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Molecular dynamics simulations of sliding friction in a dense granular material

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Abstract. Friction in a dense two-dimensional granular material is studied by molecular dynamics simulations. Initially the particles are ordered in a triangular lattice where the top layer feels a constant vertical pressure and horizontal velocity field. The dynamics of the material at low velocities is found to be characterized by avalanche-type motion during short time intervals followed by long stationary periods of internal stress buildup. At low external pressures, the time-averaged shear stress is found to be nearly constant for low values of the normal pressure and proportional to the load for higher pressures.

1. Introduction

The behaviour of sliding friction and its origin is a subject of fundamental interest and of great practical importance. For rigid bodies, the Coulomb relation [1] expressing proportionality between the shear stress and the load is well known. In the theory of plastic materials there are also several models which lead to Coulomb-like friction laws [2]. Even on the atomic scale, a recent molecular dynamics simulation [3] has indicated proportionality between average load and shear stress for a Cu tip forced to slide in various directions on a Cu(111) surface. A weak dependence on the sliding velocity was also reported in this work. For more complex types of material a velocity dependence of the friction force is also well established [4, 5].

Granular materials, like sand or micron-sized glass spheres, constitute a bridge between the atomic and macroscopic length scales. At such length scales several macroscopic phenomena have their origin. The dynamics of granular materials have recently attracted considerable experimental and theoretical attention. Much focus has been on gravitational driven flow on an inclined plane with respect to fluctuations in density and flow profiles [6–8]. In shear induced motion, stick-slip dynamics of glass spheres have recently been reported [9–12]. This type of dynamics is also seen in simulations by Thompson and Grest [13]. They found that, for constant load, the shear stress becomes asymptotically independent of the shear velocity, an indication that Coulomb friction might work well.

In the present paper we study the flow behaviour and friction of a two-dimensional granular material with a short-range particle–particle attraction in addition to the conventional particle repulsion and friction models [5–8]. The object is to investigate the Coulomb relation using particles containing some of the main features of plastic metals

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like near incompressibility, realistic elastic modulus and density as well as the fact that the particles are predominantly in a solid phase. In particular, we focus on the dynamics of the stick-slip motion and on the time-averaged friction as a function of normal pressure on the top layer of the material. All simulations are reported in 'system units' where the velocity is measured in m s^{-1} and the pressure unit is 1 Pa. This is obtained by e.g. choosing mass unit $m_0 = 10^{-18}$ kg and length unit defining the particle radius $l_0 = 10^{-6}$ m.

2. The model

The simulation model is shown in figure 1: N_l^2 two-dimensional spheres are placed on top of a stationary surface and each of the top layer particles feels a constant pressure $p_\perp$ directed downwards. The black bottom layer particles are stationary and represent a surface. The horizontal velocity, $v_{\rm fr}$, of the top-layer particles is fixed and constant. Periodic boundary conditions in the horizontal direction are applied for all moving particles. The constant velocity of the top-layer particles induces a shear force on the other particles which again results in global displacement in the horizontal direction.

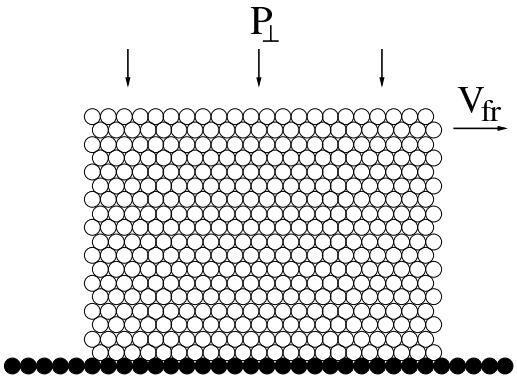

Figure 1. Simulation model. N_l spherical particles are subject to a pressure from the top layer and a shear force due to the top layers' motion. From below, the particles are bound by a stationary surface (black particles).

The model is not complete until the forces between the particles have been specified. In simulations between atoms such forces may be derived from first principles. When the active particles are built up of millions of atoms the forces are less obvious. Since plastic metals to a good approximation are incompressible, we adopt a Hooke's law repulsion with a very high repulsion constant. This guarantees that particles cannot penetrate each other significantly. Since the top boundary conditions perform work on the system, some interparticle friction mechanism has to be imposed to mimic heat transport. In the present work we follow the original model of Cundall and Strack [14] and introduce a friction force proportional to the relative velocity between two interaction particles. The force between two particles i, j acting in the direction $\boldsymbol{n}_{ij}$ defined by the line connecting the sphere centers can thus be written as,

$$\boldsymbol{F}_{ij}^n = [k_{\rm n}(|\boldsymbol{r}_{ij}| - 2r) - \gamma_{\rm n}|\boldsymbol{v}_{ij}^n|]\boldsymbol{n}_{ij} \qquad (|\boldsymbol{r}_{ij}| < 2r + {\rm d}r)$$

Here r is the radius of the spheres, $|\boldsymbol{r}_{ij}|$ is the distance between the spheres, $k_{\rm n}$ is the elastic spring constant, $\gamma_{\rm n}$ is the interparticle local friction coefficient and $|\boldsymbol{v}_{ij}^n|$ is the relative velocity component between particle i and j in the direction along $\boldsymbol{n}_{ij}$ [14].

Rotational motion is induced by the shear force,

$$\boldsymbol{F}_{ij}^{s} = \min(\gamma_s|\boldsymbol{v}_{ij}^{s}|, |\mu\boldsymbol{F}_{ij}^{n}|)\boldsymbol{s}_{ij}$$

where $\boldsymbol{s}_{ij}$ is the unit right-hand sense vector perpendicular to $\boldsymbol{n}_{ij}$ [9] and γ_s is the local shear friction coefficient and μ is the interparticle local Coulomb friction coefficient. Thus the particles may roll or slide against each other depending on the size of the relative velocity in the $\boldsymbol{s}_{ij}$ direction.

In order to probe the 'global' friction behaviour for a vide range of external pressures the elastic spring constant is taken to be large in order to prevent the spheres from penetrating and passing each other. In all simulations we have thus chosen $k_n = 5 \times 10^6$ whereas modest values of the other parameters ($\gamma_n = 10^3$, $\gamma_s = 30$, $\mu = 0.5$) have been used. In the present simulations the attraction range has been chosen small enough to keep only nearest neighbour attractions i.e. d$r = 0.05$. This value guarantees that the spheres stick together

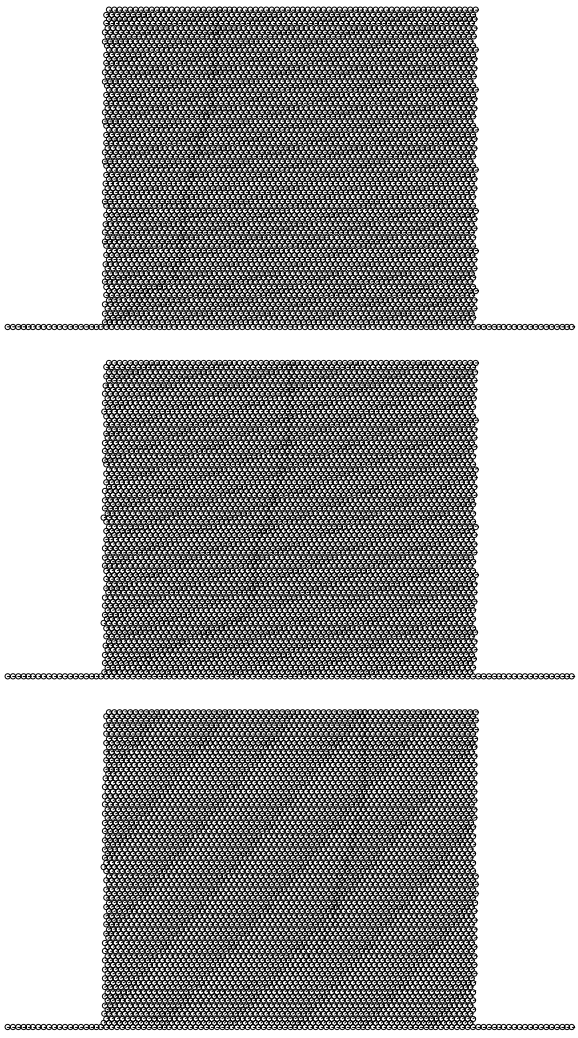

Figure 2. Flow profiles of a simulation of 4041 spheres. The dark spheres are initially placed to the left in the simulation slab.

and form a solid at zero external pressure. Alternatively, a similar mechanism could have been obtained using a weaker long range attraction as given by e.g. Lennard–Jones forces. The integration is carried out through the 'leap-frog' steps [15]. A very small time step $dt = 0.0001$ has been necessary to ensure converged results since the local fluctuations in accelerations may become very large, particularly for large samples and high external top pressure. Each simulation starts with all particles at rest except the top-layer ones.

3. Results

In figure 2 three snapshots of a simulation of 5041 spheres are shown. The dark 'line' contains the spheres initially placed on top of each other to the left of the simulation slab. Two features can be seen from the figure. The particles near the top layer move with the same velocity as the topmost layer. The particles touching the surface are near stationary and the layers are moving gradually slower with decreasing distance to the surface. In the intermediate region the front is less regular. The vertical front from the top is separated by 'slip zones' which are a signature of local avalanche-like stress releases to be discussed in detail in the following.

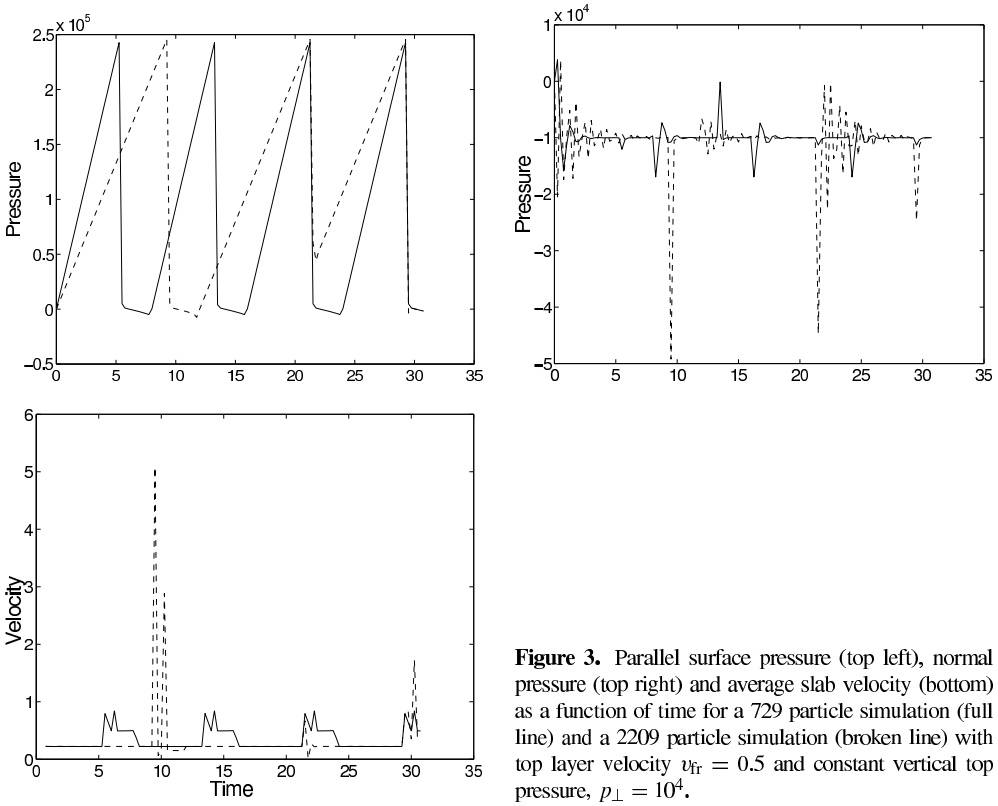

Figure 3. Parallel surface pressure (top left), normal pressure (top right) and average slab velocity (bottom) as a function of time for a 729 particle simulation (full line) and a 2209 particle simulation (broken line) with top layer velocity $v_{fr} = 0.5$ and constant vertical top pressure, $p_{\perp} = 10^4$.

In figure 3 the shear (upper) and normal (middle) pressure of the material at the lower surface as a function of time is plotted for external pressure $p = 10^4$ and a horizontal velocity $v = 0.5$. The full line is a simulation of 729 particles and the broken curve is a simulation of 2209 particles. The shear stress of the surface is seen to build up linearly with time until a critical value (2.5×10^5) is reached. This value is independent of the

number of particles in the simulation. At that point an avalanche is released resulting in a sharp increase of the average velocity of the material over a very short time interval. The avalanche may take place in one or several layers depending on the system size. The large system shows much larger fluctuations in velocity and pressure during the avalanche. This is associated with the ability to store more energy. It is interesting to note that the maximum pressure before an avalanche (critical slip pressure) is independent of the number of particles in the simulation whereas the time, ΔT, between each avalanche is proportional to the system size, i.e. the number of particles in the simulation. Associated with the slip, one or several beats of the normal pressure onto the stationary surface are seen in the middle panel. These beats would probably, in a real surface, cause large local temperature fluctuations.

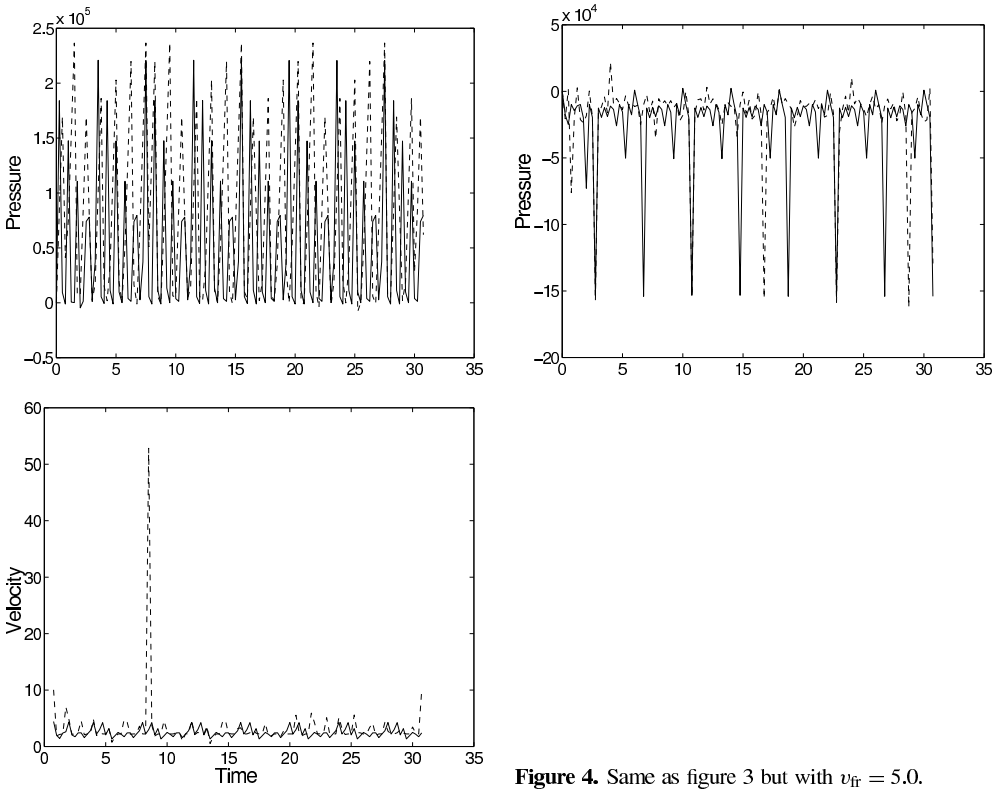

Figure 4. Same as figure 3 but with $v_{\mathrm{fr}} = 5.0$.

In figure 4 the simulation of figure 3 is shown for a much faster top layer velocity $v = 5.0$. The stick–slip behaviour is much more erratic here with a period shorter typically by a factor of 10. An interesting distribution of four periodic critical shear stress values seems to repeat itself regularly for the smallest simulation. The beats of the normal pressure onto the surface are much stronger in figure 4 and the velocity becomes less regular.

In figure 5 the velocity dynamics is displayed in more detail for a 729 particle simulation at $v = 0.5$ with three slip events shown. The variable '$y + 20$' measures the number of layers above the surface. The slip is seen to take place in all layers of the material but with varying peak velocity. During the slip events some particles even get a temporary negative horizontal velocity due to collisions. After the avalanche, a period with fast collective motion of all particles equal to the top layer particles v_{fr} occurs until the particles close to the surface finally slow down.

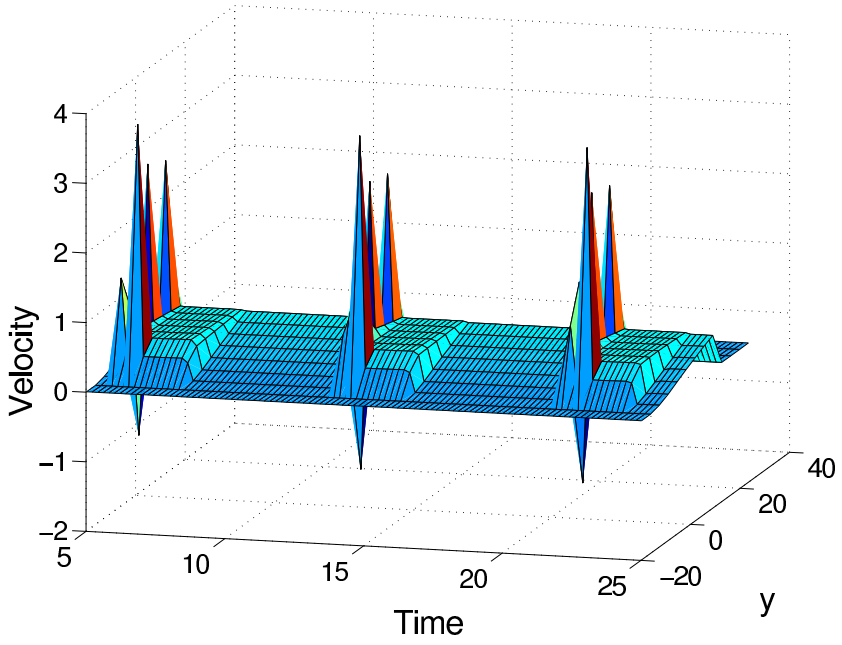

Figure 5. Particle velocity as a function of time and layer number (y) above the stationary surface.

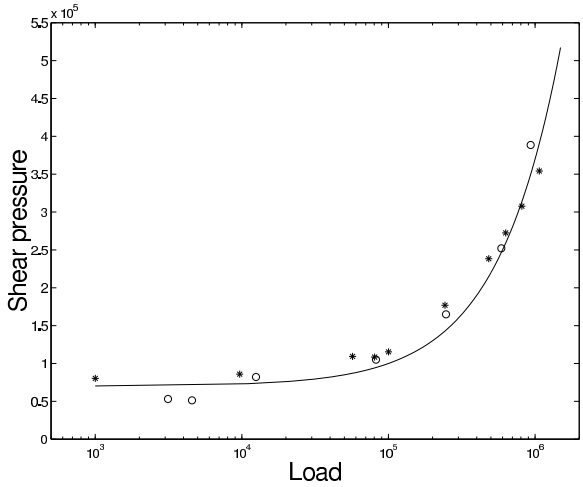

Figure 6. The average shear pressure as a function of normal pressure. The line refers to the fit $y = 0.7 + 0.3x$; $*$, simulations with $v_{fr} = 5.0$, $\circ$, simulations with $v_{fr} = 0.5$.

The average shear stress taken over several stick–slip cycles may now be calculated for a range of external loads from the order of 10 to 10^6. In figure 6 average values for $v = 0.5$ and $v = 5.0$ are shown together with a full curve which represents a fit to the data by the formula $y = 0.7 + 0.3x$. No qualitative difference is observed in the average properties at the two velocities in the high-pressure region of the data. At high pressures the Coulomb relation thus works well, whereas at low external pressure a constant average friction is

seen. The transition between these two extremes is seen to occur at pressures around 10^5 i.e. where the force between the particles is of the order of the spring constant.

4. Conclusion

In the present paper we have reported simulations of the dynamics of a granular material on a rough surface subject to external pressure. The simulations have displaced stick–slip motion in qualitative agreement with experiments. The period between each slip is found to increase with the number of particles in the simulation while the critical slip pressure is independent of the number of particles. The slip process has been found to behave like a short avalanche with velocities several orders of magnitude greater than the constant boundary velocity. The time-averaged shear stress as a function of external pressure thus becomes constant at low pressure. At a sufficiently high value of the external pressure, the critical slip pressure starts to increase giving rise to a Coulomb-like friction law.

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