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ON THE INSTABILITY OF UNIFORM SHEAR FLOW UNDER LONG WAVELENGTH PERTURBATIONS*

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1. Introduction. Uniform shear flow is considered as a prototype non-equilibrium state used to analyze fluid properties outside the domain of linear response. In this state, 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. This is an idealized version of shear flow between parallel plates; in a realistic shear flow (Couette flow), the velocity profile is also linear but with density n and temperature T fields not uniform. The uniform shear flow is generated by periodic boundary conditions in the local Lagrangian frame (Lees–Edwards boundary conditions) [6], which do work on the system and lead to a monotonous increase of temperature in time (viscous heating). This effect can be accounted for by the introduction of a thermostat, so that a steady state is achieved. These boundary conditions present important advantages from both theoretical and simulation points of view; more specifically, the absence of a hydrodynamic boundary layer and the possibility of emulating bulk effects for small real systems. The uniform shear flow has been studied by many different methods during the past fifteen years. Rheology and transport far from equilibrium have been analyzed at a fundamental level [3]. In addition, molecular dynamics simulations at finite densities have revealed a transition from fluid symmetry to an ordered state at sufficiently high shear rates [2]. Although its physical mechanism is still not well understood, this transition has been attributed to a short wavelength hydrodynamic instability.

Our objective here is to review recent work showing that uniform shear flow is also unstable at sufficiently long wavelengths for any finite value of the shear rate. First, a hydrodynamic linear analysis of the Navier–Stokes equations demonstrates that there is a critical wavevector, $k_c(a)$, such that for $k < k_c(a)$ perturbations around uniform shear flow grow exponentially in time [4]. This qualitative result applies without restriction to the atomic force law, density, or temperature. On the other hand, the hydrodynamic equations derived from a low density kinetic model confirm this result for states far from equilibrium [5]. And finally, numerical solution of this kinetic model obtained via Monte Carlo simulation shows a transition from uniform shear flow to a non-steady spatially inhomogeneous state [8].

2. Stability analysis. The Navier-Stokes equations are obtained from the exact conservation laws for the average mass, energy, and momentum densities, together with the linear (approximate) constitutive equations for the associated fluxes, namely, Fourier's law and Newton's viscosity law for the heat and momentum fluxes, respectively. These equations correctly describe the dynamics of a fluid close to equilibrium and on sufficiently large space and time scales. In particular, the Navier–Stokes equations linearized about the reference macroscopic state of uniform shear flow describe

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how small perturbations of the velocity, temperature, and densities fields evolve for small values of the shear rate a. To simplify the analysis and to focus on the instability, the following is restricted to the special case $k_z = k_x = 0$, i.e., spatial perturbations only along the velocity gradient. Moreover, the detailed form of the thermostat is not required at this level. Direct calculation demonstrate that for any fixed and finite a and for sufficiently small k ($k < k_c(a)$) there exist unstable modes which monotonically grows in time [4]. This statement holds for any atomic interaction potential, density, or temperature. The details of the calculation can be found in [8].

The above results apply only for small values of the shear rate a. The stability analysis can be extended to larger shear rates using the hydrodynamic equations derived from a more fundamental kinetic theory. In this context, the Boltzmann equation for the one-particle velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$ provides the adequate framework for studying nonequilibrium phenomena in dilute gases, but the intricacy of its collision term has made the search for explicit solutions a formidable task. In particular, the full velocity distribution function is not known for uniform shear flow. On the other hand, the nonlinear BGK model is a good approximation of the Boltzmann equation, even far from equilibrium. In addition, the exact stationary solution for uniform shear flow in presence of a thermostat has been obtained [9], and a variant of the Chapman-Enskog method can be used to study normal solutions for states near uniform shear flow. For this state the BGK equation reads

$$\left(\frac{\partial}{\partial t} - aV_y \frac{\partial}{\partial V_x} - \alpha(a) \frac{\partial}{\partial \mathbf{V}} \cdot \mathbf{V}\right) f(\mathbf{r}, \mathbf{v}, t) = -\nu \left[f(\mathbf{r}, \mathbf{v}, t) - f_\ell(\mathbf{r}, \mathbf{v}, t)\right] . \tag{2.1}$$

Here $\mathbf{V}$ is the peculiar velocity, $\mathbf{V} \equiv \mathbf{v} - \mathbf{U}$, $\alpha(a)$ is a constant (Gaussian) thermostat parameter, f_ℓ is the local equilibrium distribution, and ν is an average collision rate. In reference [5], the generalized hydrodynamic equations linearized about the reference state are derived for the case of Maxwell molecules ($\phi(r) \sim r^{-4}$). The results are now valid to order k^2. A long wavelength instability for any value of a is found again.

3. Monte Carlo simulation. To confirm the stability analysis based on the BGK equation, a Monte Carlo simulation can be used to numerically solve the kinetic model. The simulation will also allow us to investigate the asymptotic state of the system. This technique is a variant of Bird's direct simulation method [1], and its reliability to reproduce the exact time evolution of the velocity distribution has been clearly assessed. In fact, there have been several accurate tests of this method for uniform shear flow far from equilibrium [7]. In the simulation, the volume of the system is divided into cells of a typical size much smaller than the mean free path. At $t = 0$, N particles are introduced with positions and velocities sampled statistically from a specified initial distribution function. Time is advanced in discrete steps Δt much smaller than the mean free time. The free motion and the collisions are uncoupled over the interval Δt. In the streaming stage, all the particles are displaced according to their velocity components. Those particles crossing the boundaries are reentered according to the boundary conditions. Before proceeding to the next free displacement, a representative set of collisions is computed in each cell. The velocity of each particle p is replaced with a probability $\nu(n_p, T_p)\Delta t$ by a new velocity sampled from the local equilibrium distribution $f_\ell(\{n_p, T_p, \mathbf{U}_p\}; \mathbf{v})$. Here, n_p, T_p, and $\mathbf{U}_p$ are the density, temperature, and flow velocity in the cell containing particle p. The whole process is iterated for many time steps and the computed quantities are averaged over an ensemble of different replicas.

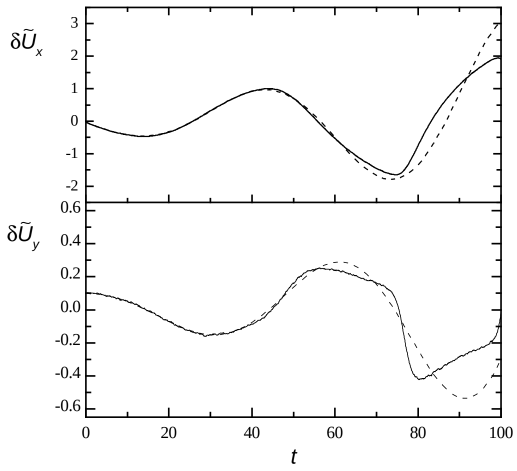

FIG. 3.1. Plot of $\delta\widetilde{U}_x(t)$ and $\delta\widetilde{U}_y(t)$. The solid lines are simulation results and the dashed lines correspond to the hydrodynamic analysis.

Henceforth, we take ν_s^{-1} and $\sqrt{2k_BT_s/m}$ as units of time and speed, respectively. Here, m is the mass of the particle and the subscript s refers to quantities in the reference state of uniform shear flow. In our simulations we have considered a system of size $L = 2\pi/k$, with $k = 0.1$, along the y-direction at a shear rate $a = 0.5$. This corresponds to conditions for which the hydrodynamic equations are unstable [5]. At $y = \pm L/2$ the Lees–Edwards (periodic) boundary conditions [6] were used to drive the shear flow. One local and two global (Gaussian) thermostats were implemented in the simulations. The local thermostat was chosen such that all viscous heating proportional to perturbations in the density and temperature fields also were compensated. For the first global thermostat, the parameter α was defined as in the reference state, i.e., $\alpha = -aP_{s,xy}/2K_s$, where $P_{s,xy}$ and K_s are the xy stress tensor element and the kinetic energy density in the uniform shear flow, respectively. The second global thermostat rescales the velocity of every particle in each time step, maintaining the average temperature constant (as usually done in molecular dynamics). Both theory and Monte Carlo simulations indicate that the details of the perturbed dynamics depend on the thermostat used, but the mechanism of the instability is insensitive to its choice. Consequently, only the results using global thermostats are presented here. At $t = 0$, the particle velocities corresponding to the exact solution of (2.1) are modified to introduce harmonic perturbations in the fields, $\delta\mathbf{U}(y,0)$, $\delta n(y,0)$, $\delta T(y,0)$.

Figure 3.1 shows $\delta\widetilde{U}_x(t) \equiv \delta U_x(-L/4,t)$ and $\delta\widetilde{U}_y(t) \equiv \delta U_y(-L/4,t)$ as functions of time. The good agreement between the results obtained from the hydrodynamic calculation and the Monte Carlo simulation demonstrates that the instability is not a consequence of the assumptions behind the hydrodynamic analysis, and also that these equations provide an accurate description of the initial stage of the instability.

Simulations performed for much longer times show that, after a transient period of length $t \approx 100$, a stable oscillatory state behavior of the hydrodynamic fields appears, suggesting the wave character of the asymptotic state. The period of the velocity oscillations is $\tau \simeq 54$, twice that of the scalar fields. We have also analyzed the profiles of these quantities at relevant times. Figure 3.2 shows the spatial variation of the velocity field at $t' = t - t_0 = 0, 0.14\tau, 0.25\tau, 0.36\tau$, and 0.5τ, where t_0 has been

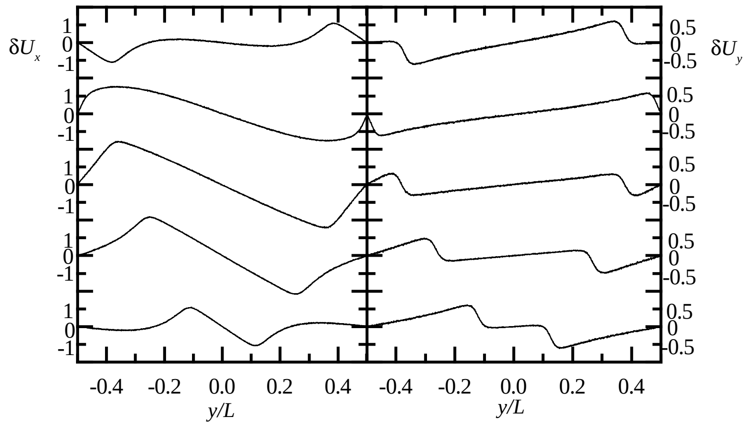

FIG. 3.2. $\delta U_x(y,t')$ and $\delta U_y(y,t')$ as a function of y for (from top to bottom) $t' = 0, 0.14\tau, 0.25\tau, 0.36\tau$, and 0.5τ.

chosen to assure the transient time is over and also with the criterion that $\delta\widetilde{U}_x(t) = 0$ at $t' = 0$. Inspection of the figure indicates that several invariance relations are verified [8].

4. Conclusions. In summary, the results reported here and in [4, 5, 8] clearly show that the uniform shear flow is unstable at sufficiently large wavelengths without restriction to the molecular interaction potential, density, or temperature. Previous studies via simulation have not seen this instability due to finite system sizes. On the other hand, the Monte Carlo simulation has been used to test the theoretical predictions of the hydrodynamic equations, showing that they are accurate on the time scale for which the linear analysis is valid. At longer times an asymptotic spatially non-uniform state is identified. The evolution of its spatial structure can be described as a periodic standing wave represented by the superposition of two symmetrical waves travelling in opposite directions.

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