sigma_r\eta_r)^{-1}$. If the flow has a characteristic length scale L, we write the Boltzmann equation in scaled variables as

$$Kn\left[\frac{\partial\varphi}{\partial t}+\eta_i\frac{\partial\varphi}{\partial x_i}\right]=\int_{\zeta_i}\int_{\Omega}\left(\varphi(\zeta_i')\varphi(\eta_i')-\varphi(\zeta_i)\varphi(\eta_i)\right)g\frac{\partial\sigma}{\partial\Omega}d\Omega d\zeta_i=\int_{\zeta_i}\left(\varphi(\zeta_i')\varphi(\eta_i')-\varphi(\zeta_i)\varphi(\eta_i)\right)g\sigma_T(g)d\zeta_i, \tag{1}$$

where the scaled velocity distribution function φ is normalized to the scaled local number density n, η_i and ζ_i are scaled molecular velocities, primes indicate post-collision velocities, Ω is the scattering solid angle, and $Kn \equiv \lambda_r/L$ is the Knudsen number. For many practical calculations it is sufficient to assume that the differential collision cross section is isotropic so that it can be integrated immediately over all scattering solid angles to give the total collision cross-section as in the last part of Eq. (1). There is no external flow length scale in homogeneous relaxation or in a simple shock calculation, so $Kn = 1$ for the cases examined in this work.

Variable hard sphere (VHS) molecules are commonly used in engineering simulations and in scaled form may be represented by $\sigma_T = g^{-\kappa}$, where the exponent κ is typically fractional. Hard-sphere molecules correspond to the case $\kappa = 0$, and Maxwell-type molecules to the case $\kappa = 1$. In this paper we restrict ourselves to "Maxwell" molecules in the computations.

We use a conservative time-splitting scheme [11] to solve Eq. (1) (with $Kn = 1$):

$$\Delta\varphi \equiv \frac{\partial\varphi}{\partial t}\Delta t=(\Delta\varphi)_{convection}+(\Delta\varphi)_{collision}=\left[-\eta_i\frac{\partial\varphi}{\partial x_i}\Delta t\right]+\left[(\Delta\varphi)_{replenishing}-(\Delta\varphi)_{depleting}\right] \tag{2}$$

$$(\Delta\varphi)_{depleting}=\Delta t\int_{\zeta_i}\varphi(\zeta_i)\varphi(\eta_i)g\sigma_T d\zeta_i=\Delta t\,\varphi(\eta_i)\int_{\zeta_i}\varphi(\zeta_i)g\sigma_T d\zeta_i, \tag{3}$$

$$(\Delta\varphi)_{replenishing}=\Delta t\int_{\zeta_i}\varphi(\zeta_i')\varphi(\eta_i')g\sigma_T d\zeta_i, \tag{4}$$

It is straightforward to evaluate the depleting term using Eq. (3), but evaluating the replenishing term via Eq. (4) is more difficult. In principle it is obtained from all velocity pairs (η_i', ζ_i') that result in a post-collision velocity of η_i (and any ζ_i) subject to the constraints imposed by the mass, momentum, and energy conservation equations. It is simpler to evaluate the replenishing term at each velocity by computing the outcomes of depleting collisions (either directly or via a statistical approximation). The sum of all depletion outcomes that result in a particular velocity then gives the replenishing term for that velocity [2].

DISCRETE VELOCITY REPRESENTATION

In the discrete approximation used in this paper $\eta_i = (I, J, K)\beta$ where I, J, K are integers and $\beta \equiv \Delta\eta/\eta_r$ is the velocity space scaled discretization parameter. For an efficient computation β cannot be too small, and we use $\beta =$ 0.5–0.7 typically, so that a Maxwellian distribution at T_r is well represented by $|I, J, K| \le 5$. Note that a velocity grid $[-5, 5]^3$ has $N_V = 11^3$ grid points in 3-D velocity space. Moments of the discrete distribution are computed from direct sums. For later reference note that the scaled entropy of the discrete distribution is defined by

$$S \equiv -\beta^3\sum_{I,J,K}\varphi_{IJK}\ln\varphi_{IJK} \tag{5}$$

where a constant factor that only shifts the absolute entropy is omitted.

Because we restrict ourselves to homogeneous relaxation test cases in this paper we omit further consideration of the convective step. If we use a scaled computational time-step $\Delta t = \delta$, then for the collision step we have

$$\varphi_{IJK}^{M+1}(N)=\varphi_{IJK}^{M}(N)+\left(\Delta\varphi_{IJK}^{M}\right)_{collision}, \tag{6}$$

with an explicit expression for the depleting collision term:

$$\left(\Delta\varphi_{IJK}^{M}\right)_{depleting} = \beta^3\ \delta\ \varphi_{IJK}^{M} \sum_{I_1,J_1,K_1} \varphi_{I_1J_1K_1}^{M}\, g\sigma_T\ . \tag{7}$$

Reference [2] used a computation scheme for efficient evaluation of the replenishing term of the collision integral within the discrete velocity representation while conserving mass, momentum, and energy exactly. Figure 1a is a 2-D representation illustrating the basic idea. The depletion of the distribution functions at velocity η_i at (I, J, K) and ζ_i at (I_1, J_1, K_1) due to collisions are mapped to another pair of points on the grid consistent with momentum and energy conservation. For elastic collisions of equal mass particles this corresponds to a pure rotation of the relative velocity vector g_i about the center of mass. All possible outcomes lie on a sphere with diameter g (in 3-D velocity space). For a discrete grid the sphere having the initial two points on its surface has a limited set of other grid points on its surface, as shown by the points lying on the circumference of the circle in Fig. 1a. The set of possible outcomes generally increases as the diameter of the sphere increases but there are relatively few outcomes for points that are close to each other, and there are no possible outcomes if the points are adjacent (e.g. vectors corresponding to dashed circle in Fig. 1). This limitation of collision outcomes on a discrete grid artificially limits the rate at which non-equilibrium distributions can relax. It is a particular problem for a coarse discretization (desirable for computational speed) because the distribution function tends to be concentrated at relatively few grid points. This would be an even bigger problem when dealing with collisions between components of a gas mixture, as the masses of the different components are rarely in a simple proportion that would allow one to use a discrete velocity scheme. An arbitrary rotation of the relative velocity vector about the center of mass (say from g to g'' on Fig. 1a) is consistent with the mechanical conservation laws, but would place some of the distribution function off the fixed velocity grid. The contribution to the fixed grid points in velocity space is needed for the calculation of the replenishing collision integral. We now examine the possibility of projecting the arbitrarily rotated portion of the distribution function back onto the fixed grid in velocity space while preserving mass, momentum, and energy.

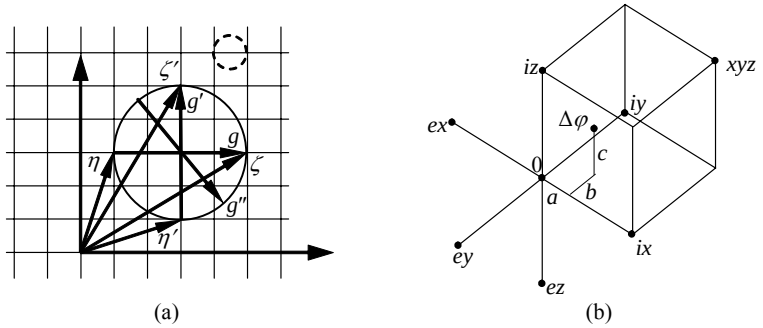


FIGURE 1. (a) 2-D representation of elastic collisions on a discrete velocity grid (b) 3-D interpolation stencil

For a constant mesh spacing it is easy to show that the problem can be reduced to the end point being at some point inside a unit cube in velocity space at location (a, b, c) relative to the origin which is the closest grid point (Fig. 1b). Let $f_j \equiv \Delta\varphi_j / \Delta\varphi; j = 0\ldots4$, be the fraction of $\Delta\varphi$ to be interpolated back onto the grid points chosen. We have 5 constraint equations (mass, x-, y-, and z-momentum equations and energy) and we choose the origin, unit points ix, iy, iz, and the diagonal point from the origin xyz. The constraint equations can be expressed in matrix form as

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 3 \end{pmatrix} \begin{pmatrix} f_o \\ f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix} = \begin{pmatrix} 1 \\ a \\ b \\ c \\ a^2+b^2+c^2 \end{pmatrix} \quad \begin{matrix} \text{Mass} \\ x-\text{Momentum} \\ y-\text{Momentum} \\ z-\text{Momentum} \\ \text{Energy} \end{matrix} \tag{8}$$

This matrix is singular because $c_5 = c_2 + c_3 + c_4 - 2c_1$, where c_i is column i, and hence no solution is possible except for the special cases a, b, c = 0 or 1, i.e. the point is on a corner. One can show that a singular matrix results from the choice of any 5 points on the corners of the unit box surrounding the interpolating point. However, it is possible to obtain a unique interpolation onto the grid using the 5 conservation equations with a fifth point that is *outside* the box. Referring to Fig. 1b, one could use any one of *ex*, *ey*, or *ez*. Algebraic solution of the resulting equations shows that $f_j < 0$ for the external point which could be interpreted as negative mass. This result may be explained as follows. When we take some mass at a specified velocity and attempt to split it into several component

masses with different velocities while conserving mass and momentum, then the components have kinetic energy relative to the center of mass. If total kinetic energy is to be conserved then the relative kinetic energy can only be cancelled by negative mass. In order to minimize the negative contributions at any grid point we use a symmetric 7-point stencil consisting of the origin (the closest grid point), 3 "interior" points from the *x*-, *y*-, and *z*-corners of the box containing the original point, and three "exterior" *x*-, *y*-, and *z*-points. We constrain the negative changes at the exterior points to be the same. The resulting interpolating equations are

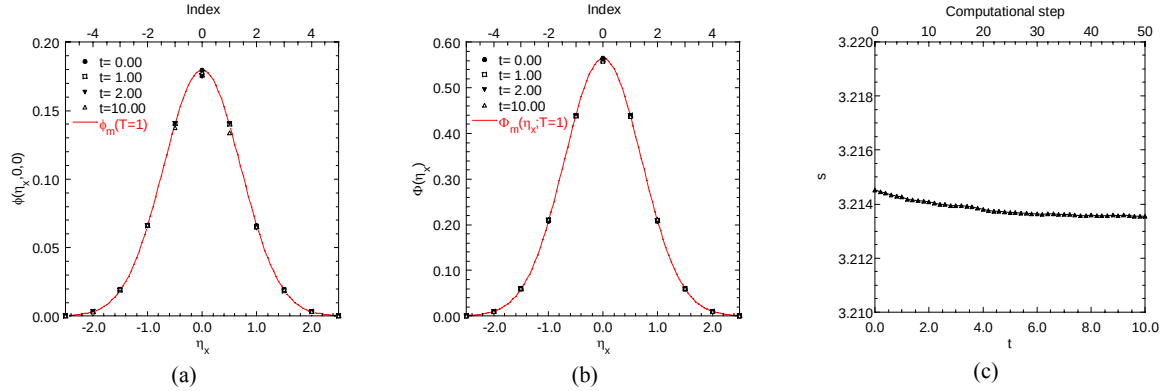
$$f_0 = \left(1 - a^2 - b^2 - c^2\right) \geq 0;\ f_e \equiv -\frac{1}{6}\left(|a| + |b| + |c| - a^2 - b^2 - c^2\right) \leq 0;$$
$$f_{ix} = \left(|a| + f_e\right);\ f_{iy} = \left(|b| + f_e\right);\ f_{iz} = \left(|c| + f_e\right);\ -0.5 \leq a, b, c < 0.5 \tag{9}$$

The choice of the origin as the closest grid point gives the constraint on the magnitudes of *a*, *b*, *c*. Note that the $f_{i\alpha}$, α = *x*, *y*, *z* are generally positive but become negative when, e.g. $|a|$ is small while $|b|$, $|c|$ are large. The interpolation is explicit and can be performed rapidly. It only needs to be done once for each collision pair because if η_i' gives fractional remainders *a*, *b*, *c* relative to the nearest grid point, then ζ_i' gives fractional remainders –*a*, –*b*, –*c* and all f are symmetric in *a*, *b*, *c*.

The stencil of points used here is the 3-D analog of one of the two stencils used in the 2-D scheme of Honma, *et al.* [12]. However, they calculated the distribution function at points off the grid by interpolation in order to estimate the replenishing integral via Eq. (4). The other interpolation stencil used in [12] is the four corners of the box containing a point which cannot be used in a projection that preserves the collision invariants.

NUMERICAL RESULTS

We present some numerical calculations to demonstrate that the interpolation scheme does not produce unphysical results even though it seems to involve negative mass corrections. In a calculation on a finite velocity space, the arbitrary rotation of the post-collision vector could result in points being mapped outside the velocity domain of interest with consequent loss of mass. Also, interpolation to grid points near the velocity domain boundary result in external points of the interpolation scheme that lie just outside the domain. Because mass is conserved across the entire set of interpolation points this could lead to an artificial increase of mass inside the domain. In principle this problem can be avoided by making the velocity space so large that there is a very large buffer zone of points with negligible φ but this is not an efficient computational strategy. For a reasonable domain size and a Maxwellian test distribution one finds that a small subset of the points near the edge of the domain have negative values of φ after evaluating the collision integral by this method. These points are set to zero, which results in fractional *n*, *T* errors $O(10^{-5})$ per computational step. To prevent error accumulation a simple explicit correction is used to ensure that density, momentum and energy are conserved across the distribution during the collision process. It should also be noted that evaluation of the depleting collisions via Eq. (7) is $O(N_V^2)$ which is inefficient. Because the replenishing collision integral is being computed statistically there should be no loss in accuracy of the total collision integral if the depleting term is also evaluated statistically by a method of $O(N_V)$. This would make the method more efficient computationally. All the calculations reported here are made using Eq. (7) for the depleting term in the integral, with scaled velocity grid size $\beta = 0.5$, and computational time step $\delta = 0.2$.



(a) (b) (c)

FIGURE 2. Variation of an initial Maxwellian distribution with repeated application of the collision integral scheme proposed (a) Sections of the Maxwellian distribution in η_y-η_z plane (b) Projection of distribution on η_x-axis (c) Variation in entropy.

Figure 2 shows that a discrete Maxwellian velocity distribution remains Maxwellian after repeated evaluation of the collision integral. There is a slight variation in individual values of φ because of the statistical nature of the computation of the replenishing integral. This can be seen in Fig. 2a which shows the section of the distribution function in the η_y-η_z plane. However, the 1-D projection, e.g. $\Phi(\eta_x)$, of the distribution $\varphi(\eta_x,\eta_y,\eta_z)$ onto any axis is stable. The entropy decreases slightly initially (note highly expanded entropy scale in Fig. 2c) because the initial distribution was based on an analytic Maxwellian, and the computation with mass, momentum, and energy conservation enforced, truncates the Maxwellian and artificially restricts the entire distribution to a finite region in velocity space.

The Bobylev-Krook-Wu non-equilibrium distribution [13,14] is a useful test case as the homogeneous relaxation to equilibrium is known analytically for Maxwell molecules. In scaled variables

$$\varphi_{BKW}(\eta,t)=\frac{1}{2K(\pi K)^{3/2}}\left(5K-3+\frac{2(1-K)}{K}\eta^2\right)\exp\left(-\frac{\eta^2}{K}\right);\ K=\left[1-0.4\exp\left(-\frac{t}{6}\right)\right]. \tag{10}$$

Figures 3a and b compare the analytic solution to distribution functions computed numerically on a $[-5,5]^3$ grid in velocity space, with $\beta=0.5$. It can be seen that there is reasonably good agreement between the theoretical curves and the numerically computed section in the η_y-η_z plane and also the projection onto the η_x-axis of the distribution. Equivalent results are obtained in other sections. The computed entropy variation shown in Fig. 3c also shows good agreement with the value calculated from the analytical distribution.

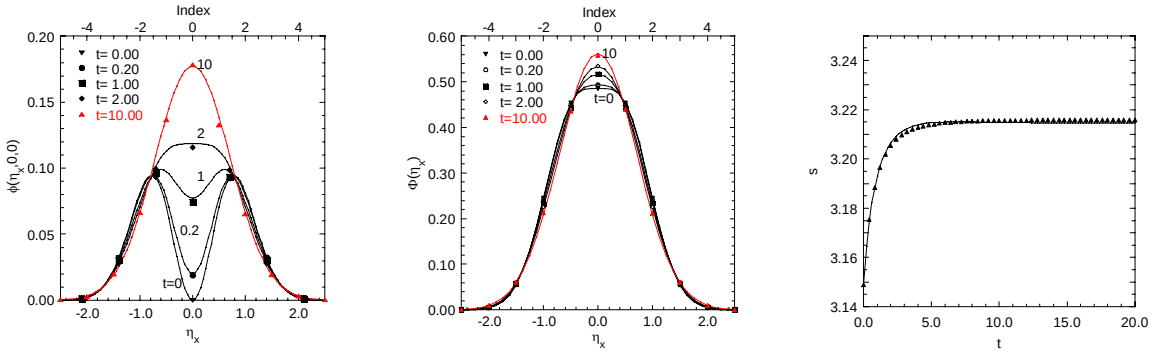


FIGURE 3. Computed relaxation of the Bobylev-Krook-Wu distribution compared with the analytic solution Eq. (10). The solid line is the analytic solution, the points are from the collision integral calculations on a $[-5,5]^3$grid using this scheme. (a) Section of the distribution in η_y-η_z plane; (b) Projection of distribution on η_x-axis; (c) Variation in entropy.

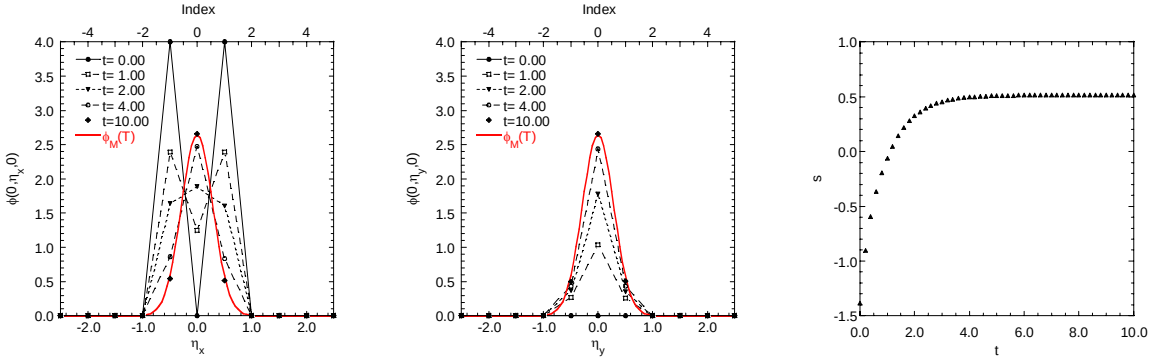


FIGURE 4. Computed relaxation of the double "delta-function" distribution of Eq. (11) computed on a $[-5,5]^3$ grid using the scheme proposed. The bold solid line is a Maxwellian computed at the initial kinetic temperature. (a) Section of the distribution in η_y-η_z plane; (b) Section of the distribution in η_x-η_z plane; (c) Variation in entropy.

The final test case consists of an initial distribution with all the mass concentrated at two nodes separated by a single grid point:

$$\varphi(\eta_i,t=0)=0.5/\beta^3 \text{ if } \eta_i=(-1,0,0)\beta \text{ and } (1,0,0)\beta;\ =0 \text{ otherwise.} \tag{11}$$

This distribution has n = 1 and a kinetic temperature T = 0.1667 for β =0.5. Figure 4 shows the relaxation of this initial distribution to equilibrium. Figures 4a and 4b show sections of the distribution in the η_y–η_z and η_x–η_z planes respectively. It can be seen that by scaled time t = 10 the distribution in either section is very close to being a Maxwellian computed at the initial kinetic temperature. Note that β = 0.5 is a very coarse velocity space discretization for T = 0.1667 and only very few velocity space points have non-zero φ. However, the arbitrary rotation of the post-collision vector enables the distribution to relax to equilibrium smoothly. Figure 4c shows the smooth increase in entropy as the distribution relaxes. The low final entropy of the final Maxwellian relative to the value for the first two test cases is consistent with the low temperature.

A particularly difficult test case consists of an initial distribution with all the mass concentrated at two adjacent nodes, e.g.

$$\varphi(\eta_i, t=0) = 0.5/\beta^3 \text{ if } \eta_i = (0,0,0)\beta \text{ and } (1,0,0)\beta;\ = 0 \text{ otherwise.} \tag{12}$$

As noted in the discussion above (see Fig. 1) the distribution would be invariant under standard discrete velocity schemes. Because the initial distribution is so pathological there appears to be no satisfactory explicit time integration scheme with conservation enforced on every step. An implicit time integration scheme appears to be necessary in this case, at least for early times. This will be considered in future work.

CONCLUSIONS

The procedure to generate post-collision velocities with arbitrary rotations of the relative velocity vector has been demonstrated to work on several test problems. The mapping of the post-collision points back onto the grid is unique. The associated negative masses are not a problem unless the initial distribution is confined to a single pair of adjacent points in velocity space. Mass, momentum, and energy conservation can be enforced locally provided the distribution function has a sufficient number of non-zero points in velocity space. The procedure satisfactorily preserves a Maxwellian distribution and does not create or destroy entropy in this case. The computed relaxation of the Bobylev-Krook-Wu distribution agreed well with the analytic results, and the entropy production matched the theoretical results. The post-collision velocity interpolation scheme can be used for Boltzmann equation calculations on gas mixtures. This interpolation scheme can also be used to map from one velocity grid to another in adaptive schemes for the Boltzmann equation where the velocity grid is adapted to the local temperature for example.

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