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Analysis on the stability of the uniform shear flow from a Monte Carlo simulation of the Boltzmann equation

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Abstract

The Boltzmann equation with Lees–Edwards boundary conditions is solved from a Monte Carlo simulation for Maxwell molecules. The solution relaxes to the exact one for uniform shear flow. Thus, the latter is stable even for shear rates at which the fourth degree moments diverge.

The uniform shear flow (USF) is one of the simplest states to study nonequilibrium phenomena. It consists of a flow in the x direction with a constant velocity field gradient in the y direction (i.e., $\partial u_i/\partial r_j = a_{ij} = a\delta_{ix}\delta_{jy}$) and a uniform density and temperature. In this state, rheological properties have been analyzed from computer simulations [1] and from a theoretical point of view [2]. In addition, computer simulations for *dense* fluids indicate that the USF is *unstable* beyond a certain critical value of the shear rate a [3]. These simulations show that, at sufficiently large shear rates, the particles are ordered into strings directed along the flow.

For a dilute gas of Maxwell molecules (r^{-4} potential) under USF, Ikenberry and Truesdell derived exact explicit expressions for the shear viscosity and the viscometric functions from the Boltzmann equation [4]. Recently, this solution has been extended to the analysis of the time evolution of the fourth degree velocity moments [5,6]. It was proved that these moments diverge in time for shear rates larger than $a_c = 6.845\tau^{-1}$, where τ is an effective mean free time. In Ref. [5] the possibility was suggested that this *singular* behavior might be connected with a transition from USF to a state with a more complex space dependence. The elucidation of this point requires solving the *inhomogeneous* Boltzmann equation [8],

$$\left(\frac{\partial}{\partial t} + (V_i + a_{ij}r_j)\frac{\partial}{\partial r_i} - \frac{\partial}{\partial V_i}(\alpha V_i + a_{ij}V_j)\right) f = J[f,f], \tag{1}$$

with boundary conditions compatible with the USF, namely the Lees–Edwards periodic boundary conditions [7],

$$f(\boldsymbol{r},\boldsymbol{V},t)|_{y=-L/2} = f(\boldsymbol{r},\boldsymbol{V},t)|_{y=+L/2}. \tag{2}$$

In these equations, $V_i \equiv v_i - a_{ij}r_j$, α is a constant thermostat parameter, f is the one-particle velocity distribution function, J denotes the nonlinear collision operator, and L is the size of the system. Notice that the variable $\boldsymbol{V}$ represents the velocity referred to a Lagrangian frame moving with the linear velocity field characteristic of the USF. As a consequence, a necessary condition for USF is that $\boldsymbol{U}(\boldsymbol{r},t) \equiv \langle \boldsymbol{V} \rangle$ vanishes and $n(\boldsymbol{r},t)$ and $T(\boldsymbol{r},t) \equiv (m/3k_B)\langle (\boldsymbol{V}-\boldsymbol{U})^2 \rangle$

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are uniform. More general, the distribution function $f(\boldsymbol{r}, \boldsymbol{V}; t)$ becomes homogeneous in the USF state. The solution of the problem defined by Eqs. (1) and (2) is a very hard task, even for Maxwell molecules. Nevertheless, this problem can be "solved" by using the direct simulation Monte Carlo (DSMC) method developed by Bird [9]. The reliability of the DSMC method to reproduce the exact time evolution of the second and fourth degree moments for Maxwell molecules has been recently assessed [10].

The aim of this Letter is to perform Monte Carlo simulations for the inhomogeneous problem described by Eqs. (1) and (2) for Maxwell molecules. The question we want to address is whether, by starting from inhomogeneous (in the Lagrangian frame) initial conditions, the distribution function evolves towards a homogeneous state or not. The first possibility would imply that the USF is stable, so that the singular behavior found in Refs. [5,6] would not be associated with any transition to a more ordered state. On the other hand, if the USF were unstable, the stable state would be inhomogeneous with respect to the y axis. In fact, beyond the transition observed in dense fluids, the particles are arranged in layers normal to the y direction [3,11]. For this reason, we will restrict ourselves to solutions to Eqs. (1) and (2) of the form $f(y, \boldsymbol{V}, t)$.

The thermostat parameter α is chosen as the one that keeps the temperature constant in the long-time limit of the USF. Its shear-rate dependence is given by $\alpha = \frac{2}{3}\tau^{-1}\sinh[\frac{1}{6}\cosh^{-1}(1 + 9a^2\tau^2)]$ [6]. In the following, we use units such that $\tau = 1$, $\overline{T}_0 = 1$, $2k_B\overline{T}_0/m = 1$, and $\overline{n} = 1$, where the bar denotes average over space and the subscript 0 refers to the initial condition. In the DSMC method [9], one has to specify the width ΔL of each layer, the time-step Δt, the number of molecules N and the number of realizations $\mathcal{N}$. Here we have taken $\Delta L = 10^{-1}$, $\Delta t = 3 \times 10^{-3}$, $N = 5 \times 10^4$, and $\mathcal{N} = 5$. Furthermore, an angular cutoff $\chi = 0.8°$ is introduced in the collisions. Finally, the size of the system has been taken as $L = 10$.

For the sake of illustration, we consider here initial conditions of the local equilibrium form, i.e.,

$$f(y, \boldsymbol{V}, 0) = n_0(y)\left(\frac{m}{2\pi k_B T_0(y)}\right)^{3/2} \times \exp\left(-m\frac{[\boldsymbol{V} - \boldsymbol{U}_0(y)]^2}{2k_B T_0(y)}\right), \quad (3)$$

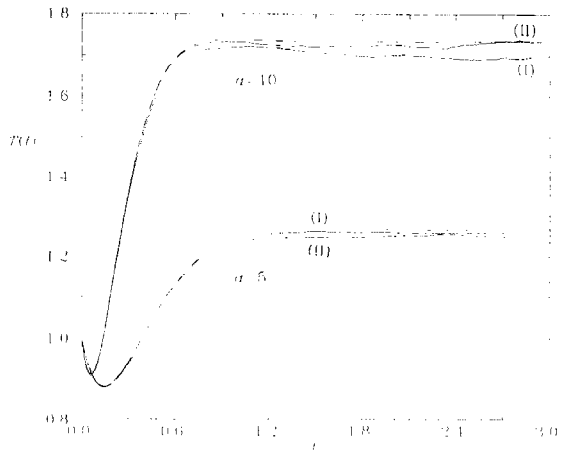

Fig. 1. Time evolution of the average temperature $\overline{T}(t)$ for $a = 5$ and $a = 10$, starting from the initial conditions (I) and (II). The dashed line refers to the exact solution for the USF.

with: (I) $n_0(y) = 1 + 0.06y$, $T_0(y) = \frac{50}{49}(1 - 0.04y)$, $\boldsymbol{U}_0(y) = 0$, and (II) $n_0(y) = 0.8 + 0.024y^2$, $T_0(y) = 1 - 0.04y$, $\boldsymbol{U}_0(y) = 0$. The average temperature $\overline{T}(t)$ is plotted in Fig. 1 for the shear rates $a = 5$ and $a = 10$, by starting from the initial conditions (I) and (II). We also show the evolution of $\overline{T}(t)$ obtained from the Ikenberry–Truesdell solution [4] corresponding to the initial condition (3) with $n_0(y) = 1$, $T_0(y) = 1$, and $\boldsymbol{U}_0(y) = 0$. We observe that the behavior of $\overline{T}(t)$ is hardly sensitive to the choice of the initial condition. In fact, $\overline{T}(t)$ tends towards a stationary value with a relaxation time that practically coincides with the one predicted in the USF case, namely $(1 + 3\alpha)^{-1}$ [6]. This relaxation time decreases as the shear rate increases, so that it is 0.256 for $a = 5$ and 0.163 for $a = 10$. A similar behavior has also been found for the element $\overline{P}_{xy}(t)$ of the pressure tensor.

The fact that the *average* temperature $\overline{T}(t)$ behaves in a similar way as the exact temperature of the USF is not sufficient to imply that the system evolves towards a homogeneous state. In order to investigate this point, one needs to analyze the hydrodynamic profiles $n(y)$, $T(y)$, and $\boldsymbol{U}(y)$. Figs. 2 and 3 show the profiles of $U_x(y)$ and $T(y)$, respectively for $a = 5$ and the initial condition (I) at $t = 0$, 11 and 110. For the sake of clarity, we have removed the fluctuations by fitting the simulation points to cubic polynomials. It is apparent that by the time $t = 11$, at which the average temperature $\overline{T}(t)$ has already reached its stationary value,

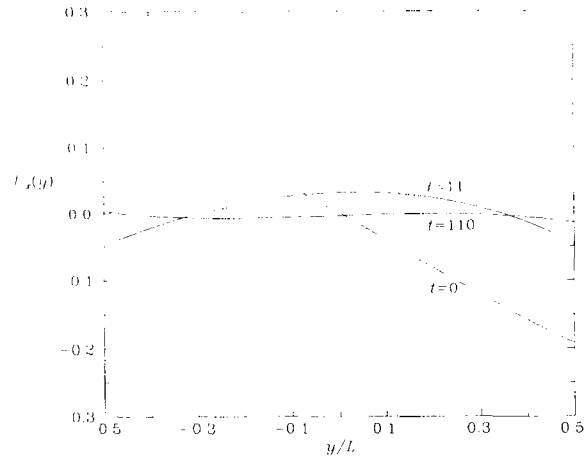

Fig. 2. Smoothed profile of $U_x(y)$ at $t = 0$, 11, and 110 for $a = 5$, starting from initial condition (I).

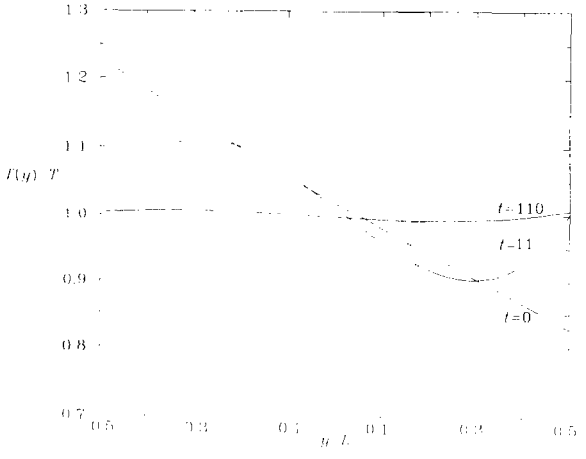

Fig. 3. The same as in Fig. 2, but for $T(y)/\overline{T}$.

the profiles are still evolving towards a homogeneous state. The latter has practically been reached by the time $t = 110$. Figs. 2 and 3, along with similar figures for $n(y)$ and the momentum flux (pressure tensor), clearly show that the USF is a stable state for $a = 5$ (at least at a hydrodynamic level). In fact, the shear viscosity measured from $\overline{P}_{xy}$ at $t = 110$ agrees well with its known exact value, which is about 8.6 times smaller than the Navier–Stokes value (shear thinning effect). It must be noticed that the shear rate $a = 5$ is smaller than the critical value $a_c = 6.845$, so that the fourth degree moments converge to stationary values in the USF state [5,6]. From that point of view, the

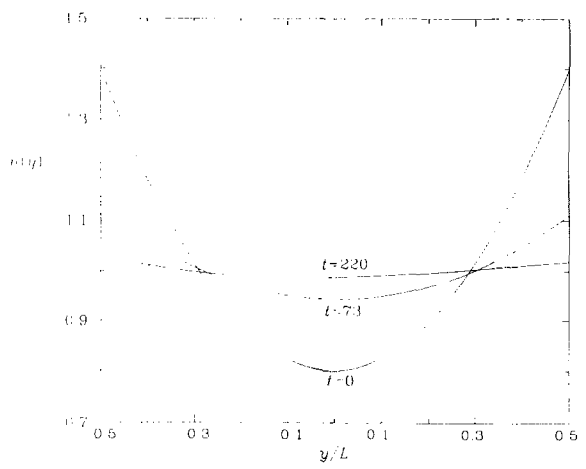

Fig. 4. Smoothed profile of $n(y)$ at $t = 0$, 73, and 220 for $a = 10$, starting from initial condition (II).

stability at $a = 5$ does not rule out a possible connection between the divergence of the fourth degree moments and an instability of the USF for $a > a_c$.

To analyze the above possibility, we have considered the hydrodynamic and momentum flux profiles for $a = 10$. For instance, Fig. 4 shows the (smoothed) profile $n(y)$ starting from the initial condition (II) for $t = 0$, 73, and 220. The results indicate that the profiles tend again towards a homogeneous state, although with a characteristic time larger than in the case $a = 5$. The fluctuating hydrodynamic profiles at $t = 220$ are presented in Fig. 5. They are fully consistent with homogeneous quantities. The large fluctuations in the temperature are due to the fact that, for long times, the high-velocity population is quite important (so that $\langle V^4 \rangle$ diverges in time for $a = 10$). The size of the thermal fluctuations explains why $\overline{T}$ at $t = 220$ does not coincide with the value expected from Fig. 1. However, the reduced shear viscosity measured at $t = 220$ again agrees well with its exact value, which is about 20 times smaller than the Navier–Stokes viscosity.

In summary, our simulation results show that the USF state is *stable* for a dilute gas of Maxwell molecules described by the inhomogeneous nonlinear Boltzmann equation. This conclusion is supported by the evidence that, starting from inhomogeneous (in the Lagrangian frame) initial conditions, the hydrodynamic fields relax towards uniform values, even for large shear rates (such as $a = 10$). In this uniform regime, the transport coefficients (e.g., the shear vis-

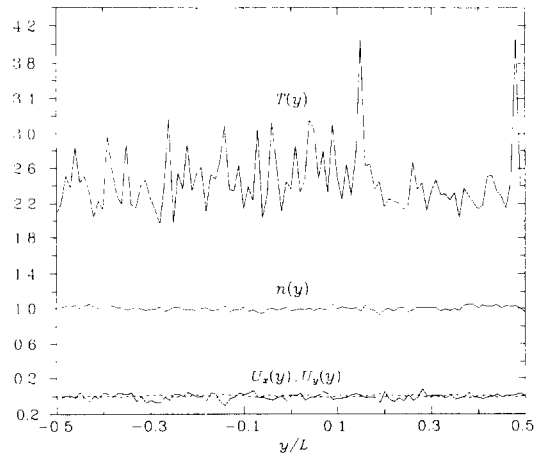

Fig. 5. Fluctuating profiles of $T(y)$, $n(y)$, $U_x(y)$, $U_y(y)$ (dashed line) at $t = 220$ for $a = 10$, starting from initial condition (II).

cosity) measured in the simulation agree well with the ones predicted theoretically in the USF. These results indicate that the singular behavior of the fourth degree moments for $a > 6.845$ [5,6] is *not* associated to an instability of the USF. In fact, recent analytical results [12] show that, for any shear rate, there exist diverging moments of sufficiently high degree. For instance, all the moments of degree larger than 4 diverge if $a > 2.346$.

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