REPORT R-348 APRIL, 1967

CSL COORDINATED SCIENCE LABORATORY

NUMERICAL STUDIES OF STRONG SHOCK WAVES PART IX: ERROR ANALYSIS FOR A MACH NUMBER OF 2.5

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This work was supported in part by the Joint Services Electronics Program (U.S. Army, U.S. Navy, and U.S. Air Force) under Contract No. DA 28 043 AMC 00073(E); and in part by the Office of Naval Research under Contract No. N00014-66-C0010-A01

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Abstract

Data from 43 computer runs makes possible a study of the Monte Carlo, iterative solutions of the Boltzmann difference equations for a strong shock wave ($M_1 = 2.5$). Estimates have been made of errors associated with iterative convergence, Monte Carlo sampling, number of stations in the shock and variations of the zero-th iterate.

Specific results are summarized at the end of the Report.

List of Symbols

1. Basic Set

Variables and Functions (Nordsieck units used throughout)

$a = a(\bar{v},n)$ $b = b(\bar{v},n)$	parts of the collision integral, (a-bf)
$f = f(\bar{v},n)$	velocity distribution function
f', F, F'	$f(\bar{v}',n)$, $f(\bar{V},n)$, $f(\bar{V}',n)$
I	number of iterations
J	number of stations in the shock
j	ordinal number of station in the shock wave- $j = 0,1,\cdots(J-1)$
$K_1 = v_m/v$	scaling parameter
M_1	upstream Mach number
N_7	2^{N_7} = number of collisions in the Monte Carlo sample
n	particle density
$\hat{n}$	reduced particle density, $(n-1)/(n_2-1)$
$\delta\underline{n}$	$(n_2-1)/(J-1)$
n'	dn/dx
$\underline{n}'$	Monte Carlo value of n'
r	ordinal number of the collision sample
s	ordinal number of velocity bin- $s = 0,1,\cdots 225$
v_x	component of $\bar{v}$ perpendicular to the shock wave
v_{xa}	value of v_x measured relative to the shock wave
$v_\perp$	component of $\bar{v}$ parallel to the shock wave

$\bar{v}$	molecular velocity
$\bar{v}$, $\bar{v}'$	velocities of molecules entering a collision
$\bar{V}$, $\bar{V}'$	velocities of molecules leaving a collision
x	position coordinate measured perpendicular to the shock wave

Subscripts etc.

c or 1	indicates "cold" or upstream side of shock
h or 2	indicates "hot" or downstream side of shock wave
m	refers to "machine" units of velocity, $v_m = K_1 v$
MC or _	Monte Carlo
M-S	Mott-Smith
___\(<___)	indicates $v_{xa} > (<) 0$
j	station j
s	velocity bin s
I	number of iterations

2. Operators Used in this Report

The operands are functions typified by F(j,s,I,J,r,u) where F may depend on one or more of the indicated parameters. Each operator also involves one or more of these six parameters.

$\delta_I F$	$F(j,s,I,J,r,u) - F(j,s,I-1,J,r,u)$
$\delta_J F$	$F_{AV}(j,s,I,J,r,u) - F_{AV}(j',s,I,J',r',u)$ where $[j/(J-1)] = [j'/(J'-1)]$
$\delta_u F$	$F(j,s,I,J,r,u) - F(j,s,I,J,r,u')$ where u,u' refer to different zero-iterates
$F_{jr} = \rho_{jr} F$	rms value, taken w.r.t. s, of F(j,s,I,J,r,u)
$F_r = \rho_r F$	rms value, taken w.r.t. $j = 1,2\cdots(J-2)$, of F_{jr}

$F_r^* = \rho_r^* F$	rms value, taken w.r.t. j=0,1,$\cdots$(J-1), of F_{jr}
$\rho_j F_{AV}$	rms value, taken w.r.t. s, of $AV_{js} F$
$AV_j F_{jr}$	mean, for a set of four values of r, of F_{jr}
AVF_r	mean, for a set of four values of r, of F_r
$F_{AV} = AV_{js} F$	mean of a sample of four values of F(j,s,I,J,r,u)
$\sigma_{js} F$	sample standard deviation, for a set of four values of r, of F(j,s,I,J,r,u)
$\epsilon_{js} F = 0.442\ \sigma_{js} F$	"likely" error of the mean of a sample of four values of F(j,s,I,J,r,u)
$\sigma_j F$	$\rho_j(\sigma_{js} F)$
$\epsilon_j F$	$\rho_j(\epsilon_{js} F)$

Introduction

In an earlier report[1] we analyzed the random and systematic errors of various Monte Carlo evaluations of the Boltzmann collision integral for a system near the condition of equilibrium. In the present report we discuss several types of errors connected with solution of the Boltzmann difference equations for a system far from equilibrium, namely, for a strong shock wave ($M_1 = 2.5$). Two discoveries in 1966 made possible this error analysis and subsequent calculation of solutions[2,3]: in April 1966 we found that use of "fixed" samples of collisions produced a visible convergence of our iterative solution of the Boltzmann difference equations; and in November 1966 we discovered the doubly-exponential nature of the convergence process. Both aspects of convergence will be discussed here.

The error analysis is based primarily on a set of 43 runs totaling 60 hours of computer time. There were four independent runs for each of the combinations of the parameters J and N_7 in Table 1 and an additional set of 11 runs designed to test the uniqueness of the solutions obtained. The computing time for a standard run (J = 9 stations, 12 iterations, and a collision sample size of $2^{N_7} = 2^{15}$) is 3.5 hours. In analyzing these runs we assume that the random Monte Carlo errors are proportional to $N_7^{-\frac{1}{2}}$, and we seek to find how the errors depend upon J, the number of stations in the shock, and upon I, the number of iterations. From this information we can derive the optimum values of J and N_7 that should be used in making studies of shock structure with our present computer program. Our understanding of the dependence upon J and I of the errors in iterative solutions of the Boltzmann equation will be aided in the future by analysis of solutions of

Table 1

Parameters for Shock Wave Calculations

Number of stations J \ N_7*	13	15	17
3	X	X	X
5	X	X	X
9	X	X	

*The size of the collision sample is 2^{N_7}.

the Krook equation that we have recently calculated by the same iterative process.

The principal results of the study of errors are listed in the Summary at the end of the Report.

The Boltzmann Difference Equations

The Boltzmann differential equation, in Nordsieck units,[2] is

$$v_{xa}(df/dx) = a-bf \tag{1}$$

where f is the velocity distribution function and (a-bf) is the collision integral. The functions to be calculated, f, a and (bf) depend upon x, the position variable, and upon two components of the molecular velocity, v_x and $v_\perp$, which lie perpendicular and parallel, respectively, to the plane of the shock. (All three components of $\bar{v}$ must be considered in the evaluation of the collision integral.) The boundary conditions are

$$\begin{aligned} f &\to f_c(\bar{v}) \quad , \quad x \to -\infty \\ f &\to f_h(\bar{v}) \quad , \quad x \to +\infty \end{aligned} \tag{2}$$

where $f_c(\bar{v})$ and $f_h(\bar{v})$ are the velocity distribution functions characteristic of the known equilibrium conditions far up- and down-stream of the shock wave. The symbol v_{xa} in Eq. (1) refers to the x component of molecular velocity relative to the shock.

The corresponding set of 226 Boltzmann difference equations, to be solved by iteration,[2] is

$$f_{j\pm1,s} = \{f_{j,s}[v_{xa}(\underline{n}'_j + \underline{n}'_{j\pm1}) - b_j\delta\underline{n}] +$$

$$(a_j + a_{j\pm1})\delta\underline{n}\}/[v_{xa}(\underline{n}'_j + \underline{n}'_{j\pm1}) + b_{j\pm1}\delta\underline{n}]. \qquad (3)$$

In Eq. (3) j refers to the position or station in the shock (j = 0,1,...,J-1 where J is the number of stations in the shock); s refers to the velocity bin (s = 0,1,...,225) in the two dimensional velocity space (v_x, $v_\perp$); $\underline{n}'_j$ is the value of the density gradient at the j-th station, calculated by numerical integration of the Monte Carlo values of (a-bf)/v_{xa}; and $\delta\underline{n} = (n_h - n_c)/(J-1)$ is the increment of a new independent variable $\underline{n}$ defined by the values of $\underline{n}'_j$. The plus (minus) signs in the subscripts are used[4] for velocity bins at positive (negative) values of v_{xa}, the total number of bins being 226.

Each term in the collision integral (a-bf) of Eq. (1) has been replaced in Eq. (3) by a Monte Carlo estimate, $a_{j,s}$, $(bf)_{j,s}$. Thus

$$a(\bar{v},x) \rightarrow a_{j,s} = 2^{-N_7} \mathcal{J}_1 \sum_{\text{sample}} \varkappa_1 FF' \qquad (4)$$

$$b(\bar{v},x)f(\bar{v},x) \rightarrow (bf)_{j,s} = 2^{-N_7} \mathcal{J}_1 \sum_{\text{sample}} \varkappa_1 ff' \qquad (5)$$

where $\mathcal{J}_1$ and $\varkappa_1$ are defined in Reference 2, Sect. 5. The $a_{j,s}$, $b_{j,s}$ are derived from the a_{AN}, b_{AN} of that reference by a small, least squares correction that insures conservation of the fluxes of mass momentum and energy. The number of collisions in the Monte Carlo sample, for one station, is 2^{N_7}.

We distinguish three types of Monte Carlo collision samples:

a) statistically independent samples for each interior station and iteration;

b) a set of independent samples for the (J-2) interior stations, this set repeated for each iteration of a given run;

c) the same collision sample for each interior station and iteration.

We used the first type of sampling until April 1966, obtaining iterations whose convergence was somewhat in doubt because of a large sampling "noise" caused by the stochastic nature of Eqs. (3). We devised the second type of sampling in April 1966 and have used it extensively since then. The "fixed" set of samples in this method corresponds to a fixed, non-stochastic set of difference equations, Eq. (3). The visible convergence of the iterations with this type of sampling follows a simple, doubly-exponential law. (See discussion in a later section.) The statistical properties of the Monte Carlo sampling are recovered by analyzing four runs made for four independent sets of samples for each value of J and N_7. The third type of sampling, which we have seldom used, might yield more rapid convergence of the iterations than the second method but probably also larger Monte Carlo fluctuations among the different runs.

Our present error analysis is based wholly on sampling of the second type. Twelve iterations (that is I = 0 to 12) were made in each of the 43 runs described in the Introduction.

Notation

We use five operators in describing our error analysis. These operators are AV, σ, ρ, ϵ, and δ. The first two operators form the mean and (sample) standard deviation of the four values of a function generated by the four "fixed" sample sets described in the previous section. The third operator, ρ, forms the root mean square, over velocity space or over the internal stations, of the values of a function. The fourth operator, ϵ, forms one-half the difference between the 50% confidence limits derived from four values of a function. We call this quantity the "likely" error to distinguish it from the "probable" error that is calculated from a sample much larger than four. For a sample of four values of a quantity F the ratio of ϵF to σF is equal to 0.442.

The fifth operator, δ, forms a set of differences, for each velocity bin, from two sets of values of a function of $\bar{v}$. For example, $\delta_I f$ gives the change in f from iteration (I-1) to I. Subscripts I, J, and u on the operator δ correspond, respectively, to changes in the ordinal number of the iteration I, in the number of stations J, and in the set of values of f_{js} that are used to start a run or series of iterations. (The subscript u is a mnemonic for the "uniqueness" runs to be discussed later.) Subscripts j, s, r on AV, ρ, σ, and ϵ indicate the variables remaining after the operation has been performed. (These subscripts on the operators do not correspond to specific values of the subscripts.) Thus, ρ_{jr} implies a root mean square operation over s only, and ρ_r implies a root mean square operation over the interior stations j and s, for a given sample set r. Unless otherwise specified it may be assumed that each quantity discussed in the error analysis depends upon I, J, N_7, and M_1.

The symbols ⟶ and ⟵ refer to $v_{xa} > 0$ and $v_{xa} < 0$ (or to the "forward and backward integration").

Convergence of Iterations

We are concerned in this section with the quantity

$$\delta_I f = f(j, s, I, J, r, u) - f(j, s, I-1, J, r, u), \qquad (6)$$

that is, the change of the velocity distribution function from one iteration to the next. We shall discuss, in several numbered subsections, the behavior of various quantities derived from it with the help of the operators defined in the previous section.

The rms values of f will be needed in our discussions and are well represented by the values of $(\rho_j f_{AV})$ given in Table 2 where f_{AV}, for each velocity bin and station, is the average value, for I = 12 and across the four independent runs, and the rms operation applies to the bins in velocity space.

1. $\rho_r(\delta_I f)$ = rms$(\delta_I f)$ w.r.t. s and j for one run. The dependence upon I of this quantity (and also of the similar quantity $\rho_r(\overleftarrow{\delta_I f})$) can apparently be represented as a sum of two exponentials

$$\rho_r(\delta_I f) = A_1 \exp(-\alpha_1 I) + A_2 \exp(-\alpha_2 I), \qquad \alpha_1 > \alpha_2 \ . \qquad (7)$$

(This representation was tested, for three of the 43 runs, for both $\rho_r(\delta_I f)$ and for $\rho_r(\overleftarrow{\delta_I f})$.) The first term is generally negligible compared to the second for $I \geq 6$. The average values of α_1 and α_2 over the three runs are 1.5 and 0.16, respectively.

From Eq. (7) we can show that, for $I \geq 6$,

$$[\rho_r(f_I - f_\infty)/\rho_r(\delta_I f)] = [\exp(\alpha_2)-1]^{-1} \cong 5.7 \qquad (8)$$

Table 2

Rms Values of f_{AV}

($J = 9$, $M_1 = 2.5$, $N_7 = 15$)

j	$\rho_j f_{AV}$	$\overrightarrow{\rho_j f_{AV}}$	$\overleftarrow{\rho_j f_{AV}}$
0	0.1396	0.1793	0.00026
1	0.1286	0.1650	0.0109
2	0.1206	0.1540	0.0206
3	0.1157	0.1464	0.0312
4	0.1135	0.1420	0.0413
5	0.1143	0.1408	0.0514
6	0.1178	0.1429	0.0614
7	0.1240	0.1484	0.0718
8	0.1349	0.1593	0.0843

where f_∞ is the extrapolated value of f_I as $I \to \infty$. We can thus estimate the "convergence error," $\rho_r(f_I - f_\infty)$, for a given value of $I \geq 6$ and a given sample set or run r, directly from the quantity $\rho_r(\delta_I f)$ that measures the change from iteration (I - 1) to iteration I.

2. $AV_j[\rho_{jr}(\delta_I f)]/_{I=12}$. This quantity varies from 1.6×10^{-5} to 2.7×10^{-4} as we change N_7, J, and j. It generally increases as J goes from 5 to 9 and as N_7 decreases. The Monte Carlo fluctuations of $\rho_{jr}(\delta_I f)$, as measured by $\epsilon_j[\rho_{jr}(\delta_I f)]$, amount to about 25% of $AV_j[\rho_{jr}(\delta_I f)]$ so that $AV_j[\rho_{jr}(\delta_I f)]$ is generally well-determined.

3. $AV[\rho_r(\delta_I f)]$. This average value is obtained from four independently determined values of the quantity discussed in subsection 1. It is about proportional, for J = 3,5 and I = 12, to $(J \cdot 2^{-N_7/2})$. For I = 3 or 12 and J = 9 it seems to be independent of N_7, and it also seems to be independent of J for $N_7 = 13$. It is equal to 0.12×10^{-3} for J = 9 and $N_7 = 15$.

If we assume that the value $\alpha_2 = 0.16$ corresponds to the behavior of $AV[\rho_r(\delta_I f)]$ as well as of $\rho_r(\delta_I f)$, for J = 9 and $N_7 = 15$, then we can estimate that the "convergence error," after 12 iterations, and averaged over all internal stations, is 6.6×10^{-4}, or 0.6% of the rms value of f for all bins and stations.

4. A special discussion is needed for the behavior of the error at the boundaries of the shock wave. We shall use, as before, the subscripts c and h to refer to the "cold" and "hot" sides of the shock. The quantities of interest to us are then:

$$\delta_I f_c = \overleftarrow{f}_{Ic} - \overleftarrow{f}_c, \qquad \delta_I f_h = \overrightarrow{f}_{Ih} - \overrightarrow{f}_h \tag{9}$$

Note that $\overleftarrow{f}_c$ and $\overrightarrow{f}_h$ are known boundary values of f, whereas f_{Ic} and f_{Ih} are obtained by backward and forward integration with respect to the independent variable x(or n, the particle density). The quantity $\delta_I f_c$ (or $\delta_I f_h$) measures, for each velocity bin, the accumulated errors in integrating backward from the hot side (or forward from the cold side) across the shock for the velocity bins with negative (or positive) values of v_{xa}. The number of values of $\delta_I f_c$ and the number of values of $\delta_I f_h$ is each less than 226. The sum of these two numbers is 226, however, corresponding as it should to the total number (226) of velocity bins and to the number of first order difference equations solved. The accumulated errors, $\delta_I f_c$ and $\delta_I f_h$ include quadrature errors (systematic and random) in calculating (a-bf) and quadrature errors in the integration process with respect to x or n. The accumulated errors are reduced by the "homing" tendency of this integration process.

The size of the quantities $AV[\rho_r(\delta_I f_c)]$ and $AV[\rho_r(\delta_I f_h)]$ (which could also be written $AV_j[\rho_{jr}(\delta_I f)]_{j=0}$ and $AV_j[\rho_{jr}(\delta_I f)]_{j=J-1}$) indicate how well, on the average, our solutions of the Boltzmann difference Eq. (3) satisfy the boundary conditions Eq. (2). The values of these quantities, for J = 9, N_7 = 15 and I = 12, are 1.0×10^{-3} and 3.7×10^{-3}. Noting that the maximum values of $\overleftarrow{f}_c$ and $\overrightarrow{f}_h$ are 1.9×10^{-3} and 0.56, respectively, we see that the solutions of the Boltzmann difference equations do satisfy the boundary conditions accurately, in the sense that large fractional errors in f occur only for a very small proportion of molecules.

The dependence on J and N_7 of the errors at the boundaries are also interesting. We find for the cold boundary that

$$AV[\rho_r(\delta_I f_c)] \cong 10^{-3}[-0.19 + 0.10\ J + 0.29 \times 2^{(-N_7+15)/12}] \qquad (10)$$

The indicated variations with J and N_7 are probably two or three times the "likely error." For $N_7 = 15$ and $J = 9$ the Monte Carlo (random or N_7-dependent) error $\overleftarrow{\sigma_j f} \cong 1.8 \times 10^{-3}$ near the cold side of a shock[5] whereas the Monte Carlo part of $AV[\rho_r(\delta_I f_c)]$ is less than 0.36×10^{-3}. The "homing" tendency of the integration method thus decreases the Monte Carlo error by a factor of five or more in the last "backward" integration step. The average "residual" error (as $N_7 \to \infty$) on the cold side, that is, the quantity $10^{-3}(-0.19 + 0.10\ J)$ is quite small but so is f_c. (Note that $\overleftarrow{\rho_j f_c} = 0.26 \times 10^{-3}$.) Thus although the fractional residual error here is large, it is large only for a very small part of the molecules, as noted before.

We find for the hot side of the shock that

$$AV[\rho_r(\delta_I f_h)] \cong 10^{-3}[2.9 + 0.8 \times 2^{(-N_7+15)/12}] \qquad (11)$$

(average over J)

The uncertainties of the two coefficients amount to 0.3×10^{-3} and 0.2×10^{-3}. Increase of J tends to produce an increase of $AV[\rho_r(\delta_I f_h)]$. This increase is especially marked for $N_7 = 17$ where the change of J from 3 to 5 increases $AV[\rho_r(\delta_I f_h)]$ by more than five times the "likely error." Near the hot side of the shock, for $J = 9$ and $N_7 = 15$, the Monte Carlo (random) error $\overrightarrow{\sigma_j f} \cong 2.5 \times 10^{-3}$, whereas the Monte Carlo part of $AV[\rho_r(\delta_I f_h)]$ is less than 0.9×10^{-3}. The "homing" tendency thus decreases the Monte Carlo error by a factor of more than two in the last "forward" integration step. The "residual error" on the hot side, 2.9×10^{-3}, is the same as the Monte Carlo error in the center of the shock and amounts to only 1.8% of $\overrightarrow{\rho_j f_h}$, the rms value of $\overrightarrow{f}$ at the hot side of the shock.

At both the cold and hot sides of the shock, the increase of "residual error" ($N_7 \rightarrow \infty$) with J cannot be due to accumulated quadrature error with respect to j, for this error should decrease as J increases. The increase may be due to small systematic errors in (a-bf), accumulated in integration w.r.t. n across the shock and reduced by the "homing" tendency.

Monte Carlo Errors

The standard deviation of f_{js} across the four sets of collision samples measures the random part of the Monte Carlo error for each station j and velocity bin s because the systematic part of the error is nearly the same for the four samples. We assume that the values of $\sigma_{js}f$, $\overrightarrow{\sigma_j f}$ and $\overleftarrow{\sigma_j f}$ derived from the sample of four runs are equal, within a factor of two, to the values that would be derived from a large number of quadruple runs. We shall discuss in turn these various measures of Monte Carlo error. The calculations are made for I = 12 because we are primarily interested in the random errors of our best values of f_{js}.

1. $\sigma_{js}f$, the sample standard deviation of f_{js}. Isolines of this quantity are approximately spherically symmetrical and are, therefore, unlike the isolines of either f or (a-bf) in the interior of the shock. For four independent runs, with $N_7 = 15$, $\sigma_j f$ equals 2×10^{-3} near the boundaries and equals 3×10^{-3} near the center of the shock, corresponding to "likely errors" $\epsilon_j f$ of 0.9×10^{-3} and 1.3×10^{-3} and fractional "likely errors" $\epsilon_j f/\rho^*_j f_{AV}$ of 7×10^{-3} and 12×10^{-3}.

The random and systematic parts of the fractional Monte Carlo error in (a-bf) for conditions near equilibrium can be calculated from the data in Reference 1. The random part is equal to 0.026 for $N_7 = 15$, while the systematic part is smaller by a factor of 1.7. If we assume that the same factor obtains for the two kinds of Monte Carlo errors in f in the non-equilibrium conditions of the shock wave, then the fractional standard deviation[6] in f, owing to systematic errors in the Monte Carlo evaluation of a collision integral, would amount to 9×10^{-3} and 15×10^{-3} near each boundary and near the center of the shock, respectively. The estimate 9×10^{-3} is smaller than the fractional residual, 18×10^{-3}, at the hot boundary, estimated in the previous section.

2. $(\overrightarrow{\sigma_j f}/\overleftarrow{\sigma_j f}) \cong 2$ for various j and J. Thus the random errors in f for $v_{xa} > 0$ and $v_{xa} < 0$ are not very different. The fractional (random) "likely error" in f is large (greater than 15%) only where f is very small, that is, for a very small proportion of the molecules, a result similar to that found for the errors at the boundaries.

Convergence with Respect to J

The key quantity here is

$$\delta_J f = [f_{AV}(j,s,I,J,r,u) - f_{AV}(j',s,I,J',r',u)] \qquad (12)$$

The corresponding values of j and j' are those for which $[j/(J-1)] = [j'/(J'-1)]$, i.e., those for which the particle densities n_j and $n_{j'}$ are equal.

1. The isolines of $\delta_J f$ in velocity space form definite patterns, but the value of this quantity, for various individual velocity bins for any given position in the shock, is generally not significantly different from zero.

2. $\rho_j(\delta_J f)$ is significantly different from zero only for J = 3, J' = 5, N_7 = 17, that is, for a run with a very large collision sample. In this one case $\rho_j(\delta_J f)/\sigma_j f = 1.8$. Thus the effect on f_{js} of increasing the number of stations beyond J = 5 is definitely less than the Monte Carlo random errors, for N_7 = 15.

We can see interesting details of the shock structure[3] for J = 9 that are not visible for J = 5, but until runs are made with larger collision samples it is necessary to run with J > 9 only if we want a more detailed picture than is given by J = 9 of the variation of f as a function of position in the shock. We also note that for J = 9 and N_7 = 15, a set of four runs (each of 12 iterations and using "fixed" sets of collision samples) takes 14 hours, which is a reasonable investment of computer time for one value of the Mach number.

We therefore conclude that the optimum values of J and N_7, for calculating shock structures from four independent runs with our present program, are J = 9 and N_7 = 15.

3. We examined the effect of J on two macroscopic quantities, n' = dn/dx and M_9 (which is proportional to the lateral temperature). For n' the only statistically significant effect due to J is a 14% decrease of n' (three times the "likely error") for $\hat{n}$ = 3/4 as J is changed from 5 to 9. For M_9 the effect of increasing J from 3 to 5 (for $\hat{n}$ = 1/2) or from 5 to 9 (for $\hat{n}$ = 1/4, 1/2, 3/4) is a significant increase of M_9 by about 0.015 (or about 1%)

for each of these postions in the shock

Further studies are needed, like those of the Krook equation mentioned in the Introduction, before the effect of J is understood well enough so that extrapolation to $J = \infty$ (and calculation of bounds to the j-quadrature error) are possible. Our results are consistent, however, with a j-quadrature error in M_9 that is inversely proportional to (J-1), with a value of this error, for $J = 9$ and $\hat{n} = 1/2$, of -0.008 or -0.6% of M_9.

Uniqueness (J = 3)

The key equation is

$$\delta_u f = f(j,s,12,J,r,u) - f(j,s,12,J,r,u') \qquad (13)$$

The argument u refers to a run with Mott-Smith starting values of f. The argument u' refers to a run with different starting values of f namely, to values of f(j,s,12,J,r',u), obtained after 12 iterations from Mott-Smith starting values, for a sample set r'. The $\delta_u f$ calculated from such a pair of runs represents the sensitivity of the final values of f to the choice of random numbers used in the various iterations.

1. Eleven runs were made for $N_7 = 13$ and 15, $J = 3$, and for various sets of collision samples, r and r'. The isolines of $\delta_u f$ show, for $N_7 = 15$, a fractional deviation (because of the different paths or starting conditions) of 0.5% or less, with a median value of 0.35%. The isolines of $\delta_u f$ for $N_7 = 13$ give larger deviations by about the expected factor of two. The fractional deviation increases, in the outer one-third of the two dimensional velocity space and in certain directions, as v decreases. The directions in which this increase takes place depend upon the choice of r, r' and N_7.

2. $\rho_r(\delta_u f) \cong 2.1 \times 10^{-4}$ (averaged over three uniqueness tests for $N_7 = 15$). Therefore, $\rho_r(\delta_u f)/AV[\rho_r(\delta_I f)] \cong 7$ for $J = 3$ and $\rho_r(\delta_u f) \cong 1.2 \times$ ("iterative convergence error"). We can thus conclude that the uniqueness runs (effect of variation of path) and the iterations (convergence rate) yield about the same estimate of convergence error after 12 iterations.

3. Similar uniqueness runs should be made for $J = 5$, $J' = 9$ when the convergence or the Monte Carlo calculations have been speeded up by new techniques that have been devised but not yet tested.

Summary

1. The convergence during the iterations follows a doubly exponential law from which we estimate the rms convergence error, for $J = 9$ and $N_7 = 15$, after 12 iterations and averaged over all internal stations in the shock, as 0.6% or less of the velocity distribution function f.

2. The boundary conditions are satisfied, for the same values of J and N_7, 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 largest value of f in the shock is unity.) There is definite evidence of the "homing" tendency provided by the stable integration process used in integrating numerically with respect to position in the shock. There is no statistically significant evidence at the boundaries of quadrature error in this integration process.

3. For internal stations the fractional "likely" error in f (owing to the Monte Carlo sampling) is, on the average, close to one percent for $N_7 = 15$, independent of the number of stations J. Random fractional errors in f are larger than 15% only where $f \ll 1$.

4. For individual velocity bins, there is no significant change of f, compared to the random Monte Carlo error, as J is changed from 3 to 9 for $N_7 = 15$. The corresponding changes in the lateral temperature and in the density gradient are small and not often significant.

5. Tests of the uniqueness of the solutions of the difference equations lead to about the same estimate of convergence error as was derived from the convergence of the iterations.

6. The optimum values of the parameters for the present program and $M_1 = 2.5$ are $J = 9$ and $N_7 = 15$, corresponding to a 3.5 hour computer run for 12 iterations.

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4. This technique of "forward and backward" integration insures stability of the numerical integration process with respect to the independent variable n (or x).

5. See the next section for a discussion of the random errors in f in the interior of the shock.

6. We specify standard deviations rather than "likely" errors here because of the non-random nature of the systematic errors.

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Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)*
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2a. REPORT SECURITY CLASSIFICATION
Unclassified

2b. GROUP

3. REPORT TITLE
NUMERICAL STUDIES OF STRONG SHOCK WAVES PART IX: ERROR ANALYSIS FOR A MACH NUMBER 2.5

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

5. AUTHOR(S) *(First name, middle initial, last name)*
Hicks, B.L. & Smith, M.A.

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
April, 1967	22	6

8a. CONTRACT OR GRANT NO.
DA 28 043 AMC 00073(E)
b. PROJECT NO. 20014501B31F; Also in part ONR N00014-66-C0010-A01
c.
d.

9a. ORIGINATOR'S REPORT NUMBER(S)
R-348

9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*

10. DISTRIBUTION STATEMENT
DISTRIBUTION OF THIS REPORT IS UNLIMITED.

11. SUPPLEMENTARY NOTES

12. SPONSORING MILITARY ACTIVITY
Joint Services Electronics Program
thru U. S. Army Electronics Command
Fort Monmouth, New Jersey 07703

13. ABSTRACT

Data from 43 computer runs makes possible a study of the Monte Carlo, iterative solutions of the Boltzmann difference equations for a strong shock wave ($M_1 = 2.5$). Estimates have been made of errors associated with iterative convergence, Monte Carlo sampling, number of stations in the shock and variations of the sero-th iterate.

Specific results are summarized at the end of the report.

DD FORM 1 NOV 65 1473 (PAGE 1)
S/N 0101-807-6811

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Boltzmann Equation						
Collision Integral						
Monte Carlo						
Statistical Sampling						
Distribution Function						
Shock Wave						
Translation Relaxation						
Pseuto-shock						
Eleastic Sphere						
Convergence						
Iteration Scheme						