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Direct Simulation and the Boltzmann Equation

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The direct simulation Monte Carlo method for the numerical solution of problems in rarefied gas dynamics is described and discussed. It is shown that the procedures adopted in this method can be directly related to the Boltzmann equation and that the two are entirely consistent. It is concluded that the results obtained from the method constitute a solution of the Boltzmann equation.

I. INTRODUCTION

A numerical method, generally called the direct simulation Monte Carlo method, has been developed for the study of rarefied gas flows.¹⁻⁸ Significant refinements have been made in the method over the past six years and the results of the more recent calculations are in excellent agreement with available experimental data. The general approach during the development of the method has been the physical simulation of the real gas flow rather than the solution of the equations describing the flow. Applications of the method can, therefore, be regarded as numerical experiments and, as a consequence, there has been confusion about the relationship between the results and a hypothetical exact solution of the Boltzmann equation.

It can be argued that the basic assumptions of the method concerning the molecular structure of the gas are common to the Boltzmann equation and that the physical modeling leads to an "implicit" solution of the Boltzmann equation. However, it has been clear that the results have not been accepted as having the authority that would be accorded to an explicit numerical solution of the Boltzmann equation. In fact, it has often been suggested that there is an element of arbitrary choice associated with the random sampling techniques in the Monte Carlo method, and that this could possibly be identified with a distortion of the Boltzmann equation. If this were the case, the results of the simulation could only be justified by comparison with experiment and the method could not be applied with confidence when this support is lacking.

The purpose of this paper is to show that there is a direct and unambiguous relationship between the random sampling technique and the Boltzmann equation. It follows that there is nothing arbitrary about the simulation procedures and the results given by the method constitute an exact numerical solution of the Boltzmann equation.

The method is described in the following section on the assumption that the gas comprises a single species with molecules obeying an inverse power law of repulsion. This model includes hard sphere and Maxwell molecules as special cases, but the method is not restricted to it. Applications have been made to the flow of binary gas mixtures,⁴ and molecules with internal degrees of freedom are currently being treated. The numerical requirements for the proper implementation of the method are now well defined and are also discussed. It should be emphasized that the method is quite distinct from the Monte Carlo methods developed by Havilland⁹ and by Hicks and Nordsieck.¹⁰

II. DESCRIPTION OF SIMULATION TECHNIQUE

The direct simulation Monte Carlo method is a technique for the computer modeling of a real gas flow by several thousand simulated molecules. The velocity components and position coordinates of the simulated molecules are stored in the computer and these are modified with time as the molecules are concurrently followed through representative collisions and boundary interactions in simulated physical space.

The initial state of the gas is specified and boundary conditions designed to produce the required flow are applied at zero time. The flow is always unsteady, but the boundary conditions may be such that a steady flow is obtained as the large time state of the unsteady flow. The simulated region is divided into a network of spatial cells with dimensions Δx , such that the change in flow properties across each cell is small. Time is advanced by discrete steps of magnitude Δt small compared with the mean free time per molecule. Both Δx , and Δt may vary with time and position.

The molecular motion and the collision processes are uncoupled over the time interval Δt by the repeated application of the following procedure:

(i) All the molecules are moved through distances appropriate to their instantaneous velocity components and Δt .

(ii) A representative set of collisions, appropriate to Δt , is computed among the molecules, and the pre-collision velocity components of those molecules involved in the collisions are replaced by the post-collision values.

Therefore, along any molecular path, collisions can only occur at intervals that are integral multiples of Δt . Since Δt is small compared with the mean free time, the resulting distortion of the path is small.

The collisions must be a representative sample of those occurring in the corresponding flow of a real gas. The procedure for a gas of point center of repulsion molecules is as follows:

(a) Since the change in flow properties across a cell is small, the molecules in a cell at any instant may be regarded as a sample of the molecules at the location of the cell. This means that the relative positions of the molecules in the cell may be disregarded and any pair of molecules chosen at random forms a possible collision pair. However, the collision probability is proportional to $g^{(\nu-5)/(\nu-1)}$ where g is the magnitude of the relative velocity and ν is the exponent in the force law. The randomly chosen pair must, therefore, be retained or rejected according to this probability.

(b) When a pair of molecules is retained for collision, appropriate random impact parameters are chosen and the post-collision velocity components are calculated.

(c) A time counter is conveniently kept for each cell and, for each collision, it is advanced by an amount

$$\Delta t_c = (2/N_c)[\pi W_m^2 (2\kappa)^{2/(\nu-1)} n g^{(\nu-5)/(\nu-1)}]^{-1}. \quad (1)$$

Here, N_c is the total number of molecules in the cell, W_m is the cutoff value of the dimensionless impact parameter, κ is the constant in the force law, and n is the number density. Sufficient collisions are computed in each cell to keep the time counters concurrent with the over-all time parameter.

The cell network usually forms a convenient reference for the periodic sampling of the macroscopic gas properties. The only one of these that is required in the method itself is the number density which appears in Eq. (1). The fluxes of the various molecular properties may, of course, be sampled at the boundaries.

A major advantage of the simulation method is

that boundary conditions are specified in terms of the probable behavior of the individual molecules encountering the boundary, rather than by the form of the distribution function in the vicinity of the boundary. For collisions with solid surfaces, any desired surface interaction law is readily applied.

Finite computer storage imposes limitations on both the total number of simulated molecules and the number of cells. The statistical scatter in the results is inversely proportional to the square root of the sample size. An ensemble average may be taken over repeated independent calculations of an unsteady flow in order to reduce the scatter to an acceptable level. If the flow becomes steady at large times, the required sample size may be built up by time averaging at sufficiently long intervals for the individual samples to be independent. It has generally been found that the scatter in the results is consistent with the total sample size irrespective of whether this is obtained from, for example, 100 samples with an average of 10 molecules per cell or 10 samples with 100 molecules per cell. It will be shown in Sec. III that the number of molecules per cell (N_c) should be such that the factor $2/N_c$ in Eq. (1) is small compared with unity. In practice, a great deal depends on the degree of nonequilibrium. For flows which involve comparatively small departures from equilibrium, consistent results may be obtained with as few as four molecules per cell. On the other hand, it has been found that there should be at least 20 simulated molecules per cell when computing the upstream region of a very strong shock wave.

Experience also shows that no spurious effects are introduced by the computational approximations of finite Δx and Δt as long as these satisfy the individual criteria discussed earlier and an additional condition that the ratio $\Delta x/\Delta t$ should not be large compared with the speed of propagation of acoustic disturbances. The reason for this additional condition is readily seen if one considers the example of a shock wave moving to the right. At a particular time, the leading edge will have just penetrated the left-hand boundary of some cell. Since the actual locations of the molecules in a cell are disregarded when computing the collisions for a cell, one of the disturbed molecules at the far left of the cell may collide with one in the undisturbed gas near the right-hand boundary. This latter molecule will then be affected by the wave and could move into the next cell to the right when all the molecules are moved. It is, therefore, possible that a spurious signal could be propagated with speed $\Delta x/\Delta t$. However, this

would require a highly improbable sequence of collisions affecting molecules near the boundaries of successive cells, and it has been found that this ratio must be several times the shock speed before the profile is affected. Moreover, the effective ratio may be reduced by placing a restriction on the spacing of molecules when choosing possible collision pairs.

The method has been applied to a wide variety of problems and there has never been any sign of instability in its operation. When the above requirements regarding sample size, cell dimensions, and time step are satisfied, the results are independent of these quantities and are altogether consistent and repeatable. The underlying physical assumptions of molecular chaos and an ordering of molecular dimensions such that only binary collisions need be considered are common to the Boltzmann equation.

III. RELATIONSHIP TO THE BOLTZMANN EQUATION

The Boltzmann equation for a monatomic gas is usually written

$$\frac{\partial(nf)}{\partial t} + u_i \frac{\partial(nf)}{\partial x_i} + F_i \frac{\partial(nf)}{\partial u_i} = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2(f'f'_1 - ff_1)g\sigma d\Omega dU_1, \quad (2)$$

where $f(u_i, x_i, t)$ is the normalized distribution function, u_i is the molecular velocity, σ is the differential cross section, $d\Omega$ is an element of solid angle, F_i is an external force per unit mass, and dU is an element of velocity space. The subscript 1 denotes the collision partner and the prime denotes the post-collision quantities. In the case of point center of repulsion molecules,

$$\sigma d\Omega = W(2\kappa/g^2)^{2/(\nu-1)} dW d\epsilon, \quad (3)$$

where W is the nondimensional impact parameter in the center of mass frame and ϵ is the azimuthal angle. The total cross section is

$$\begin{aligned} \int_0^{4\pi} \sigma d\Omega &= \int_0^{2\pi} \int_0^W W \left(\frac{2\kappa}{g^2} \right)^{2/(\nu-1)} dW d\epsilon \\ &= \pi W_m^2 \left(\frac{2\kappa}{g^2} \right)^{2/(\nu-1)}. \end{aligned}$$

The appropriate form of the Boltzmann equation is, therefore,

$$\begin{aligned} \frac{\partial(nf)}{\partial t} + u_i \frac{\partial(nf)}{\partial x_i} + F_i \frac{\partial(nf)}{\partial u_i} \\ = \pi W_m^2 (2\kappa)^{2/(\nu-1)} \int_{-\infty}^{\infty} n^2(f'f'_1 - ff_1)g^{(\nu-5)/(\nu-1)} dU_1. \end{aligned} \quad (4)$$

The right-hand side of this equation is the collision term and the left-hand side states that, in the absence of collisions, nf remains constant if one moves along with the molecules in phase space. In the Monte Carlo method, the distribution function is replaced by a finite number of simulated molecules located, at any instant, at particular points in phase space. The path of these molecules is followed exactly in phase space and the left-hand side of the Boltzmann equation is obviously satisfied.

The collision term is conveniently subdivided into the gain and loss terms, the latter representing the rate of scattering by collisions out of the phase space element $dU dX$ per unit volume of the element. This rate may be derived from the Monte Carlo procedure by the following argument.

The spatial cell in the simulated flow may be regarded as the element dX of physical space and the set of N_c molecules in the cell defines the distribution function f . The number of molecules of class u within the cell at time t is $nf dU dX$ or $N_c f dU$. Now consider a collision between a molecule of this class with one of class u_1 . The probability of finding a molecule in class u_1 is $f_1 dU_1$ and the time interval that would be added to a counter kept *only* for collisions of the class u molecule is given from Eq. (1) as

$$\Delta t_c = [\pi W_m^2 (2\kappa)^{2/(\nu-1)} n g^{(\nu-5)/(\nu-1)}]^{-1}. \quad (5)$$

The collision rate for collisions of molecules of class u with those of class u_1 follows as

$$N_c f dU f_1 dU_1 \pi W_m^2 (2\kappa)^{2/(\nu-1)} n g^{(\nu-5)/(\nu-1)}$$

or

$$\pi W_m^2 (2\kappa)^{2/(\nu-1)} n^2 f f_1 g^{(\nu-5)/(\nu-1)} dU_1 dU dX.$$

The total rate of scattering out of the class u per unit volume in phase space is obtained by integrating the class u_1 over all velocity space and dividing by $dU dX$, i.e.,

$$\pi W_m^2 (2\kappa)^{2/(\nu-1)} \int_{-\infty}^{\infty} n^2 f f_1 g^{(\nu-5)/(\nu-1)} dU_1 \quad (6)$$

which agrees with the loss term in Eq. (4).

It is apparent that the Monte Carlo method would be more directly comparable to the Boltzmann equation if a time counter was assigned to each molecule and was advanced by the interval given by Eq. (5) for each collision. Instead, a single time counter is kept for all the N_c molecules within the cell and, since each collision involves two molecules, the factor $2/N_c$ enters Eq. (1) as compared with Eq. (5). It is also necessary to decide which of the

many molecules in the cell are to be chosen for the "next" collision. The above analysis of the loss term shows that the only property of the individual molecules that contributes to the term is the relative velocity between the pair raised to the power $(\nu - 5)/(\nu - 1)$. This leads directly to step (ii) (a) in the description of the method in Sec. II. While the procedures for the selection of the collision pair and the advancing of the time parameter have been justified separately, it is shown in the next section that their combination leads to the correct collision frequency irrespective of the form of the distribution function.

The advancing of a time counter by the appropriate time interval is a means of obtaining a representative set of collisions over a long time. However, the resultant spacing in time of the individual collisions is correlated directly with the probability of occurrence of each collision, depending only on the relative velocity between the collision partners. This is physically unreal since the actual collision interval will also depend on the relative locations of the individual molecules. This undesirable direct correlation is effectively removed if the number of molecules in a cell is large, so that the factor $2/N_c$ which multiplies each time increment is small compared with unity. Referring to the simulation of a very strong shock wave as an example, at the leading edge of the wave there will be a few molecules affected by the wave and these will have large relative velocities with respect to the undisturbed molecules. An unlikely collision between two undisturbed molecules would add a comparatively long interval to the time counter for that cell. If the number of molecules in the cell were very small, this interval could be larger than the over-all mean collision time. It has been found that there is a slight distortion of the upstream region of very strong shock waves unless there are at least 20 molecules per cell.

The gain term in the Boltzmann equation is derived by analogy with the loss term through the existence of inverse collisions for simple models of monatomic molecules. The Monte Carlo method deals with a *closed set* of molecules from which both collision partners are selected, and the pre-collision velocity components are replaced by the post-collision values. This means that the correct choice of collision pairs, as demonstrated by the analysis of the loss term, together with the appropriate random selection of impact parameters automatically assures the correct "gain term." This holds irrespective of the existence of inverse collisions. The Monte

Carlo method can, therefore, be readily extended to molecules with internal degrees of freedom.

IV. COLLISION FREQUENCY

The direct simulation Monte Carlo method deals with sets of molecules in elements of physical space, while the dependent variable in the Boltzmann equation describes the molecules in an element of phase space. It would, therefore, be expected that the most direct comparison would be based on a quantity obtained from the Boltzmann equation through integration over velocity space. The obvious choice is the over-all collision frequency in the gas.

The Boltzmann result is obtained from the loss term which is first multiplied by $dU dX$ to convert it to the collision rate for molecules of class u . It is then integrated over all velocity space to give the over-all collision rate for the element dX of physical space as

$$\pi n^2 W_m^2 (2\kappa)^{2/(\nu-1)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f f_1 g^{(\nu-5)/(\nu-1)} dU dU_1 dX.$$

The number of molecules in the element is $n dX$, so the mean collision rate per molecule is

$$\zeta = \pi n W_m^2 (2\kappa)^{2/(\nu-1)} g^{(\nu-5)/(\nu-1)}. \quad (7)$$

Now turning to the Monte Carlo method, there are N_c molecules in a particular cell and the total number of possible collision pairs is $N_p = N_c(N_c - 1)/2$. Therefore, g has a set of possible values g_m , where $m = 1, \dots, N_p$. Now, let g_0 be some fixed reference value of g which, to a particular time t , has a probability of occurrence P . Since the pairs are chosen with probability proportional to $g^{(\nu-5)/(\nu-1)}$, the probability of occurrence of g_m is

$$P(g_m/g_0)^{(\nu-5)/(\nu-1)}.$$

The total number of collisions to this time is obtained by summing over all possible collision pairs, i.e.,

$$\sum_{m=1}^{N_p} P\left(\frac{g_m}{g_0}\right)^{(\nu-5)/(\nu-1)} = \left(\frac{P}{g_0^{(\nu-5)/(\nu-1)}}\right) \sum_{m=1}^{N_p} g_m^{(\nu-5)/(\nu-1)}. \quad (8)$$

Equation (1) shows that the time will be

$$t = \sum_{m=1}^{N_p} \left(\frac{2}{N_c}\right) \cdot \{\pi n W_m^2 (2\kappa)^{2/(\nu-1)} g_m^{(\nu-5)/(\nu-1)}\}^{-1} P\left(\frac{g_m}{g_0}\right)^{(\nu-5)/(\nu-1)}$$

and, since g_m disappears,

$$t = P(2/N_c) [\pi n W_m^2 (2\kappa)^{2/(\nu-1)} g_0^{(\nu-5)/(\nu-1)}]^{-1} N_p. \quad (9)$$

The total number of collisions per unit time is, therefore,

$$\left(\frac{N_c}{2}\right)\pi n W_m^2 (2k)^{2/(\nu-1)} \left(\frac{1}{N_p}\right) \sum_{m=1}^{N_p} g_m^{(\nu-5)/(\nu-1)}$$

or

$$(N_c/2)\pi n W_m^2 (2k)^{2/(\nu-1)} \overline{g^{(\nu-5)/(\nu-1)}}.$$

Since each collision involves two molecules, the mean collision rate per molecule is

$$\zeta = \pi n W_m^2 (2k)^{2/(\nu-1)} \overline{g^{(\nu-5)/(\nu-1)}} \quad (10)$$

which is identical to the result obtained from the Boltzmann equation.

V. MOLECULAR MAGNITUDES AND STATISTICAL FLUCTUATIONS

The significant quantities are the effective molecular diameter σ (assumed constant in this discussion), the mean distance between molecules $d = n^{1/3}$, and the molecular mean free path λ given by $(2^{1/2}\pi\sigma^2n)^{-1}$ in an equilibrium gas. The "dilute-gas" assumption on which the Boltzmann formulation depends is customarily expressed through the ordering $\lambda \gg d \gg \sigma$. Both λ/d and d/σ may be related to the number of molecules in a cubic element with linear dimensions equal to λ . In fact, $\lambda/d > 10$ and $d/\sigma > 7$ each correspond to

$$n\lambda^3 > 10^3. \quad (11)$$

For molecular dimensions based on the coefficient of viscosity, a typical value of $n\lambda^3$ for a gas under standard conditions is 10^4 ; therefore, at density n ,

$$n\lambda^3 = 10^4(n_0/n)^2. \quad (12)$$

In applications of the Monte Carlo method a typical cell dimension is $\lambda/3$, with approximately 30 simulated molecules per cell. For a cubic cell this corresponds to the limit of Eq. (11). Larger cells and/or a smaller number of molecules are frequently employed and it might appear that this would infringe the dilute gas assumption. However, there are several independent reasons why this is not so.

(i) A molecular "size" enters the simulation only through Eq. (1) which effectively determines the collision frequency. As far as the molecular motion and boundary interactions are concerned, the molecules are assumed to have negligible dimensions. In fact, it is valid to consider each simu-

lated molecule as representing an arbitrary number of real molecules with the velocity components and position coordinates of the simulated molecules being mean values. This approach is adopted when "weighting factors" are applied to the molecules in order to equalize sample sizes in the simulation of gas mixtures with large concentration ratios, or flows which necessarily involve large variations in cell volume.

(ii) The cell dimensions are completely specified only in three-dimensional flows. In the case of a two-dimensional flow, the simulation may be regarded as applying to an arbitrarily thin "slice" of the real flow. The thickness of the slice could be chosen such that the number of simulated molecules corresponds with the actual number. The cross-sectional area of a one-dimensional flow is similarly adjustable.

The second argument leads to a physical interpretation of the statistical fluctuations. When the thickness of a two-dimensional region or the cross-sectional area of a one-dimensional region are chosen so that the number of real and simulated molecules are equal, the scatter is physically real and should not be regarded as an "error." It would, of course, be desirable to increase the dimensions of the simulated region to such an extent that the scatter is negligible. However, the standard deviation of the scatter falls only as the square root of the sample size and practical limitations on computer time mean that a certain level of scatter must be tolerated. This places a limit on the smallness of a disturbance that can be studied, since the "signal" must be distinguished from the inevitable "noise."

A three-dimensional flow does not have any unspecified dimensions and the scatter has physical meaning only when the number of simulated molecules is consistent with Eq. (12). This equation shows that the number of molecules in a region with dimensions of the order of the mean free path is inversely proportional to the square of the density. At very low densities, the number of molecules in the simulated flow will be extremely small compared with the real number. However, in the case of a shock wave at standard density, the number and, therefore, the fluctuations in the simulated flow could well correspond exactly with those in the real flow.

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