

Exact Direct-Simulation-Scheme for the Boltzmann Equation/Correlation of Molecular Velocities Subject to Renewal Processes

By

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Abstract: The correlation of velocity between the molecules in a simulation cell is lessened by a renewal process such that new uncorrelated molecules come into the cell and some correlated ones go out of the cell. Moreover, if a portion of the cell boundary is a diffusely reflecting wall, the molecules are subject to another renewal process; each time a molecule is incident on the wall, its velocity is renewed. It is shown that the correlation coefficient between the velocities of the molecules subject to these renewal processes is $O(N^{-1})$ no matter how large the time may be, where N is the number of the molecules in the cell; by choosing a large N one can make the correlation coefficient as small as one desires. This fact assures that the exact direct-simulation method is applicable to the calculation of steady flows, which are obtained as the large time states of unsteady flows. Also, the expressions for correlation functions are obtained. These are necessary for the estimation of the sampling interval used in obtaining the time-averaged data of the steady flows.

Contents

1. Introduction
2. Renewal Process due to Molecular Exchange
 - 2.1. Correlation Coefficient
 - 2.2. Correlation Functions
3. Renewal Process due to Diffuse Reflection
 - 3.1. Analysis Based on a Model Renewal Process
 - 3.1.1. Model Process
 - 3.1.2. Correlation Coefficient
 - 3.1.3. Correlation Functions
 - 3.2. Simulation Calculations
 - 3.2.1. Renewal Rate
 - 3.2.2. Simulation Data
4. Concluding Remarks

1. Introduction

It is now possible to obtain exact, though numerical, solutions of the Boltzmann equation by use of the new direct-simulation method proposed by the author [1, 2]. It was in fact shown in ref. 2 that the velocity-distribution function determined by use of Nanbu's method agrees up to three places of decimals with the exact

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solution discovered by Krook and Wu [3]. Note, however, that it is only if the correlation of velocity between a simulated molecule and its collision partner is very weak that the obtained simulation solutions become the exact solutions of the Boltzmann equation. (Unless the correlation is weak, the assumption of molecular chaos would not be satisfied.) It was shown that the correlation coefficient ρ between the two molecules increases with τ/N , where N is the number of simulated molecules and τ is the time measured in units of mean free time per molecule [4]. In calculating collisional relaxations of nonequilibrium gas the time τ is $O(1)$ since the molecular system settles down into an equilibrium after a few collisions. If one chooses N such that $\tau/N \ll 1$ in the simulation calculation, ρ is very small and hence the obtained solutions are the exact solutions [5].

Consider the simulation calculation of steady flows. In the direct-simulation method the flow is always unsteady and a steady flow is obtained as the large time state of the unsteady flow. In this case the time τ at which the flow practically becomes steady is much greater than unity. It seems, however, that if ρ increases with the time τ , the condition $\rho \ll 1$ would never hold as $\tau \rightarrow \infty$. That is, the calculation of the steady flows seems to be impossible. The purpose of the present work is to show that this is not true, i.e., to show that the direct-simulation method is applicable also to the calculation of the steady flows. In ref. 4 the expression for ρ is obtained for a closed system of molecules across the boundary of which no exchange of molecules takes place. Contrary to this, such exchange does take place in an actual simulation cell, i.e., fresh molecules come into the cell and correlated molecules go out of the cell. We call this situation as follows: the velocities of the molecules in the cell are subject to a renewal process. Moreover, if a portion of the cell boundary is a diffusely reflecting wall, the molecular velocities are subject to another renewal process. That is, each time a molecule collides with the wall, it is emitted with a renewed velocity uncorrelated to the incident velocity. We show that if the molecular velocities are subject to one of the renewal processes, the correlation coefficient ρ is at most $O(N^{-1})$ no matter how large the time τ may be; by use of a large N , ρ can be made as small as one desires. This fact makes it possible to calculate the steady flows by use of the direct-simulation method.

We consider the renewal process due to the molecular exchange and that due to the diffuse reflection separately. Molecules are assumed to be Maxwell molecules.

2. Renewal Process due to Molecular Exchange

To make the problem tractable without loss of its essential character, the process of the exchange of molecules across the cell boundary is replaced by a much simpler model of a renewal process; it occurs with the probability $\phi \Delta\tau$ that in the time interval $\Delta\tau$ each molecule in the cell disappears and immediately reappears with a renewed velocity, i.e., a velocity uncorrelated to the one at the moment of disappearance. Here, ϕ is the rate of renewal. Clearly, disappearance

corresponds to going out of the cell and reappearance to coming into the cell. Thanks to this model, there is no necessity to take into consideration the collisionless free molecular motions. Moreover, a set of molecules in the cell can be regarded as if it were a closed system, for the number of molecules in the cell is constant at any time.

It is assumed that initially there is a uniform flow of velocity U to the x -direction of Cartesian coordinates system, and that the initial distribution function is spherically symmetrical in space of peculiar velocity.

2.1. Correlation Coefficient

Here we consider the correlation of velocity between a molecule and its collision partner. Thanks to the introduction of the renewal model we can now extend the previous theory [4]. We consider the fate of a set of N molecular velocities $\{c_{i,0}; i=1, 2, \dots, N\}$ sampled from the initial velocity-distribution function $f(c, 0)$, where c is the molecular velocity. Let C be the peculiar velocity, and $f(c, 0)$ is a function of $C(=|C|)$ from the assumption of spherical symmetry. Write $C=c-U$. Here is treated the case of $U_\alpha=\delta_{\alpha x}U$, where $U_\alpha(\alpha=x, y, z)$ is the α -component of U and $\delta_{\alpha x}$ is the Kronecker delta. Let $c_{i,n}$ be the velocity of i th molecule at time point $\tau=n\Delta\tau$, $\Delta\tau$ being the time step. (In this paper the dimensionless time τ denotes $\theta\tau$ in ref. 4. Roughly speaking, τ is the time measured in units of mean free time per molecule.) The process $\{c_{i,n}; i=1, 2, \dots, N\}$ is defined by the recurrence relation

$$c_{i,n+1}=X_{i,n}c_{i,n}^*+(1-X_{i,n})(c_{i,n}+Z_{i,n}), \quad (1)$$

where $X_{i,n}$ is a random variable whose probability law is given by

$$P[X_{i,n}=1]=P_r, \quad (2a)$$

$$P[X_{i,n}=0]=1-P_r. \quad (2b)$$

Here $P[A]$ denotes the probability of the event A and P_r is the probability of renewal. It is given by $P_r=\phi\Delta\tau$, $\phi(>0)$ being a constant. If $X_{i,n}=1$, then $c_{i,n+1}=c_{i,n}^*$, i.e., $c_{i,n}^*$ denotes a renewed velocity. Here we consider the case when $c_{i,n}^*$ is a random sample from the probability density $f(c, 0)$. If $X_{i,n}=0$, the renewal process does not occur. The variable $Z_{i,n}$ is defined in ref. 4. (Note that capital C in the definition must be replaced by lower case c .) It is a function of four random variables $Y_{i,n}$, $J(i, n)$, $\beta_{i,n}$, $\epsilon_{i,n}$, so that $c_{i,n+1}$ is now a function of six random variables $X_{i,n}$, $c_{i,n}^*$, $Y_{i,n}$, $J(i, n)$, $\beta_{i,n}$, $\epsilon_{i,n}$. Note that the members in a set $\{X_{i,n}; i=1, 2, \dots, N; n=0, 1, 2, \dots\}$ are independent identically distributed random variables. This is true also for $\{c_{i,n}^*\}$, $\{Y_{i,n}\}$, $\{J(i, n)\}$, $\{\beta_{i,n}\}$ and $\{\epsilon_{i,n}\}$. Moreover, these sets are mutually independent.

If $P_r=0$, eq. (1) is reduced to the starting eq. (1) of ref. 4. Since the probabilistic analysis of eq. (1) is analogous to that in ref. 4, we here omit it and present only resulting expressions. Since the initial velocities $c_{i,0}$ are sampled from $f(c, 0)$, the expectation $E(c_{i\alpha,0})$ is

$$E(c_{i\alpha,0}) = \delta_{\alpha x} U,$$

where $c_{i\alpha,0}$ is the α -component of $\mathbf{c}_{i,0}$. It can easily be shown by means of mathematical induction that for any n

$$E(c_{i\alpha,n}) = \delta_{\alpha x} U, \quad (n=0, 1, 2, \dots) \quad (3)$$

where we have used $E(c_{i\alpha,n}^*) = \delta_{\alpha x} U$, which is a result from the fact that $\mathbf{c}_{i,n}^*$ is also sampled from $f(\mathbf{c}, 0)$.

Next we consider the variance $\text{Var}(c_{i\alpha,n})$ and the covariance $\text{Cov}(c_{i\alpha,n}, c_{j\alpha,n})$ of $i \neq j$. The latter represents the correlation of velocities of any two randomly chosen molecules. In a system of Maxwell molecules, the collision partner of a molecule is chosen randomly from the rest. That is, $\text{Cov}(c_{i\alpha,n}, c_{j\alpha,n})$ represents the correlation of velocities of two molecules which are going to collide. Using eq. (3), we have

$$\begin{aligned} \text{Var}(c_{i\alpha,n}) &= E(c_{i\alpha,n}^2) - \delta_{\alpha x} U^2, \\ \text{Cov}(c_{i\alpha,n}, c_{j\alpha,n}) &= E(c_{i\alpha,n} c_{j\alpha,n}) - \delta_{\alpha x} U^2. \quad (i \neq j) \end{aligned}$$

At $n=0$,

$$\text{Var}(c_{i\alpha,0}) = RT (\equiv V_0), \quad (4a)$$

$$\text{Cov}(c_{i\alpha,0}, c_{j\alpha,0}) = 0, \quad (i \neq j) \quad (4b)$$

where R is the gas constant per unit mass and T is the temperature, which is independent of α because of spherical symmetry of $f(\mathbf{c}, 0)$. Equation (4b) can be obtained by noting that $\mathbf{c}_{i,0}$ and $\mathbf{c}_{j,0}$ are independently sampled from $f(\mathbf{c}, 0)$. It can be shown by mathematical induction that $\text{Var}(c_{i\alpha,n}) = V_0$ holds at any n and $C_n = \text{Cov}(c_{i\alpha,n}, c_{j\alpha,n})$ satisfies the recurrence relation

$$C_{n+1} = (1 - p - 2P_r)C_n + pV_0, \quad (5)$$

where $p = (2/N)\Delta\tau$ and terms of order $(\Delta\tau)^2$ are disregarded. By noting that $C_0 = 0$, the solution of eq. (5) is

$$C_n = \frac{pV_0}{p + 2P_r} [1 - (1 - p - 2P_r)^n]. \quad (6)$$

Define the correlation coefficient by

$$\rho_n = \frac{\text{Cov}(c_{i\alpha,n}, c_{j\alpha,n})}{[\text{Var}(c_{i\alpha,n})\text{Var}(c_{j\alpha,n})]^{1/2}},$$

and we have $\rho_n = C_n/V_0$. Consider the limit of $\Delta\tau \rightarrow 0$ by requiring that $\tau = n\Delta\tau$ is fixed, and write $\rho(\tau; N, \phi)$ in place of ρ_n . We have

$$\rho(\tau; N, \phi) = (1 + N\phi)^{-1} \{1 - \exp[-2(\phi + N^{-1})\tau]\}. \quad (7)$$

Note that $\rho(\tau; N, 0)$ is the expression derived in ref. 4. The correlation coefficient $\rho(\tau; N, \phi)$ increases monotonically from 0 to

$$\rho(\infty; N, \phi) = (1 + N\phi)^{-1}. \quad (8)$$

It is easy to show that $\partial\rho/\partial\phi < 0$ for $\tau > 0$. Hence,

$$\rho(\tau; N, \phi) < \rho(\tau; N, 0) \quad \text{for } \phi > 0. \quad (9)$$

That is, the renewal process lessens the correlation. Note that $\rho(\tau; N, \phi) < \rho(\infty; N, \phi) < (N\phi)^{-1}$. Usually $N \gg 1$, and hence the correlation coefficient is at most $O(N^{-1})$ at any time. This forms a marked contrast to the result in ref. 4. That is, in case of $\phi = 0$ we see from eq. (7) that however large N may be, $\rho(\tau; N, \phi) \simeq 1$ for $\tau \gg N$.

The expressions of the covariances of different components of velocity take the same forms as those for $\phi = 0$, i.e.,

$$\text{Cov}(c_{i\alpha, n}, c_{i\beta, n}) = 0, \quad (\alpha \neq \beta) \quad (10a)$$

$$\text{Cov}(c_{i\alpha, n}, c_{j\beta, n}) = 0, \quad (\alpha \neq \beta, i \neq j) \quad (10b)$$

hold at any n .

2.2. Correlation Functions

As before [4], consider the covariance functions

$$F(n, n+h) = \text{Cov}(c_{i\alpha, n}, c_{i\alpha, n+h}), \quad (11a)$$

$$G(n, n+h) = \text{Cov}(c_{j\alpha, n}, c_{i\alpha, n+h}). \quad (i \neq j) \quad (11b)$$

These represent the correlation of velocities at two time points $n\Delta\tau$, $(n+h)\Delta\tau$, where $h\Delta\tau$ is the lag. Expression (11a) denotes the case when the two velocities belong to a single molecule, whereas expression (11b) denotes the case when they belong to two different molecules; (11a) may be called the autocovariance function and (11b) the cross-covariance function. The covariance functions are indispensable to examine ergodicity of simulation solutions [6]. It can be shown by use of eq. (1) that $F(n, n+h)$ and $G(n, n+h)$ are subject to the following recurrence relations.

$$F(n, n+h+1) = (1 - P_r)F(n, n+h) - \frac{1}{2}(N-1)p\Delta(n, n+h), \quad (12a)$$

$$G(n, n+h+1) = (1 - P_r)G(n, n+h) + \frac{1}{2}p\Delta(n, n+h), \quad (12b)$$

where $\Delta(n, n+h) = F(n, n+h) - G(n, n+h)$, and terms of order $(\Delta\tau)^2$ are disregarded. Initial conditions for eqs. (12) are

$$F(n, n) = V_0, \quad G(n, n) = C_n.$$

The solutions of eqs. (12) are

$$\mu(n, n+h) = \xi^h - \left(\frac{N-1}{N} \right) (1 - \rho_n) (\xi^h - \zeta^h), \quad (13a)$$

$$\nu(n, n+h) = \xi^h \rho_n + \frac{1}{N} (1 - \rho_n) (\xi^h - \zeta^h), \quad (13b)$$

where $\xi = 1 - \phi \Delta\tau$, $\zeta = 1 - (\phi + 1)\Delta\tau$, $\mu(n, n+h) = F(n, n+h)/V_0$ is the autocorrelation function and $\nu(n, n+h) = G(n, n+h)/V_0$ is the cross-correlation function. Write $\tau = n\Delta\tau$ and $\eta = h\Delta\tau$ and take the limit of $\Delta\tau \rightarrow 0$. Writing $\mu(\tau, \tau + \eta; N, \phi)$ and $\nu(\tau, \tau + \eta; N, \phi)$ in place of $\mu(n, n+h)$ and $\nu(n, n+h)$, we then have

$$\mu(\tau, \tau + \eta; N, \phi) = e^{-\phi\eta} \left\{ 1 - \left(\frac{N-1}{N} \right) [1 - \rho(\tau; N, \phi)] (1 - e^{-\eta}) \right\}, \quad (14a)$$

$$\nu(\tau, \tau + \eta; N, \phi) = e^{-\phi\eta} \left\{ \rho(\tau; N, \phi) + \frac{1}{N} [1 - \rho(\tau; N, \phi)] (1 - e^{-\eta}) \right\}. \quad (14b)$$

Since these correlation functions depend on τ through $\rho(\tau; N, \phi)$, the stochastic process defined by eq. (1) is not stationary.

If $\phi > 0$, then $\rho(\tau; N, \phi) < \rho(\tau; N, 0)$ from inequality (9), hence the quantity in curly brackets of eq. (14a) is less than $\mu(\tau, \tau + \eta; N, 0)$. We now have, for $\phi > 0$ and $N \neq \infty$

$$\mu(\tau, \tau + \eta; N, \phi) < e^{-\phi\eta} \mu(\tau, \tau + \eta; N, 0). \quad (15)$$

That is, the renewal process reduces the autocorrelation function at least by a factor $e^{-\phi\eta}$. Since $\rho(\tau; N, \phi) \rightarrow 0$ as $N \rightarrow \infty$, we have from eqs. (14)

$$\mu(\tau, \tau + \eta; \infty, \phi) = e^{-(\phi+1)\eta} = e^{-\phi\eta} \mu(\tau, \tau + \eta; \infty, 0), \quad (16a)$$

$$\nu(\tau, \tau + \eta; \infty, \phi) = 0. \quad (16b)$$

Consider the case of

$$\phi \sim O(1), \quad N \gg 1 \quad \text{and} \quad \tau \gg 1. \quad (17)$$

We then have $\rho(\tau; N, \phi) \simeq (N\phi)^{-1}$ from eq. (7). Substituting this into eqs. (14) and neglecting the terms of $O(N^{-2})$, we have

$$\mu(\tau, \tau + \eta; N, \phi) \simeq e^{-(\phi+1)\eta} + \frac{1}{N} \left(1 + \frac{1}{\phi} \right) e^{-\phi\eta} (1 - e^{-\eta}), \quad (18a)$$

$$\nu(\tau, \tau + \eta; N, \phi) \simeq \frac{1}{N} \left(1 + \frac{1}{\phi} - e^{-\eta} \right) e^{-\phi\eta}. \quad (18b)$$

Since the right-hand sides of eqs. (18) do not depend on τ , the stochastic process defined by eq. (1) becomes stationary in case of (17). In case of $\phi = 0$ it was shown that it is for $\tau \ll N$ that the process is stationary [4]; there exists an upper limit of τ for $\phi = 0$. This forms a marked contrast to the fact that stationariness condition is always satisfied for $\phi \sim O(1)$ and $N \gg 1$ in so far as $\tau \gg 1$. The stationariness condition for $\phi \sim O(1)$ makes it much easier to obtain accurate time-averaged values of macroscopic observables. Assume that the state of gas has reached a stationary state at $\tau = \tau_\infty \gg 1$. Choose a lag η_0 such as $\exp[-(\phi+1)\eta_0] \ll 1$; data of the observables at the time points $\tau, \tau + \eta_0$ are almost uncorrelated. The time-averaged observables can be obtained by averaging a sequence of the data at time points $\tau = \tau_\infty + (m-1)\eta_0$ ($m = 1, 2, \dots, M$). Usually, MN is called

the sample size. In order to lessen the statistical fluctuations of the time-averaged observables, M must be chosen as large as possible. In case of $\phi=0$, the upper limit of τ severely restricts M . Since there is no such restriction on M in case of $\phi \sim O(1)$, however, we can obtain the time-averaged observables with the fluctuations small as far as we require.

The expressions for the covariance functions of different components of velocity take the same form as before [4], i.e.,

$$\begin{aligned} \text{Cov}(c_{i\alpha, n+h}, c_{i\beta, n}) &= 0, & (\alpha \neq \beta) \\ \text{Cov}(c_{i\alpha, n+h}, c_{j\beta, n}) &= 0, & (\alpha \neq \beta, i \neq j) \end{aligned}$$

hold for any h .

3. Renewal Process due to Diffuse Reflection

We discuss the strength of the correlation in reference to the molecular boundary conditions at the solid wall. First the results of a probabilistic analysis based on a model of the renewal process are presented. Next the data from actual simulation calculations are presented and discussed in relation to the results from the analysis.

3.1. Analysis Based on a Model Renewal Process

3.1.1. Model Process

It occurs frequently that a portion of the boundary of a simulation cell consists of a solid wall. As a simplest model of such a cell, we consider a gas in a vessel whose dimension is of the order of mean free path. Spatial non-uniformity of gas properties can be neglected in this small vessel. Let initial temperatures of both the gas and wall be T_0 . It is assumed that the initial velocity distribution function is spherically symmetrical in velocity space but is not always Maxwellian. Consider the case when the wall temperature is suddenly raised (or lowered) to T^* at time zero and is kept constant after that. We are concerned with the fate of N simulated molecules. Let $\mathbf{c}_{i,n}$ and $\mathbf{x}_{i,n}$ be the velocity and position of i th molecule at time point $\tau = n\Delta\tau$.

Whether a molecule strikes the wall or not must be judged by examining its position at each time-point. However, the treatment of actual molecular displacement is postponed until Sec. 3.2. We here dispense with the treatment by introducing a stochastic model of molecular reflection at the wall. The model is analogous to that used in Sec. 2; with the probability $\phi\Delta\tau$ each molecule strikes the wall, ϕ being a constant common to all molecules. Now the process $\{\mathbf{c}_{i,n}; i=1, 2, \dots, N\}$ is defined by eq. (1).

As to $\mathbf{c}_{i,n}^*$, we consider a simplest model:

$$\mathbf{c}_{i,n}^* = W_{i,n} \mathbf{c}_{i,n} + (1 - W_{i,n}) \mathbf{v}_{i,n}, \quad (19)$$

where $W_{i,n}$ is a random variable whose probability law is given by

$$P[W_{i,n}=1]=1-\zeta_D, \quad (20a)$$

$$P[W_{i,n}=0]=\zeta_D. \quad (20b)$$

We call ζ_D the percentage of diffuse reflection and $(1-\zeta_D)$ the percentage of specular reflection. A set of velocities $\{v_{i,n}: i=1, 2, \dots, N; n=1, 2, \dots\}$ is assumed to be independent of $\{c_{i,n}\}$ and to be a random sample of a random variable v whose probability density is spherically symmetrical in velocity space. We now have $E(v_{i\alpha,n})=0$ and

$$\begin{aligned} \text{Var}(v_{i\alpha,n}) &= V^* (=RT^*), \\ \text{Cov}(v_{i\alpha,n}, v_{i\beta,n}) &= 0, \quad (\alpha \neq \beta) \end{aligned}$$

where $v_{i\alpha,n}$ is the α -component of $v_{i,n}$ and T^* is the wall temperature. Of course, V^* or T^* is independent of i , α , and n . Note that seven sets of random variables $\{W_{i,n}\}$, $\{v_{i,n}\}$, $\{X_{i,n}\}$, $\{Y_{i,n}\}$, $\{J(i, n)\}$, $\{\beta_{i,n}\}$, $\{\varepsilon_{i,n}\}$ are mutually independent. Note that eq. (19) is nothing but a model. If a molecule is specularly reflected, its velocity is not $c_{i,n}$ but the component of velocity perpendicular to the wall is reversed. However, the velocity of the reflected molecule is perfectly correlated to $c_{i,n}$. This is the reason why the first term in eq. (19) will do as a specular reflection model. Similarly, if a molecule is diffusely reflected, the probability density of its velocity is not spherically symmetrical. However, the velocity of the molecule is independent of $c_{i,n}$ as $v_{i,n}$ is.

From the starting eqs. (1) and (19) we can now obtain expressions for variance, covariance, and covariance functions. We present only the final results.

3. 1. 2. Correlation Coefficient

Write

$$V(\tau) = \text{Var}(c_{i\alpha,n}), \quad (21a)$$

$$C(\tau, N) = \text{Cov}(c_{i\alpha,n}, c_{j\alpha,n}), \quad (i \neq j) \quad (21b)$$

where $\tau = n\Delta\tau$. If the limit of $\Delta\tau \rightarrow 0$ is taken by fixing τ , we have

$$V(\tau) = V^* + (V_0 - V^*) \exp(-\phi^*\tau), \quad (22a)$$

$$C(\tau; N) = V^* \{A_1 + A_2 \exp(-\phi^*\tau) - (A_1 + A_2) \exp[-2(\phi^* + N^{-1})\tau]\}, \quad (22b)$$

where $V_0 = \text{Var}(c_{i\alpha,0}) = RT_0$, $\phi^* = \zeta_D\phi$, and

$$A_1 = \frac{\varepsilon}{1+\varepsilon}, \quad A_2 = \frac{2\varepsilon}{1+2\varepsilon}(\omega-1)$$

with $\varepsilon = 1/(N\phi^*)$ and $\omega = V_0/V^* = T_0/T^*$. The correlation coefficient $\rho(\tau; N)$ is given by $C(\tau; N)/V(\tau)$. In case of $\zeta_D = 0$, the limit $\varepsilon \rightarrow \infty$ must be taken. If $\omega = 1$, then $V(\tau) = V_0$, hence $\rho(\tau; N)$ takes the form

$$\rho(\tau; N) = (1 + N\phi^*)^{-1} \{1 - \exp[-2(\phi^* + N^{-1})\tau]\}. \quad (\omega = 1) \quad (23)$$

In case of $\zeta_D = 1$ we have $\phi^* = \phi$, so that eq. (23) agrees with eq. (7). We see from eq. (23) that $\rho(\tau; N)$, which is at most $(1 + N\phi^*)^{-1}$, decreases drastically as

ϕ^* or ζ_D increases because of $N \gg 1$.

It is important to pay attention to the maximum value of $C(\tau; N)$. If $\omega \leq 1$, then $C(\tau; N)$ takes the maximum of V^*A_1 at $\tau = \infty$. If $\omega > 1$, however, $C(\tau; N)$ for any $\zeta_D \neq 0$ takes the maximum at a finite τ . For simplicity, we show this fact in a special case. The number N is large in usual simulation calculations. Consider the case of $\varepsilon \ll 1$ (or $N \gg 1$ and $\zeta_D \neq 0$). Neglect of terms of $O(\varepsilon)$ in eq. (22b) yields

$$C(\tau; N)/C(\infty; N) = 1 + 2(\omega - 1)e^{-\phi^*\tau} - (\omega - 1)e^{-2\phi^*\tau}, \quad (24)$$

where $C(\infty; N) = \varepsilon V^*$. The right hand side of eq. (24) is a quadratic function of $e^{-\phi^*\tau}$. We see that $C(\tau; N)$ takes the maximum $[\omega^2/(2\omega - 1)]\varepsilon V^*$ at $\tau = \phi^{*-1} \ln[(2\omega - 1)/(\omega - 1)]$. Since the maximum increases with ω , it is desirable to increase the number N and hence reduce ε in simulating a hot gas in a cold vessel.

Covariances for different components of velocity vanish, i.e.

$$\begin{aligned} \text{Cov}(c_{i\alpha, n}, c_{i\beta, n}) &= 0, & (\alpha \neq \beta) \\ \text{Cov}(c_{i\alpha, n}, c_{j\beta, n}) &= 0, & (\alpha \neq \beta, i \neq j) \end{aligned}$$

3.1.3. Correlation Functions

Write

$$\begin{aligned} F(\tau, \tau + \eta; N) &= \text{Cov}(c_{i\alpha, n}, c_{i\alpha, n+h}), \\ G(\tau, \tau + \eta; N) &= \text{Cov}(c_{j\alpha, n}, c_{i\alpha, n+h}), \quad (i \neq j) \end{aligned}$$

where $\tau = n\Delta\tau$ and $\eta = h\Delta\tau$, h being a non-negative integer. If the limit of $\Delta\tau \rightarrow 0$ is taken by fixing τ and η , we have

$$F(\tau, \tau + \eta; N) = e^{-\phi^*\eta} \left\{ V(\tau) - \frac{N-1}{N} [V(\tau) - C(\tau; N)](1 - e^{-\eta}) \right\}, \quad (25a)$$

$$G(\tau, \tau + \eta; N) = e^{-\phi^*\eta} \left\{ C(\tau; N) + \frac{1}{N} [V(\tau) - C(\tau; N)](1 - e^{-\eta}) \right\}. \quad (25b)$$

The autocorrelation function is given by $F(\tau, \tau + \eta; N)/[V(\tau)V(\tau + \eta)]^{1/2}$ and the cross-correlation function is given by $G(\tau, \tau + \eta; N)/[V(\tau)V(\tau + \eta)]^{1/2}$.

Covariance functions for different components of velocity vanish, i.e.

$$\begin{aligned} \text{Cov}(c_{i\alpha, n+h}, c_{i\beta, n}) &= 0, & (\alpha \neq \beta) \\ \text{Cov}(c_{i\alpha, n+h}, c_{j\beta, n}) &= 0. & (\alpha \neq \beta, i \neq j) \end{aligned}$$

3.2. Simulation Calculations

In Sec. 3.1. we introduced a renewal model and dispensed with the treatment of molecular positions $\{\mathbf{x}_{i, n}\}$. We here make actual simulation calculations by taking $\{\mathbf{x}_{i, n}\}$ into consideration. We direct our attention to the case of $T^* = T_0$ since it is only in this case that the exact solution of the Boltzmann equation is known. Let a gas of temperature T_0 be initially in equilibrium. Clearly, the

exact solution is the Maxwellian distribution for temperature T_0 . Let the vessel be a cube a side of which is equal to the mean free path λ_0 . Before presenting simulation data we give an expression for the renewal rate ϕ , which is necessary to discuss the data in reference to the analytical results in Sec. 3. 1.

3.2. 1. Renewal Rate

For a while, let a side of the cube be of length $2L$. Take the origin of the Cartesian coordinates system at the center of the cube and let (X_x, X_y, X_z) be the coordinates of a molecule. Since X_α ($\alpha=x, y, z$) is uniformly distributed, the probability density $g(x_\alpha)$ of X_α is given by

$$g(x_\alpha) = (2L)^{-1} \quad \text{for } |x_\alpha| \leq L. \quad (26)$$

Of course, $g(x_\alpha) = 0$ for $|x_\alpha| > L$. Let (C_x, C_y, C_z) be the molecular velocity. (Capital letters are used here since they are random variables.) Strictly speaking, the probability density of (C_x, C_y, C_z) is given by the Maxwellian distribution only at time $t=0$. (Here, t is the dimensional time.) Since this is, however, approximately true at any time insofar as the correlation coefficient is small, let the probability density $f(c_\alpha)$ of C_α be always

$$f(c_\alpha) = (2\pi RT_0)^{-1/2} \exp\left(-\frac{c_\alpha^2}{2RT_0}\right). \quad (27)$$

Define the event A_α by $A_\alpha = \{|X_\alpha + C_\alpha \Delta t| > L\}$, where Δt is the dimensional time-step. We have [7]

$$\begin{aligned} \phi \Delta \tau &= P[A_x \cup A_y \cup A_z], \\ &= P[A_x] + P[A_y] + P[A_z] - P[A_x A_y] \\ &\quad - P[A_y A_z] - P[A_x A_z] + P[A_x A_y A_z]. \end{aligned} \quad (28)$$

Since A_x, A_y, A_z are mutually independent and a symmetry relation $P[A_x] = P[A_y] = P[A_z]$ holds, eq. (28) becomes

$$\phi \Delta \tau = 3P[A_\alpha] - 3\{P[A_\alpha]\}^2 + \{P[A_\alpha]\}^3. \quad (29)$$

The probability $P[A_\alpha]$ is given by

$$P[A_\alpha] = 1 - 2 \int_0^{2L/\Delta t} f(c_\alpha) dc_\alpha \int_{-L}^{L-c_\alpha \Delta t} g(x_\alpha) dx_\alpha. \quad (30)$$

Substitution of eqs. (26) and (27) into (30) yields

$$P[A_\alpha] = \operatorname{erfc} a + a^{-1} \pi^{-1/2} [1 - \exp(-a^2)], \quad (31)$$

where $a = 2L/[\Delta t(2RT_0)^{1/2}]$ and erfc is the complementary error function. From ref. 8, $\operatorname{erfc} a = \alpha^{-1} \pi^{-1/2} \exp(-a^2)$ as $\Delta t \rightarrow 0$, so that

$$P[A_\alpha] = \frac{\lambda_0}{2\pi^{1/2}L} \Delta \hat{t}, \quad (32)$$

where $\Delta\hat{t} = \Delta t(2RT_0)^{1/2}/\lambda_0$. Substituting eq. (32) into (29) and neglecting the terms of $O(\Delta\hat{t})$, we have

$$\phi\Delta\tau = \frac{3\lambda_0}{2\pi^{1/2}L} \Delta\hat{t}. \quad (33)$$

The relation between \hat{t} and τ should be given here. The nondimensional time τ is defined by

$$\tau = [2\pi A_1(5)n(2b/m)^{1/2}]t, \quad (34)$$

where $A_1(5) = 0.4219$, n is the number density, b is the constant in the potential law, and m is the mass of a molecule. The time $\hat{t} [=t(2RT_0)^{1/2}/\lambda_0]$ is in essence the time measured in units of mean free time. We define λ_0 by $\lambda_0 = (2^{1/2}n\bar{\sigma}_M)^{-1}$, where $\bar{\sigma}_M$ is the momentum-transfer cross-section averaged over the Maxwellian distribution. It is [9]

$$\bar{\sigma}_M = 4A_1(5)(2\pi b/mRT_0)^{1/2}.$$

Now \hat{t} takes the form

$$\hat{t} = [8A_1(5)n(2\pi b/m)^{1/2}]t. \quad (35)$$

We have from eqs. (34) and (35)

$$\hat{t} = (4/\pi^{1/2})\tau. \quad (36)$$

Using eq. (36) and setting $2L = \lambda_0$, we have from eq. (33)

$$\phi = 12/\pi. \quad (37)$$

3.2.2. Simulation Data

Initial positions and velocities of N simulated molecules are sampled from eqs. (26) and (27) respectively. All molecules are then moved freely over the time step $\Delta\hat{t}$. If a molecule lies outside the cube at $\hat{t} = \Delta\hat{t}$, it is reflected at the wall diffusely with probability ζ_D and specularly with probability $(1 - \zeta_D)$. Consider, e.g., the diffuse reflection at $x = -\lambda_0/2$; the velocity of the reflected molecule is sampled from the probability density

$$\frac{1}{2\pi R^2 T_0^2} c_x \exp\left(-\frac{c_x^2 + c_y^2 + c_z^2}{2RT_0}\right) \quad (c_x > 0).$$

Note that the density is not spherically symmetrical. The reflected molecule is moved freely over $\Delta\hat{t} - (\Delta\hat{t})_1$, where $(\Delta\hat{t})_1$ is the time taken for the molecule to arrive at the wall. If the molecule lies outside the cube at $\hat{t} = \Delta\hat{t}$, it must again be reflected at the wall. The positions of all molecules at $\hat{t} = \Delta\hat{t}$ are determined in this way.

Next intermolecular collisions are calculated by fixing the molecular positions. The collision probability P_c per molecule over the time step $\Delta\hat{t}$ is

$$P_c = \frac{\pi^{1/2}\beta_0^2}{4A_1(5)} \left(\frac{N-1}{N}\right) \Delta\hat{t},$$

where $\beta_0=2.391$, which is the cut-off value of the dimensionless impact parameter corresponding to the cut-off angle of 2° . The time step Δt is chosen to be 0.01, for which $P_c=0.06$. Determination of the post-collision velocities completes the calculation of the first time step. Time is advanced up to $600\Delta t=6$. All calculations from $t=0$ to 6 are repeated (S/N) times, where the sample size S is fixed at 10^5 for any N .

Although the exact solution of the Boltzmann equation is the Maxwellian distribution for temperature T_0 , there may appear a distortion in the velocity distribution determined by means of the simulation calculations because of increased correlation of velocity between two molecules. As a measure of the distortion we consider, as before [4], a set of moments M_{2k} of c^{2k} ($k=1, 2, \dots, 5$), c being the molecular speed. The exact solution gives at any time

$$M_{2k}=(2RT_0)^k(2k+1)!!/2^k,$$

where $(2k+1)!!=1\cdot 3\cdot 5\cdots(2k+1)$. Let \tilde{M}_{2k} be the moments resulting from the simulation calculations. The deviations of the ratios \tilde{M}_{2k}/M_{2k} from unity reflect the strength of the correlation of velocity. Note that since the sample size S is finite, the data M_{2k}^* sampled from the exact solution also show fluctuations. The data M_{2k}^*/M_{2k} lie with the probability of 99% within the bound [4]

$$\left| \frac{M_{2k}^*}{M_{2k}} - 1 \right| \leq 2.58 \left[\frac{1}{S} \left(\frac{M_{4k}}{M_{2k}^2} - 1 \right) \right]^{1/2}. \quad (38)$$

Here is presented only some representative data of the actual simulation calculations. Figure 1 shows \tilde{M}_{2k}/M_{2k} for $N=100$ and $\zeta_D=0$. (The data are shifted upward by $(1-0.2k)$ for each k .) The correlation coefficient ρ is the one calculated from eq. (23) with $\phi^*=0$. Each two dashed lines containing a solid line represent the bound (38) of M_{2k}^*/M_{2k} . If the data \tilde{M}_{2k}/M_{2k} go outside the bound, it is almost certain that the error of the data is no small owing to the increased correlation. We see that the data for $\rho < 0.04$ lie within the bound (38). Figure 2 shows the data for $N=50$ and $\zeta_D=0$. The data for $\rho < 0.035$ lie within the

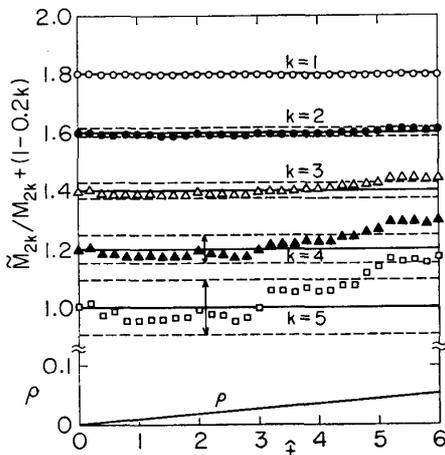


Fig. 1. Simulation data of even moments for $N=100$ and 100% specular reflection. Each two dashed lines containing a solid line represent the theoretical bound of fluctuations. The lowest curve represents the correlation coefficient.

bound. Figure 3 shows the data for $N=50$ and $\zeta_D=1$. The correlation coefficient ρ can be obtained from eqs. (23) and (37); it is very small, i.e., $\rho < 0.005$ at any time. We see that the data for all k 's lie within the bound at any time. That is, the simulation solution is the exact solution of the Boltzmann equation at any time. Figure 4 shows the data for $N=20$ and $\zeta_D=0.2$. The data for $\rho < 0.05$ lie within the bound. Figure 5 shows the data for $N=20$ and $\zeta_D=1$. The correlation coefficient is $\rho < 0.013$ at any time. The data are always within the bound. It is to be emphasized that these correct data are obtained by using only 20 simulated molecules.

The behavior of the data from the actual simulation calculations can be discussed successfully in reference to the approximate analysis in Sec. 3.1. It is concluded that if the correlation coefficient is less than a few percent, the simulation solutions are the exact solutions of the Boltzmann equation.

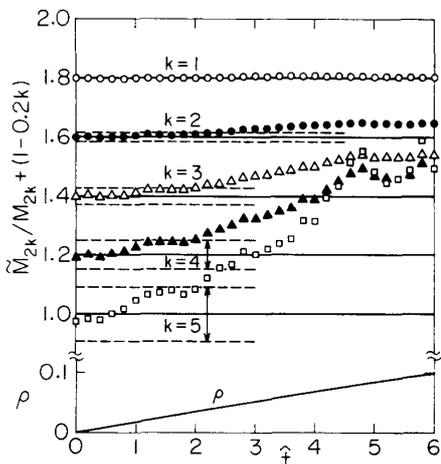


Fig. 2. Simulation data of even moments for $N=50$ and 100% specular reflection. See also the caption of Fig. 1.

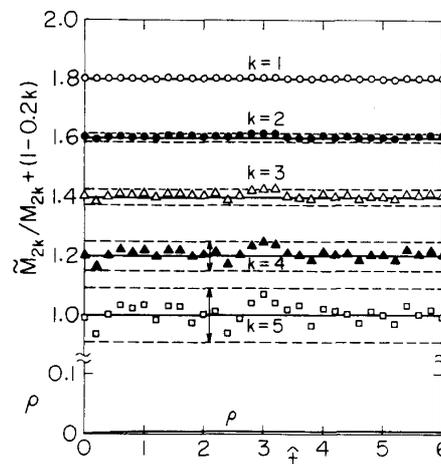


Fig. 3. Simulation data of even moments for $N=50$ and 100% diffuse reflection. See also the caption of Fig. 1.

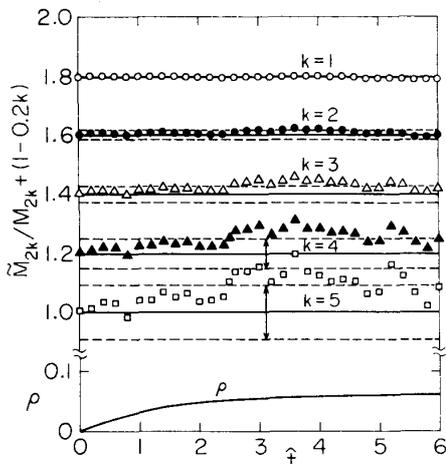


Fig. 4. Simulation data of even moments for $N=20$ and 20% diffuse and 80% specular reflection. See also the caption of Fig. 1.

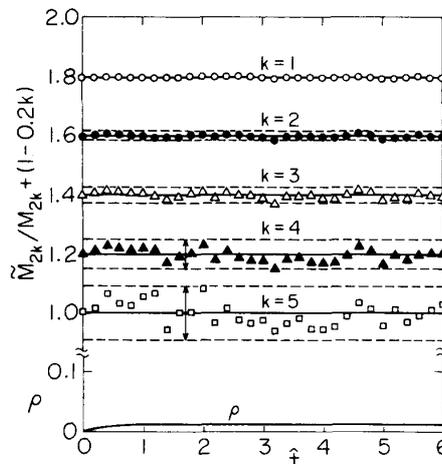


Fig. 5. Simulation data of even moments for $N=20$ and 100% diffuse reflection. See also the caption of Fig. 1.

4. Concluding Remarks

Now one can obtain exact solutions of the Boltzmann equation by using the new direct-simulation method proposed by the author. It is known, however, that it is only if the correlation of velocity between a molecule and its collision partner is very weak that the solutions from simulation calculations agree with the exact solutions. In this paper the correlation is examined for the molecules in a simulation cell. These molecules are subject to a renewal process such that new uncorrelated molecules come into the cell and some correlated ones go out of the cell. Moreover, if a portion of the cell boundary is a diffusely reflecting wall, the molecules are subject to another renewal process; the velocity of a molecule incident on the wall is renewed each time it collides with the wall.

It has been shown that for the molecules subject to such renewal processes the strength of the correlation is of order N^{-1} no matter how large the time may be, where N is the number of the molecules in the cell. This fact assures that the direct-simulation method is also applicable to the calculation of steady flows. That is, if the simulation calculation is made by use of such a large N that the effect of the correlation is negligibly small, the obtained solution is the solution of the Boltzmann equation even at a large time when the steady flow is already established.

The expressions for correlation functions are also obtained; these are useful for estimating the sampling interval used in obtaining the time-averaged data of the steady flows.

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