Simulation of the Enskog equation *à la* Bird

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(Received 27 November 1996; accepted 12 March 1997)

We present a modification of a recently proposed Monte Carlo simulation method [J. M. Montanero and A. Santos, Phys. Rev. E **54**, 438 (1996)] to numerically solve the Enskog equation for a dense hard-sphere fluid. While in the original method momentum and energy are conserved by collisions only on average [as happens with Nanbu's scheme of the direct simulation Monte Carlo (DSMC) method for solving the Boltzmann equation], the modified algorithm (that extends Bird's null-time-counter version of the DSMC method) preserves exactly the conservation laws. Both methods are applied to fluids under shear for a wide range of densities. The agreement with the theoretical predictions for the shear viscosity and the viscometric coefficients is found to be excellent. © *1997 American Institute of Physics.* [S1070-6631(97)00507-2]

In the context of dilute gases, the Boltzmann equation (BE) (Ref. 1) provides an adequate description for states arbitrarily far from equilibrium. In this low-density regime, the information contained in the BE is valid even for large gradients of the hydrodynamic fields, beyond the range of applicability of the hydrodynamic equations. Nevertheless, because of the mathematical complexity of the BE, only a limited number of exact solutions are known.[2] If one is mainly interested in a semiquantitative description, the above difficulty can be overcome by the use of simplified kinetic models.[3] Otherwise, one must resort to numerical methods, the favorite of which is the so-called direct simulation Monte Carlo (DSMC) method,[4] first introduced by Bird in 1963. The DSMC method has proven to be a very reliable and useful tool to analyze nonequilibrium states of dilute gases. A number of different schemes of this algorithm have been proposed, two of the most widely used ones being Bird's null-time-counter (NTC),[4] and Nanbu's.[5]

In 1992, Enskog[6] modified the BE for hard spheres in an attempt to incorporate finite-density effects. He introduced two significant changes: (a) the finite distance between the centers of a colliding pair, and (b) the increase of the collision frequency due to excluded volume effects. More specifically, the Enskog equation (EE) for the distribution function f reads[1,6]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right)f(\mathbf{r},\mathbf{v},t)=\sigma^2\int d\mathbf{v}_1\int d\hat{\boldsymbol{\sigma}}\,\Theta(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})\times[\chi(\mathbf{r},\mathbf{r}-\boldsymbol{\sigma})f(\mathbf{r},\mathbf{v}',t)\times f(\mathbf{r}-\boldsymbol{\sigma},\mathbf{v}_1',t)-\chi(\mathbf{r},\mathbf{r}+\boldsymbol{\sigma})\times f(\mathbf{r},\mathbf{v},t)f(\mathbf{r}+\boldsymbol{\sigma},\mathbf{v}_1,t)]. \quad (1)$$

Here, $\Theta(x)$ is the Heaviside function, $\boldsymbol{\sigma}=\sigma\hat{\boldsymbol{\sigma}}$ (σ being the diameter of a sphere), $\mathbf{g}\equiv\mathbf{v}-\mathbf{v}_1$, $\mathbf{v}'=\mathbf{v}-(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})\hat{\boldsymbol{\sigma}}$, and $\mathbf{v}_1'=\mathbf{v}_1+(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})\hat{\boldsymbol{\sigma}}$. In the standard Enskog theory (SET),[1] $\chi(\mathbf{r},\mathbf{r}\pm\boldsymbol{\sigma})=\chi(n(\mathbf{r}\pm\frac{1}{2}\boldsymbol{\sigma}))$, where $\chi(n)$ is the equilibrium pair correlation function at contact and $n(\mathbf{r})$ is the number density field. In the revised Enskog theory (RET),[7] developed by van Beijeren and Ernst, $\chi(\mathbf{r},\mathbf{r}\pm\boldsymbol{\sigma})$ is identified with the local equilibrium pair correlation function in a nonuniform state, so that it is a functional of the density field. From Eq. (1) one can obtain the balance equations for the densities of mass, $mn(\mathbf{r},t)$, momentum, $mn(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)$, and kinetic energy, $\frac{3}{2}n(\mathbf{r},t)k_BT(\mathbf{r},t)$, with explicit expressions for the kinetic and collisional transfer parts of the corresponding fluxes. By means of the standard Chapman–Enskog method,[1] one gets the Navier–Stokes constitutive equations and identifies the transport coefficients.

Needless to say, the EE is even more difficult to solve than the BE. Recently, simplified kinetic models that keep the essential features of the EE have been proposed.[8] As in the case of the BE, a different approach consists of solving the EE by means of a numerical Monte Carlo algorithm in the same spirit as the DSMC method of solving the BE. The implementation of this objective is not straightforward. A first attempt by Alexander, Garcia, and Alder[9] gives the correct equation of state but does not reproduce the Enskog transport coefficients. We have recently developed an extension of the DSMC method, the Enskog simulation Monte Carlo (ESMC) method,[10] that is fully consistent with the transport coefficients derived from the EE.[11,12] In the low-density limit, this ESMC method reduces to Nanbu's scheme of the DSMC method.[5] The key difference between Bird's and Nanbu's schemes is that, in the latter, only one of the two particles involved in a collision changes its velocity, so that momentum and energy are conserved only on average. This might lead to a bias in the statistical errors,[13] forcing the use of very large values for the number N of simulated molecules. Although we have not observed any problem associated with the lack of detailed conservation of momentum and energy in our ESMC method *à la* Nanbu (hereafter, referred to as the ESMC1 method), it is highly desirable to adapt it to preserve the exact conservation laws. The objective of this paper is to describe this modified ESMC method *à la* Bird

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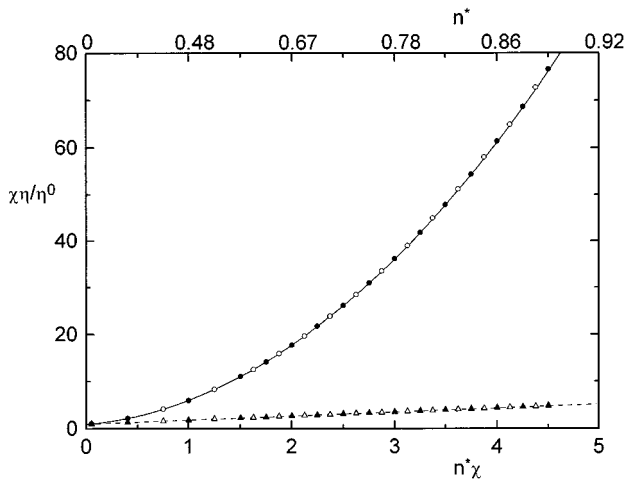

FIG. 1. Plot of $\chi\eta/\eta^0$ (circles and solid line) and of $\chi\eta^k/\eta^0$ (triangles and dashed line) as functions of $n^*\chi$. The open and solid symbols are the results obtained from the ESMC1 and ESMC2 methods, respectively. The lines are the theoretical predictions. The upper scale corresponds to the reduced density n^*, according to the Carnahan–Starling equation of state.

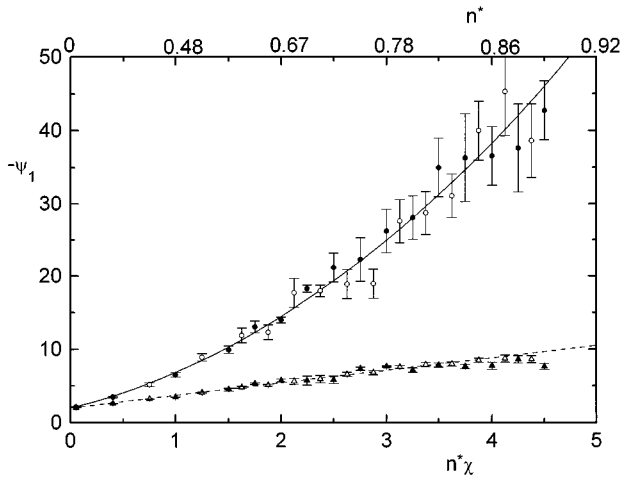

FIG. 2. The same as in Fig. 1, but for $-\Psi_1$ and $-\Psi_1^k$.

(hereafter, referred to as the ESMC2 method) and compare both of them with analytical results obtained from the EE for the uniform shear flow (USF) state.

As in DSMC,[4] in the ESMC method N simulated particles are contained in a volume V split into cells with a typical size ΔL much smaller than both the mean-free path and the characteristic hydrodynamic length. The number N has a statistical meaning, so that the ratio N/V does not coincide, in general, with the physical average density of interest, $\overline{n}$; consequently, the ratio $\nu \equiv \overline{n}/(N/V)$ is a technical parameter that can be chosen independent of the physical density $\overline{n}$. The ''local'' density of cell I is $n_I=(N_I/V_I)\nu$, where N_I and V_I are the number of particles and volume of cell I, respectively. The positions and velocities are updated in two stages (convection and collisions) that are decoupled for a time step Δt much smaller than both the mean time between collisions and the hydrodynamic time. In the convection stage, the particles move freely (under the possible action of an external force) and those leaving the volume are reentered in accordance with the boundary conditions. The only distinction between the ESMC1 and the ESMC2 methods appears in the treatment of the collision stage. In ESMC1,[10] the following steps are taken for every particle $i=1,\ldots,N$: (1) a given direction $\hat{\boldsymbol{\sigma}}_i$ is chosen at random with equiprobability; (2) a test particle j belonging to the cell J that contains the point $\mathbf{r}_i+\sigma\hat{\boldsymbol{\sigma}}_i$ is chosen at random with equiprobability; (3) the collision between particles i and j is accepted with a probability equal to $\Theta(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\omega_{ij}$, where $\mathbf{g}_{ij}\equiv\mathbf{v}_i-\mathbf{v}_j$ and $\omega_{ij}\equiv\sigma^2 4\pi(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\chi(\mathbf{r}_i,\mathbf{r}_i+\sigma\hat{\boldsymbol{\sigma}}_i)n_J\Delta t$; and (4) if the collision is accepted, the postcollision velocity $\mathbf{v}_i'=\mathbf{v}_i-(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\hat{\boldsymbol{\sigma}}_i$ is assigned to particle i, once the collision stage *has finished* for all the particles. Notice that the role of particle j is to sample the velocity distribution in the cell J, so that its velocity is not changed. In the modified method (ESMC2) we propose here, the collision stage is inspired in Bird's NTC algorithm.[4] For each cell I, a sample of $\frac{1}{2}N_I\omega_{\max}$ particles are chosen at random with equiprobability, where $\omega_{\max}$ is an upper bound of the set $\{\omega_{kl}\}$, k being any particle of cell I and l any particle of those cells separated a distance σ from I. For each particle i of this sample, the following steps are taken: (1) a given direction $\hat{\boldsymbol{\sigma}}_i$ is chosen at random with equiprobability; (2) a particle j belonging to the cell J that contains the point $\mathbf{r}_i+\sigma\hat{\boldsymbol{\sigma}}_i$ is chosen at random with equiprobability; (3) the collision between particles i and j is accepted with a probability equal to $\Theta(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\omega_{ij}/\omega_{\max}$; and (4) if the collision is accepted, the post-collision velocities $\mathbf{v}_i'=\mathbf{v}_i-(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\hat{\boldsymbol{\sigma}}_i$ and $\mathbf{v}_j'=\mathbf{v}_j+(\hat{\boldsymbol{\sigma}}_i\cdot\mathbf{g}_{ij})\hat{\boldsymbol{\sigma}}_i$ are *immediately* assigned to particles i and j, respectively. In both methods, the physical quantities are evaluated in every cell by averaging over the particles inside that cell and also over an ensemble of $\mathscr{N}$ different realizations. In particular, the kinetic and collisional transfer contributions of the local pressure tensor are obtained, in each realization, as

$$\mathsf{P}_I^k=\frac{\nu}{V_I}\,m\sum_{i\in I}(\mathbf{v}_i-\mathbf{u}_I)(\mathbf{v}_i-\mathbf{u}_I), \tag{2}$$

$$\mathsf{P}_I^c=-c\,\frac{\nu\sigma}{V_I\Delta t}\,m\sum_{i\in I}(\mathbf{v}_i'-\mathbf{v}_i)\hat{\boldsymbol{\sigma}}_i\,. \tag{3}$$

In Eq. (2), $\mathbf{u}_I=N_I^{-1}\Sigma_{i\in I}\mathbf{v}_i$ is the local velocity. In Eq. (3), the summation restricts to particles involved in accepted collisions and $c=\frac{1}{2}$ (ESMC1) or $c=1$ (ESMC2). Finally, the SET is implemented by making $\chi(\mathbf{r}_i,\mathbf{r}_i+\sigma\hat{\boldsymbol{\sigma}}_i)=\chi(n_{I'})$, where the cell I' is the one containing the point $\mathbf{r}_i+\frac{1}{2}\sigma\hat{\boldsymbol{\sigma}}_i$; in the RET, $\chi(\mathbf{r}_i,\mathbf{r}_i+\sigma\hat{\boldsymbol{\sigma}}_i)$ must be computed from the knowledge of the density in al cells, $\{n_K\}$.

The ESMC1 method has been shown to reproduce correctly the shear viscosity,[10,11] the viscometric coefficients,[11] and the thermal conductivity[12] given by the EE. To check the validity of the ESMC2 method proposed in this paper, we have applied it to the USF state. This nonequilibrium state is characterized by a constant density, a uniform temperature, and a linear velocity profile: $\mathbf{u}(\mathbf{r})=ay\hat{\mathbf{x}}$, where a is the constant shear rate. The appropriate boundary conditions leading to this state are Lees–Edwards's,[14] which can be seen as periodic boundary conditions in the local Lagrangian frame.[15] Since the density is uniform, there is no distinction

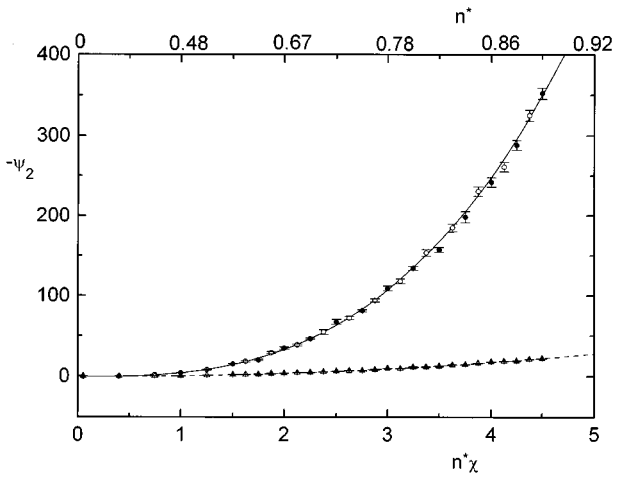

FIG. 3. The same as in Fig. 1, but for $-\Psi_2$ and $-\Psi_2^k$.

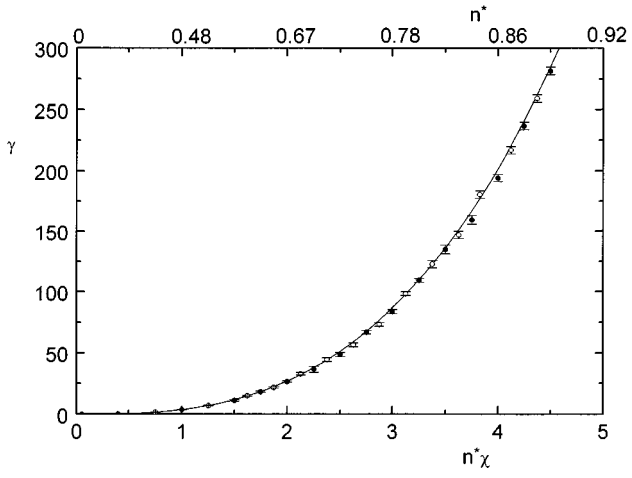

FIG. 4. The same as in Fig. 1, but for γ.

between the SET and the RET in this state. We have solved the EE for USF by means of the ESMC2 method for $0.05 \leqslant n^*\chi \leqslant 4.5$, that, according to the Carnahan–Starling equation of state,[16] is equivalent to the range $0.047 \leqslant n^* \equiv n\sigma^3 \leqslant 0.891$. In all the cases, the system had a size $L = 20\lambda$ (where $\lambda = \sigma/\sqrt{2}\pi n^*\chi$ is the generalized mean-free path) along the y axis and was split into 100 layers of equal width (i.e., $\Delta L = 0.2\lambda$). We have considered $N = 10^5$ particles, a time step $\Delta t = 10^{-2}\tau$ (where $\tau = \eta^0/\chi n k_B T$ is an effective mean time between collisions, η^0 being the Boltzmann viscosity), and $\mathcal{N} = 20$ replicas. Since the temperature increases due to viscous heating effects, Δt decreases with time (roughly as t^{-1}) and so does the reduced shear rate $a^* \equiv a\tau$.

In the simulations, the kinetic and collisional parts of the pressure tensor P have been evaluated as functions of time. From them, we have obtained the (Navier–Stokes) shear viscosity

$$\chi \frac{\eta}{\eta_0} = \lim_{a^* \to 0} \frac{-P_{xy}}{n k_B T a^*}, \tag{4}$$

and the (Burnett) viscometric coefficients

$$\Psi_1 = \lim_{a^* \to 0} \frac{P_{yy} - P_{xx}}{n k_B T a^{*2}}, \quad \Psi_2 = \lim_{a^* \to 0} \frac{P_{zz} - P_{yy}}{n k_B T a^{*2}},$$

$$\gamma = \lim_{a^* \to 0} \frac{p - p_0}{n k_B T a^{*2}}. \tag{5}$$

The coefficients $\Psi_{1,2}$ measure normal stress effects, while γ measures the increase of the nonequilibrium hydrostatic pressure $p = \frac{1}{3}\,\mathrm{Tr}\mathsf{P}$ from its equilibrium value p_0. In practice, the limit $a^* \to 0$ has been replaced by an average over the interval $0.04 < a^* < 0.06$. Figures 1–4 show the comparison between the simulation data and the theoretical predictions; in addition to the total values of the shear viscosity and viscometric coefficients, their kinetic contributions (denoted with the superscript k and defined in Ref. 10) are also shown. In the case of the viscometric coefficients, the theoretical results correspond to a recent perturbative solution of the EE through second order in the shear rate and fourth order in the velocity moments.[17] Also shown are the simulation data obtained in Ref. 11 with the ESMC1 method. As one can see, the agreement is very good in both cases.

In summary, the two simulation Monte Carlo methods (ESMC1 and ESMC2) are equally useful to solve numerically the EE. While the ESMC1 method proposed in Ref. 10 reduces to Nanbu's DSMC method[5] in the limit of dilute gases, the ESMC2 method proposed in this paper becomes Bird's NTC version of the DSMC method[4] in the same limit. Apart from the problems that Nanbu's method might present if N is not sufficiently large,[13] the choice between both algorithms is mainly a matter of taste. A key factor to prefer one over the other is computational efficiency. In our application to the USF state, we have found the ESMC2 method to be typically twice as efficient as the ESMC1 method.

ACKNOWLEDGMENTS

The authors are grateful to A. Frezzotti for insightful discussions and for calling Ref. 13 to our attention. This research has been supported by the DGICYT (Spain) through Grant No. PB94-1021 and by the Junta de Extremadura (Fondo Social Europeo) through Grant No. EIA94-39.

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