Monte Carlo simulation of the Boltzmann equation for uniform shear flow

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The Boltzmann equation is numerically solved by means of the Direct Simulation Monte Carlo method for molecules interacting via repulsive $r^{-\mu}$-potentials under uniform shear flow far from equilibrium. The non-Newtonian shear viscosity is found to be rather insensitive to the interaction model. The results show that the divergence of velocity moments of degree equal to or larger than four obtained from an exact solution for Maxwell molecules [Phys. Rev. Lett. **71**, 3971 (1993)] is also present for other interaction potentials. © *1996 American Institute of Physics.* [S1070-6631(96)03307-7]

One of the rare cases for which the nonlinear Boltzmann equation allows an exact analysis is the uniform shear flow (USF). In this state,[1] the only non-zero hydrodynamic gradient is $\partial u_x/\partial y = a$, where $\mathbf{u}(\mathbf{r})$ is the flow velocity and a is the constant shear rate. Moreover, this state becomes spatially homogeneous in the Lagrangian frame, i.e. $f(\mathbf{r},\mathbf{v},t) = f(\mathbf{V},t)$, where f is the velocity distribution function and $\mathbf{V} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity. In principle the USF state is not steady since the temperature increases in time (viscous heating). In order to prevent this effect, an artificial ''drag'' force of the form $\mathbf{F}^{\text{th}} = -m\alpha\mathbf{V}$ is usually introduced.[2]

In 1956, Ikenberry and Truesdell[3] obtained explicitly the second-degree moments (pressure tensor) for arbitrary values of the shear rate as a function of time, in the special case of Maxwell molecules, namely particles interacting via an r^{-4}-potential. Recently, the fourth-degree moments have also been obtained.[1,4] In contrast to the regular behavior of the pressure tensor, the fourth-degree moments diverge beyond a critical shear rate $a_c \simeq 6.845\nu$ (ν being an effective collision frequency). This singular behavior extends to higher-degree moments, the values of the critical shear rate being a decreasing function of the degree.[5] A natural question is whether the above singular behavior also appears for other interaction potentials. Except for Maxwell molecules, the moment hierarchy cannot be solved exactly, so that the problem becomes untractable from an analytical point of view. In order to overcome these difficulties, in this Brief Communication we use the Direct Simulation Monte Carlo (DSMC) method[6] to numerically solve the Boltzmann equation for repulsive interactions of the form $\phi(r) \propto r^{-\mu}$, with $\mu = 4,6,8,12$, and ∞. This method has proved to exhibit a good agreement with the exact solution for Maxwell molecules under USF.[7,8]

Under the assumptions established above for the USF, the Boltzmann equation can be written as[1]

$$\frac{\partial}{\partial t} f - aV_y \frac{\partial}{\partial V_x} f - \alpha \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} f) = J[f,f]. \tag{1}$$

The second term on the left-hand side represents an inertial force $\mathbf{F}^{\text{in}} = -maV_y\hat{\mathbf{x}}$ due to the Lagrangian frame, while the third term represents the thermostat force $\mathbf{F}^{\text{th}}$. Since the problem is spatially homogeneous in the Lagrangian frame, only the velocities $\mathbf{V}_i, i = 1, \ldots, N$ of a system of N particles need to be stored. The main quantities are the pressure tensor,

$$\mathsf{P} = \frac{mn}{N} \sum_{i=1}^{N} \mathbf{V}_i \mathbf{V}_i \tag{2}$$

and, more generally, velocity moments of the form

$$\langle V^{\ell} \rangle = \frac{1}{N} \sum_{i=1}^{N} V_i^{\ell}. \tag{3}$$

We have also computed the marginal distribution $\Phi_x(V_x)$, where $\Phi_x(V_x)\Delta V_x$ is the fraction of particles having velocities $\mathbf{V}_i$ such that $V_{iy} > 0$ and $V_x - \frac{1}{2}\Delta V_x < V_{ix} < V_x + \frac{1}{2}\Delta V_x$. As usually done in the DSMC method, the above quantities are averaged over an ensemble of $\mathcal{N}$ replicas. In our simulations, we have taken $N = 5 \times 10^4$ particles and a time-step $\Delta t = 0.003\nu^{-1}$, where $\nu = nk_BT/\eta_{\text{NS}}$, η_{NS} being the Navier-Stokes shear viscosity. Henceforth, we take ν^{-1} and $\sqrt{2k_BT/m}/\nu$ as the unit of time and the unit of length, respectively. In the analysis of the time evolution of second-degree moments the number of replicas has been $\mathcal{N} = 25$ for $\mu \neq 4$ and $\mathcal{N} = 100$ for $\mu = 4$; in the case of higher moments, $\mathcal{N} = 70$ and 200, respectively. In the evaluation of the distribution function we have taken $\Delta V_x = 0.012$ and instead of averaging over different replicas, we have averaged over time intervals.

The main transport coefficient is the nonlinear shear viscosity $\eta = -P_{xy}/a$. Although the hydrodynamic definition of this coefficient is only meaningful in the long-time limit (steady-state), it is interesting to introduce a time-dependent η in order to analyze its transient regime. In Fig. 1, we plot the reduced shear viscosity $\eta^* = \eta/\eta_{\text{NS}}$ as a function of time for $a = 6$. Also shown is the exact curve for Maxwell molecules, although it is hardly distinguishable from the simulation data for this interaction. It is clear that most of the influence of the potential has been scaled out by the choice of the reduced quantities. This is particularly remarkable if one

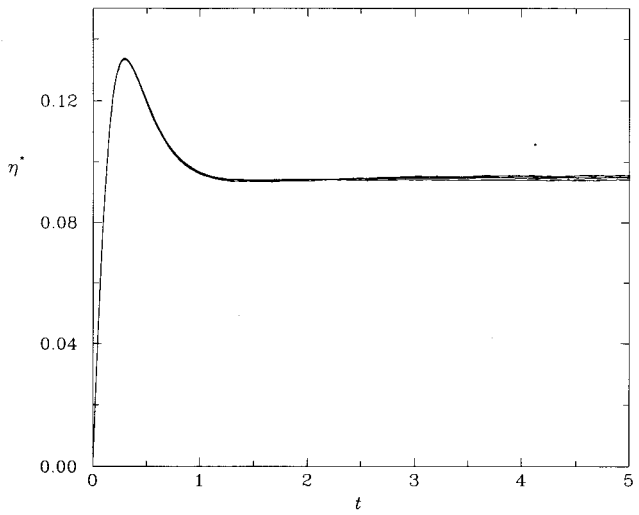

FIG. 1. Time evolution of the reduced shear viscosity, obtained by simulation, at shear rate $a=6$ and for (from bottom to top) $\mu=4,6,8,12$, and ∞ (solid lines). The dashed line corresponds to the exact solution for Maxwell molecules ($\mu=4$).

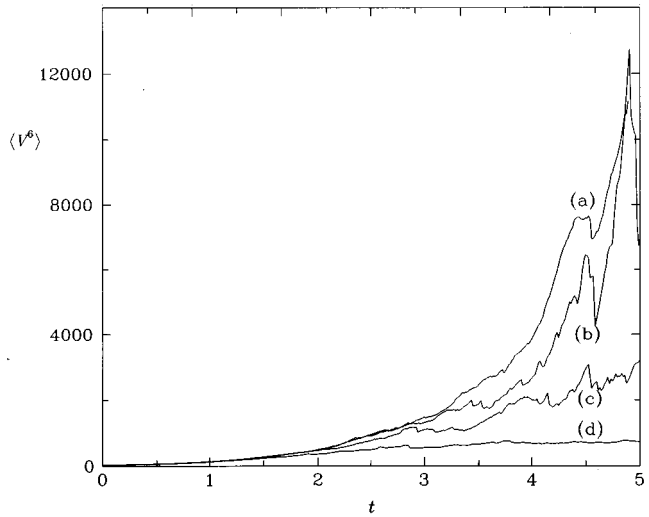

FIG. 3. Time evolution of $\langle V^6\rangle$, obtained by simulation, at shear rate $a=7.33$ and for (a) $\mu=4$, (b) $\mu=8$, (c) $\mu=12$, and (d) $\mu=\infty$.

takes into account that at $a=6$ the non-Newtonian effects are very important ($\eta^*\approx 0.1$). This hydrodynamic value slightly increases as the interaction becomes harder.

Figure 2 shows the time evolution of the fourth-degree moment $\langle V^4\rangle$ at $a=7.33$ and for $\mu=4,8,12$, and ∞. We observe again a good agreement between exact[1] and simulation results for Maxwell molecules. The fact that the data for $\mu=6$ (not shown in Fig. 2 for the sake of clarity) and $\mu=8$ practically overlap with those for $\mu=4$ indicates that $\langle V^4\rangle$ at $a=7.33$ diverges for those cases as well. Nevertheless, the data for $\mu=12$ and $\mu=\infty$ seem to reach stationary values. The interesting question is whether this is also true for moments of a degree higher than 4. As a matter of fact, in the particular case of Maxwell molecules,[5] $\langle V^4\rangle$ converges but $\langle V^6\rangle$ diverges for shear rates within the range $2.346<a<6.845$. The evolution of $\langle V^6\rangle$ is shown in Fig. 3. This moment seems to diverge in time for $\mu=12$, while it still reaches a stationary value for hard spheres. The absence of divergence of the moments $\langle V^4\rangle$ and $\langle V^6\rangle$ at $a=7.33$ for hard spheres ($\mu=\infty$) might be due to the fact that the shear rate is not sufficiently large and/or the degree of the moments is not sufficiently high. In order to shed light on this point, in Fig. 4 we plot $\langle V^\ell\rangle$, $\ell=4,6,8,$ and 10, at $a=10$ and for hard spheres. It is evident that the moments considered reach steady-state values after a few collision times. These values are, on the other hand, much larger than the equilibrium ones. For instance, $\langle V^{10}\rangle\sim 10^8$ at $a=10$, while $\langle V^{10}\rangle=\frac{10\ 395}{32}$ at equilibrium. On the basis of the results shown in Fig. 4, we can conjecture that *all* the velocity moments are convergent for any shear rate in the case of hard spheres.

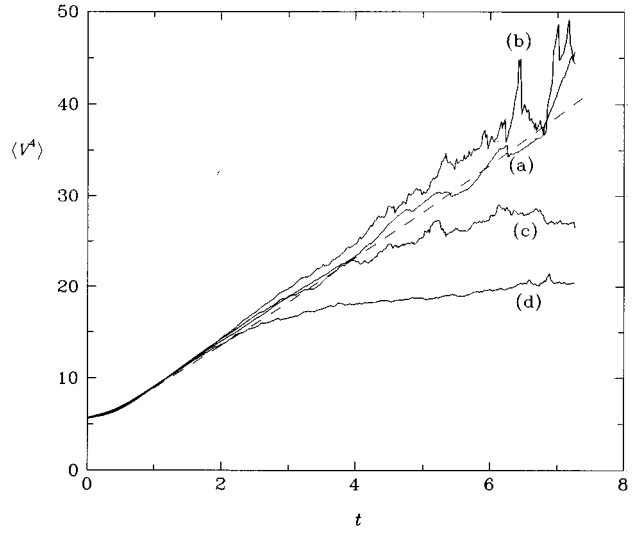

FIG. 2. Time evolution of $\langle V^4\rangle$, obtained by simulation, at shear rate $a=7.33$ and for (a) $\mu=4$, (b) $\mu=8$, (c) $\mu=12$, and (d) $\mu=\infty$. The dashed line is the exact solution for Maxwell molecules ($\mu=4$).

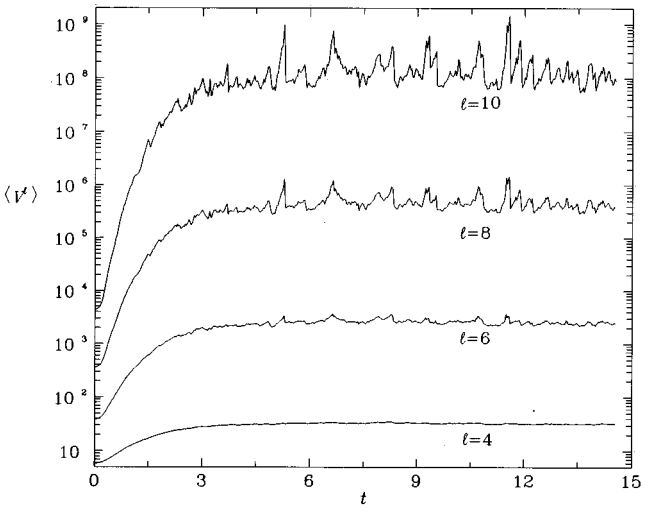

FIG. 4. Time evolution of $\langle V^\ell\rangle$, $\ell=4,6,8,$ and10 at shear rate $a=10$ and for hard spheres ($\mu=\infty$).

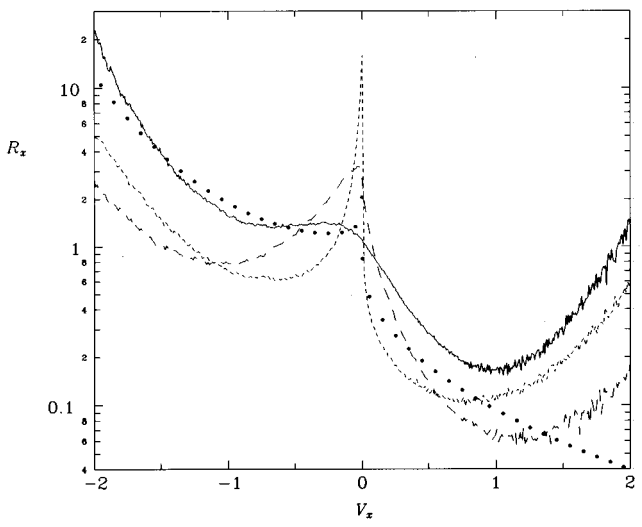

FIG. 5. Plot of the reduced velocity distribution function $R_x(V_x)$ at $a=7.33$ for $\mu=4$ (—), $\mu=8$ (– – –), and $\mu=\infty$ (- - -). The functions have been averaged over the time interval $13<t<14.5$. The dotted line represents the stationary solution of the BGK kinetic equation.

Apart from the analysis of the velocity moments, a complete description of the state of the system requires the knowledge of the velocity distribution function. This function is not explicitly known, even in the case of Maxwell molecules, but can be obtained from the simulation results. Figure 5 shows $R_x(V_x)=\Phi_x(V_x)/(\frac{1}{2}\pi^{-1/2}e^{-V_x^2})$ at $a=7.33$ for $\mu=4,8$, and ∞. We have also included the exact solution of the BGK kinetic equation.[9] The distortion from local equilibrium is significant in all the cases ($R_x \neq 1$), but an important influence of the interaction potential on the shape of the distribution function is observed. The BGK distribution, which is independent of the interaction model, reproduces fairly well the main qualitative features of the distribution functions.

In summary, we have solved the Boltzmann equation for repulsive $r^{-\mu}$-potentials in the USF state by means of the DSMC method. The results show that, by a convenient scaling of the physical quantities, the nonlinear shear viscosity is rather insensitive to the choice of the interaction potential. In contrast, the shape of the velocity distribution function is clearly affected by the interaction considered. In particular, as the hardness of the interaction increases, so does the concentration of particles with velocities close to zero. The main conclusion of this Brief Communication is that the known divergence of the moments for Maxwell molecules at sufficiently large shear rates[4,5] is also present for other interactions. On the other hand, this phenomenon is less notorious as the interaction is harder and seems to disappear in the limit of hard spheres. A possible physical scenario is the following one. The viscous heating [which is produced in the Lagrangian frame by the nonconservative force $\mathbf{F}^{\text{in}}$ in Eq. (1)] is only *globally* controlled by the thermostat force $\mathbf{F}^{\text{th}}$. This means that the *relatively small* high-velocity population may increase in time. This increase can be compensated for if collisions involving high-velocity particles are sufficiently frequent, so that the energy is redistributed. As the interaction becomes harder, the collision frequency for high-velocity particles increases and the energy redistribution is more efficient. This is consistent with a stationary high-velocity tail of the form $f(\mathbf{V})\sim V^{-5-\sigma(a,\mu)}$, where $\lim_{a\to 0}\sigma(a,\mu)=\lim_{\mu\to\infty}\sigma(a,\mu)=\infty$ and $\lim_{a\to\infty}\sigma(a,\mu)=0$. This algebraic decay leads to the divergence of moments of degree $k\geqslant 2+\sigma(a,\mu)$. The verification of this scenario by means of simulation is a very hard task, since it requires the accurate determination of the high-velocity population. In that region, a huge number of particles are needed to achieve a small noise/signal ratio. We plan to undertake this study in the near future.

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