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On the Accuracy of Monte Carlo Solutions of the Nonlinear Boltzmann Equation

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ABSTRACT

Nordsieck's Monte Carlo method of evaluating the Boltzmann collision integral made possible, for the first time, solutions of the nonlinear Boltzmann equation for many kinetic-theory problems of interest. This paper summarizes an extensive series of numerical studies directed toward understanding and evaluating the various errors in these solutions. A generally useful technique permits estimation of the random part of the Monte Carlo error in any quantity derivable from the computed values of the velocity distribution function or from the two parts of the Boltzmann collision integral. Some of the systematic errors can be evaluated.

The Boltzmann equation has been solved by the Monte Carlo method on the CDC 1604 computer for three problems, the pseudoshock, the shock wave, and heat transfer in a rarefied gas. The errors in the velocity distribution function, in the collision integral, and in moments of each of these functions are discussed in the paper for the first and second problems. In the solution of the shock problem for a Mach number of 2.5, the random errors in the velocity distribution function and the collision integral amount to 2% or less, and random errors in moments of these functions range from 0.03 to 2.7%.

I. INTRODUCTION

At present there is only one method of solving the non-linear Boltzmann equation in kinetic theory, the Monte Carlo method of Nordsieck [1]. The method has been applied to several kinetic theory problems: to the pseudoshock [1], [2], to the shock wave [1], [3], and, in recent, unpublished research, to heat transfer in rarefied gases [4]. Analysis of the errors inherent in the method is an important part of applying it to these or other problems because an understanding of the errors is needed as a basis for designing Monte Carlo calculations of known

accuracy, for interpretation of the results of these calculations, and for comparison with other studies, both experimental and theoretical.

To solve the nonlinear Boltzmann equation for a given problem requires the calculation and interpretation of a large number of quantities. In the shock-wave problem, for any one Mach number, it is necessary to calculate about 2,000 values of each of three functions of position and velocity (the velocity distribution function and the two parts of the Boltzmann collision integral) and about 200 values of the moments of these functions. Error analysis requires even more computation; the values of the functions and moments must be recalculated for each combination of parameters relevant to the numerical method. A complete error analysis, based on such calculations, should make it possible to understand how the random and systematic errors in each of the many quantities are affected by the various parameters of the numerical method, in particular, by the Monte Carlo sample size, by the number of cells in each of several relevant spaces, and by the nature of the initial approximation used in iterative solution of the Boltzmann equation.

At present a study of these errors must rely primarily upon numerical methods. Purely analytical methods are not suitable for evaluating the errors of so many quantities and indeed are not possible until at least approximate solutions of the nonlinear Boltzmann equation have been obtained by numerical methods.

In our studies of the nonlinear Boltzmann equation, we have been collecting and analyzing data on errors since 1963. The present paper summarizes the analyses that have been described in Coordinated Science Laboratory reports and contains new analyses of "quasi-equilibria" and of the errors of moments of the velocity distribution function and of the collision integral. Our analysis of random errors is relatively complete: all random errors introduced because of our use of the Monte Carlo method (rather than some conventional quadrature method that is, of necessity, much slower) can be easily evaluated. As in any large numerical quadrature problem, it is difficult to evaluate systematic errors, but several types of systematic error are now well understood and are described in the paper.

In subsequent sections of the paper we shall consider the Monte Carlo method of evaluating the Boltzmann collision integral, errors in this method, and errors in the solution of two kinetic-theory problems described by the nonlinear Boltzmann equation, the pseudoshock and the strong shock wave. It is feasible, on a CDC 1604 computer, to get solutions of these problems with an accuracy of the order of 1 %.

II. The Boltzmann Equation and its Solution

The classical, low-density phenomena of kinetic theory are described by the molecular distribution function $f(x, t, \mathbf{v})$, which depends upon the single space

variable x, the time variable t, and the molecular velocity $\mathbf{v}$. The particle density n is given by

$$n(x, t) = \int f(x, t, \mathbf{v})\, d\mathbf{v}. \tag{1}$$

The velocity distribution function satisfies the nonlinear Boltzmann equation

$$v_x \frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} = \int (d\mathbf{k}/4\pi) \int d\mathbf{v}'(FF' - ff') \mid \mathbf{k} \cdot (\mathbf{v}' - \mathbf{v}) \mid = a - bf \tag{2}$$

and, for any particular problem, the boundary conditions peculiar to that problem. It is convenient to use the notation $(a - bf)$ for the so-called Boltzmann collision integral on the right-hand side of Eq. (2) to emphasize that the second term is proportional to f. The two terms $a = a(x, t, \mathbf{v})$ and $b = b(x, t, \mathbf{v})$ are positive, facts useful in the design of a method of solution of the equation. The two terms correspond to the effect of the collisions in increasing and decreasing, respectively, the number of molecules of velocity $\mathbf{v}$. The unit vector $\mathbf{k}$ in the integrand lies along the line of centers for a collision. The differential collision cross-section $\mid \mathbf{k} \cdot (\mathbf{v}' - \mathbf{v}) \mid$ is that for elastic sphere molecules, the case that we have treated in solving the nonlinear Boltzmann equation.

In Eqs. (1) and (2), and throughout the paper, the unit of x is $\lambda/\sqrt{2}$, the unit of velocity v is $\pi c/2$ and the unit of f is f_m where λ, c and f_m are, respectively, the values of the mean free path, the mean molecular speed and the maximum value of f in an appropriate reference gas. The units of all other quantities can be expressed in terms of the units of x, v, and f.

The only method of obtaining detailed and accurate solutions of the Boltzmann equation, Eq. (2), for conditions far from thermal equilibrium, is that of Nordsieck [1]. For any kinetic-theory problem the first step in this method is the calculation of values of each part of the collision integral by carefully designed, fair, Monte Carlo sampling of the integrand over the five-dimensional $(\mathbf{v}, \mathbf{k})$ space covered by the collision integral. The Monte Carlo method thus computes the rate of change of $f(x, t, \mathbf{v})$ produced by a large set of randomly chosen molecular collisions in the five-dimensional space. For the problems of interest here f, a, and $a - bf$ are functions of v_x and $v_\perp$ only. Each part, a and bf, of the collision integral is therefore evaluated for each x and t and for each of 226 values of a molecular velocity vector $\mathbf{v} = (v_x, v_\perp)$ where v_x and $v_\perp$ are cylindrical coordinates in velocity space. The end points of the 226 velocity vectors lie at the centers of 226 cells or bins in the two-dimensional velocity space shown in Fig. 1.

The 226 values of a and of bf are computed (in parallel) by the present program in 2.5 minutes on the CDC 1604 computer with statistical fluctuations in $(a - bf)$ of 2.6% for a sample of 3.2×10^4 collisions. In many applications of the Monte Carlo method we have made least square corrections of these Monte Carlo

values of a and of bf in order that conservation equations could be satisfied exactly. These corrections might also be useful for methods of evaluation of the collision integral other than the Monte Carlo method, for no numerical quadrature method is wholly free of systematic error.

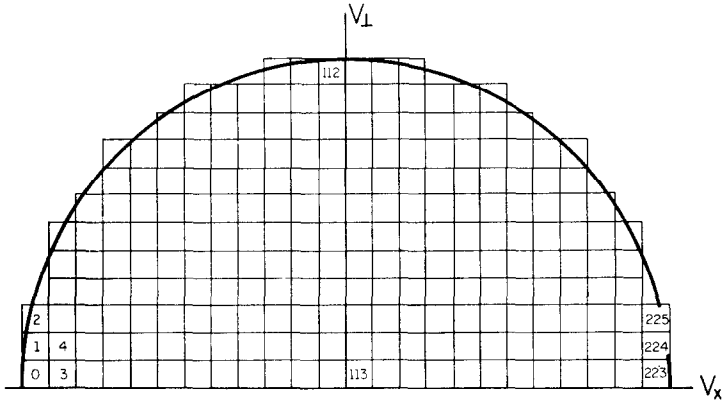

FIG. 1. Bins in velocity space. The velocity distribution function f and the collision integral $(a - bf)$ are functions of the cylindrical coordinates v_x and $v_\perp$ in the velocity space.

The other steps in solving the Boltzmann equation are peculiar to the particular kinetic-theory problem being studied. If the properties of the gas are independent of position as in problems of translational relaxation (see Section IV), then the velocity distribution function $f(t, \mathbf{v})$ for discrete times $t = t_1, t_2 \ldots$ is obtained by forward numerical integration in time of the values of the collision integral obtained by the Monte Carlo method. If the properties of the gas are independent of time, as in the case of the steady shock wave (see Section V), then the velocity distribution function $f(x, \mathbf{v})$ is obtained for discrete positions $x = x_1, x_2 \ldots$ by an appropriately designed, stable iteration process. In each type of problem we approximate a solution of the Boltzmann *differential* equation by solving stochastic, nonlinear, Boltzmann *difference* equations whose coefficients depend on the Monte Carlo collision samples. In each type of problem, we compute moments of f, a, and bf by fourth order numerical quadrature.

For any kinetic theory problem it is necessary to evaluate the errors both in the Monte Carlo step of the solution of the Boltzmann equation and in the later steps involving numerical integration with respect to x, t, or $\mathbf{v}$. Random errors, generated by the Monte Carlo sampling, are propagated throughout the calculations and appear in the calculated values of f, a, bf and their moments. These random errors are easy to evaluate, as will be shown later. Systematic errors, generated in

the Monte Carlo (or any other) method of evaluation of a and bf and in the other steps of the numerical method, can be evaluated only incompletely at present.

III. Errors Related to the Monte Carlo Evaluation of the Collision Integral

A. *Studies of "Hits/Bin"*

Nordsieck's Monte Carlo evaluation [1] of the Boltzmann collision integral was carefully designed to yield fair sampling over the space of the Boltzmann integrand, within the limitations imposed by the finite number of velocity bins chosen, namely 226, and by the finite number of intervals used for each of the various relevant angle variables. One series of tests, made in 1963–65, evaluated the fairness of the sampling under these limitations by counting the number of collisions (i.e., the number of "hits/bin") that affects each of the 226 velocity bins in $(v_x, v_\perp)$ space. For these tests the integrand of the collision integral was replaced by a constant so that the number of "hits/bin" generated by the program would be uniform over velocity space if the sampling was fair. The distribution was found to be uniform (within the 2.6% fluctuations to be expected for the 226 bins and the size of the samples used) for molecules both entering and leaving the collisions and throughout the important part of the velocity space, that is, for molecular speeds up to 96% of the maximum speed allowed in the sampling. The distribution is not uniform (i.e., it falls off by as much as 40%) in the outer 4% of this maximum molecular speed because the efficiency and fairness of the Monte Carlo sampling [1] depends upon rejecting those few random collisions that produce molecular speeds larger than the maximum speed allowed in the calculations. This nonuniformity produces only unimportant errors in the values of the collision integral computed by the Monte Carlo method (see Sect. 3.2) because the rejected collisions involve only those molecules whose values of f or of a and bf are very small.

B. *Accuracy of Monte Carlo Estimates of a and bf*

1. *Applicability of Error Studies to Gases Near to and Far from Thermal Equilibrium.* For a gas *in* or very *near* thermal equilibrium, as near the boundaries of a strong shock wave, the two parts, a and bf, of the collision integral are equal and can be computed analytically, making possible direct determination of the accuracy of the Monte Carlo estimates of a and bf. The results of such error studies, made in 1963–65, will be discussed in this section. Both systematic and random errors will be described. Using the method of Section III.D, which was

developed after 1965, we could also calculate now the *random* errors in *a*, *bf* and *a-bf* for each velocity bin and for each station in the *interior* of a shock of any strength.

The error studies described in this section apply *directly* only to Monte Carlo estimates for a gas near thermal equilibrium. For a gas *far* from thermal equilibrium, as in the interior of a strong shock wave, the values of the two parts of the collision integral, *a* and *bf*, can be computed at present only by the Monte Carlo method. Although there are thus no independent calculations which may be used to test the Monte Carlo estimates directly, it is, nevertheless, possible to make a partial assessment of the accuracy of the Monte Carlo estimates of *a* and of *bf* because the variations of the functions $f(x, \mathbf{v})$ over velocity space are roughly similar in shape for the different positions in the interior of a shock wave. The *fractional* errors (random and systematic) in the Monte Carlo calculations of *a* and *bf* from values of $f(x, \mathbf{v})$ will then be approximately constant across the shock. In the interior of a strong shock, *a-bf* is comparable in size to *a* or *bf*, and we would expect the fractional errors of *a-bf* in the interior to be not much larger than the fractional errors of *a* or of *bf* there. For a weak shock or near the boundaries of a strong shock, where $|\, a\text{-}bf \,| \ll a$, our qualitative argument gives us no information about the fractional errors in *a-bf*. We note, however, that Nordsieck's Monte Carlo evaluation of *a-bf* to give smaller absolute errors for a gas near equilibrium than for one far from equilibrium.

It should be emphasized that knowledge of both the *absolute* and the *fractional* errors in such basic quantities as *f*, *a*, and *a-bf* is a prerequisite to thorough understanding of the reliability of Monte Carlo or any other solution of the shock problem. The accuracy of calculation of any one derived property, like one of the moments to be discussed in later sections, may depend more strongly, however, on the fractional errors in the basic quantities than on the absolute errors, or vice versa.

2. *Error Studies for Gases in Thermal Equilibrium.* In the 1963–65 studies we used Maxwell–Boltzmann equilibrium values of *f*, for the hot and cold sides of a shock wave for a Mach number of 2.5, and made computer runs for two sizes of collision sample, namely, a sample of 4.4×10^4 collisions for which random errors dominate, and a sample of 7.0×10^5 collisions for which systematic errors dominate. From this set of runs it was possible to estimate the random and systematic errors in the Monte Carlo evaluation in each of the two parts of the collision integral and also to judge the effects of rejection of collisions, of the sharp peak in the velocity distribution function on the cold side of the shock, and of using various linear combinations of the Monte Carlo estimates of *a* and of *bf*.

The most important results were obtained by analyzing the random and systematic errors of three ratios, $(a/bf)_{AN}$, a_{AN}/a_n, and $(bf)_{AN}/a_n$. The correct value

of each ratio is of course one. The subscript AN in these ratios refers to the best linear combination [1] of Monte Carlo estimates of a or bf. The subscript n refers to analytical values of a, which were calculated by the program with an accuracy of better than 0.2 % except for a few bins.

The variation of these ratios over velocity space may be illustrated by plotting a contour map for one of them, $(a/bf)_{AN}$, as in Fig. 2. The contours are shown

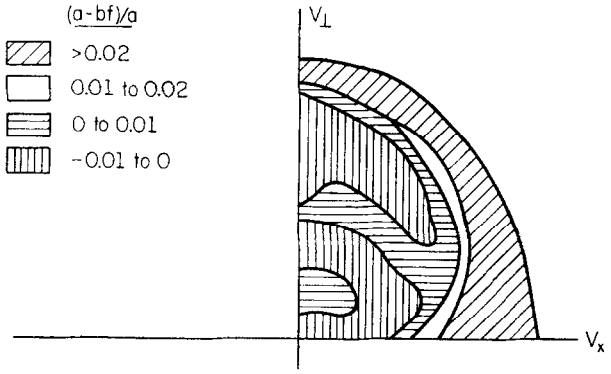

FIG. 2. Fractional systematic errors $(a - bf)/a$ in the Monte Carlo calculation of the collision integral for a gas in thermal equilibrium on the hot side of a shock wave. The Monte Carlo sample contained 5.2×10^6 collisions. Least-square corrections of $(a - bf)$ were made.

only for the right half of velocity space because of their symmetry with respect to the $v_\perp$ axis. Data for this figure was obtained in a recent run made with a large enough sample (5.2×10^5 collisions) so that the random errors are again smaller than the systematic errors. In this run the values of $(a\text{-}bf)$ were corrected by the least-square procedure mentioned in Sect. 2, which reduces the systematic errors by about a factor of two. The least-square correction was not used in the 1963–65 runs which are the source of data for the remainder of this section,

The systematic errors in $(a/bf)_{AN}$ shown in Fig. 2 lie in the range -1 to $+1$ % except in the outer part of the velocity space and in a few small, isolated regions not shown in the figure. The details of the variation over velocity space of these systematic errors are characteristic of the numerical quadrature formulas implied by the Monte Carlo method of evaluating a and bf.

Further analysis of the errors may be divided into three parts. In the first part, the means and variances of the three ratios are analyzed for the inner 85 % of the velocity space. In the second part, the errors in the outer 15 % of the velocity space, which are affected by the rejection of collisions (Section III.A), are analyzed. In the third part, errors of eight other ratios are studied.

The first part of the analysis requires separation of the random and systematic

errors in the inner 85% of the velocity space. We therefore assumed that the systematic error is not a function of sample size; that the Monte Carlo fluctuations (or random errors) are proportional to $N^{-1/2}$, where N is the sample size, but do not depend strongly on v (this was verified in later calculations); and that the random and systematic errors are independent of one another. On the basis of these assumptions it was possible to resolve the random and systematic errors with the results shown in Table I.

TABLE I

RANDOM AND SYSTEMATIC ERRORS IN MONTE CARLO ESTIMATES OF THE COLLISION INTEGRAL[a,b]

	Mean	Standard Deviations systematic	random
$(a/bf)_{AN}$	1.012	0.0182	0.026
a_{AN}/a_n	1.026	0.0091	0.089
$(bf)_{AN}/a_n$	1.017	0.0050	0.093

[a] The subscripts AN and n refer, respectively, to the best Monte Carlo estimate and to the analytical calculations of a or bf for the hot side of the shock wave. Least squares corrections (Sec. V.A. 5.1) of the Monte Carlo estimates were not made.

[b] The Monte Carlo sample contained 3.2×10^4 collisions.

The means of each of the three ratios differ from unity by less than 2.7%, and the (systematic) standard deviations S_s of the ratios are less than 1.9%. This level of *systematic* error of about 2% is what was intended in Nordsieck's design of his Monte Carlo method. Correlation of the Monte Carlo errors in a_{AN} and $(bf)_{AN}$ reduces the deviation from unity of the mean value of $(a/bf)_{AN}$ but does not reduce the value of the (systematic) standard deviation. The least-square correction, as noted earlier, reduces the systematic errors in $(a/bf)_{AN}$, shown in Table I, by a factor of two and reduces substantially the systematic errors in the values of moments of $(a\text{-}bf)$.

The first part of the analysis also yielded comparisons of these *systematic* errors for the cold and hot sides of the shock. The sharp peak of the equilibrium velocity distribution on the cold side produces larger quadrature errors in a and in bf than on the hot side. Thus the deviation from unity of the mean value of $(a/bf)_{AN}$ is larger by a factor of three for the cold side than for the hot side, about what would be expected from the smaller number of velocity bins effective in the Monte Carlo evaluation of the collision integral on the cold side. The value of S_s is larger on the cold side by a factor of four.

Nordsieck designed the Monte Carlo evaluation of the collision integral to

produce a positive correlation between the *random* errors of a and bf. In Table I the values of standard deviation S_r representing the random errors, for a sample of 3.2×10^4 collisions, show clearly the resulting cancellation of errors. If there were no cancellation, the random errors in a_{AN}/a_n and $(bf)_{AN}/a_n$ would yield a value of $0.129 = (0.089^2 + 0.093^2)^{1/2}$ for the standard deviation of $(a/bf)_{AN}$, a value five times the value of 0.026 shown in Table I. We note that the random and systematic errors of the ratio $(a/bf)_{AN}$ are comparable for a sample of 3.2×10^4 collisions. It is feasible to make Monte Carlo calculations on the CDC 1604 for a sample of this size. (See Section V.A, for example.)

The second part of the analysis of the 1963–65 data was concerned with the outer 15% of the velocity space on the hot side of the shock. In this region the rejection of collisions produces on the average a systematic error of -7% in $(a/bf)_{AN}$, a much smaller error than the 40% reduction in hits/bin in the outer part of this region. (See Section III.A.) On the cold side of the shock rejection of collisions causes negligible errors in $(a/bf)_{AN}$.

In the third part of the analysis we studied errors in Monte Carlo values of eight other ratios in addition to the three discussed above. We shall quote just two results of this analysis here. First, the pure quadrature error (in the calculation of bf, for example) does not include interpolation errors caused by sampling collisions on a discrete velocity space and amounts to 0.4% on the hot isde of the shock where the velocity space is well-filled. Second, the various interpolation errors appear to be larger by factors of from two to seven than the pure quadrature error. The analysis of these different sources of systematic error has led to an improved Monte Carlo method that will be described elsewhere.

C. *Quasi-Equilibria.*

Another test of the Monte Carlo method of evaluation of the nonlinear Boltzmann collision integral is afforded by the study, made early in 1967, of certain quasi-equilibria. In this study the translational relaxation is calculated, for a gas which is initially in thermal equilibrium, by a version of our Monte Carlo method in which a *fixed, finite* collision sample is used. A stable *quasi*-equilibrium is reached (within the equivalent of a few collisions per molecule) which exhibits the pecularities characteristic of the fixed, finite sample and other effects related to our implementation of the Monte Carlo method. For this test the Monte Carlo calculation of the collision integral included the least-square correction which forces conservation of density and energy. (See Sections IV and V for discussions of other applications of this technique.)

Quasi-equilibria were studied for four independent samples for each of three different sizes of collision sample. The comparison function used was the ratio f_Q/f_{eq} of the values of f for the quasi- and true equilibria because this ratio exhibits

any differences between the quasigas described by our Monte Carlo method and the real gas in thermal equilibrium at the same density and temperature. It was found that the mean value of this ratio is not significantly different from one and that the standard deviation of the ratio, for the inner half of the velocity space, amounts to 0.02 for a sample of 3.2×10^4 collisions. Contour lines of f_Q/f_{eq} are shown in Fig. 3 for one of the samples of 3.2×10^4 collisions. As in Fig. 2 the

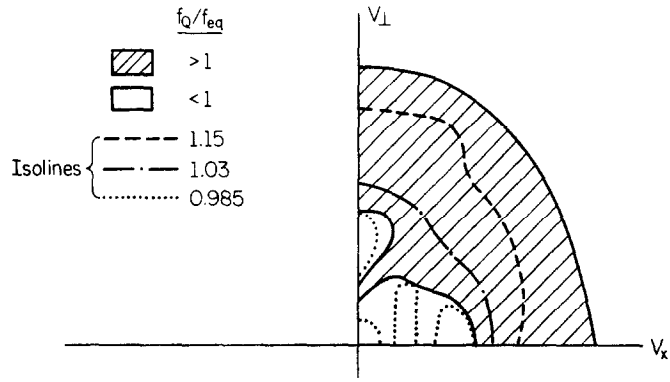

FIG. 3. Comparison of a quasi-equilibrium velocity distribution $f_Q(v_x, v_\perp)$ and an equilibrium velocity distribution $f_{eq}(v_x, v_\perp)$. The distribution $f_Q(v_x, v_\perp)$ is a Monte Carlo solution of the Boltzmann equation for a (fixed) Monte Carlo sample of 3.2×10^4 collisions.

contour lines are symmetrical with respect to the $v_\perp$ axis and are therefore not given for the left half of velocity space. The shape of the contour lines suggests the complicated nature of the variation of the ratio over velocity space, a variation that depends in its details upon the sample chosen. Except for large v, where a and bf are small, the ratio differs substantially from unity only for a small number of velocity bins. This behavior is typical of the quasi-equilibrium values of f even for much smaller samples than 3.2×10^4.

D. *Estimation of the Likely Error*

A new method of evaluating the random error, caused by Monte Carlo sampling, in *any* quantity derived from the Monte Carlo estimates of the values of the collision integral was used to obtain the estimates of random error given in later sections. For a given kinetic-theory problem the method requires finding a solution of the Boltzmann difference equations and their auxiliary boundary conditions for each of N independent sets of Monte Carlo samples of molecular collisions. Each quantity X derivable from the solution is then represented by N independent

estimates, from which can be derived the mean and "likely error" of the mean.[1] The symbol $\epsilon_N X$ denotes the "likely error," estimated in this way, of the quantity X.

The "likely error" ϵ_4 ($N = 4$) will be used in Sects. V.D and V.F to represent our estimate of the Monte Carlo errors. For this value of N, $\epsilon_4 X = 0.442\, S(X)$ where S is the sample standard deviation of the quantity X. For most of our calculations we have found that $N = 4$ yields an adequate understanding of the Monte Carlo or random error in each of the large number of calculated quantities that are of interest. These estimates could be refined as much as needed, with no increase in computing time, by further subdivision of a collision sample and calculation of statistically independent solutions of the difference equations for each of the new subsets. The estimate of "likely error" would then be changed to that for a sample of some standard size by scaling in proportion to the inverse square root of the size of the subset.

Because of the ease with which these methods of estimating the "likely error" can be applied, we may say that use of the Monte Carlo calculation of the Boltzmann collision integral, rather than of some (nonexistent) *direct* quadrature method, imposes no new handicap because of new and unknown errors: the errors that are not easily evaluated are, as in all similar numerical quadrature problems, the systematic errors.

IV. Relaxation Calculations

The first solution of the nonlinear Boltzmann equation was found in 1964–65 for a relaxation problem which we call the pseudoshock. Brief accounts of this solution have been published [1], [2]. Less accurate solutions have been made by another method [5].

In the pseudoshock problem a homogeneous gas relaxes toward thermal equilibrium from an initial condition described by a bi-modal velocity distribution function. A Mach number M, proportional to the half distance between the two peaks of the bi-modal distribution, measures the initial departure from equilibrium. Computer runs were made for values of M from 0.5 (near equilibrium initially) to 6.0 (far from equilibrium initially). The Monte Carlo values of $(a\text{-}bf)$ were corrected slightly, by the least-square procedure, to keep the time derivatives of the density and energy equal to zero, a behavior to be expected in the relaxation of a real gas. In each run, unlike the quasi-equilibrium runs, a different, independent sample (containing 10^4 collisions) was used for each step of the forward integration in time of the Boltzmann equation.

[1] The "likely error" $\epsilon_N X$ is defined as one-half of the difference between the 50% confidence limits for a sample of N values of a variate X. As $N \to \infty$, $\epsilon_N X$ approaches the probable error.

One of the important questions about the calculated pseudoshock concerns the behavior of the gas for large values of the time: are the Monte Carlo fluctuations stable during the asymptotic approach to equilibrium? We found that the fluctuations in the computed solutions are stable. They become dominant only when representative moments of the velocity distribution function approach to within 0.1–0.2% of their equilibrium values, which requires, on the average, two to four collisions for each molecule. The asymptotic values of representative moments, estimated from the runs, agree with the known analytical values to within 0.4% or better except for $M = 6$. Without the least-square corrections of $(a\text{-}bf)$ the runs slowly diverged. The corrections thus serve to stabilize the calculations and to yield accurate asymptotic behavior by having removed, to a large extent, the effects of the residual systematic errors in the Monte Carlo evaluation of the collision integral.

A second and physically important question about the pseudoshock concerns the behavior of representative moments of f *during* the relaxation: how well is the relaxation of these functions described by a single, exponential relaxation process? A realistic answer to this question requires some assessment of the errors in the numerical method; therefore, the random errors of two representative moments were estimated by a method similar to that described in Section III.D. A study of the systematic errors showed that the errors in the forward integration process could be neglected compared to the other errors.

The respresentative moments of f that were examined were $nt_\perp/\pi$ (where $t_\perp$ is the lateral temperature) and the Boltzmann function H. The two functions measure in different ways the time-dependent departure of the relaxing gas from thermal equilibrium. We studied the logarithmic slopes of the relaxation curves of these two functions for five different values of the parameter M. The logarithmic slope of the $t_\perp$ curve was found to have the value 0.354 with a "likely error" of 0.004 and showed no statistically significant deviations from this value over one or two decades of relaxation *or* with change of the parameter M. A similar result was obtained for the logarithmic slope of the H curve, the value here being 0.561 with a "likely error" of 0.008. We may then answer the second question as follows: in these runs with samples of 10^4 collisions, there is no statistically significant evidence of more than one relaxation time for either function nor of dependence of relaxation rate upon the parameter M.

V. Shock-Wave Calculations

A. *General Remarks*

Solution of the nonlinear Boltzmann equation for the shock wave is more difficult than for the pseudoshock in several respects: new techniques must be

added to the numerical methods of integrating the Boltzmann equation; there are more parameters of the numerical method that must be optimized; and the calculations are more time-consuming by an order of magnitude. It is also more difficult to find other reliable solutions of the Boltzmann equation, even in limiting cases, with which the Monte Carlo solutions can be compared. In spite of these greater difficulties we have solved the Boltzmann equation with our present computer program (in the sense of Section II) for Mach numbers of 1.4, 2.5, and 4. We are able to estimate the random errors of any calculated quantity, by the method described in Section III.D, and to estimate some of the systematic errors associated with convergence of the iterations, integrations across the shock and variations of the zeroth iterate. These various random and systematic errors will be discussed in Sections V.B–F.

The several new techniques needed to solve the shock problem may be described briefly. The first technique (1958, Nordsieck[2]) is that of stable numerical integration in the forward direction for $v_x > 0$ and in the negative direction for $v_x < 0$. The second technique (1963) is the use of the number density n as independent variable in place of x, which also makes a necessary contribution to the stability of the iterative solution of the Boltzmann equation for the shock wave. The third technique (1966) is the use of a fixed set of collision samples for a given run, rather than a new and independent set of samples for each iteration. This technique makes visible the convergence of the iterative process, a convergence which is obscured by fluctuations when independent samples are used for each successive iteration. The fourth technique (1965) represents a simple extension of one used for the pseudoshock and quasi-equilibrium calculations: the Monte Carlo values of the collision integral are corrected slightly at each station in the shock, by a least-square procedure, to make equal to zero the three moments of the collision integral that correspond to the gradients of the fluxes of mass, momentum and energy.

With the help of these techniques the Boltzmann equation was solved by the Monte Carlo method in 1966 for a Mach number of 2.5 and in 1967 for Mach numbers of 1.4 and 4.0. The errors in the solution for the Mach number of 2.5 are what we shall discuss here. Four statistically independent runs were made, each of which entailed 12 iterations. Values of f, a, bf, and their moments were calculated for $J = 9$ stations or positions in the shock wave. For each run a fixed set of seven independent collision samples was used to evaluate the two parts of the collision integral for the seven interior stations and for each of the 226 velocity bins. Four independent sets each consisting of seven independent collision samples were used for the four runs. The sample size for each station in each run was 2^{N_7} with $N_7 = 15$. These four runs supplied all the information

[2] The numbers in parentheses indicate when the several techniques were first used.

necessary to calculate the mean and "likely error" of the mean of any quantity of interest for a composite sample with $N_7 = 17$. In an attempt to estimate some of the systematic errors, 39 additional runs were made for other values of J and N_7 and also for various initial approximations to the solution.

For $M_1 = 2.5$, $J = 9$, and $N_7 = 15$ the contribution of each of the various sources of error to the error in f for any one velocity bin is of the order of 1 %. These values of J and N_7 correspond to a 4.5-hour computer run for 12 iterations on the CDC 1604.

B. *Convergence of the Iterations*

For each station the deviation in f, from one iteration to the next, indicates what we may call the *iteration error* in the solution of the Boltzmann difference equation. To get a satisfactory measure of this error we calculated the rms value, taken over velocity space, of this deviation at *each* station in the shock wave. For the sake of brevity we shall discuss here another rms value taken *both* over velocity space and over the seven interior stations in the shock wave. We denote this rms measure of the iteration error by $\delta_I f$.

Semilogarithmic plots of $\delta_I f$ against the number of iterations (for several values of J and N_7) showed that the decrease of the error followed a doubly exponential law. In the first and rapid part of the decrease, the value of $\delta_I f$ is reduced by a factor of 30 or more in three iterations, and the Monte Carlo estimates of $(a\text{-}bf)$ become noticeably less noisy, that is, the contour lines of this function in velocity space become smoother. In the subsequent, slow part of the variation of $\delta_I f$ it decreases by a factor of about 1.5 in three iterations. This part of the variation is apparently connected with the small corrections in a and bf being made to force conservations of mass, momentum and energy fluxes [6]. Study of the slow part indicated that the *convergence* error (that is, the rms deviation between $f/I = 12$ and the exact solution of the difference equations, averaged over all internal stations in the shock) amounts to 0.6 % of the rms value of f, for $J = 9$ and $N_7 = 15$.

In our subsequent discussion we shall use values of f, a and $(a\text{-}bf)$, and their moments that were calculated for the twelfth iteration.

C. *Random and Systematic Errors at the Boundaries*

The solution $f(n, \mathbf{v})$ of the Boltzmann equation for a shock wave should satisfy boundary conditions at the upstream and downstream boundaries of the shock, that is, $f(n, \mathbf{v})$ should be identically equal to the known Maxwell-Boltzmann velocity distribution functions there. The Monte Carlo solutions are obtained by starting for each velocity bin with the correct value of f at one boundary and

integrating across to a second boundary. The total error, caused by the accumulation in the integration of errors of all kinds, is measured by the deviations of the computed values at the second boundary from the known and correct values.

Our results show that the boundary conditions are satisfied, for $J = 9$ and $N_7 = 15$, within rms errors in f of 1.0×10^{-3} and 3.7×10^{-3} at the cold and hot sides of the shock, respectively. The systematic part of each of these errors is about $\frac{2}{3}$ of the total. (As a basis of comparison we note that the largest value of f in the shock is unity, and the rms value of f, for the whole interior of the shock, is 0.12.) Fractional errors at the boundaries are larger than 15% only for bins for which $f \ll 1$. There is definite evidence of the "homing" tendency provided by the stable integration process. The systematic errors may, therefore, be larger in the *interior* of the shock than these figures for the boundaries would indicate.

The numerical integration across the shock is a second-order integration process. The corresponding local quadrature errors should therefore vary like $(J - 1)^{-2}$, where J is the number of stations. It was not possible to separate unambiguously this quadrature error in f from other errors at the boundaries for our Monte Carlo solution of the Boltzmann equation for the shock wave. We were, however, able to evaluate this quadrature error in solutions of the Krook equation for the shock, made with the *same* numerical integration program. For the Krook equation the systematic errors in f at the cold boundary decrease as J increases, like quadrature errors to be expected from a second-order integration toward this boundary. The systematic errors at the hot boundary of the Krook shock appear to decrease less rapidly as J increases than would be expected for a second-order process. We do not yet know the detailed explanation of this difference of behavior of the errors for the forward and backward integration.

D. *Random and Systematic Errors in the Interior of the Shock*

Values of $\epsilon_4 f$, the "likely error" in the mean value of f, were computed for each velocity bin and for each station in the interior of the shock by the method of Section III.D. The sample corresponding to the means contains 2^{17} collisions. Contour lines of the random fractional error $(\epsilon_4 f)/f$ were constructed for each station with the help of the computer program. The contour lines for the center of the shock are shown in Fig. 4. The random fractional error does not vary much over velocity space at this station nor does it vary much at other stations except next to the cold side of the shock.

The rms value (taken over all 226 bins in velocity space) of the "likely error" near the cold and hot boundaries of the shock amounts to 1.0×10^{-3}. Near the center of the shock (corresponding to Fig. 4) this error increases to 1.3×10^{-3}. Division of each of these values of the error by the corresponding rms values of f yields fractional errors, near the boundaries and near the center of the shock

respectively, of 7×10^{-3} and 12×10^{-3}. The value of the random fractional error calculated from the quasi-equilibrium runs of Section III.C, for the same value of N_7, namely 17, and expressed as a "likely error," is 4×10^{-3}. These two estimates of the Monte Carlo or random errors in f agree within the uncertainty of the estimates of each.

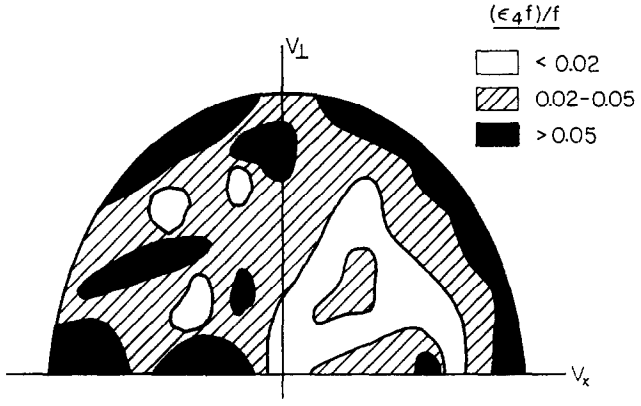

FIG. 4. Fractional random errors in the velocity distribution function for the center of a shock wave ($M = 2.5$). The function and its random errors were calculated from Monte Carlo solutions of the Boltzmann equation for four sets of Monte Carlo samples, each sample containing 2^{15} collisions.

The rms "likely error" for the velocity bins that require forward integration ($v_x > 0$) is larger by a factor of two than the value for the bins requiring backward integration ($v_x < 0$). Random fractional errors in f are larger than 15% only for the bins for which $f \ll 1$, as was found also for the end stations (Section V.C).

The effect of interval size (governed by the number of stations J) was studied by comparing, for $J = 3$, 5, and 9, the values of f and $(a\text{-}bf)$ for individual bins and by comparing the values of two moments of f and of $(a\text{-}bf)$. For the individual velocity bins there is no significant change of f compared to the "likely error," for $N_7 = 15$, as J is changed from 3 to 9. The changes in $\mathcal{M}_9$, which is a moment of f that is proportional to the lateral temperature $t_\perp$, are small and seldom significant. The changes in dn/dx, a moment of $(a - bf)$, are also small and not often significant. A study of solutions of the Krook equation, made with the same numerical integration program, showed that the variations of $\mathcal{M}_9$ and dn/dx with J could be described by polynomials of the second degree in $(J - 1)^{-1}$.

E. *Uniqueness of the Solutions*

A direct test of the uniqueness of our solutions of the Boltzmann equation by the Monte Carlo method is afforded by making runs with different starting approxi-

mations and comparing the values of f or of its moments after 12 iterations. This test has also been used in an extensive study [4] made with almost the same computer program, of solutions of the Krook equation for the shock wave for $J = 9$. It was found there that using Navier–Stokes instead of Mott-Smith values of f as zeroth iterate produced an rms change in the solution of the Krook equation that decreased by the twelfth iteration to 3.6×10^{-4}.

Our study of the effects of starting approximations upon solutions of the Boltzmann equation was more limited than for the Krook equation. As the computer runs are long, J was set at 3 rather than 9. The question related to uniqueness that we asked was this: what variations in the solution are obtained after 12 iterations with *one set* of fixed collision samples when the starting approximations are the various sets of values of f obtained after 12 iterations made with various independent sets of fixed samples? The variations of the solutions can be described in terms of the rms value (over all velocity bins of the one interior station) of the deviation in f among three runs for $N_7 = 15$ made with these different starting approximations. This rms value was equal to 2×10^{-4}, corresponding to an average fractional deviation of about 0.2 %. These numbers indicate that the variety of starting conditions tested produces deviations, after twelve iterations, about equal to the estimated convergence error after twelve iterations and smaller by a factor of ten than the Monte Carlo fluctuations for the same sample size.

F. *Errors in the Moments of f and of $a - bf$*

Except in our studies, the velocity distribution function f and the Boltzmann collision integral $a - bf$ are seldom calculated explicitly for any model of the shock wave and cannot at present be determined experimentally. A limited amount of information about *moments* of these functions has, however, been obtained by various means:

(a) Many moments of f have been calculated for *non-Boltzmann* models of the shock wave (like the Krook model).

(b) According to Boltzmann's theorem, the Boltzmann flux

$$\mathcal{M}_{10} = \int v_x f \log f \, d\mathbf{v}$$

must, if calculated from an exact solution of the Boltzmann equation, decrease monotonically through the shock wave.

(c) Two moments of f can be determined experimentally as functions of position in the shock, the number density n [Eq. (1)] and the moment

$$\mathcal{M}_9 = (n/\pi) \int v_\perp{}^2 f \, d\mathbf{v},$$

which is related to a measured gas temperature.

Comparison of our solutions of the Boltzmann equation for the shock wave with these results can, therefore, be made only in terms of the *moments* of f or of $a - bf$, and it is necessary to understand the errors in our calculations of these quantities.

Tables II and III summarize part of the information about errors of the moments of f, a, and $(a - bf)$ that can be derived from our Monte Carlo solution of the Boltzmann equation for a Mach number of 2.5. The values, computed for $J = 9$ stations and 2^{17} collisions, are listed for each of five positions in the shock, spaced at equal intervals of the (reduced) number density $\hat{n} = (n - n_1)/(n_2 - n_1)$ where n_1 and n_2 are the values of n at the cold and hot sides of the shock, respectively. For the three interior positions in the shock, $\hat{n} = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$, the quantities given are the values of the moments $\mathscr{M}_k$, $\mathscr{M}'_k$, and their likely errors $\epsilon_4\mathscr{M}_k$, $\epsilon_4\mathscr{M}'_k$. (See Section III.C). At the end positions, $\hat{n} = 0, 1.0$, other quantities are listed whose significance will be indicated later.

The eleven moments of f and of $a - bf$ that are tabulated are defined by the weight factors $\Phi_k(v) = v_x^{r_k}v^{s_k}$ listed at the top of each column in the two tables. (The index $k = 1, 2, \ldots 11$ is used in our computer calculations as a convenient shorthand to distinguish among the moments, and will be used for the same purpose here.) The moments are arranged according to the degree of the weight factor Φ_k, and the two "logarithmic moments" are listed last.

We shall discuss the random errors first. The moments $\mathscr{M}_2$, $\mathscr{M}_3$, $\mathscr{M}_4$ in Table II are almost constant (i.e., "conserved") as $\hat{n}$ varies. Their derivatives are exactly equal to zero because the least-squares correction method outlined in Section V.A forces them to be zero. Vanishing of these derivatives $\mathscr{M}'_2$, $\mathscr{M}'_3$, $\mathscr{M}'_4$, which are moments of df/dx, does not imply that the corresponding moments $\mathscr{M}_2$, $\mathscr{M}_3$, $\mathscr{M}_4$, derived from f by numerical integration, will be *exactly* constant.

The values of the "likely error" for $\mathscr{M}_k$ and $\mathscr{M}'_k$ in Tables II and III do not vary significantly with $\hat{n}$, that is, with position *within* the shock. The errors in $\mathscr{M}_5$ correlate with the errors in the other logarithmic moment $\mathscr{M}_{10}$. Except for two moments ($\mathscr{M}_1$ and $\mathscr{M}_8$), the "likely error" in any moment $\mathscr{M}_k$ appears to be roughly the same as the "likely error" in the derivative of that moment, within, say, a factor of two; thus the values of $\epsilon_4\mathscr{M}_k$ and $\epsilon_4\mathscr{M}'_k$, averaged over the three values of $\hat{n}$ and over all k except 2, 3, 4, 7, are 0.0050 and 0.0044, respectively.[3] All of these conclusions about $\epsilon_4\mathscr{M}_k$ and $\epsilon_4\mathscr{M}'_k$ also hold for $\hat{n} = \frac{1}{8}, \frac{7}{8}$, that is, near the cold and hot sides of the shock wave, respectively.

The general level of accuracy attained in the Monte Carlo calculations may also

[3] The four derivatives $\mathscr{M}'_2$, $\mathscr{M}'_3$, $\mathscr{M}'_4$, $\mathscr{M}'_7$ are, for various reasons, equal to zero or are very small. The fractional errors in these four derivatives should not then be averaged with the fractional errors of the other derivatives, and, for the sake of uniformity the fractional errors of $\mathscr{M}_2$, $\mathscr{M}_3$, $\mathscr{M}_4$, $\mathscr{M}_7$ are not averaged with the fractional errors of the other moments.

TABLE II

MOMENTS AND THEIR ERRORS IN A STRONG SHOCK WAVE ($M_1 = 2.5$)
MOMENTS OF f: $\mathcal{M}_k = \int f \Phi_k(\bar{v})\, d\bar{v}$

$\hat{n}$	k $\Phi_k(\bar{v})$	1 1	2 v_x	3 v_x^2	9 $v_\perp^2$	4 $v_x v^2$	6 v_x^3	7 $v_x^2 v^2$	11 v_x^4	8 $v_x v^4$	5 $\ln f$	10 $v_x \ln f$
0	$\mathcal{M}_k$	1.0011	1.2890	1.8191	.3179	3.1618	2.7525	4.9901	4.4125	9.4424	−1.4994	−1.9305
	$\mathcal{M}_k - \mathcal{M}_{kn}$	.0011[a]	.0014	.0020	−.0004	.0026	.0030	.0041	.0048	.0056	.0006	.0009
$\frac{1}{4}$	$\mathcal{M}_k$	1.4291	1.2899	1.8184	.8448	3.1653	2.5578	4.9936	4.1392	9.7510	−3.1455	−2.2822
	$\epsilon_4 \mathcal{M}_k$	.0021[b]	.0003	.0006	.0041	.0011	.0020	.0015	.0041	.0116	.0086	.0055
$\frac{1}{2}$	$\mathcal{M}_k$	1.8542	1.2897	1.8183	1.3736	3.1654	2.3708	4.9906	3.8737	10.0506	−4.1933	−2.4889
	$\epsilon_4 \mathcal{M}_k$	.0022	.0001	.0006	.0055	.0011	.0018	.0025	.0029	.0105	.0081	.0034
$\frac{3}{4}$	$\mathcal{M}_k$	2.2738	1.2876	1.8170	1.9139	3.1617	2.1809	4.9949	3.6099	10.4161	−4.9859	−2.6042
	$\epsilon_4 \mathcal{M}_k$	.0015	.0006	.0008	.0044	.0009	.0023	.0025	.0026	.0130	.0055	.0025
1	$\mathcal{M}_k$	2.7019	1.2872	1.8135	2.4000	3.1510	2.0076	4.9669	3.3630	10.7161	−5.5261	−2.6326
	$\mathcal{M}_k - \mathcal{M}_{kn}$	−.0008	−.0004	−.0035	−.0072	−.0083	−.0049	−.0377	−.0233	−.1097	.0122	.0058

[a] $\mathcal{M}_{kn}$ is the correct value of $\mathcal{M}_k$, calculated analytically.

[b] $\epsilon_4 \mathcal{M}_k$ is the "likely error" in $\mathcal{M}_k$ for a sample of 2^{17} collisions (see Sec. III.D).

TABLE III

MOMENTS AND THEIR ERRORS IN A STRONG SHOCK WAVE ($M_1 = 2.5$)
MOMENTS OF (df/dx): $\mathscr{M}'_k = \int (a - bf)\, \Phi_k(\bar{v})\, d\bar{v}/v_x$

$\hat{n}$	k / $\Phi_k(\bar{v})$	1 1	2 v_x	3 v_x^2	9 $v_\perp^2$	4 $v_x v^2$	6 v_x^3	7 $v_x^2 v^2$	11 v_x^4	8 $v_x v^4$	5 $\ln f$	10 $v_x \ln f$
0	$\mathscr{M}'_k$	.0008	.0000	.0000	.0001	.0000	.0005	.0011	.0018	.0044	−.0040	−.0001
	$\mathscr{M}'_{ka}$	.4134[a]	.4500	.5794	.1523	.9966	.8296	−1.0686	1.2836	2.8472	−.3973	−.3372
$\frac{1}{4}$	$\mathscr{M}'_k$	.2794	.0000	.0000	.3440	.0000	−.1235	−.0018	−.1746	.1863	−.8064	−.1703
	$\epsilon_4 \mathscr{M}'_k$	.0041[b]	.0000	.0000	.0036	.0000	.0022	.0020	.0033	.0028	.0099	.0021
$\frac{1}{2}$	$\mathscr{M}'_k$	.3470	.0000	.0000	.4441	.0000	−.1567	.0040	−.2203	.2794	−.7472	−.1354
	$\epsilon_4 \mathscr{M}'_k$	.0050	.0000	.0000	.0053	.0000	.0022	.0025	.0048	.0020	.0067	.0023
$\frac{3}{4}$	$\mathscr{M}'_k$	.2327	.0000	.0000	.2956	.0000	−.1008	.0052	−.1375	.2298	−.3764	−.0395
	$\epsilon_4 \mathscr{M}'_k$	.0054	.0000	.0000	.0062	.0000	.0031	.0026	.0053	.0059	.0085	.0016
1	$\mathscr{M}'_k$	.0543	.0000	.0000	.0329	.0000	.0042	.0040	.0059	.0594	−.0261	.0000
	$\mathscr{M}'_{ka}$	4.2223	5.4964	2.6185	4.5726	9.7805	4.0923	−1.9503	4.6602	27.8939	−1.3622	−7.1026

[a] $\mathscr{M}'_{ka} = \int a\, \Phi_k(\bar{v})\, d\bar{v}/v_x$.

[b] $\epsilon_4 \mathscr{M}'_k$ is the "likely error" in $\mathscr{M}_k$, for a sample of 2^{17} collisions (see Sec. III.D).

be indicated by giving the values of the fractional "likely errors," $(\epsilon_4 \mathscr{M}_k)/\mathscr{M}_k$ and $(\epsilon_4 \mathscr{M}'_k)/\mathscr{M}'_k$, averaged over all moments except[3] those designated by 2, 3, 4, and 7. The average value of $(\epsilon_4 \mathscr{M}_k)/\mathscr{M}_k$ for the seven remaining moments is 0.0016, which is seven times smaller than the value of the fractional "likely error" of f, namely, 0.012, given in Section V.D for the center of the shock. The ratio of these two errors would be about $(226)^{1/2} \cong 15$ if the random errors of f for the various velocity bins were uncorrelated and f were nearly constant over velocity space. The average value of $(\epsilon \mathscr{M}'_k)/\mathscr{M}'_k$ for the seven moment of $a - bf$ is 0.02 which is about 13 times larger than the corresponding average fractional error for the moments of f. These conclusions about the fractional "likely errors" also hold for $\hat{n} = \frac{1}{8}$, near the cold side of the shock but not for $\hat{n} = \frac{7}{8}$, near the hot side of the shock, where many of the derivatives $\mathscr{M}'_k$ become small.

The generally small values of these representative random errors of the moments of f and $a - bf$ show that the Monte Carlo solutions of the nonlinear Boltzmann equation provide an excellent basis for studying the properties of strong shock waves and other systems that are far from thermal equilibrium.

Our analysis of the systematic errors is much less complete than our analysis of random errors, but certain information about the systematic errors has been obtained. In Table II we show the numerical quadrature errors $(\mathscr{M}_k - \mathscr{M}_{kn})$ at the two end stations, $\hat{n} = 0$, 1.0. The errors are less than 0.3 %, except for the high-order moments $\mathscr{M}_7$, $\mathscr{M}_8$, $\mathscr{M}_{11}$ at $\hat{n} = 1.0$. Since quadrature errors (except for the logarithmic moments) vary almost linearly across the shock, they can be compared, in the interior of the shock, with the "likely errors" that include contributions only from random errors. We notice that the "likely error" of any one moment in the interior of the shock ($\hat{n} = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$) is generally less than the numerical quadrature error on the hot side of the shock ($\hat{n} = 1.0$). The "likely errors" of each of the three "conserved" moments, $\mathscr{M}_2$, $\mathscr{M}_3$, $\mathscr{M}_4$, in the interior of the shock are generally much smaller than the quadrature errors at the two end stations.

In Table III we give the values at the end stations of $\mathscr{M}'_k$, the moments of the Monte Carlo ($a - bf$), and the corresponding moments $\mathscr{M}'_{ka}$ of the Monte Carlo a.[4] The differences from zero of the values of $\mathscr{M}'_k$ indicate the combined effects of the systematic errors in the Monte Carlo calculation (with least-square corrections) of $a - bf$ at the end stations and of the errors in numerical quadrature over velocity space to obtain the moments. Except for $\mathscr{M}'_1$ and $\mathscr{M}'_5$ these errors in the $\mathscr{M}'_k$ are less than 0.8 % of the corresponding $\mathscr{M}'_{ka}$. A method devised by Yen [4] gives additional information about the systematic errors in the Monte Carlo calculation

[4] In our Monte Carlo solution of the shock problem we use the known, *analytically* computed values of a and bf at the end stations. For our present discussion of errors, however, we made *Monte Carlo* calculations of a and bf at the end stations.

of the three derivatives, $\mathscr{M}_6'$, $\mathscr{M}_7'$ and $\mathscr{M}_{11}'$ for stations in the interior of the shock. He has calculated the values of these derivatives, both analytically and by accurate Monte Carlo calculations for several interior stations in a Mott-Smith shock for $M_1 = 2.5$. He finds that the systematic errors in $\mathscr{M}_6'$ and $\mathscr{M}_{11}'$ are probably less than 2% but that the systematic error in $(\mathscr{M}_7' - \mathscr{M}_{11}')$ ranges from 4% to 25%.

VI. Concluding Remarks

As illustrated in the paper, the random errors can be determined for *any* function derived from the Monte Carlo calculations of the distribution function and of the Boltzmann collision integral. Only a few types of systematic error can be determined at present: for example, the systematic errors in Monte Carlo calculation of the collision integral for a gas at or near thermal equilibrium; the iteration error (for $M_1 = 2.5$) in the solution of the Boltzmann equation for the shock wave; numerical quadrature error in calculating moments throughout the shock wave; and certain errors in derivatives of moments at the boundaries and in the interior of the shock wave.

Much more analysis and calculation must be undertaken and completed before we can calculate an upper bound, for any given problem, to the difference between the solution of the Boltzmann difference equations used in the Monte Carlo method and the solution of the Boltzmann differential equation. But even before such a bound is determined we can assume that the solutions of the difference equations are similar, in many respects, to the solutions of the differential equation, both because of the inherent soundness of Nordsieck's Monte Carlo method and because so many of the errors that have already been computed are small.

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