Velocity Profiles in Repulsive Athermal Systems under Shear

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We conduct molecular dynamics simulations of athermal systems undergoing boundary-driven planar shear flow in two and three spatial dimensions. We find that these systems possess nonlinear mean velocity profiles when the velocity $u$ of the shearing wall exceeds a critical value $u_c$. Above $u_c$, we also show that the packing fraction and mean-square velocity profiles become spatially-dependent with dilation and enhanced velocity fluctuations near the moving boundary. In systems with overdamped dynamics, $u_c$ is only weakly dependent on packing fraction $\phi$. However, in systems with underdamped dynamics, $u_c$ is set by the speed of shear waves in the material and tends to zero as $\phi$ approaches $\phi_c$. In the small damping limit, $\phi_c$ approaches values for random close-packing obtained in systems at zero temperature. For underdamped systems with $\phi < \phi_c$, $u_c$ is zero and thus they possess nonlinear velocity profiles at any nonzero boundary velocity.

We will answer several important questions in this letter. First, does the packing fraction of the system strongly influence the shape of the velocity profiles? Most previous simulations investigating velocity profiles in sheared systems have been performed either near random close-packing as in simulations of granular materials \cite{3} or at high density as in studies of Lennard-Jones liquids \cite{4} and glasses \cite{5,6}. However, a systematic study of the role of density has not been performed. Nonlinear mean velocity profiles have been found at both high density and near random close packing, but it is not clear whether the same physical mechanism is responsible in both regimes.

We also consider the influence of the speed $u$ of the shearing wall on the mean velocity profiles. Results from previous simulations of glassy systems \cite{10,11} indicate that a critical velocity $u_0$ exists below which the mean velocity profiles become nonlinear \cite{12}. In these systems, the yield stress $\Sigma_{yv}$ at constant shear stress (shear stress required to move the boundary at nonzero velocity) is larger than the yield stress $\Sigma_{yv}$ at constant velocity (shear stress in the limit of zero velocity). When the shear stress is between these two values, part of the system can flow while other parts remain nearly static. In this letter, we concentrate instead on the larger $u$ regime, and ask whether the velocity profiles remain linear for all $u > u_0$.

![Graph showing shear stress vs. velocity](image)

FIG. 1: Shear stress $\Sigma$ vs. velocity $u$ of the wall moving at constant velocity (circles) and constant stress (squares) for a 2D underdamped system with linear spring interactions at $\phi = 0.85$. $\Sigma_{ys}$ is the yield stress at constant stress. Previous studies \cite{10,11} have shown that mean velocity profiles can switch from nonlinear to linear as $u$ increases above $u_0$, where $u_0$ is the wall velocity at $\Sigma = \Sigma_{ys}$. We will show below that the mean velocity profiles become nonlinear again when $u > u_c$, where $u_c \geq u_0$ is always satisfied.

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as a function of height \(y/L\).

Particles were implemented in all directions. Following the quench, periodic boundary conditions were imposed to zero temperature [13] using the conjugate gradient dynamics (1).

During the quench, the systems were sheared for a strain of 5 to remove initial transients and then quantities like velocity, pressure, and shear stress (obtained from the microscopic pressure tensor [13]), and local packing fraction were measured as a function of distance \(y\) from the stationary wall. Averaged quantities were obtained by sampling between strains of 5 to 10.

Bulk and boundary particles interact via the following pairwise, finite-range, purely repulsive potential: \(V(r_{ij}) = \epsilon (1 - r_{ij}/\sigma_{ij})^{\alpha}/\alpha\), where \(\alpha = 2, 5/2\) correspond to harmonic and Hertzian spring interactions, \(\epsilon\) is the characteristic energy scale of the interaction, \(\sigma_{ij} = (\sigma_i + \sigma_j)/2\) is the average diameter of particles \(i\) and \(j\), and \(r_{ij}\) is their separation. The interaction potential is zero when \(r_{ij} \geq \sigma_{ij}\). Our results were obtained over a range of packing fraction from \(\phi = [0.58, 0.80]\) in 3D and \(\phi = [0.75, 1.0]\) in 2D, which allows us to probe packing fractions both above and below random close-packing [13]. The units of length, energy, and time are \(\sigma, \epsilon\), and \(\sigma\sqrt{m/\epsilon}\), respectively.

For athermal or dissipative dynamics, the position and velocity of each particle are obtained by solving [16]

\[
m \frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i - b \sum_j (\vec{v}_i - \vec{v}_j),
\]

where \(\vec{F}_i = -\sum_j dV(r_{ij})/dr_{ij} \hat{r}_{ij}\), the sums over \(j\) only include particles that overlap \(i\), \(\vec{v}_i\) is the velocity of particle \(i\), and \(b > 0\) is the damping coefficient. Although for the present discussion we neglect the particles’ rotational degrees of freedom, we have shown that including these does not qualitatively change any of our results [13].

The dynamics can be changed from underdamped to overdamped by tuning the dimensionless damping coefficient \(b^* = b\sigma/\sqrt{\epsilon m}\) above \(b^*_c = \sqrt{2}\). Frictionless granular materials and model foams can be studied using \(b^* < b^*_c\) [16] and \(b^* \gg b^*_c\) [18], respectively.

Three physical parameters, the packing fraction \(\phi\), the velocity \(u\) of the moving boundary, and the dimensionless damping coefficient \(b^*\), strongly influence the shape of the mean velocity profile. First, we find that a critical boundary velocity \(u_c\) exists that separates linear from therefore rough and amorphous. Results did not depend on the thermal quench rate provided the systems were sheared long enough to remove initial transients.

Shear flow in the \(x\)-direction with a shear gradient in the \(y\)-direction was created by moving all particles in the top wall at fixed velocity \(u\) in the \(x\)-direction relative to the stationary bottom wall. Therefore, particles in the walls do not possess velocity fluctuations. During the shear flow, periodic boundary conditions were imposed in the \(x\)- and \(z\)-directions (in 3D). The system-size was varied in the range \(N = [256, 3072]\) to assess finite-size effects. Only small sample sizes were required in the \(x\) and \(z\) directions. In contrast, more than \(\approx 50\) particle layers were required in the shear-gradient direction to remove finite-size effects. Most simulations were carried out using \(L_x = L_z = 18\sigma\) and \(L_y = 72\sigma\), where \(\sigma\) is the small particle diameter. The systems were sheared for a strain of 5 to remove initial transients and then quantities like velocity, pressure, and shear stress (obtained from the microscopic pressure tensor [13]), and local packing fraction were measured as a function of distance \(y\) from the stationary wall. Averaged quantities were obtained by sampling between strains of 5 to 10.

In order to demonstrate these results, we performed a series of molecular dynamics simulations of soft repulsive athermal systems undergoing boundary-driven shear flow under conditions of fixed volume, number of particles \(N\), and velocity of the top shearing wall \(u\). The systems were composed of \(N/2\) large particles and \(N/2\) small particles with equal mass \(m\) and diameter ratio 1.4 to prevent crystallization and segregation. Initial states were prepared by quenching the system from random initial positions to zero temperature [13] using the conjugate gradient method [14] to minimize the system’s total potential energy. During the quench, the systems were sheared in all directions. Following the quench, particles with \(y\)-coordinates \(y > L_y (y < 0)\) were chosen to comprise the top (bottom) boundary. The walls were

![FIG. 2: (a) Average velocity \(\langle u\rangle\) (normalized by \(u\)) in the flow direction, (b) local packing fraction \(\phi\), and (c) velocity fluctuations \(\delta v\) in the \(x\)- (solid lines) and \(y\)-directions (symbols) as a function of height \(y/L\) from the stationary wall in a 2D system with harmonic spring interactions and underdamped dynamics (\(b^* = 0.01\)) at \(\phi = 0.85\). In each panel, 4 boundary velocities are shown; triangles, diamonds, squares, and circles correspond to \(u = 0.075, 0.15, 0.37,\) and 0.75, respectively. The inset to (c) compares velocity fluctuations in the \(x\)- and \(y\)-directions at \(u = 0.75\).]
nonlinear flow behavior. For $u < u_c$ (but not in the quasistatic flow regime), the mean velocity profiles in the flow direction are linear; however, when $u > u_c$ they become nonlinear. The width of the shearing region decreases as $u$ continues to increase above $u_c$. This is shown in Fig. 2(a) for an underdamped ($b^* < b^*_c$) system in 2D with harmonic spring interactions at $\phi = 0.85$. As $u$ is increased above $u_c \approx 0.08$, the mean velocity profiles $\langle v_x(y) \rangle$ become more and more nonlinear. When the boundary velocity has increased to $u = 0.75$, approximately 80% of the system is nearly static, while the remaining 20% undergoes shear flow.

We also monitored the local packing fraction and mean-square velocity fluctuations (or kinetic temperature) during shear. These are shown for the same dense system with underdamped dynamics in Fig. 2(b) and (c). We find that when the mean velocity profile is linear, the packing fraction and velocity fluctuations are spatially uniform. Moreover, the velocity fluctuations in the $x$- and $y$-directions are identical. However, when the boundary velocity exceeds $u_c$, the packing fraction and mean-square velocity profiles become spatially dependent. In this regime, the compressional forces induced by the shearing boundary are large enough to cause dilation. The system becomes less dense near the shearing wall and more compact in the nearly static region. In addition, the shearing wall induces a kinetic temperature gradient with velocity fluctuations larger near the shearing boundary. The kinetic temperature also becomes anisotropic with $\langle \delta v_x^2 \rangle < \langle \delta v_y^2 \rangle$ when $u > u_c$. Thus, several phenomena occur simultaneously as the boundary velocity is increased above $u_c$: 1) the velocity profile becomes nonlinear, 2) the system dilates near the shearing boundary and compacts in the bulk, and 3) the kinetic temperature becomes higher near the shearing wall.

We have measured the critical wall velocity $u_c$ as a function of packing fraction $\phi$ for systems with underdamped dynamics and harmonic and Hertzian spring interactions in 2D and 3D. These measurements are shown in Fig. 3. We find that $u_c$ is nearly constant at large $\phi$ but then decreases sharply as $\phi$ approaches a critical packing fraction $\phi_c$. For $\phi < \phi_c$, $u_c = 0$ with $\phi_c \approx 0.81 - 0.82$ in 2D for harmonic and Hertzian springs and $\phi_c \approx 0.61$ in 3D for harmonic springs. We expect that Hertzian springs will give a similar result for $\phi_c$ in 3D. These values for $\phi_c$ are close to recent measurements of random close packing in systems at zero temperature \[13\]. We have also measured $u_0$ in underdamped systems \[17\], and $u_0$ decreases strongly near random close packing, but for all systems studied $u_0 \leq u_c$. In particular, we find that when $u = 0$, $u_0 = 0$ also.

A possible interpretation of the critical wall velocity $u_c$ can be obtained by comparing the time it takes the system to shear a unit strain to the time it takes a shear wave (with speed $u_T$) to traverse the system and return to the shearing boundary. This simple argument predicts $u_c = u_T/2$. $u_T$ can be obtained by studying the transverse current correlation function $C_T(\omega, k)$ as a function of frequency $\omega$ and wavenumber $k = 2\pi n \sigma/L_x$ ($n$ integer) and the resulting dispersion relation $\omega_T(k)$ \[19\]. In Fig. 3 we compare $u_T = \omega_T / dk$ (for $n = 3$ to 12) and $u_c$ as a function of $\phi$ for both potentials in 2D and for harmonic springs in 3D \[20\]. Although deviations occur close to $\phi_c$, we find that $u_c$ agrees very well with $u_T/2$ over a wide range of $\phi$.

What is the shape of mean velocity profiles in dilute underdamped systems with $\phi < \phi_c$? Since $u_c$ is zero below $\phi_c$, we expect that mean velocity profiles in these dilute systems are nonlinear for all nonzero $u$. This is indeed what we find for all systems studied. Fig. 4 shows the mean velocity profiles for a 2D underdamped system at $\phi < \phi_c$ over three decades in $u$. In contrast to the behavior in dense systems, the velocity profiles are not monotonic in $u$. However, there is a range of boundary velocities (one decade) over which the velocity profiles collapse onto a common exponential profile. A robust exponential profile has also been found over a wide range of shear rates in experiments of granular materials \[2\]. Similarly to the systems characterized by large $\phi$, low $\phi$ ones are accompanied by spatially-dependent packing fraction and mean-square velocity profiles.

Boundary-driven shear flow in underdamped systems is, however, substantially different from that in underdamped systems since velocities of neighboring particles

![FIG. 3: Critical velocity $u_c$ of the moving wall versus packing fraction $\phi$ in (a) 2D and (b) 3D systems with harmonic (circles) and Hertzian (squares) spring interactions. The open and filled symbols correspond to $b^* = 0.01$ and $b^* = 5$, respectively. For underdamped systems, we plot $u_T/2$ for harmonic (small circles) and Hertzian (small squares) spring interactions, where $u_T$ is the shear wave speed.](image-url)
as the dissipation increases at fixed $u$. Three boundary velocities are shown; squares, downward triangles, and pluses correspond to $u = 0.38, 0.038$, and $7.7 \times 10^{-3}$, respectively. The inset shows that there is a wide range of velocities are shown; squares, downward triangles, and pluses correspond to $u = 0$ from 0.0077 (leftward triangles) to 0.077 (circles) over which the velocity profiles collapse.

are strongly coupled. Fig. 4 shows that in the overdamped limit ($b^* \gg b^*$), the critical boundary velocity is nearly independent of $\phi$ over the studied range in both 2D and 3D. We also find that $u_c$ increases linearly with $b^*$, thus the velocity profiles tend toward linear profiles as the dissipation increases at fixed $u$.

In this letter we present results of molecular dynamics simulations of repulsive athermal systems undergoing boundary-driven shear flow in 2D and 3D. We demonstrate that a critical boundary velocity $u_c$ exists (at large $u$) that signals the onset of spatial inhomogeneity. When $u$ exceeds $u_c$, the mean velocity profiles become nonlinear, the system becomes dilated near the moving wall and compressed near the stationary wall, and the system possesses a nonuniform kinetic temperature profile with higher temperature near the moving wall. For underdamped systems, $u_c$ is nearly constant at large $\phi$ but decreases strongly at lower $\phi$ until it vanishes at $\phi_c$. $\phi_c$ depends on the damping coefficient but approaches recent estimates of random close-packing [13] in the small damping limit. In this limit, $u_c$ is determined by the speed of shear waves in the material, $u_T$. When $u$ exceeds $u = u_T/2$, large shear strain occurs before shear waves are able to traverse the system. In the overdamped limit, $u_c$ is nearly independent of $\phi$ over the studied range and scales linearly with the damping coefficient $b^*$.

Possible future directions include adding friction to the model in Eq. 1 which would allow us to make more direct contact with experiments on granular materials [1, 2]. Are nonlinear velocity profiles more likely to occur in systems with frictional particles? How does the propagation of shear waves change in that case? We are currently investigating these important questions.

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