Monte Carlo simulation for molecular gas dynamics

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Abstract. The dynamics of low-density flows is governed by the Boltzmann equation of the kinetic theory of gases. This is a nonlinear integro-differential equation and, in general, numerical methods must be used to obtain its solution. The present paper, after a brief review of Direct Simulation Monte Carlo (DSMC) methods due to Bird, and Belotserkovskii and Yanitskii, studies the details of the DSMC method of Deshpande for mono as well as multicomponent gases. The present method is a statistical particle-in-cell method and is based upon the Kac-Prigogine master equation which reduces to the Boltzmann equation under the hypothesis of molecular chaos. The proposed Markoff model simulating the collisions uses a Poisson distribution for the number of collisions allowed in cells into which the physical space is divided. The model is then extended to a binary mixture of gases and it is shown that it is necessary to perform the collisions in a certain sequence to obtain unbiased simulation.

Keywords. Low density flow; Boltzmann equation; Kac-Prigogine master equation; collision dynamics; Monte Carlo method; unbiased and consistent estimator.

1. Introduction

With the advent of space vehicles flying at altitudes of several hundred kilometers or more, it has become necessary to study aerodynamics at low densities. The chief parameter that governs such flows is the Knudsen number Kn, which is the ratio of the mean free path of molecules between collisions (say λ) to a characteristic linear dimension of the body in flight (say L). Figure 1 shows the variation of λ with altitude in the International Tropical Reference Atmosphere (ITRA) (Ananthasayanam & Narasimha 1986). It is seen that for $L \simeq 1$ m, the Knudsen number Kn $\simeq 1$ at an altitude of 110 km. At much lower altitudes, Kn is small and by
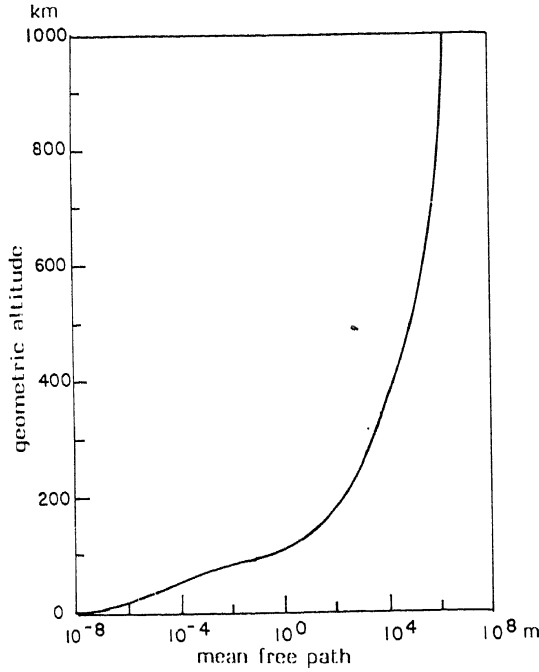
Figure 1. Variation of mean free path with altitude in the International Tropical Reference Atmosphere (1986).

implication the number of intermolecular collisions (in volume L^3) is much larger than the molecular impacts with the body. Consequently, the gas is very nearly in thermodynamic equilibrium everywhere and may be treated as obeying the laws of classical gas dynamics to a good approximation. In the opposite limit of a large Knudsen number, the molecules hardly collide among themselves; the 'free molecule' flow that results is then dominated by molecular impacts with the body and the gas is everywhere far from thermodynamic equilibrium. The molecular gas dynamics regime starts roughly when $Kn = O(1)$ and continues all the way upto $Kn \rightarrow \infty$. In this regime the governing equation is the well-known Boltzmann equation of the kinetic theory of gases. This is a nonlinear integro-differential equation governing the spatio-temporal evolution of the one-particle velocity distribution function $f(t, \mathbf{x}, \mathbf{v})$, and is given by

$$(\partial f/\partial t) + \mathbf{v} \cdot (\partial f/\partial \mathbf{x}) + \mathbf{F} \cdot (\partial f/\partial \mathbf{v}) = \int [f(\mathbf{v}')f(\mathbf{w}')$$

$$-f(\mathbf{v})f(\mathbf{w})]gb \, db \, d\varepsilon \, D\mathbf{w}, \qquad (1)$$

where $\mathbf{v}$ is the molecular velocity, $\mathbf{x}$ is the position vector, $\mathbf{F}$ is the external force per unit mass; $\mathbf{v}$, $\mathbf{w}$ are the precollision velocities of a colliding pair; b is the impact parameter; ε is the angle between the plane of motion and a reference plane (see figure 2), and $D\mathbf{w}$ is an infinitesimal volume in velocity space. Further, in (1) we have written $f(\mathbf{v})$ in place of $f(t, \mathbf{x}, \mathbf{v})$ and shown only one integration symbol for brevity. The velocities $\mathbf{v}'$, $\mathbf{w}'$ are functions of $\mathbf{v}$, $\mathbf{w}$, ε and the scattering angle θ (see figure 2) and are given by

$$\mathbf{v}' = \mathbf{v} + \mathbf{k}(\mathbf{k}, \mathbf{g}), \quad \mathbf{w}' = \mathbf{w} - \mathbf{k}(\mathbf{k}, \mathbf{g}), \qquad (2)$$
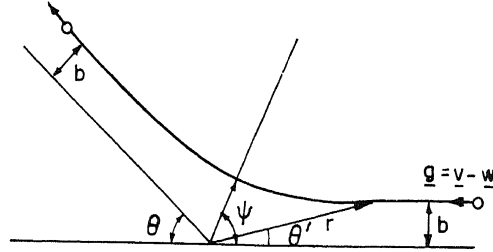
Figure 2. Trajectory of a particle in a central force field.

where 　g = relative velocity of colliding pair = v − w 　　　　(3)

and **k** is the unit vector given by

$$k = [\cos(\theta/2)\cos\varepsilon, \cos(\theta/2)\sin\varepsilon, \sin(\theta/2)]. \qquad (4)$$

The scattering angle θ has to be determined by the two-body collision dynamics and, in general, depends on the impact parameter b, relative speed g and the intermolecular force law.

It is clear that obtaining a solution of (1) for bodies in low density flows is a formidable task and no exact solution to (1) is known except when the gas is everywhere in thermodynamic equilibrium. Over the last several years the statistical-particle-in-cell method or the Monte Carlo method for obtaining the numerical solution of the Boltzmann equation has been developed and successfully applied to a variety of low density flows, some of the most recent examples being hypersonic transitional flows by Moss (1986) and Advanced Orbital Transfer Vehicle (AOTV) entry flows by Bird (1986). We will consider in the following sections of the paper the basics of DSMC (Direct Simulation Monte Carlo) and some aspects of its application to free molecule as well as transitional flows. The development of various computer codes and the Kac-Prigogine equation based DSMC were undertaken under various ISRO*-sponsored research contracts spanning the period from 1970 to 1983.

2. Free molecule drag calculation by Monte Carlo

In free molecule flows the intermolecular collision term in (1) is zero, and the flow field changes because of molecular impacts with the body. It is then possible to calculate the drag and lift coefficients as well as the Stanton number by simply calculating the momentum and energy transferred to the body by the impacts. In fact, assuming diffuse reflection at the body surface the free molecule drag coefficient C_{Dfm} for an arbitrary body is given by

$$C_{Dfm} = 1/(\tfrac{1}{2}\rho_\infty U_\infty^2 A_{\text{ref}}) \int dS(p) \int_{v_n > 0} D\mathbf{v}[v_n^2 + v_n(\pi R T_w/2)^{\frac{1}{2}} \cdot n_x(p)$$

$$+ v_{t1} v_n t_{1x}(p) + v_{t2} v_n t_{2x}(p)] F_\infty, \qquad (5)$$

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where ρ_∞ = density in the free stream,

A_{ref} = reference area,

F_∞ = the free-stream Maxwellian distribution

$$= n_\infty(\beta_\infty/\pi)^{3/2} \exp\left[-\beta_\infty(\mathbf{v} - \mathbf{U}_\infty)^2\right], \tag{6}$$

n_∞ = free stream number density,

$\beta_\infty = 1/(2\,R\,T_\infty)$, T_∞ = free stream temperature,

R = gas constant per unit mass,

$\mathbf{U}_\infty$ = mean velocity in the free stream,

∂B = body surface,

$dS(p)$ = elementary area on ∂B around point P,

$D\mathbf{v} = dv_1\,dv_2\,dv_3$ = infinitesimal volume in velocity space (v_1, v_2, v_3),

$n_x(p)$, $t_{1x}(p)$, $t_{2x}(p)$ are respectively the x-components of normal vector $\mathbf{n}$ and $\mathbf{t}_1$, $\mathbf{t}_2$ are two tangent vectors to the body surface ∂B at the point P, and v_n, v_{t1}, v_{t2} are the corresponding components of velocity $\mathbf{v}$.

The limits of integration with respect to $\mathbf{v}$ in (5) are defined by $v_n > 0$. By defining the characteristic function $X(v_n) = 1$, if $v_n > 0$, $= 0$ otherwise, the integral in (1) can be written in the compressed form

$$C_{Dfm} = \int_{\partial B} dS(p) \int\!\!\int\!\!\int_{-\infty}^{+\infty} D_F(\mathbf{v}, p) X(v_n) D\mathbf{v}, \tag{7}$$

where

$$D_F(\mathbf{v}, p) = [v_n^2 + v_n(\pi R\,T_w/2)^{\frac{1}{2}}\,n_x(p) + v_{t1}v_n t_{1x}(p) +$$
$$+ v_{t2}v_n t_{2x}(p)]\,F_\infty/(\tfrac{1}{2}\rho_\infty U_\infty^2 A_{ref}).$$

The sample mean Monte Carlo estimator for C_{Dfm} can now be constructed as follows. First, we choose a finite volume Ω in velocity space in such a way that the contribution to C_{Dfm} due to velocities falling outside Ω is negligibly small. For example, Ω can be taken as a cube centred around $\mathbf{U}_\infty$ and having sides equal to several times the mean thermal speed $1/\beta_\infty^{1/2}$. The body surface is then divided into several elemental surfaces $A_1, A_2 \ldots A_N$ as shown in figures 3 and 4 where the SLV-3 surface is paneled. Then the sample mean Monte Carlo estimator for C_{Dfm} is given by

$$C_{Dfm} = (\Omega_A/N) \sum_{i=1}^{N} D_F(v_i, p_i) X(v_{ni}) (A_i/A) \tag{8}$$

where P_i is a point uniformly distributed on the SLV-3 surface, v_i is a random velocity vector uniformly distributed within the volume Ω, and A is the total area of all the panels on the body. Figure 5 shows the free molecule drag coefficient of SLV-3 with zero angle of attack and diffuse reflection using the above sample mean Monte Carlo estimator at various speed ratios. Also shown in the same figure is the scatter of the estimator. The statistical scatter is always present in any Monte Carlo estimator and is a very characteristic feature of the Monte Carlo method. The details of surface paneling, drawing of random numbers, estimation of variance,
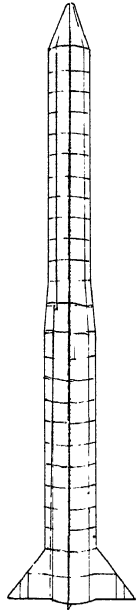
Figure 3. Paneling of SLV-3 surface (side view).

use of variance reduction techniques and calculation of drag coefficients for various bodies including SLV-3 are given in Deshpande & Subba Raju (1973).

3. DSMC method for the Boltzmann equation

3.1 *Introduction*

For the purpose of Monte Carlo simulation of (1) we drop the $\mathbf{F} \cdot (\partial f/\partial \mathbf{v})$ term and the equation becomes

$$(\partial f/\partial t) + \mathbf{v} \cdot (\partial f/\partial \mathbf{x}) = J(f, f)$$

$$= \int [f(t, \mathbf{x}, \mathbf{v}')f(t, \mathbf{x}, \mathbf{w}') - f(t, \mathbf{x}, \mathbf{v})f(t, \mathbf{x}, \mathbf{w})]g\sigma(\Omega, g)\,D\mathbf{w}\,d\Omega,$$
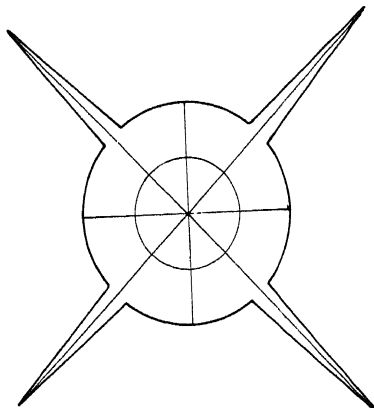
$$(9)$$

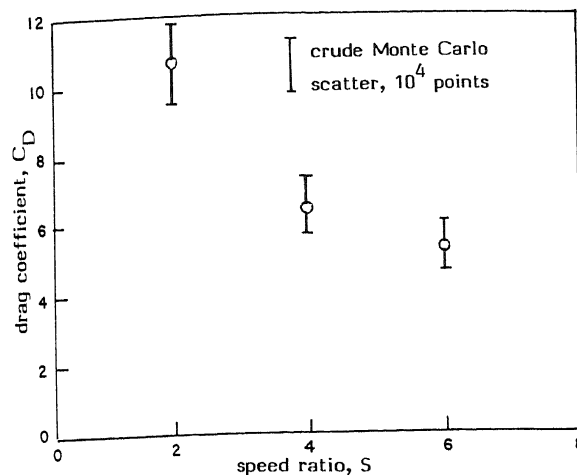**Figure 4.** Approximate representation of SLV-3 base (enlarged).

Figure 5. Drag coefficient for SLV-3 at zero angle of attack in free molecule flow, diffuse reflection.

where $\sigma \, d\Omega$ is the differential scattering cross section, $d\Omega = \sin \theta \, d\theta d\varepsilon$ is the infinitesimal solid angle, and θ is the scattering angle. In terms of impact parameter b introduced in §1 we have $\sigma \, d\Omega = b \, db d\varepsilon$. The most difficult problem in seeking a solution of (9) has been the tackling of the quadratic nonlinear collision term $J(f, f)$. Among different numerical methods used the DSMC of Bird (1970, 1976) has been very successful in handling a variety of multidimensional flows in aerospace engineering. The faithfulness of the Time Counter (TC) strategy of Bird has always been doubted (Deshpande 1978; Pullin 1974; Yanitskii 1973). For example, Yanitskii (1973) has shown that the collision-relaxation model of Bird is not satisfactory in the sense that Bird's method distorts the actual distribution of the number of collisions q and further that the method gives a biased value of the mathematical expectation of q. This bias becomes vanishingly small as the number of molecules per cell tends to infinity. Further, Deshpande (1976) has pointed out that while trying to simulate the collision term Bird (1970) suggests that a time counter be kept for each class of molecules whose velocity vectors fall within $\mathbf{v}$ and $\mathbf{v} + d\mathbf{v}$. On the other hand, in all applications of this method to specific flow problems, a time counter is kept for each cell in physical space, that is, for all molecules in a physical cell. No analysis is made regarding the possible approximation involved. Bird (1970) has observed that the Monte Carlo would be more directly comparable to the Boltzmann equation if a time counter is kept for each molecule and suitably advanced. We will show that for faithful simulation it is *not* necessary to keep a time counter for each cell[†].

The motivation for the Kac-Prigogine based DSMC arose from the above doubts concerning the faithfulness of the TC strategy of Bird. The connection between the master equation and the Boltzmann equation was exploited by Deshpande (1976) to develop an RCN (random collision number) strategy. The theoretical basis of the unbiasedness and consistency of the RCN method was studied in considerable detail

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[†] In a private communication with the author in 1976 Bird stated that he no longer speculates on the possibility of using a separate time counter for each molecule.

by Deshpande (1978). A modified RCN (MRCN) method was developed by Deshpande *et al* (1979) to keep the computing task proportional to the number of particles by using the sampling technique to determine the expected number of collisions per cell. A considerably simpler and transparent proof of the Kac-Prigogine-equation-based DSMC method of Deshpande was given by Deshpande (1982) in a paper at a workshop on Monte Carlo methods. This method was later extended to multicomponent mixtures by Deshpande (1983). Further, the above DSMC method was made computationally more efficient by Deshpande & Subba Raju (1981) by using operator splitting.

It may be noted here that Belotserkovskii & Yanitskii (1975) were the first to use the master equation to develop the statistical particle in cell method, termed the tracer method by Yen (1985). Their method is different from that of Deshpande (1976) in that Belotserkovskii & Yanitskii (1975) use a time counter while Deshpande uses the Poisson distribution to draw the allowed number of collisions in a cell. A review of different DSMC methods is given by Yen (1985) and by Nanbu (1986). As we shall see later some comments of Nanbu (1986) about Deshpande's method are not entirely correct. We shall study here the theoretical basis of the Kac-Prigogine equation-based DSMC of Deshpande for mono and multicomponent gases.

3.2 *Kac-Prigogine master-equation-based* DSMC

We write the Boltzmann equation (9) as

$$(\partial f/\partial t) = (\partial f/\partial t)_{\text{con}} + (\partial f/\partial t)_{\text{col}} \tag{10}$$

where

$$(\partial f/\partial t)_{\text{con}} = \text{streaming term} = -v \cdot (\partial f/\partial x), \tag{11}$$

$$(\partial f/\partial t)_{\text{col}} = \text{collision term} = J(f, f). \tag{12}$$

Using the operator splitting theory of Yanenko (1971) we construct the solution of (9) in two steps as:

$$(\partial f/\partial t) = (\partial f/\partial t)_{\text{con}}, \overline{f^{n+1}} = O_{\text{con}}(\Delta t)f^n = f^n + \Delta t(\partial f/\partial t)_{\text{con}}^n, \tag{13}$$

$$(\partial f/\partial t) = (\partial f/\partial t)_{\text{col}}, f^{n+1} = O_{\text{col}}(\Delta t)\overline{f^{n+1}}$$

$$= \overline{f^{n+1}} + \Delta t J(\overline{f^{n+1}}, \overline{f^{n+1}}), \tag{14}$$

where f^n = velocity distribution at the time level n, and $\overline{f^{n+1}}$ is the solution at the intermediate time level. The solution $\overline{f^{n+1}}$ given by (13) is the solution when the collision term is dropped and hence will represent the free molecule flow, while (14) is the solution with only the collision term present and thus represents the solution of the homogeneous Boltzmann equation. The decoupling between the collision and streaming is possible due to the splitting and the resultant solution

$$f^{n+1} = O_{\text{con}}(\Delta t) O_{\text{col}}(\Delta t) f^n + O(\Delta t^2)$$

$$= O_{\text{col}}(\Delta t) O_{\text{con}}(\Delta t) f^n + O(\Delta t^2), \tag{14a}$$

is only first-order accurate in time. It is now necessary to develop methods for solving the split equations or equivalently for constructing the solution operators O_{con} and O_{col}.

The solution operator O_{con} can be easily constructed as follows. We choose a sufficiently large box (see figure 6) around a body to approximate the infinite flow field. The computational domain is then divided into a network of cells (or finite volumes), the molecules outside the box are assumed to obey the free stream velocity distribution which in many cases is the Maxwellian distribution defined by (6). Several thousands of molecules are distributed initially in the box with their positions distributed in space and their velocities are uniformly drawn from the free stream Maxwellian distribution. Once the initialization is over the simulation of $(\partial f/\partial t) + \mathbf{v} \cdot (\partial f/\partial \mathbf{x}) = 0$ is done by moving along the characteristics

$$(df/ds) = (\partial f/\partial t)(dt/ds) + (\partial f/\partial \mathbf{x}) \cdot (d\mathbf{x}/ds),$$

$$(dt/ds) = 1, \quad (d\mathbf{x}/ds) = \mathbf{v}, \tag{15}$$

that is, we just move the molecules with their velocities over the time interval Δt. During this movement the molecules may quit the box, may hit the body and get reflected, and thus transfer momentum and energy to the body. The various possibilities are taken care of by developing (1) a subroutine for influx of molecules into the box through the boundaries, (2) a subroutine for determining the intersection of the molecular trajectory with the body surface, (3) a subroutine for obtaining reflected velocities after impact with the body, and (4) a subroutine for arranging a molecular list according to the cell numbers they occupy. Subroutines CONV and ARANG were developed by Deshpande *et al* (1977) and validated against available results for a cone and cone-cylinder in a free molecule flow.

3.3 *Simulation of collisions*

The Markoff process for the simulation of the homogeneous Boltzmann equation (12) is based on the Kac-Prigogine model

$$\frac{\partial P_0}{\partial t} = \frac{1}{\text{Vol}} \sum_{1 < j < k < N} \int d\Omega_{jk}\, \sigma(\Omega_{jk}, g_{jk}) g_{jk}$$

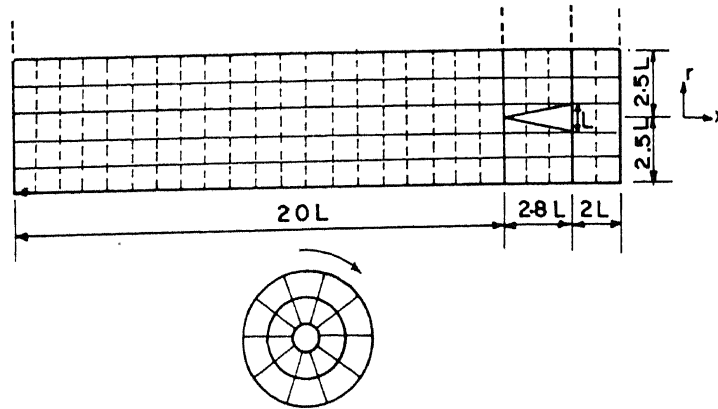$$\times [P_0(t, V'_{jk}) - P_0(t, V)], \tag{16}$$

Figure 6. Division of flow field for computing flow past a cone.

where P_0 is the N-particle velocity distribution function,

$$V = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N\}, \quad V'_{jk} = \{\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}'_j, \ldots \mathbf{v}'_k, \ldots \mathbf{v}_N\},$$

$$\mathbf{g}_{jk} = \mathbf{v}_j - \mathbf{v}_k. \tag{17}$$

The master equation (16) governs the time evolution of the N-particle distribution due to collisions among N molecules in the cell whose volume is denoted by "Vol". One of the very important properties of the Kac-Prigogine equation (16) is that under the hypothesis of molecular chaos

$$P_0(t, V) = \Phi(t, \mathbf{v}_1)\Phi(t, \mathbf{v}_2)\ldots\Phi(t, \mathbf{v}_N), \tag{18}$$

where $\Phi(t, \mathbf{v})$ is the one-particle velocity distribution function, the master equation reduces to the Boltzmann equation. Further, the molecular chaos once established perpetuates in time provided N is very large, and the initial validity of the chaos is ensured by taking

$$P_0(t_0, V) \propto F_\infty(\mathbf{v}_1)F_\infty(\mathbf{v}_2)\ldots F_\infty(\mathbf{v}_N). \tag{19}$$

F_∞ is the free stream Maxwellian defined by (6).

The relationship between the simulation method and the master equation becomes transparent if we write (16) in the form

$$(\partial P_0/\partial t) = B(O - I)P_0(t, V), \tag{20}$$

where

$$B = \text{number of binary interactions per unit volume per unit time} = \text{SUM/Vol},$$

$$\text{SUM} = \sum_{1 \leqslant i < r \leqslant N} \int g_{ir}\sigma(\Omega_{ir}, g_{ir})\, d\Omega_{ir}, \tag{21}$$

$$OP_0 = \sum_{1 \leqslant j < k \leqslant N} \int p_{jk}(\sigma_{jk}, g_{jk})P_0(V'_{jk})\, d\Omega_{jk}, \tag{22}$$

$$p_{jk}(\Omega_{jk}, g_{jk}) = [g_{jk}\sigma(\Omega_{jk}, g_{jk})]/\text{SUM}, \tag{23}$$

$$I = \text{identity operator}.$$

The operator O gives OP_0 which is the new N-particle velocity distribution after one collision. Everytime there is a collision the N-particle velocity distribution undergoes a change $(O - I)P_0(t, V)$. As there are B binary interactions per unit time per unit volume the total change due to them will be $B(O - I)P_0$. Equation (20) is obtained by equating this change per unit time to $\partial P_0/\partial t$. A formal solution of (20) for a small time interval Δt is

$$P_0(t + \Delta t, V) = \exp(-B\Delta t)\, \exp(\Delta t BO)P_0$$

$$= \exp(-B\Delta t) \sum_{r=0}^{\infty} [(\Delta t B)^r/r!]O^r P_0(t, V). \tag{24}$$

Recognizing that

$$[(\Delta t B)^r/r!]\exp(-B\Delta t), \tag{25}$$

is a Poisson distribution, it follows from (24) that $P_0(t + \Delta t, V)$ is the mathematical expectation of $O^r P_0(t, V)$ with r obeying a Poisson distribution having a mean equal to $B\Delta t$.

The Monte Carlo simulation of the homogeneous Boltzmann equation (12) can thus be performed by the following algorithm:

(a) Calculate the binary interaction rate B by using (21), which requires relative velocity for every possible colliding pair, and the differential scattering cross-section $\sigma(\Omega, g)$.

(b) Draw a random variable r from the Poisson distribution $\exp(-B\Delta t)(B\Delta t)^r / r!$

(c) Select a pair of molecules v_j, v_k and solid angle Ω_{jk} from the probability distribution $p_{jk}(\Omega_{jk}, g_{jk})$.

(d) For the collision partners drawn in step (c) determine the post-collision velocities v'_j, v'_k from collision dynamics and replace v_j and v_k by v'_j and v'_k. The determination of the post-collision velocities requires the use of (2) which in turn requires the values of the azimuthal angle ε and the scattering angle θ. The latter can be determined from the dynamics of two-body collision.

(e) Repeat the steps (c) and (d) r times.

Several comments are in order about the Kac-Prigogine-equation-based DSMC method. First, step (a) requires the calculation of $N_c = N(N-1)/2$ pairs of relative velocities g_{jk} as j and k run from 1 to N. Hence, the collision strategy described above will require an operation count that goes like N^2. It is preferable to have an operation count that goes like N especially when N is large. However, whenever the number of molecules per cell is very large (as happens when the flow is collision-dominated) it is possible to estimate the SUM given by (21) by a sampling procedure. In order to determine SUM in such a case all that is required is to randomly draw N pairs $g_1, g_2 \ldots g_N$ corresponding to partners (i_1, r_1), $(i_2, r_2) \ldots (i_N, r_N)$, and then determine SUM by the sample mean Monte Carlo estimator

$$\text{SUM} = \sum_{j=1}^{N} \int g_j \sigma(\Omega, g_j) \, d\Omega. \tag{26}$$

Further, several variance reduction techniques can be employed (importance sampling, stratified sampling etc.) to construct an estimator for SUM having smaller variance than for the sample mean estimator (26). The sample mean estimator (26) is the basis of the MRCN method of Deshpande et al (1979). In summary, the present DSMC can be easily designed to have an operation count that is linearly related to the number of molecules in a cell. This point has not been recognised by Nanbu (1986) in his recent article on "Theoretical basis of the DSMC method" where he claims that unless the molecular model is Maxwellian, only Bird's method and Nanbu's method modified by Babovsky are of practical use as the computing task is proportional to the number of particles. This claim as we have seen is not entirely correct because in the present DSMC method also the computing task is proportional to the number of particles. Further Nanbu (1986) has stated that Deshpande (1978) "tried to derive the method from the Kac equation but his derivation is rather a kind of plausibility argument". It is difficult to know the basis of this statement. Unbiasedness and consistency of DSMC of Deshpande were proven in the report of Deshpande (1978). The analysis of the present paper is the

same as that of Deshpande (1982) and is much more transparent than the one given by Deshpande (1978) earlier. The actual calculations of low density flows past a cone at Knudsen number close to unity (see Deshpande *et al* 1978) show that the RCN strategy and the TC strategy of Bird require very nearly the same CPU time even though the RCN strategy requires an operation count that goes like N^2 instead of like N for the TC strategy. This is primarily because the number of operations required to advance the solution from one time level to the next is dominated by the convection operator O_{con} and *not* by the collision operator O_{col} for flows having Kn = O(1).

The step (a) above requires the calculation of SUM given by (21), and SUM in turn depends on the intermolecular force law. For rigid sphere molecules

$$\int_0^{2\pi} \int_0^{d} gb\,db\,d\varepsilon = \pi d^2 g,$$

where d is the diameter of the molecules. The SUM then is given by

$$\text{SUM} = \pi d^2 \sum\sum_{1 \leqslant i < j \leqslant N} g_{ij}. \tag{27}$$

For a molecular pair i, j retained for a collision the vector relative velocity g_{ij} is known. The scattering angle θ and the azimuthal angle ε in (4) are drawn with uniform distributions from the intervals $[0, \pi]$ and $[0, 2\pi]$. For these values of g_{ij}, θ, and ε, the post-collision velocities v', w' can then be determined from relations (2) and (4).

In case of molecules with soft potential having point-centres of repulsion we have,

$F = $ intermolecular force between two molecules separated by
distance $r = a/r^s$. $\tag{28}$

Defining the dimensionless impact parameter α by

$$\alpha = b[mg^2/2(s-1)a]^{1/(s-1)}$$

we obtain

$$gb\,db\,d\varepsilon = K_0 g^{\omega}\alpha\,d\alpha\,d\varepsilon, \tag{29a}$$

where

$$\omega = (s-5)/(s-1), \quad K_0 = [2(s-1)a/m]^{1/(s-1)}. \tag{29b}$$

For such molecules SUM reduces to

$$\text{SUM} = \pi\alpha_{max}^2 K_0 \sum\sum_{1 \leqslant i < j \leqslant N} g_{ij}^{\omega}, \tag{30}$$

where α_{max} is the cut-off value of the dimensionless impact parameter. The scattering angle θ for molecules with soft potentials is no longer a uniformly distributed random variable. The scattering angle θ is a function of α given by

$$\theta = \pi - 2 \int_0^{\eta_1} d\eta \, \{1 - \eta^2 - [2/(s-1)](\eta/\alpha)^{s-1}\}^{-1/2}, \tag{31}$$

where η_1 is the positive real root of the equation

$$1 - \eta_1^2 - [2/(s-1)](\eta_1/\alpha)^{s-1} = 0. \tag{32}$$

The scattering angle is determined by drawing a random number α uniformly distributed between $[0, \alpha_{max}]$, and then computing θ by the evaluation of the integral (31). This integral in general has to be computed numerically, but for some values of s closed form results are available, e.g. for a Maxwell molecule $s = 5$, and (31) reduces to

$$\theta = \pi - 2(1 - 2q^2)^{\frac{1}{2}} K(q), \tag{33}$$

where

$$q^2 = \tfrac{1}{2}\{1 - 1/[1 + (2/\alpha^4)]^{\frac{1}{2}}\},$$

and $K(q)$ is the complete elliptic integral of the first kind (Abramowitz & Stegun 1965). The above detailed algorithm about drawing random numbers g, α or θ, ε can be briefly summarized by the simplified expressions for $p(\Omega, g)$ given by

$$p(\Omega, g) = p(\theta, \varepsilon, g) = (g/\Sigma g), \text{ for rigid spheres, and}$$

$$p(\Omega, g) = p(\alpha, \varepsilon, g) = (g^\omega/\Sigma g^\omega)\,(\alpha/\pi\alpha_{max}^2), \text{ for soft potentials.}$$

3.4 *An efficient operator-split* DSMC

We have now given methods for constructing operators $O_{con}(\Delta t)$ and $O_{col}(\Delta t)$ used in advancing the solution in time. The CPU time required depends on the number of arithmetic operations involved in $O_{con}(\Delta t)$ and $O_{col}(\Delta t)$. For advancing the solution through two time steps we have to use the sequence twice, that is,

$$f^{n+2} = [O_{con}(\Delta t)\, O_{col}(\Delta t)][O_{con}(\Delta t)\, O_{col}(\Delta t)]\, f^n, \tag{34}$$

which involves two convection and collision operators. On the other hand the equivalent sequence

$$f^{n+2} = O_{col}(\Delta t)\, O_{con}(2\Delta t)\, O_{col}(\Delta t)\, f^n, \tag{35}$$

involves only one convection and two collision operators. It has been found that the sequence (35) required about half as much time as required by the sequence (34). This time saving is due to the following reason. After the convection of molecules is done the computer code has to arrange the molecular list according to cell numbers. This arrangement is done by subroutine ARANG. Such an arrangement is necessary for calling subroutine COLSN which performs collisions cell by cell. The sequence (35) makes only one call to subroutine ARANG while the sequence (34) requires two calls. This is the reason for the saving in CPU time when sequence (35) is used instead of the sequence (34). Table 1 shows a comparison between the CPU times taken by the two sequences for advancing the solution through two time steps.

4. Extension of the Kac-Prigogine based DSMC to mixture of gases

Let us consider the binary mixture of two gases denoted by subscripts a and b. The

Table 1. Comparison of CPU[i] times

Method	Subroutines (s)		Complete cycle (s)
	CONV	ARANG	
Sequence (34)	17·8	165·9	195·8
Sequence (35)	15·5	70·9	95·9

[i] Computer used is CYBER 170/730 system at VSSC, Trivandrum. The RDP = rate of data processing defined by the CPU time required to advance the solution through $2\Delta t$ per molecule is a measure of the efficiency of the numerical method. The RDP for the sequence (34) is 0·032 s per molecule per $2\Delta t$, while it is 0·016 s for the sequence (35).

relevant Boltzmann equations for the one-particle probability density functions $\Phi_a(t, \mathbf{x}, \mathbf{v})$ and $\Phi_b(t, \mathbf{x}, \mathbf{v})$ are

$$(\partial \Phi_a/\partial t) + \mathbf{v}_{a1} \cdot (\partial \Phi_a/\partial \mathbf{x}) = J(\Phi_a, \Phi_a) + J(\Phi_a, \Phi_b),$$

$$(\partial \Phi_b/\partial t) + \mathbf{v}_{b1} \cdot (\partial \Phi_b/\partial \mathbf{x}) = J(\Phi_b, \Phi_a) + J(\Phi_b, \Phi_b). \qquad (36)$$

The collision terms J are defined by

$$J(\Phi_a, \Phi_a) \equiv n_a \int |\mathbf{v}_{a1} - \mathbf{w}| \, \sigma_{aa}(\Omega, |\mathbf{v}_{a1} - \mathbf{w}|) \times$$

$$[\Phi_a(\mathbf{v}'_{a1})\Phi_a(\mathbf{w}') - \Phi_a(\mathbf{v}_{a1})\Phi_a(\mathbf{w})] \, d\Omega D\mathbf{w}, \qquad (37a)$$

$$J(\Phi_a, \Phi_b) \equiv n_b \int |\mathbf{v}_{a1} - \mathbf{w}| \, \sigma_{ab}(\Omega, |\mathbf{v}_{a1} - \mathbf{w}|) \times$$

$$[\Phi_a(\mathbf{v}'_{a1})\Phi_b(\mathbf{w}') - \Phi_a(\mathbf{v}_{a1})\Phi_b(\mathbf{w})] \, d\Omega D\mathbf{w}, \qquad (37b)$$

$$J(\Phi_b, \Phi_a) \equiv n_a \int |\mathbf{v}_{b1} - \mathbf{w}| \, \sigma_{ab}(\Omega, |\mathbf{v}_{b1} - \mathbf{w}|) \times$$

$$[\Phi_b(\mathbf{v}'_{b1})\Phi_a(\mathbf{w}') - \Phi_b(\mathbf{v}_{b1})\Phi_a(\mathbf{w})] \, d\Omega D\mathbf{w}, \qquad (37c)$$

$$J(\Phi_b, \Phi_b) \equiv n_b \int |\mathbf{v}_{b1} - \mathbf{w}| \, \sigma_{bb}(\Omega, |\mathbf{v}_{b1} - \mathbf{w}|) \times$$

$$[\Phi_b(\mathbf{v}'_{b1})\Phi_b(\mathbf{w}') - \Phi_b(\mathbf{v}_{b1})\Phi_b(\mathbf{w})] \, d\Omega D\mathbf{w}, \qquad (37d)$$

Here n_a, n_b are the number densities of species a and b, σ_{aa}, σ_{ab} etc. are cross-sections for a–a, a–b etc. collisions, and dependence of Φ_a, Φ_b on t and $\mathbf{x}$ is suppressed for brevity. The solution of (36) can be constructed in two steps by adopting the split scheme:

(i) *Convection step*
Integrate the equations

$$(\partial \Phi_a/\partial t) + \mathbf{v}_{a1} \cdot (\partial \Phi_a/\partial \mathbf{x}) = 0, \quad (\partial \Phi_b/\partial t) + \mathbf{v}_{b1} \cdot (\partial \Phi_b/\partial \mathbf{x}) = 0$$

over small time duration Δt by moving particles a and particles b with their respective velocities. This convection of the particles is exactly similar to the

convection step described earlier for monocomponent gases. We thus obtain the intermediate solution $\Phi_a^{\overline{n+1}}$, $\Phi_b^{\overline{n+1}}$, and the convection operator $O_{con}(\Delta t)$ corresponding to the solution is defined by

$$\begin{bmatrix} \Phi_a^{\overline{n+1}} \\ \Phi_b^{\overline{n+1}} \end{bmatrix} = O_{con}(\Delta t) \begin{bmatrix} \Phi_a^n \\ \Phi_b^n \end{bmatrix}. \tag{38}$$

(ii) *Collision step*

Next, construct the solution

$$\begin{bmatrix} \Phi_a^{n+1} \\ \Phi_b^{n+1} \end{bmatrix} = O_{col}(\Delta t) \begin{bmatrix} \Phi_a^{\overline{n+1}} \\ \Phi_b^{\overline{n+1}} \end{bmatrix}, \tag{39}$$

by integrating the homogenous Boltzmann equations

$$(\partial \Phi_a / \partial t) = J(\Phi_a, \Phi_a) + J(\Phi_a, \Phi_b),$$

$$(\partial \Phi_b / \partial t) = J(\Phi_b, \Phi_a) + J(\Phi_b, \Phi_b), \tag{40}$$

over time duration Δt with $\Phi_a^{\overline{n+1}}$, $\Phi_b^{\overline{n+1}}$ as initial velocity distribution functions. The solution so obtained will be first-order accurate in time.

The collision operator $O_{col}(\Delta t)$ for solving (40) is constructed using the relationship between the Boltzmann equations (40) and the Kac-Prigogine master equation. We write the master equation for a binary mixture of gases in a box of volume "Vol" as

$$(\partial P_0 / \partial t) = J(P_0)$$

$$= \frac{1}{\text{Vol}} \sum_{1 \le j < k \le N} \int |\mathbf{v}_{aj} - \mathbf{v}_{ak}| \sigma_{aa}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{ak}|) \times$$

$$[P_0(V'_{ajk}, V_b) - P_0(V)] \, d\Omega_{jk}$$

$$+ \frac{1}{\text{Vol}} \sum_{j=1} \sum_{k=1} \int |\mathbf{v}_{aj} - \mathbf{v}_{bk}| \sigma_{ab}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{bk}|) \times$$

$$[P_0(V'_{abjk}) - P_0(V)] \, d\Omega_{jk}$$

$$+ \frac{1}{\text{Vol}} \sum_{1 \le j < k \le M} \int |\mathbf{v}_{bj} - \mathbf{v}_{bk}| \sigma_{bb}(\Omega_{jk}, |\mathbf{v}_{bj} - \mathbf{v}_{bk}|) \times$$

$$[P_0(V_a, V'_{bjk}) - P_0(V)] \, d\Omega_{jk}, \tag{41}$$

where

$$V = \{V_a, V_b\}, \quad V_a = \{\mathbf{v}_{a1}, \mathbf{v}_{a2}, \dots, \mathbf{v}_{aN}\},$$

$$V_b = \{\mathbf{v}_{b1}, \mathbf{v}_{b2}, \dots, \mathbf{v}_{bM}\},$$

$$V'_{ajk} = \{\mathbf{v}_{a1}, \dots, \mathbf{v}'_{aj}, \dots, \mathbf{v}'_{ak}, \dots, \mathbf{v}_{aN}\},$$

$$V'_{bjk} = \{\mathbf{v}_{b1}, \dots, \mathbf{v}'_{bj}, \dots, \mathbf{v}'_{bk}, \dots, \mathbf{v}_{bM}\},$$

$$V'_{abjk} = \{\mathbf{v}_{a1}, \dots, \mathbf{v}'_{aj}, \dots, \mathbf{v}_{aN}, \mathbf{v}_{b1}, \dots, \mathbf{v}'_{bk}, \dots, \mathbf{v}_{bM}\}.$$

Further, $\sigma_{aa} d\Omega_{jk}$ is the differential scattering cross-section for a-a collisions, $\sigma_{ab} d\Omega_{jk}$ for a-b collisions and so on. In (41) $P_0(t, V)$ is a joint probability density function. An interesting property of (41) is that it reduces to the homogenous Boltzmann equations (36) under the hypothesis of molecular chaos. For, we then have

$$P_0(t, V) = \Phi_a(t, v_{a1})\Phi_a(t, v_{a2})\ldots\Phi_a(t, v_{aN})\Phi_b(t, v_{b1}) \times$$
$$\Phi_b(t, v_{b2})\ldots\Phi_b(t, v_{bM}). \tag{42}$$

Integrating the master equation (41) with respect to all the velocity variables except v_{a1} and observing that

$$\sum_{1 \leqslant j < k \leqslant M} \int d\Omega_{jk} |v_{bj} - v_{bk}| \sigma_{bb}(\Omega_{jk}, |v_{bj} - v_{bk}|) \times$$
$$[P_0(V_a, V'_{bjk}) - P_0(V)] Dv_{a2}\ldots Dv_{bM} = 0,$$

we obtain the first of the homogenous Boltzmann equations (36). In establishing this result we have assumed that N and M are sufficiently large so that

$$n_a \simeq (N-1)/\text{Vol}, \quad n_b \simeq (M-1)/\text{Vol}.$$

Similarly, integrating the master equation (41) with respect to all velocity variables except v_{b1} and invoking (42) we obtain the second of the homogenous Boltzmann equations (36). Thus, under the condition of molecular chaos, we obtain

$$J(\Phi_a, \Phi_a) + J(\Phi_a, \Phi_b) = \int J(P_0) Dv_{a2}\ldots Dv_{aN} Dv_{b1}\ldots Dv_{bM}, \tag{43}$$

$$J(\Phi_b, \Phi_a) + J(\Phi_b, \Phi_b) = \int J(P_0) Dv_{a1}\ldots Dv_{aN} Dv_{b2}\ldots Dv_{bM}. \tag{44}$$

These relations are very crucial to the present DSMC method for a binary mixture. These relations enable us to tackle the nonlinear Boltzmann equations through the linear Kac-Prigogine master equation. What is now required for the development of DSMC is the Monte Carlo game exactly simulating the Kac-Prigogine equation governing the time evolution of the $(N + M)$-particle probability density function $P_0(t, V)$.

It may be observed that the equivalence between (40) and (41) requires the condition of molecular chaos and even though we can ensure its satisfaction at some initial time by properly sampling the $N + M$ velocity vectors, its validity thereafter is in general not guaranteed. As time proceeds correlations between velocity vectors will appear thus destroying the chaos. However, the molecular chaos has the self-preservation property in the limit of an infinite number of particles. It is therefore possible to reduce the distortion introduced in the numerical simulation by choosing sufficiently large N and M in a cell.

The development of the Markoff model for the simulation of the master equation (41) is very similar to the case of a monocomponent gas. The details of the Markoff model for a binary mixture are given in Deshpande (1983), only a brief description is given here.

5. Markoff model for a binary mixture

For the purpose of developing the Markoff model we introduce the following probability distributions

$$P_{aajk} = P_{aa}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{ak}|) = |\mathbf{v}_{aj} - \mathbf{v}_{ak}| \sigma_{aa}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{ak}|)/S_{aa},$$

$$S_{aa} = \sum_{1 \leqslant j < k \leqslant N} \int |\mathbf{v}_{aj} - \mathbf{v}_{ak}| \sigma_{aa}(\Omega_{jk}, \mathbf{v}_{aj} - \mathbf{v}_{ak}) \, d\Omega_{jk}, \tag{45}$$

$$P_{abjk} = P_{ab}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{bk}|) = |\mathbf{v}_{aj} - \mathbf{v}_{bk}| \sigma_{ab}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{bk}|)/S_{ab},$$

$$S_{ab} = \sum_{j=1}^{N} \sum_{k=1}^{M} \int |\mathbf{v}_{aj} - \mathbf{v}_{bk}| \sigma_{ab}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{bk}|) \, d\Omega_{jk}, \tag{46}$$

$$P_{bbjk} = P_{bb}(\Omega_{jk}, |\mathbf{v}_{bj} - \mathbf{v}_{bk}|) = |\mathbf{v}_{bj} - \mathbf{v}_{bk}| \sigma_{bb}(\Omega_{jk}, |\mathbf{v}_{bj} - \mathbf{v}_{bk}|)/S_{bb},$$

$$S_{bb} = \sum_{1 \leqslant j < k \leqslant M} \int |\mathbf{v}_{bj} - \mathbf{v}_{bk}| \sigma_{bb}(\Omega_{jk}, |\mathbf{v}_{bj} - \mathbf{v}_{bk}|) \, d\Omega_{jk}. \tag{47}$$

The probability distributions P_{aajk}, P_{abjk}, and P_{bbjk} are functions of discrete variables j, k and continuous variables θ, ε. The dependence on θ, ε is because of the dependence of the distributions on Ω_{jk}.

Define operators O_{aa}, O_{ab} and O_{bb} by

$$O_{aa}P_0(t, V) = \sum_{1 \leqslant j < k \leqslant N} \int P_{aajk}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{ak}|) \times$$

$$P_0(t, V'_{ajk}) \, d\Omega_{jk}, \tag{48}$$

$$O_{ab}P_0(t, V) = \sum_{j=1}^{N} \sum_{k=1}^{M} \int P_{abjk}(\Omega_{jk}, |\mathbf{v}_{aj} - \mathbf{v}_{bk}|) \times$$

$$P_0(t, V'_{abjk}) \, d\Omega_{jk}, \tag{49}$$

$$O_{bb}P_0(t, V) = \sum_{1 \leqslant j < k \leqslant M} \int P_{bbjk}(\Omega_{jk}, |\mathbf{v}_{bj} - \mathbf{v}_{bk}|) \times$$

$$P_0(t, V'_{bbjk}) \, d\Omega_{jk}. \tag{50}$$

These operators give the $(N + M)$-particle probability density function after one collision of the type a–a, a–b, and b–b. In terms of these operators (41) can be written in the compressed form

$$(\partial P_0/\partial t) = (B_{aa}O_{aa} + B_{ab}O_{ab} + B_{bb}O_{bb} - BI)P_0(t, v), \tag{51}$$

where $B = B_{aa} + B_{ab} + B_{bb}$, $B_{aa} = S_{aa}/\text{Vol}$, $B_{ab} = S_{ab}/\text{Vol}$, $B_{bb} = S_{bb}/\text{Vol}$, and I = identity operator. Notice that as collisions are allowed the set of velocity vectors V changes which in turn causes changes in S_{aa}, S_{ab} and S_{bb}. The variables

B_{aa}, B_{ab}, B_{bb} and B therefore change with time. For small values of time duration Δt, the variables B, B_{aa}, B_{ab} and B_{bb} can be treated as constants and we can write the formal solution of (51) as

$$P_0(t + \Delta t, V)$$
$$= \exp(-B\Delta t)\exp[\Delta t(B_{aa}O_{aa} + B_{ab}O_{ab} + B_{bb}O_{bb})]P_0(t, V). \quad (52)$$

The operators O_{aa} and O_{bb} do not commute with O_{ab} and consequently

$$\exp[\Delta t(B_{aa}O_{aa} + B_{ab}O_{ab} + B_{bb}O_{bb})]$$
$$\neq \exp(\Delta t B_{aa}O_{aa})\exp(\Delta t B_{ab}O_{ab})\exp(\Delta t B_{bb}O_{bb}).$$

It is therefore not possible to develop a simulation in which b–b collisions are performed first, a–b collisions next and a–a collisions last, or for that matter any fixed sequence of collisions of various types. Expanding the exponential in (52) we obtain

$$P_0(t + \Delta t, V) = \exp(-B\Delta t) \times$$
$$\sum_{r=0}^{\infty} [(\Delta t B_{aa}O_{aa} + \Delta t B_{ab}O_{ab} + \Delta t B_{bb}O_{bb})^r/r!]P_0(t, V).$$

It is now easy to construct a Monte Carlo estimator for $P_0(t + \Delta t, V)$. We first draw a Poissonly distributed random integer r with mean $B\Delta t$ and then draw r uniformly distributed random variables $Rf_1 \ldots Rf_r$ lying in the interval $[0, 1]$. We then construct an operator O according to the following procedure. Define

$$O = O_1 O_2 \ldots O_r, \quad (53)$$

where

$$O_k = O_{aa}, \text{ if } 0 < Rf_k < B_{aa}/B,$$
$$O_k = O_{ab}, \text{ if } B_{aa}/B < Rf_k < (B_{aa} + B_{ab})/B,$$
$$O_k = O_{bb}, \text{ if } (B_{aa} + B_{ab})/B < Rf_k < 1.$$

Evidently the expectation of O defined by (53) for fixed r is

$$E\{O\} = (B_{aa}O_{aa} + B_{ab}O_{ab} + B_{bb}O_{bb})^r/B^r$$

and hence $O_1 O_2 \ldots O_r P_0(t, V)$ is an unbiased Monte Carlo estimator for $P_0(t + \Delta t, V)$ in the limit of $\Delta t \to 0$.

Now if we have a sample at time t of $N + M$ velocity vectors, which is a realization from the ensemble with probability density $P_0(t, V)$ then a realization from the ensemble with probability density $P_0(t + \Delta t, V)$ can be easily constructed using the operator sequence (53). We just let O operate on V. The operator O is an ordered product of $O_1, \ldots O_r$ and each of these factors can be any one of the operators O_{aa}, O_{ab}, O_{bb}. Hence, it is enough for the purpose of letting O operate on V if we know how transformed samples $O_{aa}V$, $O_{ab}V$ can be obtained. The procedure for obtaining the transformed sample consists in drawing a pair j, k of molecules either of a–a type, a–b type, b–b type, and the azimuth ε and scattering angle θ are then sampled from the relevant distributions. A collision is then allowed between the molecules of the pair and precollision velocities replaced by the post-collision velocities using collision dynamics.

In operating $O_1, O_2, \ldots$ etc. on V the exact order of the various operators has to be preserved and a–a collisions, a–b collisions etc. cannot be performed in any way we please without introducing a bias in the estimator. No such ordering is present for monocomponent gases. The present Markoff model for a binary mixture can be easily extended to the mixture of several components.

6. Concluding remarks

A direct simulation Monte Carlo method based on the Kac-Prigogine master equation has been developed for the numerical simulation of the Boltzmann equation. This method requires the estimation of collision-rate per unit volume. The operation count required to determine the collision can be linearly related to the number of particles by resorting to sample mean Monte Carlo estimator. This fact has not been noticed by Nanbu (1986) in his critique of the method. A computationally efficient version of the present DSMC has been developed by employing a suitable sequence of convection and collision operators. Further, the DSMC has been extended to multicomponent mixtures of gases and it has been shown that it is necessary to perform the collisions in a certain sequence to obtain unbiased simulation.

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