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MONTE CARLO EVALUATION OF THE BOLTZMANN COLLISION INTEGRAL*

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Abstract

A Monte Carlo method of solving the fundamental equation of the kinetic theory of dilute gases has been developed and successfully applied to two problems, one involving translational relaxation of a spatially homogeneous gas and the other a plane steady shock of arbitrary strength (shock strength limited only by the fineness of the velocity space mesh). This is the first and only method capable of computing the molecular velocity distribution under conditions far from equilibrium.

The essence of the problem is evaluation of the non-linear five-dimensional collision integral. Straight forward numerical quadrature would require about a year on the fastest present day computers. The computation time is reduced to a practical value, of the order of an hour, by a statistical sampling technique closely resembling the real statistical collision phenomena in the gas.

Computations to date have been restricted to elastic sphere scattering of molecules without internal degrees of freedom. Differential scattering cross-sections other than elastic sphere can be accommodated in the computer program without complications or computing time penalty. Introduction of one or two internal molecular degrees of freedom will increase the complexity and computing time, but not to an impractical degree.

Several technical problems had to be solved in order to make the method work properly. The "fairness" of the random collision-selecting process had to be designed with care and verifie'

thoroughly. Furthermore, a tendency for the theoretically conserved quantities (number of molecules, momentum and energy) to change slightly because of interpolation and quadrature errors, had to be corrected to prevent its building up significantly over many time steps or iterations. In the case of the more difficult shock wave computation, a tendency for the shock front to creep out of the computational reference frame in the course of successive iterations had to be eliminated by choosing density rather than distance normal to the shock front as independent variable. Finally, a verifiably convergent iteration scheme had to be devised for successively improving an initial trial solution. All of these technical problems have been solved. The initial trial solution so far used has been the Mott-Smith approximation.

We exhibit for the translational relaxation problem a graph of the temporal behavior of the Boltzmann function for Mach numbers ranging from 0.5 to 6. For the shock wave problem we show, for Mach number 3.0, contour plots of the Mott-Smith velocity distribution function, and of the collision integral derived from it, together with other plots characterizing the Monte Carlo solution of the problem.

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1. Introduction

The basic equation in the kinetic theory of dilute gases is the Boltzmann equation. Analytical solution of this equation has only been possible for conditions near equilibrium and for a limited number of intermolecular potentials.

The principal obstacle in the way of solving the Boltzmann equation is the nonlinearity and complexity of the collision integral in it. Evaluation of the integral by direct numerical quadrature is too slow to be useful, even on the fastest computers. The senior author therefore devised in 1955 a Monte Carlo method[1] for the numerical evaluation of the integral on digital computers. The method can be applied to any velocity distribution function. We have programmed the method for elastic sphere molecules but extensions to other molecular forces are feasible whenever the differential cross-sections are known.

Since 1955, the authors have refined and carefully tested this method and have applied it to several problems in kinetic theory.* The present paper gives the first complete account of the method. We made careful studies of accuracy which are especially important for our work because of the complexity of the collision integral and the wide usefulness of a reliable means of evaluating it. All indications are that the Monte Carlo calculations are valid to within the expected

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*These studies were first described in nine CSL reports published in the years 1962-1966.

statistical fluctuations. Lack of space prohibits detailed description of the accuracy studies here.

One problem in kinetic theory to which we have applied our Monte Carlo method is that of the "pseudo-shock," a kind of translational relaxation of molecules.[2,3] Solution of the Boltzmann equation follows easily once the Monte Carlo method permits evaluation of the necessary collision integrals, and the solution is obtained with equal ease for conditions very near and very far from equilibrium.

In a second problem, that of shock structure, a more difficult iteration procedure is necessary to solve the Boltzmann equation. We have substantial numerical evidence of the convergence of the iteration process. Even apart from the convergence question, the Monte Carlo evaluation of the collision integral can yield new and fundamental information about shock structure. In particular it is now possible:[4] a) to test any velocity distribution function proposed as an approximate solution of the Boltzmann equation for a shock wave or other flow condition; and b) to check directly the various elaborate analytical calculations involved in moment methods.

The Monte Carlo methods of Haviland[5,6] and Bird[7,8] have also been used in kinetic theory problems. Neither method evaluates collision integrals, so neither method can yield detailed, accurate, and explicit solutions of the Boltzmann equation. Bird's method is, however, nicely complementary to ours in that, though less accurate, it is at present faster than ours and is therefore already useful in problems involving more than one independent variable.

2. Outline of the Method

In the Monte Carlo method the collision integral is first replaced by an integral over a finite region of velocity space. This or similar approximations must always be used in numerical evaluation of integrals over an infinite region. The finite region, of volume R, is taken large enough so that it includes most of the molecules. The average of the integrand over R and over all values of the line-of-centers vector $\bar{k}$ is then approximated by the average of a large and fair sample of N values of the integrand. A Monte Carlo estimate of the value of the collision integral (with random errors proportional to $N^{-1/2}$) is given by the product of this average value with the volume R. Note that the integrand is a function of eight independent variables derived from the three vectors, $\bar{v}$, $\bar{v}'$, and $\bar{k}$ that define a collision. Nordsieck's Monte Carlo method enforces a fairness of the sampling in the eight-dimensional space of these variables.

3. The Boltzmann Equation

The units we shall use are the values, denoted by the subscript 1, of various properties of a reference gas. Thus n_1, T_1 are the units of number density n and temperature t. The unit length of length $\ell_1 = 1/(2\pi n_1\sigma^2)$ = (mean free path)$_1/\sqrt{2}$. The unit of velocity $c_1 = \sqrt{(2\pi kT_1/m)}$ = (mean speed)$_1$ $\times$ $(\pi/2)$. The unit of time is therefore (mean free time)$_1$ $\times$ $(\sqrt{2}/\pi)$ and of the velocity distribution function is n_1/c_1^3. In these units the Boltzmann equation

may be written

$$\partial f/\partial\tau + v_x \partial f/\partial x = \hat{a} - \hat{b}f =$$

$$\int (FF' - ff') \left| \bar{k}\cdot\bar{v}_r \right| d\bar{v}' (d\bar{k}/4\pi). \qquad (1)$$

where $f = f(\bar{v},x,\tau)$ is the velocity distribution function, x is the distance variable, and τ is the time variable; the unit vector $\bar{k}$ gives the direction of the line of centers during a collision; $\bar{v}_r = \bar{v}' - \bar{v}$; and f,f',F,F' denote the four values of f corresponding to the four velocities, $\bar{v},\bar{v}',\bar{V},\bar{V}'$. Integration is over the whole 4π solid angle in order that the $\bar{k}$ integration limits may be independent of $\bar{v}$ and $\bar{v}'$. The notation $\hat{b}f$ reminds us that this second part of the collision integral is proportional to $f(\bar{v},x,\tau)$, a fact of importance in devising a stable method of integrating the differential equation for the case of the strong shock wave.

4. Geometrical and Numerical Assumptions

To develop a specific Monte Carlo algorithm that will yield estimates of the Boltzmann collision integral we must make a number of geometrical and numerical assumptions. Most of these may be easily modified as required in the future. First, as we restrict ourselves to flows possessing axial symmetry, we represent any velocity vector $\bar{v}$ by its cylindrical components $(v_x, v_\perp, \phi)$ in velocity space. Because of the axial symmetry the velocity distribution function will not depend upon ϕ. In the sampling, however, we must still treat a collision as a full three-dimensional phenomenon.

Convenience of computer programming of the Monte Carlo scheme requires that the region R in velocity space be spanned by a fixed set of velocity cells. We therefore transform $\bar{v}$ to a new variable $\bar{v}_m$ by introducing as adjustable parameters, a shift of the origin and a velocity scale factor K_1. For any given problem these parameters are fixed so that all but 0.1%, for example, of the molecules are within R. Because of the rapid (Gaussian) decrease of density with increase of velocity, quadrature error in the velocity space is quite insensitive to the fraction of molecules excluded from R so long as that fraction is small.

The quantization of the velocity space $\bar{v}_m$ in which we define fixed cells was designed to yield accuracy of the order of 1% in the Monte Carlo estimation of the two parts of the collision integral. (The values of the components of $\bar{v}_m$ and $\bar{k}_m$ that are used in the calculations are those corresponding to the centers of the cells in $\bar{v}_m$ space and $\bar{k}_m$ space.) We choose 226 cells in the two-dimensional $(v_x, v_\perp)$ space, as shown in Fig. 1, to cover the semicircular region $v_m \leq 24$ in such a way that the area of the 226 cells is different from the area of the semicircular region by less than 0.1%. In our calculations we are concerned with those functions a, bf, and f that depend only upon the two velocity components v_x and $v_\perp$, together with either the time or position variables. Therefore, tables of 226 values of each of these functions are stored in the computer for each value of the time or position variable. As examples of the graphical representation of such functions we show, in Fig. 2, isolines of the Mott-Smith approximate

velocity distribution and the associated collision integral within a strong shock wave. The v_x axis in the figures is perpendicular to the shock front.

The quantized values of the azimuthal angle ϕ are chosen to be odd multiples of $(90^\circ/32)$ so that the range of ϕ from 0 to 2π contains 64 cells. Sixteen values each of $\sin\phi$ and $\cos\phi$ are stored in fixed tables corresponding to the range 0 to $\pi/2$. The other quadrants are introduced in the Monte Carlo calculations by randomizing signs appropriately. The unit vector $\bar{k}$ is represented by 64 sets of values of the three direction cosines. The values are chosen in such a way as to divide the first octant of the unit sphere into 64 equal parts. These 192 values of the direction cosines appear in a fixed table in the computer.

Having defined the cells we shall use in $\bar{v}$ and $\bar{k}$ space, we can now define the sampling algorithm. A sequence of pseudo-random numbers each containing 37 bits is generated by a modified Juncosa[10] process. Bits in the same number and in the sequence are practically uncorrelated over the whole repeat cycle of 2^{37} numbers. From each random number we derive a random collision by using the bits as follows: 14 bits for the vector $\bar{v}$, 14 for the vector $\bar{v}'$, and 9 for the unit vector $\bar{k}$. Successive numbers in the sequence then lead to successive and independent collisions randomly chosen from the $2^{37} \cdot (226/256)^2 = 1.07 \times 10^{11}$ cells in the eight dimensional $(\bar{v},\bar{v}',\bar{k})$ space. A collision is rejected as "unsuccessful" if either $\bar{V}$ or $\bar{V}'$, computed from $(\bar{v},\bar{v}',\bar{k})$, lies outside the region $v_m \leq 24$.

The fraction of collisions thus rejected is 0.1583. The values of $(V_x, V_\perp, V_x', V_\perp')_m$ are, in effect, rounded to values corresponding to the nearest cell center in $(v_x, v_\perp)_m$ space.

5. Various Monte Carlo Estimates of the Collision Integral

5.1 <u>The Eight Basic Estimates</u>. Let us now consider four Monte Carlo approximations to each of the functions $\hat{a}v_{\perp m}$ and $\hat{b}fv_{\perp m}$. The eight approximating functions are:

$$\underset{\sim}{a} = J_1 \langle FF'\varkappa_1 \rangle^{av}_{\bar{v}} \qquad \underset{\sim}{b}f = J_1 \langle ff'\varkappa_1 \rangle^{av}_{\bar{v}}$$

$$\underset{\sim}{a}' = J_1 \langle FF'\varkappa_1 \rangle^{av}_{\bar{v}'} \qquad \underset{\sim}{b}'f' = J_1 \langle ff'\varkappa_1 \rangle^{av}_{\bar{v}'} \tag{2}$$

$$\underset{\sim}{A} = J_1 \langle ff'\varkappa_1 \rangle^{av}_{\bar{V}} \qquad \underset{\sim}{B}F = J_1 \langle FF'\varkappa_1 \rangle^{av}_{\bar{V}}$$

$$\underset{\sim}{A}' = J_1 \langle ff'\varkappa_1 \rangle^{av}_{\bar{V}'} \qquad \underset{\sim}{B}'F' = J_1 \langle FF'\varkappa_1 \rangle^{av}_{\bar{V}'}$$

In these equations

$$J_1 = (8\pi)\ 226(K_1)^{-4}; \quad \varkappa_1 = [v_\perp v_\perp' \,|\bar{k}\cdot(\bar{v}'-\bar{v})|\,]_m \tag{3}$$

where we are using the "machine units" defined above. The symbol below each average-value sign in Eq. 2 indicates which of the four velocities is held constant in averaging over a sample of collisions. Each of the functions $\underset{\sim}{a}, \underset{\sim}{a}', \underset{\sim}{A}, \underset{\sim}{A}'$ approaches the function $\hat{a}$, and each of the functions $\underset{\sim}{b}f$, $\underset{\sim}{b}'f'$, $\underset{\sim}{B}F$, $\underset{\sim}{B}'F'$ approaches the function $\hat{b}f$ as one decreases

by one means or another the errors of various kinds. For finite errors of each type, however, the four functions of each type are distinct.

We may expect that the statistical errors in the Monte Carlo method of evaluating $\hat{a}$ and $\hat{b}f$ will decrease in proportion to $N^{-1/2}$ where N is the sample size. We may expect that the quadrature error, corresponding to the finite size of the cells in $\bar{v}$ and $\bar{k}$ spaces will decrease as the volumes of the cells are decreased. Our program permits easy variation of the cell size for the velocity space. The error owing to the neglect of a few molecules with large velocities will decrease rapidly as K_1 is decreased.

5.2 <u>Linear Combinations of the Estimates</u>. An important characteristic of the Monte Carlo method is that all of the eight functions in Eq. 2 can be evaluated simultaneously and, indeed, in any useful linear combination. For example, let us look at the evaluation of $\underset{\sim}{a}$ which is found by forming a sum over the collision sample

$$\langle FF'\varkappa_1\rangle_{\bar{v}}^{av} = M_o^{-1} \sum_{\bar{v}} FF'\varkappa_1 \tag{4}$$

where $\bar{v}$ is held constant during the summation and M_o is equal to the number of increments or hits for each velocity cell during the sampling process. Each such sum is formed by fixed point arithmetic to permit unbiased rounding of the increments.

An increment $(FF'\varkappa_1/M_o)$ in the value of the sum is made, for each random sampled collision $(\bar{v},\bar{v}',\bar{k})\rightarrow(\bar{V},\bar{V}')$, to the velocity cell labelled by the velocity $\bar{v}$. In forming $\underset{\sim}{b}f$ or $\underset{\sim}{b}'f'$ we sum

$(ff'\varkappa_1/M_o)$ similarly, again making increments in the $\bar{v}$ or $\bar{v}'$ cell, respectively. In forming $\underset{\sim}{A}$, $\underset{\sim}{A}'$, $\underset{\sim}{BF}$, $\underset{\sim}{B}'F'$, we make use of the fact that each collision (for molecules exerting central forces) has an inverse; that is, if $(\bar{v},\bar{v}',\bar{k})\rightarrow(\bar{V},\bar{V}')$ is a collision, so also is $(\bar{V},\bar{V}',-\bar{k})\rightarrow(v,v')$. Then to get $\underset{\sim}{A}$ we sum $(ff'\varkappa_1/M_o)$ over $(\bar{v},\bar{v}',\bar{k})$ while holding $\bar{V}$ constant, and similarly for $\underset{\sim}{A}'$, $\underset{\sim}{BF}$, and $\underset{\sim}{B}'F'$.

In the simultaneous calculation of the eight quantities in Eq. 2 we symmetrize the Monte Carlo summand by multiplication by $v_\perp$. This accomplishes two ends; it increases the speed of calculating the eight estimates and it makes possible achievement of good statistics for the cells near $v_\perp = 0$ because we can distribute hits uniformly over $(v_x,v_\perp)$ space and then later correct by the factor $2\pi v_\perp'$ to effect uniform a priori probability of collision over three dimensional velocity space.

The eight functions defined in Eq. 2 are basic to all considerations of Nordsieck's Monte Carlo method. In the calculations discussed in this paper, and in our study of accuracy, we considered in particular three linear combinations of these basic Monte Carlo functions. Two of these are

$$a_u = 1/2(\underset{\sim}{a} + \underset{\sim}{a}'), \tag{5}$$

$$a = 1/2[a_u(v_x,v_\perp) + a_u(-v_x,v_\perp)], \tag{6}$$

with similar equations for A_u, $(bf)_u$, ... , BF. Eq. 5 expresses an average over the two incoming (or two outgoing) molecules. Eq. 6 expresses an average of a Monte Carlo estimate of a function and of the

"reflected" estimate. In Nordsieck's Monte Carlo method the samples of $\bar{v}$ and of $\bar{v}'$ are each distributed uniformly and independently over the $(v_x, v_\perp)_m$ space ($v_m \leq 24$). In our study of hits per cell we then needed to consider only a_u, and not $\underset{\sim}{a}$ and $\underset{\sim}{a}'$ separately.

The other linear combination used is

$$a_{AN} = 1/2(a + A)$$

with a similar equation for $(bf)_{AN}$. This is an average of the Monte Carlo functions for the direct and inverse collisions which takes advantage of the uniformity of sampling in $\bar{v}$ and $\bar{V}$ spaces.

Each of the linear combinations that has been defined is relevant to the Monte Carlo method because the corresponding summands <u>in each case</u> can be computed from the two basic functions $(ff'\varkappa_1)$ and $(FF'\varkappa_1)$ with almost no additional arithmetic. <u>Therefore, the size of a Monte Carlo sample can be increased, in effect, by these exchange operations between primed and unprimed molecules, between incoming and outgoing molecules, and between a collision and its reflection</u>.

5.3 <u>Corrections that Force Conservation</u>. The starting point in deriving these corrections is the observation that accurate solutions of the Boltzmann equation must satisfy conservation equations characteristic of the problem at hand. We therefore compute the smallest corrections of the values of the 226 values of the collision integral, in a least-squares sense, that are consistent with enforcing conservation.

Why is this correction method appropriate? Any numerical quadrature method of evaluating the collision integral produces non-zero quadrature errors. There will consequently be a bias in the computed values of the two parts of the collision integral. (The neglect of a few molecules with large speeds will cause a somewhat smaller bias.) Solutions of the Boltzmann equation both for the pseudo-shock and the shock wave require repeated evaluation of the collision integral, so that uncorrected bias tends to build up unacceptable trends in the computed solutions. If, as in the case of our Monte Carlo method, the bias is not large, then the least square adjustment that we have described will produce values of the collision integral which satisfy the conservation equations and prevent, to a large extent, the drift or trend in the calculations.

6. The Computer Program

As noted above, our program at present assumes elastic sphere molecules and axial symmetry of velocity distributions. The first restriction is easily removable. The program can be modified to remove the second restriction. However, the present program without modification is directly applicable to the pseudo-shock, the shock wave and all similar problems involving only one space or time variable.

The Monte Carlo part of the program contains about 900 words (order-pairs, constants, and fixed tables). The complete program contains about 8,000 words which includes the Monte Carlo part of the

program, integration and moment programs, and many useful auxiliary programs. As noted earlier, the number of cells in the eight dimensional $(\bar{v},\bar{v}',\bar{k})$ space that is sampled is more than 10^{11}. (A direct simple, numerical quadrature of comparable accuracy would require $\sim 2 \times 10^9$ cells in a seven dimensional space.) The program computes 226 values (in parallel) of each of the functions a_{AN} and $(bf)_{AN}$, according to the Nordsieck prescription, in three minutes on the CDC 1604 with statistical fluctuations of 8%.

In any accurate method of solution of the Boltzmann equation it is necessary to add efficient methods of monitoring and judging the large volume of numerical data produced. Our calculations generally produce 226 values of each of the functions f, a, and bf for each iteration in the shock wave problem or each step in time in a relaxation problem like the pseudo-shock.

We have two monitoring devices for following this large output of data.* One monitoring device is the calculation and output of many moments of f, a, or (a-bf). Our numerical integrations in velocity space are good to much better than 1%, except for high order moments or sharply peaked integrands. We output 11 independent moments of the velocity distribution function f (including the two or three moments which should be conserved, the density, the Boltzmann function,

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*It must be remembered that in developing a method of solving a difficult equation like the Boltzmann equation it is necessary to make many more trials and test calculations than are needed for the final production run.

and its flux). We also output nine moments of a and of (a-bf), some of which, by conservation, should be zero, or, by the Boltzmann theorem, should be negative.

As a second monitoring device we output characters denoting ranges of values of each of the velocity dependent functions f, a, and bf. Approximate isolines may easily be derived from these characters and permit immediate and vivid visualization of the nature of the functions and their changes from one physical or calculational situation to another. The spacing of the isolines can be set at any appropriate level by changing the table of the reference function values that correspond to the characters output. Examples of accurate isolines, derived by such a procedure, are shown in Fig. 2.

7. Behavior of Solutions of the Boltzmann Equation

We have been particularly interested in using the Monte Carlo evaluation of the Boltzmann collision integral in calculating a translational relaxation process (the "pseudo-shock") and in trying to solve the Boltzmann equation for a shock wave. From each of these problems we have derived considerable, though indirect, support for the validity and reliability of the Monte Carlo method. In both problems we take, as absolute requirements on the validity of the method, that the appropriate conservation equations be satisfied and that the appropriate Boltzmann function decrease monotonically. Such requirements must clearly be made on physical grounds and are especially important in the absence of methods other than Monte Carlo of solving the Boltzmann equation for these problems.

Using the least square adjustments of the collision integrals we solved the pseudo-shock problem[3] and demonstrated the accuracy, stability, and convergence of the solution process, these characteristics being dependent upon the reliability of the Monte Carlo evaluation of the collision integral Fig. 3 illustrates several of the favorable characteristics of our Monte Carlo solution for this pseudo-shock. The Boltzmann function decreases monotonically, for each value of the Mach number M, and Monte Carlo fluctuations have negligible effect until late in the relaxation process. Even for the rather small samples used (10,000 collisions for each forward step in time) we were able to calculate the slope of each of the curves in Fig. 3 and show that there was no significant difference between the slopes.

It has been our objective since 1958 to solve the Boltzmann equation for shock waves using our Monte Carlo method. It has been apparent for several years that it is the convergence and stability of our iterative method of solution of the Boltzmann differential equation, rather than the difficulty in evaluating the collision integral in it, which has been impeding our progress toward solution of this problem. We have recently been using the correction method which forces the conservation equations to hold and have begun obtaining stable and convergent results in treating the internal structure of shock waves.

Let us illustrate these remarks with data for a shock wave that is described by the values of $f(\bar{v},x)$ and of $(a-bf)$ at nine positions within the shock. Fig. 4 illustrates the rapid convergence obtained for a typical Monte Carlo run for $M = 2.5$ with 2^{13} collisions

in each Monte Carlo sample used. The rms change, δf, of f from one iteration to the next, decreases by a factor of seven in the first three iterations. By the twelfth iteration the rms value of δf has decreased to 0.00013, although the largest value of f, near the cold boundary of the shock, is close to unity.

The data shown in Fig. 5 were obtained by averaging the values from four independent runs of twelve iterations each, with 2^{13} collisions in each Monte Carlo sample. It has been shown earlier[11] that the density profile n' is appropriately represented by a plot of the density gradient dn/dx against the reduced number density $\hat{n}=(n-n_1)/(n_2-n_1)$, as in Fig. 5. For a Mott-Smith shock the curve is a parabola. Even at this exploratory stage of our calculations, with samples of 2^{13}, there is some evidence that the shock is significantly asymmetrical. As expected from the Boltzmann theorem, the Boltzmann flux derived from the same four runs decreases monotonically through the shock.

Further indirect checks of the Monte Carlo evaluation of the collision integral will depend upon comparisons with accurate analytical solutions of the Boltzmann equation for very weak or very strong shock waves. The Navier-Stokes equations should describe accurately the internal structure of weak shock waves, and also the characteristics of shocks of any strength near their up- and down-stream boundaries.[11] Although it has been suggested[12] that the Mott-Smith model is asymptotically correct for strong shocks, it predicts the wrong value of the Prandtl number near the down-stream boundary.[11]

In view of the errors of the various methods we do not know at this time whether there is any value of the Mach number for which the errors of the methods would be small enough so that comparisons of the predicted details of shock structure would be meaningful. Efforts to make such meaningful comparisons are obviously important both to check further the solutions based on the Monte Carlo evaluation of the collision integral and to define the range of validity of the analytical theories.

8. Future Studies

We shall outline here briefly a variety of directions that may be taken in future research, now that there is a reliable method of evaluating the Boltzmann collision integral. These various researches may involve either modifications of our method or applications of it, and these aspects of course will often overlap.

Let us first consider modifications and studies of the Monte Carlo method which will be useful in <u>all</u> of the applications of this method that will be outlined below. These are: a) Many random collisions calculated once for all and prestored on tape or disc. Use of such prestored collisions should speed up the Monte Carlo part of the program by a factor of five on our present computer, b) Higher accuracy Monte Carlo calculations of the collision integral by using more cells in velocity space and larger samples of collisions, c) Modification of the program so that it will accept differential cross-sections corresponding to arbitrarily given intermolecular

potentials, d) Comparison of our Monte Carlo calculations of the Boltzmann collision integral for far-from-equilibrium conditions with accurate and direct numerical quadratures.

Now let us consider a whole class of kinetic theory problems for monatomic, single component gases that can be studied directly with our present Monte Carlo program and its auxiliary programs without major modification. These problems are those in which there is just one independent variable of position or time in the Boltzmann equation. Typical problems are those of translational relaxation (any such relaxation, not just that in the pseudo-shock); shock waves for a variety of Mach numbers and intermolecular potentials; and rarefied gases in which there are large gradients of temperature, velocity, or pressure (in other words, problems of heat and momentum transfer, of diffusion and thermal diffusion, and of gase subjected to strong perturbations by high-frequency sound or light).

Useful comparisons will be possible of Monte Carlo solutions of any of these problems with algebraic and substitute theories of shock structure and with appropriate approximate theories of other physical phenomena. The range of calculations we have just described could also be used as a basis for describing phenomena in non-equilibrium monatomic gases that contain a small fraction of other species. Understanding of a number of physical phenomena in these impure monatomic gases then could be aided by the results derived from the Monte Carlo calculations for monatomic gases, namely: rotational and vibrational excitation; the initiation of ionization

and of chemical reactions; electrostatic fields produced by a shock wave in a gas already slightly ionized; and the phenomena of shock precursors.

There are also interesting calculations, which hitherto have not been possible, which will require more extensive but not basic modifications of our program. One set of problems concerns phenomena in binary and multi-component mixtures of gases. Treatment of such problems requires some modifications of the algebra and bookkeeping in the Monte Carlo program to account for collisions between unlike species. A second set of problems which is closer to the interest of aerodynamicists, involves two independent variables of position or time. Problems of this type are: shock initiation; the classical problem of transient heat flow, which would provide a useful check calculation; and hypersonic flow and heat transfer in the stagnation point region and over slender bodies for Knudsen numbers less than one.

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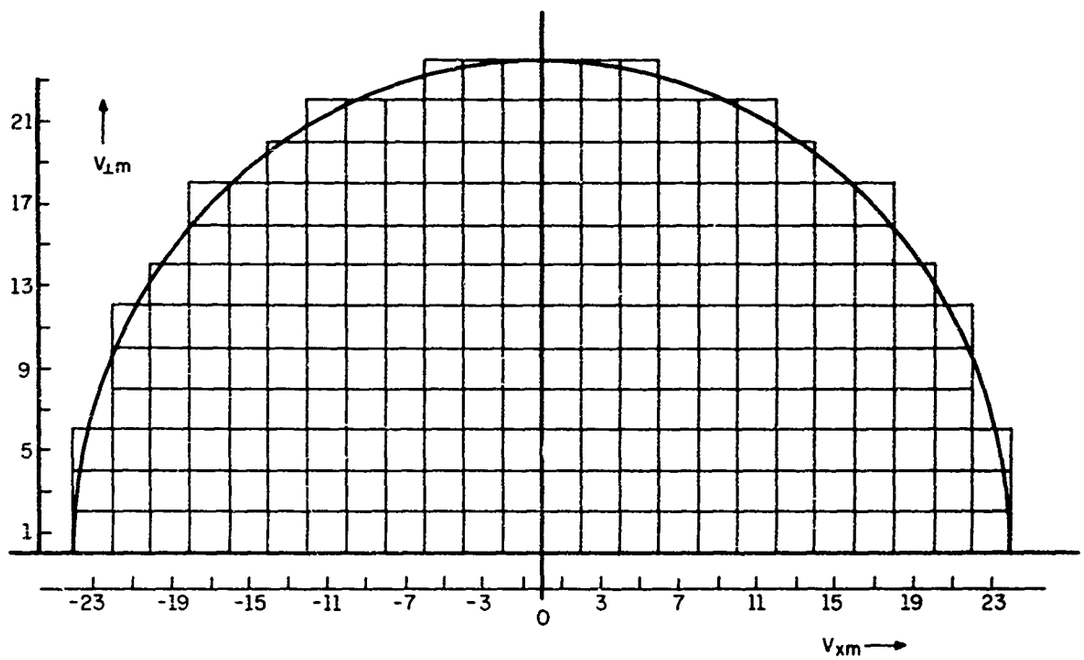

Fig. 1 Velocity Space.

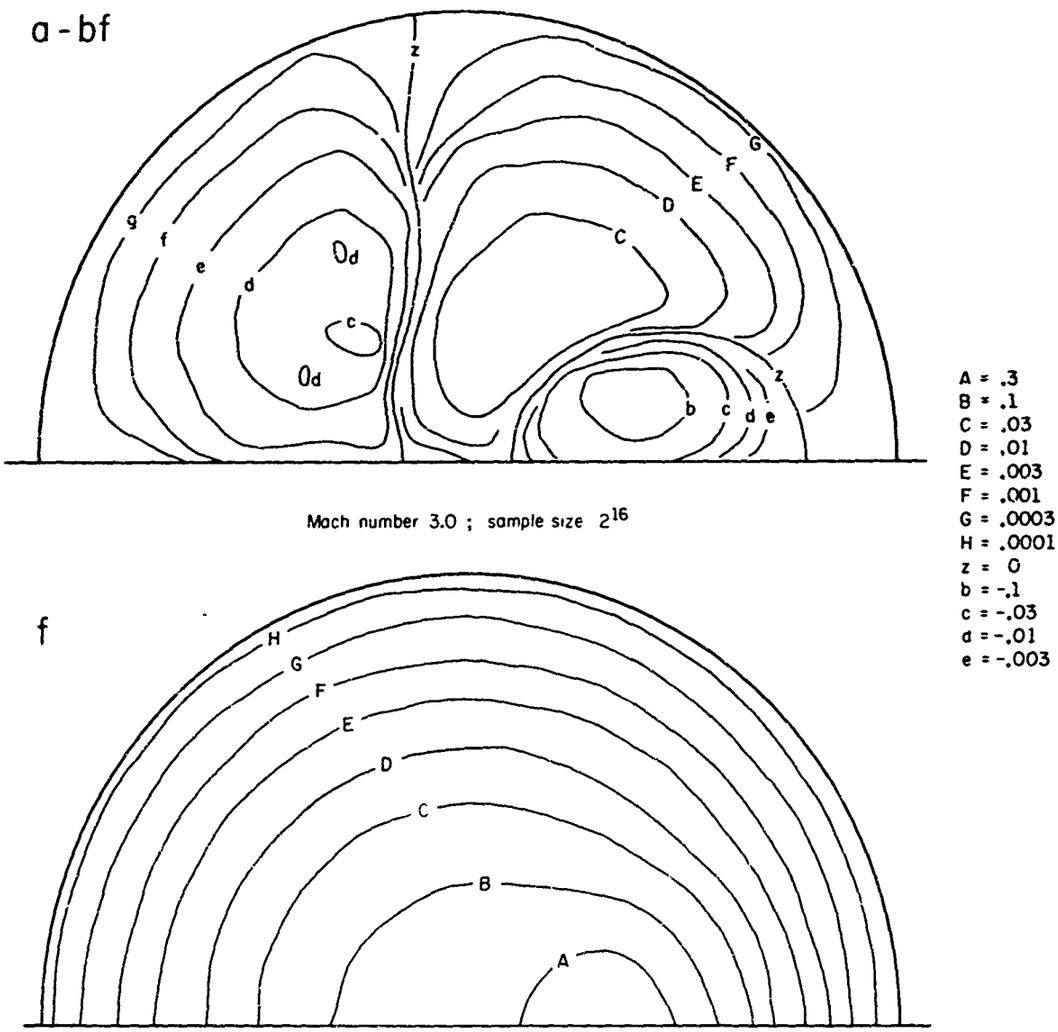

Fig. 2 Isolines of (a-bf) and f for the center of a Mott-Smith shock wave in a gas of elastic spheres. (Arbitrary units)

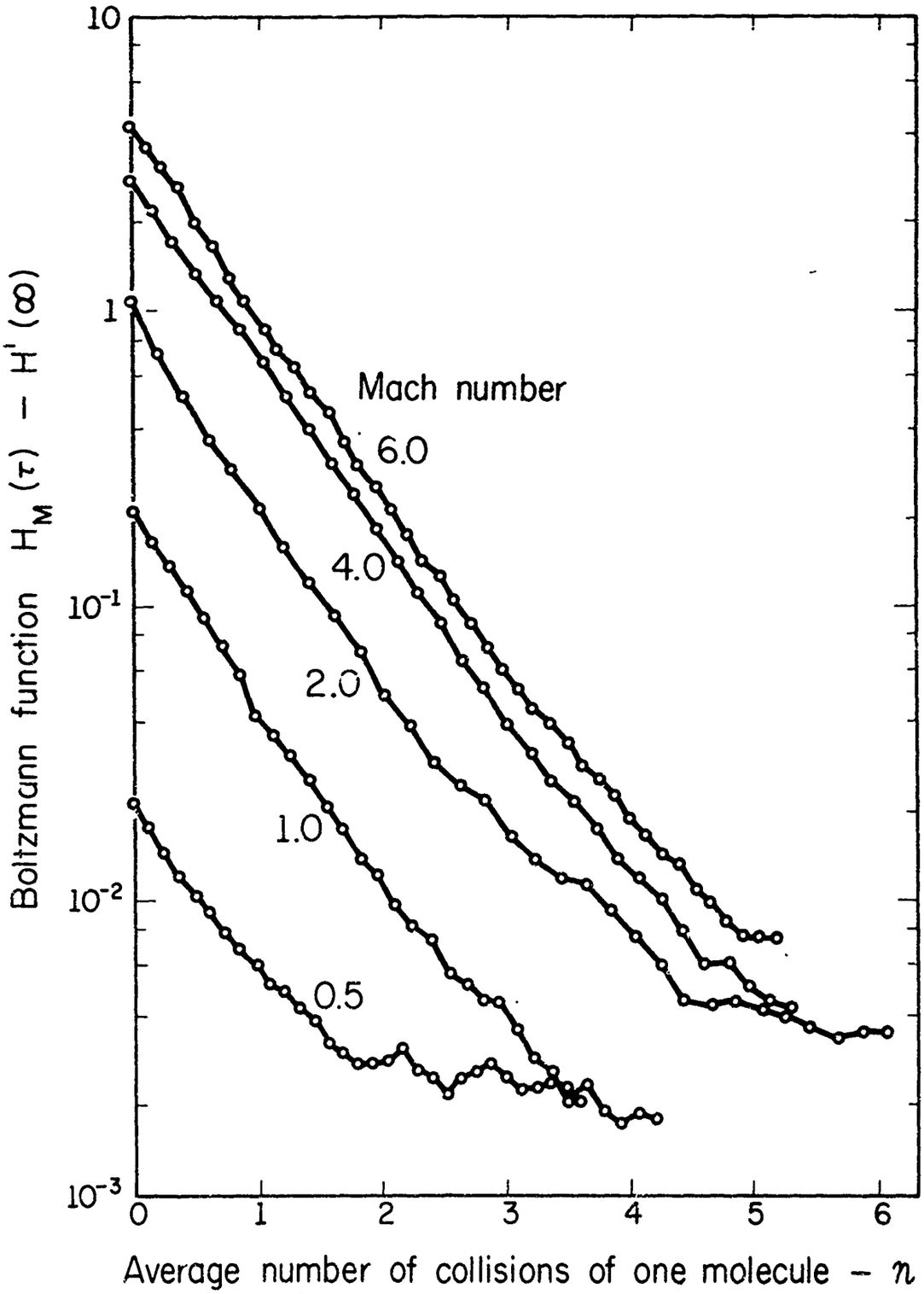

Fig. 3 Translational relaxation of the Boltzmann function. The ordinate is the excess of the value of the Boltzmann function, calculated by the Monte Carlo solution of the Boltzmann equation, over its predicted asymptotic value.

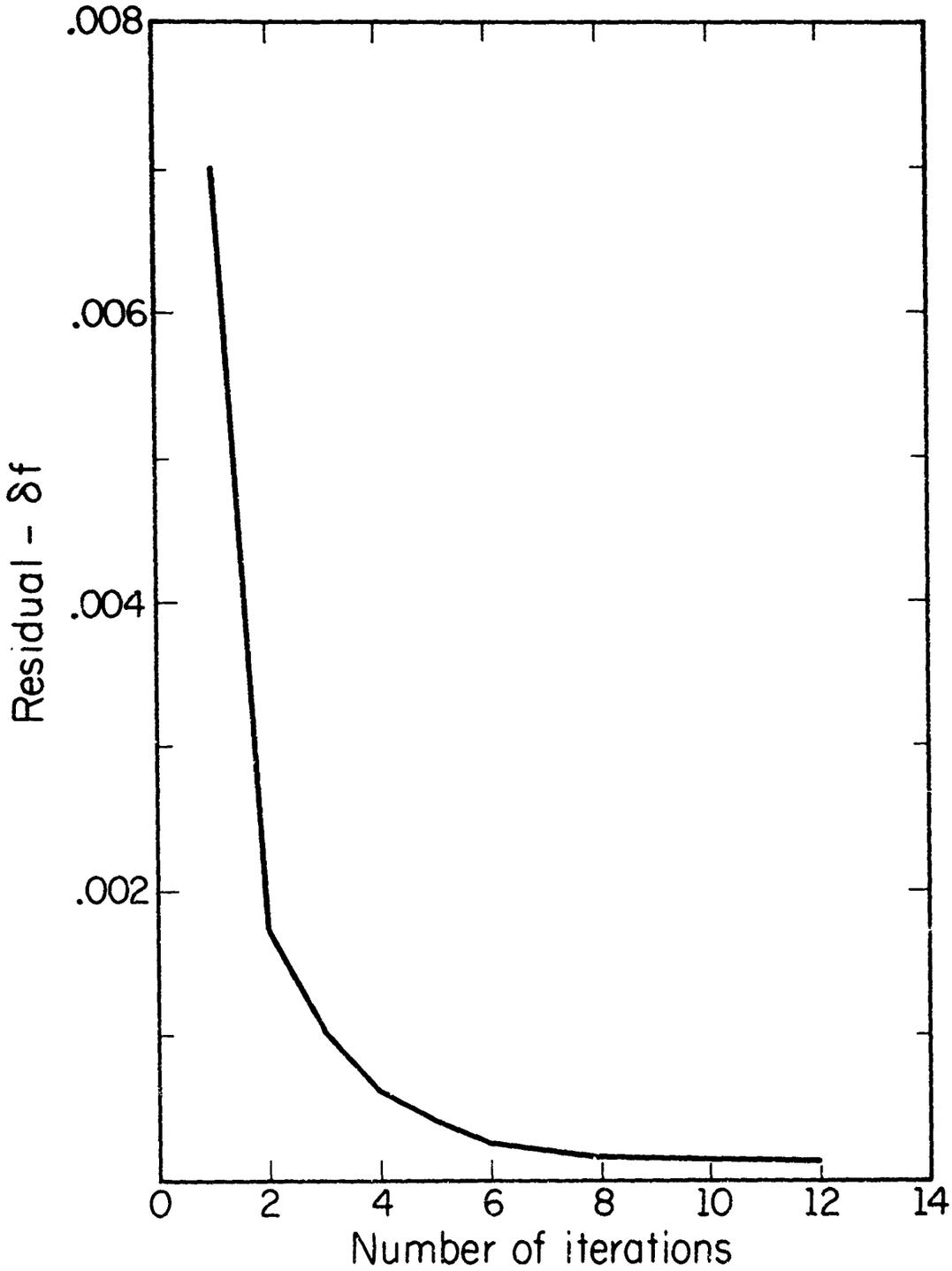

Fig. 4 Convergence of an iterative solution of the Boltzmann equation for a shock wave (Mach number 2.5).

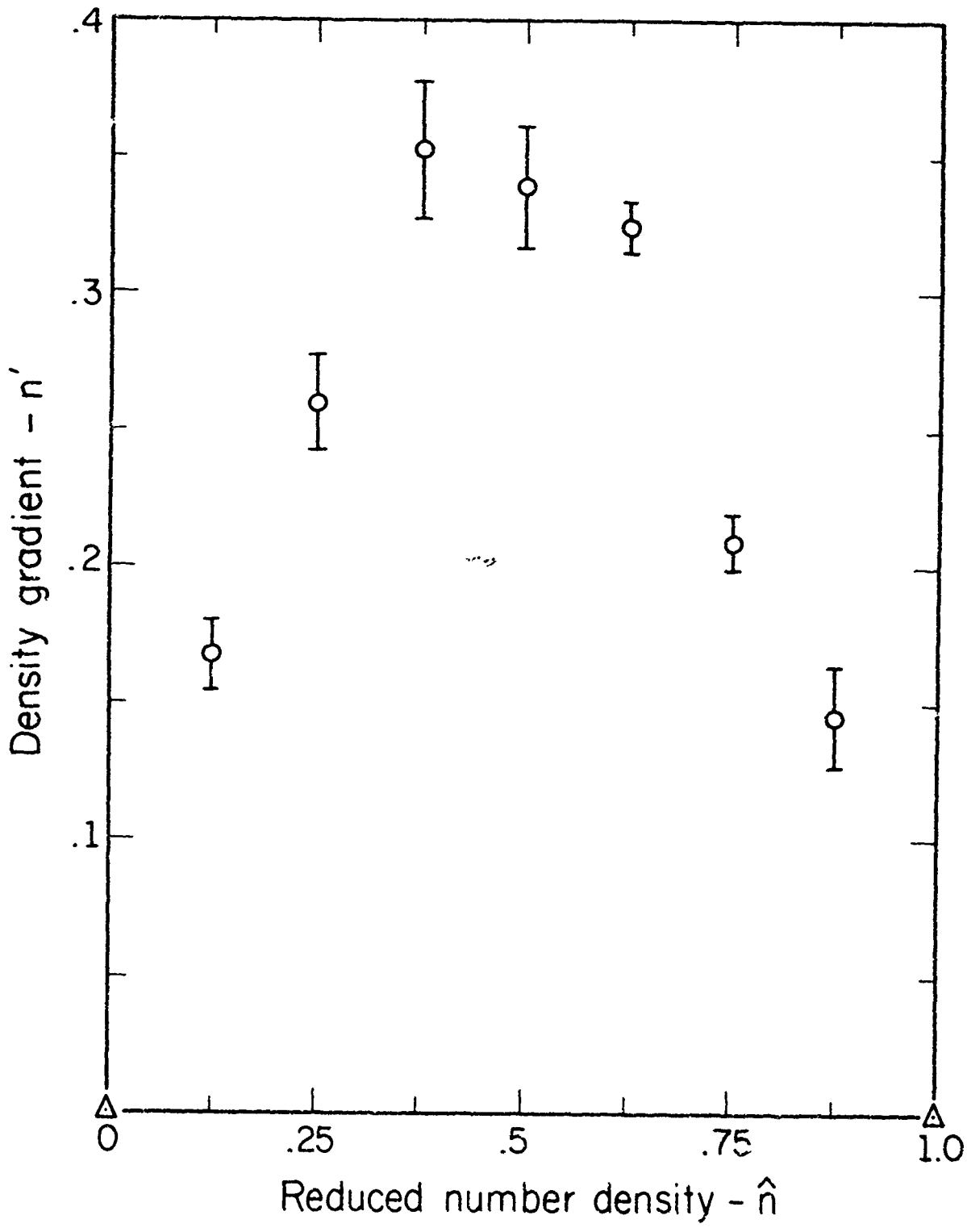

Fig. 5 The density gradient as a function of reduced number density in a shock wave (Mach number 2.5). The units are described in Section 3.

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13. ABSTRACT

A Monte Carlo method of solving the fundamental equation of the kinetic theory of dilute gases has been developed and successfully applied to two problems, one involving translational relaxation of a spatially homogeneous gas and the other a plane steady shock of arbitrary strength (shock strength limited only by the fineness of the velocity space mesh). This is the first and only method capable of computing the molecular velocity distribution under conditions far from equilibrium.

The essence of the problem is evaluation of the non-linear five-dimensional collision integral. Straight forward numerical quadrature would require about a year on the fastest present day computers. The computation time is reduced to a practical value, of the order of an hour, by a statistical sampling technique closely resembling the real statistical collision phenomena in the gas. (continued on next page)

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Abstract (continued)

Computations to date have been restricted to elastic sphere scattering of molecules without internal degrees of freedom. Differential scattering cross-sections other than elastic sphere can be accommodated in the computer program without complications or computing time penalty. Introduction of one or two internal molecular degrees of freedom will increase the complexity and computing time, but not to an impractical degree.

Several technical problems had to be solved in order to make the method work properly. The "fairness" of the random collision-selecting process had to be designed with care and verified thoroughly. Furthermore, a tendency for the theoretically conserved quantities (number of molecules, momentum and energy) to change slightly because of interpolation and quadrature errors, had to be corrected to prevent its building up significantly over many time steps or iterations. In the case of the more difficult shock wave computation, a tendency for the shock front to creep out of the computational reference frame in the course of successive iterations had to be eliminated by choosing density rather than distance normal to the shock front as independent variable. Finally, a verifiably convergent iteration scheme had to be devised for successively improving an initial trial solution. All of these technical problems have been solved. The initial trial solution so far used has been the Mott-Smith approximation.

We exhibit for the translational relaxation problem a graph of the temporal behavior of the Boltzmann function for Mach numbers ranging from 0.5 to 6. For the shock wave problem we show, for Mach number 3.0, contour plots of the Mott-Smith velocity distribution function, and of the collision integral derived from it, together with other plots characterizing the Monte Carlo solution of the problem.

Security Classification

KEY WORDS	LINK A ROLE	LINK A WT	LINK B ROLE	LINK B WT	LINK C ROLE	LINK C WT
Boltzmann equation						
collision integral						
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statistical sampling						
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