Direct simulation for a homogeneous gas

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A probabilistic analysis of the direct simulation of a homogeneous gas is given. A hierarchy of equations similar to the BBGKY hierarchy for the reduced probability densities is derived. By invoking the molecular chaos assumption, an equation similar to the Boltzmann equation for the single particle probability density and the corresponding H-theorem is derived.

I. INTRODUCTION

Direct simulation Monte Carlo method (DSMC) is a standard method for solving the Boltzmann equation numerically. In this method space is divided into cells of volume $\Delta V$ and a large number of “particles” ($N = 10^3–10^6$) represent the real gas molecules. The evolution of the gas for a short time $\Delta t$ is calculated in two steps. In the first step all particles are propagated for a time $\Delta t$ without collisions. In the second step some randomly chosen pairs of particles in the same cell are allowed to collide and change their velocities without changing their positions. Number of pairs ($n$) chosen to make collision attempts is given by the formula $n = RN^2\Delta t/2V$ where $R$ is a parameter we choose, $N$ is the number of particles in the cell and $V$ is the volume of the cell. We call $n$ number of collision attempts because not every chosen pair makes a collision. A pair is allowed to make a collision with a probability $u\sigma_T/R$, where $u$ is their relative velocity and $\sigma_T$ is the total cross section. The results are not sensitive to value of the parameter $R$ as long as it is big enough such that very few pairs violate the condition $u\sigma/R \leq 1$ since average number of successful collision attempts

$$n \langle u\sigma_T \rangle / R = RN^2\Delta t \langle u\sigma_T \rangle / 2V R = N^2 \langle u\sigma_T \rangle / 2V \Delta t,$$

is independent of $R$. Here $\langle u\sigma_T \rangle$ is the average of $u\sigma_T$ over all possible pairs. Although taking a very big $R$ is acceptable theoretically, for practical reasons $R$ should not chosen be too big either.

The original method is due mainly to G. A. Bird. A seminal paper\textsuperscript{1} of Bird gave some
heuristic arguments to justify its use. There are many good references on the subject. Ref. 2 has a good tutorial on the subject and Ref. 3 is a monograph on the subject by Bird himself which is a complete reference for the developments up to its publication year 1994. Also books on rarified gas dynamics devote many chapters to the subject and Ref. 4 and Ref. 5 are useful references in this category.

A variant of the method was derived by Nanbu starting from the Boltzmann equation. To represent the evolution of the real gas such methods should converge to the true solution of the Boltzmann equation in the limit $N \to \infty$, $∆V \to 0$, and $∆t \to 0$. Convergence proofs were given by Babovsky and Babovsky and Illner for Nanbu’s method and by Wagner for Bird’s method.

For the evolution of the velocity distribution of a spatially uniform gas there is no need to divide physical space into cells and we can just work in velocity space. Although Bird recommended dividing real space into cells for studying the spatially homogeneous gas, we will show that this division is unnecessary. If we consider velocity space only and collide random pairs, we should obtain the evolution of the velocity distribution. The purpose of this paper is to study this stochastic process.

These efforts to solve the Boltzmann equation using stochastic methods were driven by scientific applications and there was no motivation to use them as a pedagogical tool. It is surprising that similar stochastic algorithms for the homogeneous gas were conceived by people interested in using them as a pedagogical tool to demonstrate the evolution of a gas to the Maxwell-Boltzmann distribution. The earliest of such articles of which the author is aware is that of Novak-Bortz who studied the evolution of a gas of two-dimensional disks. Their algorithm is based on taking random pairs and colliding them with a probability proportional to $uσ$. Eger and Kress modified this algorithm and Bonomo and Riggi applied the modification to hard disks. There are also other papers that do not use DSMC type stochastic processes to demonstrate the Maxwell-Boltzmann distribution. Although the DSMC method was well known, these papers do not reference papers on DSMC. Apparently the idea of stochastic methods for the evolution of a homogeneous gas was conceived for pedagogical applications independently.

As mentioned, the DSMC algorithm can be used to demonstrate the approach of a velocity distribution to the Maxwell-Boltzmann distribution. The algorithm also gives an estimate of how many collisions is required to reach equilibrium and how various parameters affect
the evolution of the system.

Although direct simulation is intuitively appealing, it is not clear that direct simulation algorithms represent the evolution of a real gas. The convergence proofs we have cited are formal and difficult to read. In this paper we prove that in the direct simulation appropriately normalized single particle probability distribution satisfies the Boltzmann equation for a homogeneous gas. The proof is relatively easy and intuitively appealing and also its language is familiar to the physicist from the well known BBGKY hierarchy.\(^{15}\)

In Sec. II we consider the stochastic algorithm for a homogeneous gas. We derive a hierarchy of equations for the probability distribution of particles similar to the BBGKY hierarchy.\(^{15}\) We use the molecular chaos assumption to derive an equation similar to the Boltzmann equation for the single particle probability distribution \(f(v)\). We derive an H-theorem for \(f(v)\) and prove convergence to equilibrium. We also show how the equation for \(f(v)\) reduces to the Boltzmann equation for a particular choice of collision probabilities and derive Bird’s “time counter” and “no time counter” methods.

**II. ANALYSIS OF THE DIRECT SIMULATION ALGORITHM FOR A HOMOGENEOUS GAS**

Consider a homogeneous gas of \(N \gg 1\) molecules without internal degrees of freedom. We randomly select pairs of molecules to collide. All possible pairs have an equal probability of \(2/(N - 1)N\) to be selected. Suppose the velocities of the pair are \(v_A\) and \(v_B\). The conditional probability that after the collision they have the velocities \(v_C\) and \(v_D\) in the intervals \(d^3v_C\) and \(d^3v_D\) is \(T(v_A, v_B; v_C, v_D) d^3v_C d^3v_D\). (From now on we will denote \(d^3v\) as \(dv\) for simplicity.) We also assume the symmetries

\[
T(v_A, v_B; v_C, v_D) = T(v_C, v_D; v_A, v_B) \tag{1a}
\]

\[
T(v_A, v_B; v_C, v_D) = T(v_B, v_A; v_D, v_C). \tag{1b}
\]

The total probability is unity and therefore

\[
\int T(v_A, v_B; v_C, v_D) dv_C dv_D = \int T(v_A, v_B; v_C, v_D) dv_A dv_B = 1. \tag{2}
\]

Every selected pair makes a collision, although as we will show, by defining \(T(v_A, v_B; v_C, v_D)\) some of the collisions do not change velocities. After each collision new velocities of the
molecules are replaced by the old ones, and we select a new pair for the next collision. Of course there is the possibility of choosing the same pair with a very small probability. If that happens we let them collide again. We don’t keep record of pairs that have made collisions already.

We define \( f^{(N)}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N) \) as the probability density for the molecules. Because the molecules are indistinguishable, we require that the \( f^{(N)} \) be totally symmetric:

\[
 f^{(N)}(\mathbf{v}_1, \ldots, \mathbf{v}_i, \ldots, \mathbf{v}_j, \ldots, \mathbf{v}_N) = f^{(N)}(\mathbf{v}_1, \ldots, \mathbf{v}_j, \ldots, \mathbf{v}_i, \ldots, \mathbf{v}_N). 
\]  

(3)

We also define the reduced probability densities

\[
 f^{(M)}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M) = \int f^{(N)}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N) \, d\mathbf{v}_{M+1} \, d\mathbf{v}_{M+2} \ldots d\mathbf{v}_N.
\]  

(4)

Because we will be dealing with pairs of particles, it is useful to define

\[
 f^{(M)}_{i,j}(\mathbf{v}_A, \mathbf{v}_B) = f^{(M)}(\mathbf{v}_1, \ldots, \mathbf{v}_i = \mathbf{v}_A, \ldots, \mathbf{v}_j = \mathbf{v}_B, \ldots, \mathbf{v}_M).
\]  

(5)

That is, the velocities of the \( i, j \) pair are replaced by \( \mathbf{v}_A, \mathbf{v}_B \) in the \( f^{(M)}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M) \) where \( i, j \leq M \). We will also use the notation \( f^{(M)}(\mathbf{v}; n) \) for \( f^{(M)}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M) \) after the \( n^{th} \) collision.

The function \( f^{(N)}(\mathbf{v}; n) \) satisfies the equation

\[
 f^{(N)}(\mathbf{v}; n + 1) = \frac{1}{N(N-1)} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \int f^{(N)}_{i,j}(\mathbf{v}_A, \mathbf{v}_B; n) T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_i, \mathbf{v}_j) \, d\mathbf{v}_A \, d\mathbf{v}_B.
\]  

(6)

The meaning of Eq. (6) is clear. If \( i, j \) is the last pair of molecules that has collided, then the probability of having \( \mathbf{v}_i, \mathbf{v}_j \) pairs after the collision is the probability of having initial velocities \( \mathbf{v}_A, \mathbf{v}_B \) (represented by \( f^{(N)}_{i,j}(\mathbf{v}_A, \mathbf{v}_B) \)) multiplied by the probability of ending with \( \mathbf{v}_i, \mathbf{v}_j \) (represented by \( T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_i, \mathbf{v}_j) \)). The sum over \( i, j \) and the factor \( 1/N(N-1) \) in Eq. (6) represents the fact that all pairs are possible with probability \( 1/N(N-1) \).

If we integrate Eq. (6) over \( \mathbf{v}_{M+1}, \mathbf{v}_{M+2}, \ldots, \mathbf{v}_N \), we obtain

\[
 f^{(M)}(\mathbf{v}; n + 1) = \frac{(N-M)(N-M-1)}{N(N-1)} f^{(M)}(\mathbf{v}; n)
\]  

\[
 + \frac{2(N-M)}{N(N-1)} \sum_{i=1}^{M} \int f^{(M+1)}_{i,M+1}(\mathbf{v}_A, \mathbf{v}_B; n) T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_i, \mathbf{v}_{M+1}) \, d\mathbf{v}_A \, d\mathbf{v}_B \, d\mathbf{v}_{M+1}
\]  

\[
 + \frac{M(M-1)}{N(N-1)} \sum_{i=1}^{M} \sum_{j \neq i}^{M} \int f^{(M)}_{i,j}(\mathbf{v}_A, \mathbf{v}_B; n) T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_i, \mathbf{v}_j) \, d\mathbf{v}_A \, d\mathbf{v}_B.
\]  

(7)
The \( f^{(M)}(v; n + 1) \) depends on \( f^{(M+1)}(v; n) \); Eq. (7) represents a hierarchy of equations similar to the BBGKY hierarchy.\(^{15} \)

The first equation in the hierarchy is

\[
\begin{align*}
  f^{(1)}(v; n + 1) &= (1 - 2/N)f^{(1)}(v; n) \\
  &+ \frac{2}{N} \int f^{(2)}(v_A, v_B; n)T(v_A, v_B; v_C, v)dv_A dv_B dv_C. 
\end{align*}
\]

(8)

If we make the assumption of molecular chaos

\[
  f^{(2)}(v_A, v_B; n) = f^{(1)}(v_A; n)f^{(1)}(v_B; n),
\]

(9)

we obtain a nonlinear equation for \( f^{(1)}(v; n) \) similar to the Boltzmann equation. For large \( N \) this approximation is almost exact as shown by the following argument. The velocities \( v_1, v_2 \) can be correlated only if particles one and two have collided with each recently. But this probability is of order \( 1/N \), which implies that for large \( N \), the velocity distributions of any two particles are uncorrelated. Present personal computers can handle \( N = 10^5 - 10^6 \) so the assumption is almost exact.

The key assumption in the argument for the validity of Eq. (9) is “recently.” Two particles might be correlated for a short time, but after they have made a few collisions with other particles the correlations are expected to disappear.

Another simplification occurs for large \( N \). The factor of \( 2/N \) in Eq. (8) is small and thus we can consider \( \tau = 2n/N \) to be a continuous parameter which we call the collision time. Then \( \Delta \tau = 2/N \) and \( [f^{(1)}(v; n + 1) - f^{(1)}(v; n)]/\Delta \tau \) can be written as \( \partial f^{(1)}(v; \tau)/\partial \tau \) and Eq. (8) becomes

\[
\frac{\partial f^{(1)}(v; \tau)}{\partial \tau} = -f^{(1)}(v; \tau) + \int f^{(1)}(v_A; \tau)f^{(1)}(v_B; \tau)T(v_A, v_B; v_C, v)dv_A dv_B dv_C. \]

(10)

From now on we will suppress the superscript (1) and the collision time \( \tau \) in \( f^{(1)}(v; \tau) \). Equation (10) can be expressed as

\[
\frac{\partial f(v)}{\partial \tau} = -f(v) + \int f(v_A)f(v_B)T(v_A, v_B; v_C, v)dv_A dv_B dv_C. \]

(11)

A. The H-theorem and approach to equilibrium

By using the relation

\[
f(v) = \int f(v)f(v_C)T(v_A, v_B; v_C, v)dv_A dv_B dv_C, \]

(12)
which follows from Eq. (2) and the normalization of \( f(v_C) \), we can write Eq. (11) as
\[
\frac{\partial f(v)}{\partial \tau} = \int [f(v_A)f(v_B) - f(v)f(v_C)] T(v_A,v_B;v_C,v) \, dv_A \, dv_B \, dv_C. 
\tag{13}
\]
This form is similar to the Boltzmann equation.

We can derive an H-theorem for this equation. We define
\[
H(\tau) = \int f(v) \ln(f(v)) \, dv, 
\tag{14}
\]
and use Eqs. (1) and (13) to express \( dH/d\tau \) as
\[
\frac{dH}{d\tau} = -\frac{1}{4} \int \Psi[f] T(v_A,v_B;v_C,v) \, dv_A \, dv_B \, dv_C \, dv, 
\tag{15}
\]
where
\[
\Psi[f] = [f(v_A)f(v_B) - f(v)f(v_C)] \left[ \ln f(v_A)f(v_B) - \ln f(v)f(v_C) \right]. 
\tag{16}
\]
The function \( \Psi[f] \) can be shown to be always nonnegative. We argue that \((x - y)(\ln x - \ln y)\) is nonnegative for all positive \( x \) and \( y \); \( \ln x \) is an increasing function and thus \( x - y \) and \( \ln x - \ln y \) always have the same sign. Their product is always either positive or zero and zero occurs for \( x = y \). \( T(v_A,v_B;v_C,v) \) is intrinsically positive. Therefore the integrand is positive and \( dH/d\tau \) is negative.

Following the usual arguments of the H-theorem, the decrease of \( H \) stops only when
\[
\ln f(v_A) + \ln f(v_B) = \ln f(v) + \ln f(v_C) 
\tag{17}
\]
is satisfied, which implies that \( \ln f(v) \) is a collision invariant. If we choose \( T(v_A,v_B;v_C,v) \) such that the total momentum and energy is conserved in each collision, then \( \ln f(v) \) must be expressible as a linear combination of these collision invariants as
\[
\ln f(v) = \frac{m}{2\Theta} (v - v_0)^2 + \text{constant}, 
\tag{18}
\]
where \( \Theta \) is the temperature in energy units \((k_B = 1)\) and \( m \) is the mass of a molecule. Here \( v_0 \) is the velocity of the center of mass of the system. Hence we have shown that the system approaches the Maxwell-Boltzmann distribution.

B. Structure of \( T(v_A,v_B;v_C,v) \), and connection with the Boltzmann equation

We define new variables
\[
v_T = (v_A + v_B)/2, \quad u = v_A - v_B, \quad u = |u| 
\tag{19a}
\]
\[
v'_T = (v + v_C)/2, \quad u' = v_C - v, \quad u' = |u'|, 
\tag{19b}
\]

where \( \mathbf{v}_T \) and \( \mathbf{v}'_T \) are the center of mass velocities before and after the collision. The Jacobian of the transformation is unity and integrations can be written in terms of the new variables. Momentum conservation is imposed on \( T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_C, \mathbf{v}) \) as

\[
T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_C, \mathbf{v}) = \delta^3(\mathbf{v}_T - \mathbf{v}'_T)G(\mathbf{u}, \mathbf{u}').
\tag{20}
\]

The integral in Eq. (11) is then written as

\[
I = \int f(\mathbf{v}_A)f(\mathbf{v}_B)T(\mathbf{v}_A, \mathbf{v}_B; \mathbf{v}_C, \mathbf{v}) \, d\mathbf{v}_A \, d\mathbf{v}_B \, d\mathbf{v}_C
\tag{21a}
\]

\[
= \int f(\mathbf{v} + \frac{\mathbf{u}' + \mathbf{u}}{2})f(\mathbf{v} - \frac{\mathbf{u} - \mathbf{u}'}{2})G(\mathbf{u}, \mathbf{u}') \, d\mathbf{u} \, d\mathbf{u}'.
\tag{21b}
\]

The conditions in Eqs. (1) and (2) become for \( G(\mathbf{u}, \mathbf{u}') \):

\[
\int G(\mathbf{u}, \mathbf{u}') \, d\mathbf{u} = \int G(\mathbf{u}, \mathbf{u}') \, d\mathbf{u}' = 1,
\tag{22}
\]

\[
G(\mathbf{u}, \mathbf{u}') = G(\mathbf{u}', \mathbf{u}).
\tag{23}
\]

Energy conservation requires that \( u = u' \). If we define unit vectors \( \mathbf{\hat{u}} = \mathbf{u}/u \) and \( \mathbf{\hat{u}'} = \mathbf{u}'/u \) and the angle \( \theta \) between them as \( \cos \theta = \mathbf{\hat{u}} \cdot \mathbf{\hat{u}'} \), we can write \( G(\mathbf{u}, \mathbf{u}') \) as

\[
G(\mathbf{u}, \mathbf{u}') = \frac{\delta(u' - u)}{u^2}g(\theta, u).
\tag{24}
\]

The condition in Eq. (22) becomes for \( g(\theta, u) \):

\[
\int g(\theta, u) \, d\mathbf{\hat{n}} = 1,
\tag{25}
\]

where \( g(\theta, u) \, d\mathbf{\hat{n}} \) is the probability of scattering into the solid angle \( d\mathbf{\hat{n}} \) in the center of mass frame. Then the integral \( I \) in Eq. (21a) becomes

\[
I = \int f(\mathbf{v} + \frac{\mathbf{u}}{2} + u\mathbf{\hat{n}}/2)f(\mathbf{v} - \frac{\mathbf{u}}{2} + u\mathbf{\hat{n}}/2)g(\theta, u) \, d\mathbf{u} \, d\mathbf{\hat{n}}.
\tag{26}
\]

If we write the \( f(\mathbf{v}) \) term in Eq. (11) as

\[
f(\mathbf{v}) = \int f(\mathbf{v})f(\mathbf{v} - \mathbf{u})g(\theta, u) \, d\mathbf{u} \, d\mathbf{\hat{n}},
\tag{27}
\]

which follows from Eq. (25) and the normalization of \( f(\mathbf{v}) \), we can write Eq. (11) as

\[
\frac{\partial f(\mathbf{v})}{\partial \tau} = \int [f(\mathbf{v}_A)f(\mathbf{v}_B) - f(\mathbf{v})f(\mathbf{v} - \mathbf{u})]g(\theta, u) \, d\mathbf{u} \, d\mathbf{\hat{n}},
\tag{28}
\]
where
\[ v_A = v + \frac{u}{2} + u\hat{n}/2 \]  
\[ v_B = v - \frac{u}{2} + u\hat{n}/2, \]  
\( (29a) \)  
\( (29b) \)

Equation (28) is almost in the form of the Boltzmann equation.

The Boltzmann equation represents a dilute gas for which the collision probability is proportional to \( u\sigma_T(u) \), where \( \sigma_T(u) \) is the total cross section. We consider a large enough number \( R \) such that the ratio \( u\sigma_T(u)/R \) for a selected pair is almost always less than unity.

For \( \sigma_T(u) = \sigma_0 \) the constant \( R/\sigma_0 \) can be chosen to be a few (say five) times the rms velocity. Then when a pair is selected, we take a random number \( r \) and allow the collision to occur if \( r < u\sigma_T(u)/R \); we select another pair if \( r > u\sigma_T(u)/R \). Although this procedure insures that the collision probability is proportional to \( u\sigma_T(u) \), it appears to violate the condition in Eq. (25) that all the selected pairs have a collision. To satisfy the condition in Eq. (25) we select \( g(\theta, u) \) as
\[ g(\theta, u) = \frac{u\sigma(\theta, u)}{R} + \left( 1 - \frac{u\sigma_T(u)}{R} \right)\delta(\hat{u} - \hat{n}), \]  
\( (30) \)

where \( \sigma(\theta, u) \) is the differential cross section. The latter is related to the total cross section \( \sigma_T(u) \) by
\[ \sigma_T(u) = \int \sigma(\theta, u) \, d\hat{n} = 2\pi \int \sigma(\theta, u) \sin(\theta) \, d\theta. \]  
\( (31) \)

The second term in Eq. (30) transfers the initial velocities to the final velocities with the probability \( 1 - u\sigma_T(u)/R \) and the collision becomes a null collision. The \( \delta(\hat{u} - \hat{n}) \) requires \( \hat{u} = \hat{n} \) which implies \( u' = u \) since \( u' = u \) from the energy conservation and \( u' = u\hat{n} \), \( u = u\hat{u} \). This means \( v_A - v_B = v_C - v \). We also have \( v_A + v_B = v_C + v \) from center of mass velocity conservation. These two equations yield \( v_C = v_A \) and \( v = v_B \) and velocities have not changed. A normal collision occurs with the probability \( u\sigma_T(u)/R \). It is easy to verify that \( g(\theta, u) \) given in Eq. (30) satisfies the condition in Eq. (25).

If we substitute \( g(\theta, u) \) in Eq. (30) into Eq. (28), we obtain
\[ \frac{\partial f(v)}{\partial(\tau/R)} = \int [f(v_A)f(v_B) - f(v)f(v - u)]u\sigma(\theta, u) \, du \, d\hat{n}, \]  
\( (32) \)

where \( v_A \) and \( v_B \) were given in Eq. (29). Equation (32) is essentially the Boltzmann equation with the difference that \( f(v) \) is the probability density in velocity space whereas the
Boltzmann equation is written in terms of the probability density in both physical and velocity space. If the volume of the cell containing the molecules is \( V \), then we can write Eq. (32) for \( F(\mathbf{v}) = (N/V)f(\mathbf{v}) \) as

\[
\frac{\partial F(\mathbf{v})}{\partial t} = \int [F(\mathbf{v}_A)F(\mathbf{v}_B) - F(\mathbf{v})F(\mathbf{v} - \mathbf{u})] u\sigma(\theta, u) \, du \, d\hat{n},
\]

where \( t = \tau V/N = 2nV/RN^2 \) is interpreted as the physical time. Equation (33) is the Boltzmann equation for a homogeneous gas.

### III. DISCUSSION

Let us summarize the direct simulation Monte Carlo algorithm for solving the Boltzmann equation. We choose a sufficiently large \( R \) such that only a negligible fraction of the selected pairs (say less than one in a thousand) violate the condition \( u\sigma_T(u)/R \leq 1 \). Then we select pairs randomly and let them collide with probability \( u\sigma_T(u)/R \). The latter is achieved by generating a random number \( r \) and letting the collision occur if \( r \leq u\sigma_T(u)/R \). If a pair collides, then in the center of mass system the collision occurs within the solid angle \( d\hat{n} \) with probability \( P(\theta)d\hat{n} = [\sigma(\theta, u)/\sigma_T(u)]d\hat{n} \). Suppose that we put the \( z \)-axis along \( \mathbf{u} \) and we need to determine \( \hat{n} = \mathbf{u}'/u \), which is determined by the angles \( \theta \) and \( \phi \). To determine \( \theta \) we need to generate a random value of \( \theta \) by converting the random numbers produced by a uniform probability distribution to random numbers in the interval \((0, \pi)\) according to the probability distribution \( P(\theta) \). The \( \phi \) angles in the interval \((0, 2\pi)\) are equally likely. In this way we determine the final velocities of the particles as \( \mathbf{u}' \) and \( -\mathbf{u}' \) in the center of mass frame. By adding the center of mass velocity we find the final velocities in the lab frame. After storing the final velocities of the particles, we choose another pair and repeat the same process. The physical time is \( t = 2nV/N^2R \), where \( n \) is the number pairs chosen to make attempts for a collision. If the number of collisions in a given time is required, we can count the successful attempts for a collision. In Ref. 3 this algorithm for keeping track of the time is called the “no time counter method.”

The original method of Bird\(^3\) to keep track of the time was the time counter method. Consider a narrow interval of \( u\sigma_T(u) \) values. For a large \( n \) there will be \( \Delta n \) pairs with \( u\sigma_T(u) \) values in this interval. Of these, only \( (u\sigma_T(u)/R)\Delta n \) of them will make collisions corresponding to a time interval \((2V/N^2R)\Delta n \). Thus the elapsed time per successful attempt
\[ \Delta t = \frac{(2V/N^2R)\Delta n}{(u\sigma_T(u)/R)\Delta n} = \frac{2V}{N^2u\sigma_T(u)}. \] (34)

In the time counter method we let every pair collide, increase time by \( \Delta t \) \((t \rightarrow t + \Delta t)\) after each collision, and keep selecting pairs and colliding them until we reach the desired time. Every collision will cause a different time increment depending on the value of \( u\sigma_T(u) \). One disadvantage of this method is that if a collision with a low \( u\sigma_T(u) \) occurs, the time increment will be large. Such collisions can occur with pairs having almost equal velocities. The time counter method was declared “obsolete” in Ref. 3. But it is useful to be aware of the method since it is widely used in the past and it might come across in some papers.

If the purpose of the simulation is to demonstrate that the velocity distribution approaches the Maxwell-Boltzmann distribution, we could let all the selected pairs make a collision and the velocity distribution will converge to the Maxwell-Boltzmann distribution. This simplification corresponds to \( u\sigma_T(u)/R = 1 \) or \( \sigma_T(u) = R/u \), where the total cross section is inversely proportional to the relative velocity. Also, if it is desired to not discuss cross sections and the time tracking method, it is convenient to assume isotropic scattering in the center of mass frame. Then \( \mathbf{u}' \) can be calculated by taking a random unit vector \( \mathbf{n} \) and multiplying it by \( u \). These two simplifications make the programming easier and an undergraduate student with some programming background can write a program demonstrating the Maxwell-Boltzmann distribution.

Direct simulation methods are also applicable to radiative processes and chemical reactions and the present formalism generalizes to all these cases in a more or less straightforward fashion for homogeneous gases. Such generalizations can be a useful teaching tool and a fertile field for student projects.

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