Analysis of discretization in the direct simulation Monte Carlo

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(Received 15 October 1999; accepted 7 June 2000)

We propose a continuous-time formulation of the direct simulation Monte Carlo that allows the evaluation of the transport coefficient dependence on the time step through the use of the Green–Kubo theory. Our results indicate that the error exhibits quadratic dependence on the time step, and that for time steps of the order of one mean free time the error is of the order of 5%. Our predictions for the transport coefficients are in good agreement with numerical experiments. The calculation of the cell size dependence, first obtained by Alexander *et al.* [Phys. Fluids **10**, 1540 (1998)], is reviewed and a correction is pointed out. © *2000 American Institute of Physics.* [S1070-6631(00)00210-5]

I. INTRODUCTION

The direct simulation Monte Carlo (DSMC) has been a very useful tool for the simulation of equilibrium and nonequilibrium gas flows.[1,2] It is very attractive because it successfully ''coarse grains'' the molecular description to the hydrodynamic regime, thus offering substantial computational efficiency advantages over ''brute force'' molecular dynamics simulations. DSMC simulations have been shown[3] to converge to Boltzmann equation solutions in the limit of infinite number of particles, and vanishing cell size and time step. However, like most computational methods, in the limit of finite discretization, numerical error contaminates the solution.

In a recent paper, Ohwada[4] has shown that the DSMC procedure viewed as a splitting method applied to the *time integration* of the Boltzmann equation results in a first-order accurate description of the *distribution function*. Ohwada finds that due to error accumulation, the distribution function diverges from the correct time-evolving distribution function proportionally to the time step Δt in transient problems. This is in contrast to the results of Bogomolov[5] that had previously shown a second-order behavior.

In this paper we focus on a different class of problems. We consider problems that are steady with respect to the molecular time scale, and thus the distribution function has relaxed to a steady state. We quantify the deviation of this state from the correct nonequilibrium state by obtaining measures of the deviation of the transport coefficients from their theoretical values. We will refer to the deviation of the transport coefficients from the exact Enskog values for dilute gases (which DSMC reproduces in the limit of an infinite number of particles and vanishing time step and cell size) as the truncation error. As we now discuss, DSMC introduces a truncation error due to discretization both in space and time.

Truncation error from discretization in space results from the selection of collision partners from cells of finite size (L). In a previous paper[6] it was shown that the resulting error is proportional to the square of the cell size, with the constant of proportionality such that cell sizes of the order of one mean free path result in errors of the order of 10%. In this paper we show that DSMC commits a ''discretization crime'' by performing an instantaneous collision of the molecules that would have normally collided within a time step Δt. This shift in the collision times is shown to have two contributions to the transport coefficients by comparing DSMC with a model where collisions take place in a continuous fashion. First, the molecules that are close enough to be considered for collision during the ''collide'' part of the algorithm (in the same cell) would have been at a finite distance if they collided at the proper time; this is a source of error similar to the finite cell size effect. Second, extra fluxes are generated due to the altered trajectories of the molecules that, as a result of the discretization, collide at times other than their proper collision time.

Alexander *et al.*[6] have shown that the effects of discretization in space can be calculated by application of the Green–Kubo formulation[7] when the collision process is assumed to be continuous ($\Delta t \to 0$). Unfortunately, DSMC does not lend itself naturally to the application of this formulation for the calculation of the truncation error due to a finite time step because DSMC is a discrete-time model. In order to apply the Green–Kubo procedure we will first formulate a continuous-time model that is dynamically equivalent to DSMC.

In Sec. II we give an overview of the dynamical steps of the DSMC algorithm and review the calculation for the effect of finite cell size. In Sec. III we quantify the two sources of error arising from a finite time step and show how the error for transport coefficients can be calculated as a function of the time step. In Sec. IV we compare our predictions with simulation results, and finish with some concluding remarks in Sec. V.

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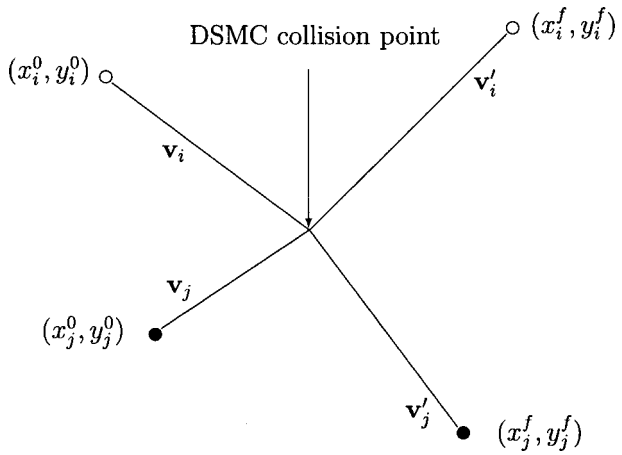

FIG. 1. Schematic of a representative collision between particles in DSMC for cell size $L\to 0$. The particles collide at $\tau=\Delta t/2$.

II. DSMC ALGORITHM AND CELL SIZE DEPENDENCE OF TRANSPORT COEFFICIENTS

In what follows we will limit our illustration to two dimensions; generalization to three dimensions follows directly. Consider two particles, i and j, that collide at time step n (Fig. 1); let their initial locations (at the start of the time step) be (x_i^0, y_i^0) and (x_j^0, y_j^0). Let τ be the time variable over which DSMC coarse grains, that is $\tau=\mathrm{mod}(t,\Delta t)$, where $t=n\Delta t+\tau$ is time. The above particles travel with velocities $\mathbf{v}_i$ and $\mathbf{v}_j$, and at $\tau=\Delta t/2$ (when collisions take place) will be in the same cell so that they are chosen as collision partners. After colliding, the particles acquire new velocities $\mathbf{v}_i'$ and $\mathbf{v}_j'$ and travel ballistically for the remainder of the time step $\tau=\Delta t/2$ to their final positions (x_i^f, y_i^f) and (x_j^f, y_j^f). Note that in our notation a time step starts $1/2\Delta t$ before the instantaneous collision process and ends $1/2\Delta t$ after the instantaneous collision process. This being purely a matter of convention has no effect on the DSMC dynamics: particles travel ballistically between collisions for a time Δt (we exclude the presence of external fields that may introduce particle accelerations) and then instantaneous collisions accounting for the whole time interval Δt take place. Our convention merely introduces a shift in the global time counter with collisions taking place at $t=\Delta t/2,\ 3\Delta t/2,\ 5\Delta t/2,\ldots$, with ballistic motion in between, instead of $t=0,\ \Delta t,\ 2\Delta t,\ldots$, with ballistic motion in between.

In the limit that $\Delta t\to 0$ we can neglect the error from the discrete nature of this algorithm and use the Green–Kubo theory[7] to evaluate the effect of cell size L on the transport coefficients. We review here the calculation of the viscosity coefficient as a function of the cell size in order to point out a correction. Following Alexander *et al.*[6] we define the stress tensor $J_{xy}(t)$ for a hard sphere system,

$$J_{xy}(t)=m\left[\sum_{i=1}^{N} u_i v_i+\sum_{c}\ \Delta u_i (y_i-y_j)\,\delta(t-t_c)\right], \tag{1}$$

where N is the number of molecules, m is the mass of the molecules, u_i, v_i are the x and y components of the velocity of molecule i, Δu_i is the change in the velocity of particle i in the x direction during collision, and Σ_c denotes the sum over all collisions, each collision occurring at t_c and involving molecules i and j. The distance (y_i-y_j) between the two molecules at collision introduces a potential contribution that is absent in the Enskog theory of dilute gases.

The viscosity is calculated using the Green–Kubo formulation as applied to hard spheres by Wainright,[7]

$$\eta=\frac{1}{VkT}\int_0^\infty ds\left[\frac{1}{t_s}\int_0^{t_s} dt\, J_{xy}(t)J_{xy}(t+s)\right], \tag{2}$$

where V is the volume, and t_s is a sufficiently long smoothing time (several time steps). Substitution of Eq. (1) into Eq. (2) yields[6]

$$\eta=\eta^K+\eta^C+\eta^P, \tag{3}$$

where the superscripts K, C, P denote kinetic, cross, and potential terms. The kinetic term is the Chapman–Enskog viscosity of a dilute gas (hard spheres of diameter σ)[6]

$$\eta^K=\frac{5\pi}{16}m\Gamma\lambda^2, \tag{4}$$

where $\Gamma=2\sigma^2 n^2\sqrt{\pi kT/m}$ is the collision rate per unit volume, and $\lambda=1/(\sqrt{2}n\pi\sigma^2)$ is the mean free path.

The cross term is zero because particle velocities are uncorrelated with their positions.[6] The potential term is given by[6]

$$\eta^P=\frac{m^2\Gamma}{2kT}\langle[(y_i-y_j)\Delta u_i]^2\rangle_c$$

$$=\frac{m^2\Gamma}{2kT}\langle(y_i-y_j)^2\rangle_c\langle(\Delta u_i)^2\rangle_c, \tag{5}$$

where $\langle\ \rangle_c$ denotes average over collisions. For a gas of uniform density, $\langle(y_i-y_j)^2\rangle_c=L^2/6$. We would like to point out that $\langle(\Delta u)^2\rangle_c=\frac{4}{3}(kT/m)$ instead of the original value of $\frac{8}{9}(kT/m)$ given in Alexander *et al.*,[6] and thus the viscosity as a function of cell size in DSMC is given by

$$\eta=\frac{5}{16\sigma^2}\sqrt{\frac{mkT}{\pi}}\left(1+\frac{16}{45\pi}\frac{L^2}{\lambda^2}\right). \tag{6}$$

The expression for the thermal conductivity given in the paper by Alexander *et al.* is not affected by this correction.

III. TIME-STEP DEPENDENCE OF TRANSPORT COEFFICIENTS

A. Equivalent continuous-time model

We now proceed to examine the case where Δt is finite and thus the DSMC algorithm becomes discrete in time. For the above formalism to be applied we propose a continuous-time model that is dynamically equivalent to DSMC.

Consider a model where the particles that according to DSMC would have collided at $\tau=\Delta t/2$ (that is, at $\tau=\Delta t/2$ were in the same cell) instead collide (each colliding pair independently) at t_c that lies uniformly between $\tau=0$ and $\tau=\Delta t$. The distribution function for the particle location relative to the DSMC collision point at collision ($\tau=t_c$) de-

pends on the difference between the collision time t_c and the DSMC collision time $\tau=\Delta t/2$: We can write the single particle distribution function (in one dimension) in the case that the collision cell is centered on $x=0$ as

$$f(x;t_c)=\int_{-L/2}^{L/2} p(\tilde{x})q(x|\tilde{x};t_c)d\tilde{x}, \tag{7}$$

where $p(\tilde{x})$ is the probability (uniform in this approximation) for a particle to be in the cell at $\tilde{x}$, and $q(x|\tilde{x};t_c)$ is the probability for a particle that is at $\tilde{x}$ at $\tau=\Delta t/2$ to be found at x at $\tau=t_c$. Due to the Maxwellian velocity distribution $q(x|\tilde{x};t_c)$ has a particularly simple form that leads to

$$f(x;t_c)=\sqrt{\frac{m}{2\pi kT(t_c-\Delta t/2)^2}}\int_{-L/2}^{L/2}\frac{1}{L}\times\exp\left(-\frac{m(x-\tilde{x})^2}{2kT(t_c-\Delta t/2)^2}\right)d\tilde{x}, \tag{8}$$

where k is Boltzmann's constant, and T is the temperature. The above expression reduces to a Maxwellian distribution (centered at $x=0$) if the cell size $L\to 0$. We can see that a finite cell size modifies the particle distribution function and, thus, strictly couples to the finite time-step truncation error. In the interest of simplicity (the effect of finite cell size can be fully quantified if the algebraic complexity is undertaken) and because the error due to a finite cell size in the limit $\Delta t\to 0$ is known,[6] we will take $L\to 0$. In this limit the relative distance in the y direction between a collision pair at collision can be written as

$$(y_i-y_j)=\left(t_c-\frac{\Delta t}{2}\right)g_y, \tag{9}$$

where $\mathbf{g}=\mathbf{v}_i-\mathbf{v}_j$ is the precollision relative velocity of the particles.

Figure 2 indicates that for this model to be dynamically identical to the DSMC implementation, colliding particles need to be shifted after their collisions by an amount that corrects for their ballistic motion with postcollision velocities instead of the precollision velocities for the appropriate amount of time $(t_c-\Delta t/2)$. The shift ensures that the molecules have final positions (x_i^f,y_i^f) and (x_j^f,y_j^f) that are the same as for DSMC (Fig. 1). The amount each molecule needs to be shifted is given by

$$\Delta\mathbf{r}_i=\left(t_c-\frac{\Delta t}{2}\right)(\mathbf{v}_i'-\mathbf{v}_i). \tag{10}$$

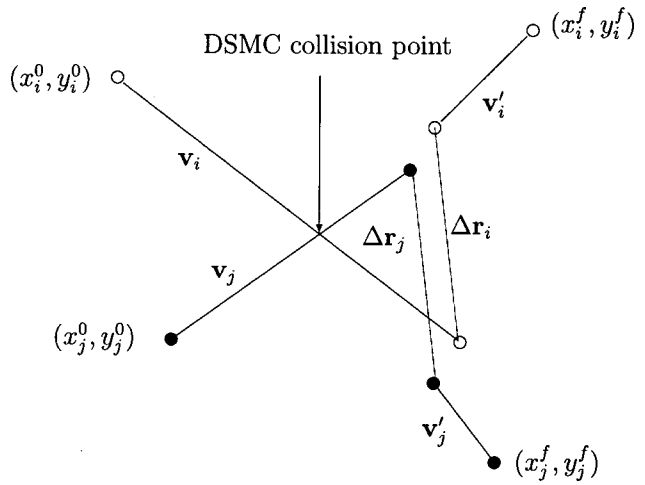

FIG. 2. Schematic of a representative collision between particles in the continuous-time model. The discontinuous jump in the trajectories represents the shift occurring along with the collision.

This shift introduces mass, momentum, and energy fluxes that contribute to ''enhanced'' transport coefficients as shown below.

B. Calculation of transport coefficients

We now present the calculation of the viscosity of the DSMC-equivalent continuous-time model as a function of the time step. Application of the Green–Kubo theory implies that steady problems are considered, at least at the autocorrelation decay time scale. This is not a very restrictive assumption since typical hydrodynamic evolution takes place at time scales much longer than the latter time scale.

The momentum flux resulting from the particle shift can be written as

$$J_{xy}^s=m\sum_c (u_i'\Delta y_i+u_j'\Delta y_j)\,\delta(t-t_c)$$
$$=m\sum_c\left(t_c-\frac{\Delta t}{2}\right)\Delta v_i g_x'\,\delta(t-t_c), \tag{11}$$

where $\mathbf{g}'=\mathbf{v}_i'-\mathbf{v}_j'$ is the postcollision relative velocity between particle i and particle j. Shifting the particles before or after collision results in the same total potential contribution to the stress tensor:

$$J_{xy}(t)=m\left[\sum_{i=1}^N u_i v_i+\sum_c (\Delta u_i(y_i-y_j)+u_i'\Delta y_i+u_j'\Delta y_j)\,\delta(t-t_c)\right] \tag{12}$$

$$=m\left[\sum_{i=1}^N u_i v_i+\sum_c [\Delta u_i(y_i+\Delta y_i-(y_j+\Delta y_j))+u_i\Delta y_i+u_j\Delta y_j]\,\delta(t-t_c)\right] \tag{13}$$

$$=m\left[\sum_{i=1}^N u_i v_i+\sum_c\left(t_c-\frac{\Delta t}{2}\right)(\Delta u_i g_y+\Delta v_i g_x')\,\delta(t-t_c)\right]. \tag{14}$$

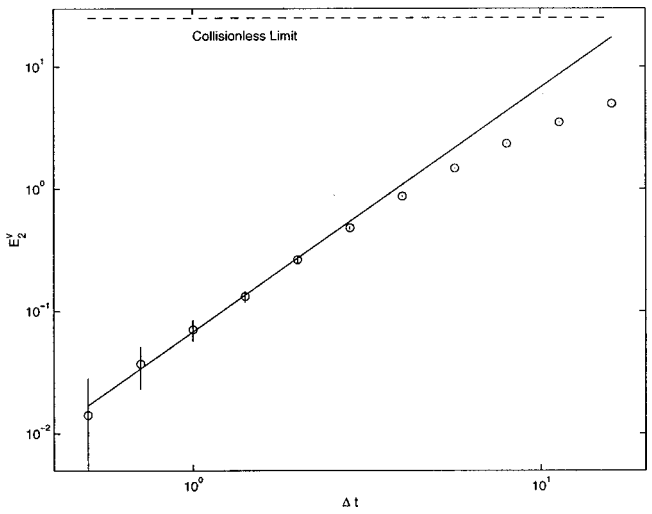

FIG. 3. Error in coefficient of viscosity as a function of the scaled (by λ/c_0) time step (from Ref. 8). Circles denote the normalized error in momentum flux (E_2^v) in the simulations of Garcia and Wagner (Ref. 8), and the solid line is the prediction of (19).

Here Δv_i is the change in velocity of particle i in the y direction due to the collision.

Application of the Green–Kubo formula (2) again results in kinetic, cross, and potential terms. The kinetic term is again the dilute gas term [Eq. (4)]. The cross term is zero because DSMC is ''centered'' in time: The contribution is proportional to $\langle (t_c-(\Delta t/2)\rangle_c$ and hence zero because

$$\int_0^{\Delta t}\left(t_c-\frac{\Delta t}{2}\right)dt_c=0. \tag{15}$$

The potential contribution can be written as

$$\eta^P=\frac{m^2\Gamma}{2kT}\left\langle\left[\left(t_c-\frac{\Delta t}{2}\right)(\Delta u_i g_y+\Delta v_i g_x')\right]^2\right\rangle_c. \tag{16}$$

This expression assumes that there is no correlation beyond the first collision between molecules. The uniform collision in time gives

$$\left\langle\left(t_c-\frac{\Delta t}{2}\right)^2\right\rangle_c=\frac{(\Delta t)^2}{12}, \tag{17}$$

whereas

$$\langle(\Delta u g_y+\Delta v g_x')^2\rangle_c=\frac{16}{5}\left(\frac{kT}{m}\right)^2. \tag{18}$$

The expression for the viscosity including the time-step contribution is thus

$$\eta=\frac{5}{16\sigma^2}\sqrt{\frac{mkT}{\pi}}\left(1+\frac{32}{150\pi}\frac{(c_0\Delta t)^2}{\lambda^2}\right), \tag{19}$$

where $c_0=\sqrt{2kT/m}$ is the most probable speed.

The calculation of other transport coefficients follows along the same lines. Potential contributions are proportional to $\langle(t_c-\Delta t/2)^2\rangle_c=(\Delta t)^2/12$ and cross contributions vanish because DSMC is centered in time. The pressure is unaffected by the time step as we would normally expect: The virial $\langle\Delta u_i(y_i-y_j)+u_i'\Delta y_i+u_j'\Delta y_j\rangle_c$ is proportional to $\langle(t_c-\Delta t/2)\rangle_c=0$.

A similar calculation for the thermal conductivity κ yields

$$\kappa=\frac{75k}{64\sigma^2}\sqrt{\frac{kT}{\pi m}}\left(1+\frac{64}{675\pi}\frac{(c_0\Delta t)^2}{\lambda^2}\right). \tag{20}$$

The diffusion coefficient can be calculated using the Einstein formula

$$D=\frac{1}{2t}\left(\frac{1}{N}\sum_i^N(x_i(t)-x_i(0))^2\right), \tag{21}$$

where a long time limit is assumed. Applying this formula to the continuous-time model reveals that the shift [Eq. (10)] for *both* colliding particles required for every collision, leads to a ''potential-like'' term $\Delta\mathbf{r}_i\delta(t-t_c)=(t_c-\Delta t/2)\Delta\mathbf{v}_i\delta(t-t_c)$ that yields an error proportional to $(\Delta t)^2$. The resulting expression for the diffusion coefficient D is

$$D=\frac{3}{8n\sigma^2}\sqrt{\frac{kT}{\pi m}}\left(1+\frac{4}{27\pi}\frac{(c_0\Delta t)^2}{\lambda^2}\right), \tag{22}$$

where n is the number density.

IV. COMPARISON WITH NUMERICAL SIMULATIONS

Garcia and Wagner[8] performed steady state and transient numerical simulations in a variety of configurations to measure the truncation error as a function of the time step. In those simulations the cell size was taken to be $L=\lambda/5$ so that the cell size contribution is negligible, and the time step was varied from $\Delta t=\lambda/(2c_0)$ to $\Delta t=16\lambda/c_0$. The error is defined as the normalized deviation in the flux corresponding to the transport coefficient with respect to the exact result. The exact result is taken to be a very accurate simulation with $\Delta t=\lambda/(8c_0)$.

Figure 3 shows the comparison between the numerical results of Garcia and Wagner for the viscosity coefficient and the theoretical prediction [Eq. (19)] for steady Couette flow. The agreement is very good for $\Delta t\to 0$. For $\Delta t\gg\lambda/c_0$ the error deviates from the quadratic time step dependence. Garcia and Wagner[8] point out that this is due to the upper bound set on the transport coefficients by the collisionless limit that is indicated on the same graph. The predictions given here for the thermal conductivity [Eq. (20)] and diffusion coefficient [Eq. (22)] are also in very good agreement with the numerical results of Garcia and Wagner[8] in steady state. The transient calculations of Garcia and Wagner also exhibit a quadratic error in the time step; however, no comparison with our results was presented.

V. CONCLUDING REMARKS

We have presented a formulation that allows the calculation of the transport coefficient dependence on the time step. The calculations predict that the error in the *transport coefficients* is of order Δt^2, and that for $\Delta t\sim\lambda/c_0$ the trun-

cation error is approximately 5%, which confirms the empirical observations that accurate solutions require a time step that is a small fraction of the mean free time. The theory presented relies on the application of the Green–Kubo theory and is thus valid for problems that appear steady at the autocorrelation decay time scale.

The results of this paper have been verified by extensive numerical simulations[8] of steady state configurations; the agreement between simulations and theory is very good for $\Delta t \to 0$. For $\Delta t \gg \lambda / c_0$ the error approaches the value set by the collisionless limit.

ACKNOWLEDGMENTS

The author would like to thank Alej Garcia and Frank Alexander for helpful discussions.

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