

# Pressure-controlled granular shear flows between bumpy planes

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**Abstract.** In this work, DEM numerical simulations of granular systems sheared between two rough counter-surfaces and under steady, constant-load conditions, have been performed. In the simulations, a collection of identical, frictionless spheres is sheared between two parallel bumpy walls moving at constant velocity in opposite direction, and the rough walls are made bumpy by gluing particles in a regular array. The main purpose of the research is to investigate the lubricant properties of granular particles in a sliding interface with multiple contact asperities, with the long-term goal of designing realistic transport systems for the industry of particulates with extremely low energy-demand. We focus particularly on high applied loads, relevant for practical applications of granular lubricants, which may lead to crystallization of the granular system with significantly increase in the shear resistance. A systematic investigation of the role played by boundary roughness on the macroscopic friction and crystallization process has been conducted, to find the best combination of micro and macro parameters to reduce shear resistance.

## 1 Introduction

In most industrial and geophysical applications involving granular fluids, e.g., hopper discharge, transport on conveyor belts, landslides, the presence of solid boundaries induces strong spatial heterogeneities and controls the flow. Granular materials exhibit complex behavior [1], especially when influenced by the presence of boundaries, and they even undergo a phase transition when subjected to external energy, with their structure changing from a random, fluid state to an ordered, crystalline state [2].

Discrete element (DEM) numerical simulations of pressure-controlled granular flows, bounded between bumpy planes,[3] have shown that there exists a minimum load above which particles crystallize. Many studies have investigated the crystallization process of granular matter, analyzing the effect of shearing[4, 5], geometry of the boundaries[6–8], inter-particle friction coefficient, applied load[9] and cyclic shear[10, 11].

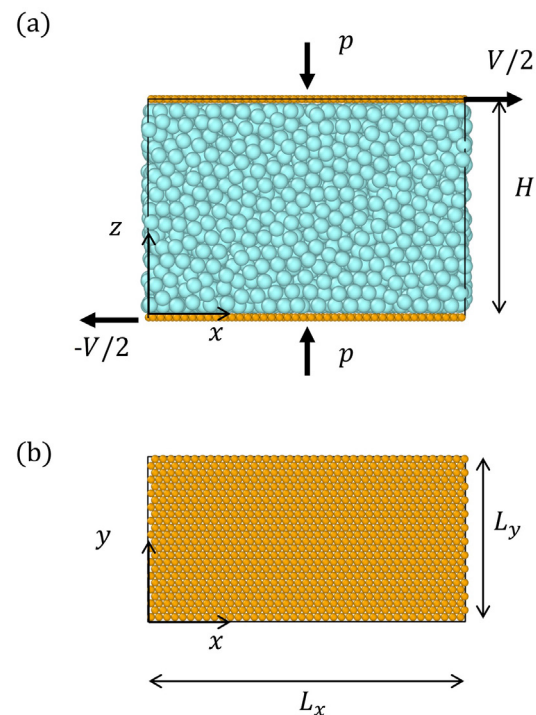
Here, we want to investigate the role played by the bumpiness of boundaries on the crystallization process of bounded granular shear flows, with particular focus on the shear resistance. To this purpose, we perform DEM simulations of steady, pressure-imposed, heterogeneous flows of identical, frictionless, inelastic spheres sheared between rigid, parallel bumpy planes, in the absence of gravity.

## 2 DEM simulations

We have performed DEM simulations of granular shear flows with the molecular dynamics platform LAMMPS<sup>1</sup>[12], by employing the linear spring-dashpot contact

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**Figure 1.** (a) Snapshot of a typical pressure-imposed simulation once the steady state is attained. Also shown is the frame of reference. (b) Top view of the bumpy plane composed of regularly arranged spheres of diameter  $d_w = 1/2$

force model and by modelling friction according to the Coulomb law. In the simulations,  $N$  identical, frictionless spheres of diameter  $d$ , mass density  $\rho_p$ , stiffness  $k$  and normal and tangential restitution coefficient  $e_n$ , are

initially placed at random in a rectangular box of size  $L_x$  and  $L_y$ , along  $x$  and  $y$ , respectively. The  $x$ ,  $y$  and  $z$  directions are the flow, gradient and vorticity directions, respectively. The granular system is sheared between two parallel planes moving relative to each other with a constant velocity  $V$ , in the absence of gravity. We apply periodic boundary conditions along the  $x$  and  $y$  directions. Both planes experience a constant pressure  $p$  along the  $z$ -axis, and can freely move vertically as rigid bodies, so that the flow height,  $H$ , changes in time and at the steady state may be different from the initial condition. A snapshot of the shear cell with the associated frame of reference is shown in Figure 1(a). The planes are constructed by gluing one layer of spheres of diameter  $d_w$  in a regular hexagonal closed-packed arrangement, at close contact and aligned with the direction of the flow, as shown in Figure 1(b).

In the simulations, all the variables are made dimensionless using  $\rho_p$ ,  $d$  and  $V$ : then e.g., lengths, velocities and stresses are given in units of  $d$ ,  $V$  and  $\rho_p V^2$ , respectively. The integration time step  $\delta t$  for the numerical integration is fixed and equal to  $t_c/50$ , that is  $\delta t \sim 7.5 \times 10^{-5}$ , where  $t_c = \min(t_c^{ij})$  and  $t_c^{ij} = \pi \left[ \frac{k}{m_{ij}} + \frac{k}{m_{ij}} \frac{(\log e_n)^2}{\pi^2 + (\log e_n)^2} \right]^{-1/2}$  is the duration of the collision between particle  $i$  and particle  $j$  for the linear spring-dashpot contact model, where  $m_{ij} = \pi d_i^3 d_j^3 / [6(d_i^3 + d_j^3)]$ , being  $d_i$  and  $d_j$  the diameter of particle  $i$  and  $j$ , respectively, equal either to  $d$  for moving particles or  $d_w$  for boundary particles. The saving time step of the simulations is set to 100 integration time steps, so that measurements are recorded at time intervals of 0.0075.

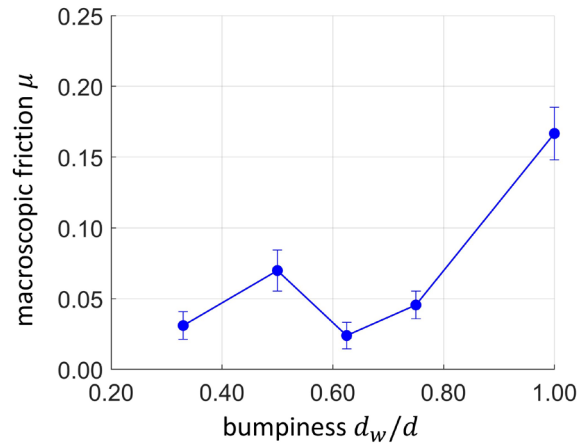
We have employed  $N = 3150$  flowing particles, with  $k = 2 \times 10^5$  and  $e_n = 0.9$ . The boundary particles are characterized by the same mechanical properties of the moving particles, i.e., same  $k$  and  $e_n$ , whereas we vary their diameter,  $d_w$ , in order to investigate the effect of the bumpiness of the boundaries, here defined as  $d_w/d$ . As a consequence, the number of boundary particles changes according to their diameter, and we also change the domain sizes  $L_x$  and  $L_y$  in order to get an integer number of boundary particles arranged in hexagonal closed-packed arrays, with zero distance between the edges of two adjacent boundary spheres.

In the simulations, the imposed pressure is  $p = 30$ , corresponding to approximately 100 kPa for velocities on the order of 1 m/s and particles with a density of around 1000 kg/m<sup>3</sup>. This value of the pressure is well above the minimum value required to observe crystallization in imposed-pressure shearing flows of frictionless spheres when the bumpiness of the walls is  $d_w/d = 1$  [3]. The influence of the bumpiness was analyzed in Ref.[3], in the case of very small applied loads, that is in non-crystallized systems.

Finally, we have measured the macroscopic friction coefficient  $\mu$  in the steady state as the time-averaged value of the ratio of the shear stress to the pressure exerted on the moving planes. This quantity is representative of the shear resistance of the granular flow, and has significant practical implications. In particular, it measures the capability of the moving spheres to act as a lubricant fluid with re-

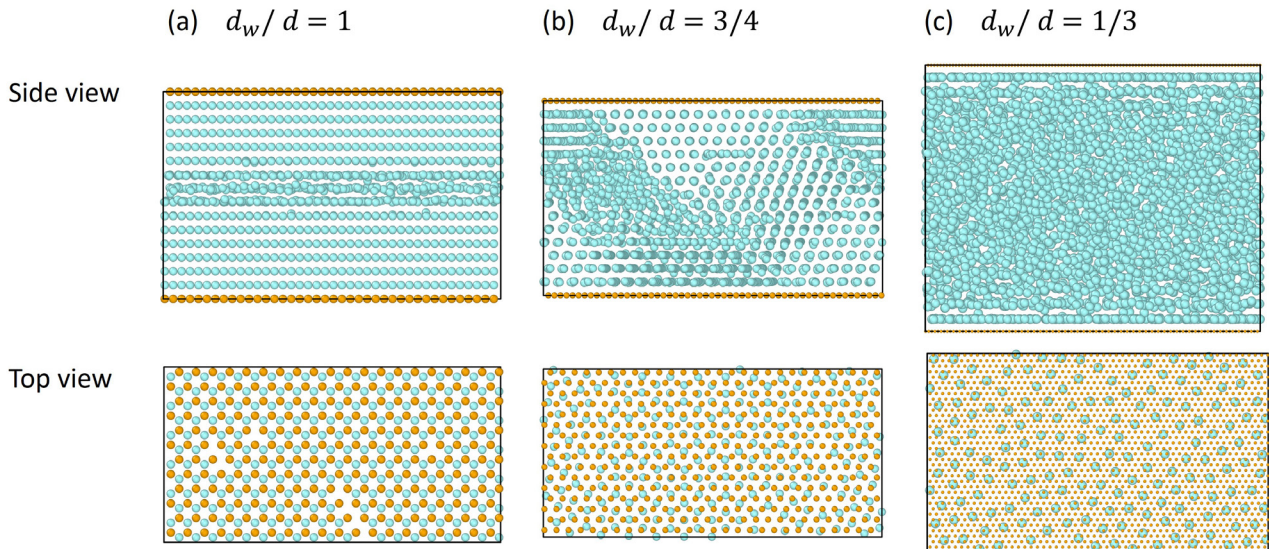
spect to the two rigid, bumpy boundaries. We consider the steady state achieved when the average kinetic energy per particle becomes approximately constant (fluctuations around the time-averaged value less than 10%).

### 3 Results



**Figure 2.** Macroscopic friction as a function of the bumpiness of the boundaries in the steady state (the error bars show the standard deviation of the fluctuations in time)

In Figure 2 we plot the macroscopic friction,  $\mu$ , measured in the steady state, as a function of the bumpiness of the walls. The macroscopic friction decreases strongly with decreasing bumpiness and shows a non-monotonic trend. When the bumpiness is equal to 1, i.e., the boundary particles have the same diameter of the moving particles, the imposed pressure is large enough to induce the formation of regular crystalline structures inside the flowing particles. In these conditions, we observe a shear band of thickness of about 2 to 3 diameters inside the flow domain, as illustrated in Figure 3(a), where the particle positions projected on the  $x$ - $z$  and  $x$ - $y$  planes are displayed for a given snapshot in the steady state. The shear band is squeezed between two blocks of crystallized particles moving as rigid bodies with the bumpy planes. The crystallized flowing particles are also perfectly aligned with the boundaries. A very similar behavior of the granular system was observed in [9], under the same shearing velocity and imposed pressure, in the case of more dissipative particles ( $e_n = 0.4$ ) and for both frictionless and frictional particles. In [9], the shear band thickness was found to be independent of the friction coefficient of the flowing particles. However, the shear band location varied with particle friction, positioning either at the center of the domain or shifting toward one of the bumpy planes. Furthermore, the crystalline structures were found to be independent of particle friction and consistently aligned with the bumpy boundaries. This alignment resulted in macroscopic geometrical friction that also remained unaffected by particle friction.



**Figure 3.** Snapshots of the particle positions projected on the  $x$ - $z$  (first row) and  $x$ - $y$  planes (second row), for frictionless flowing particles when (a)  $d_w/d = 1$ , (b)  $d_w/d = 3/4$  and (c)  $d_w/d = 1/3$ . Particle size is scaled by 50% to facilitate the view

As the bumpiness decreases to  $d_w/d = 3/4$ , the ordering at the boundaries becomes partially disrupted, and most particles transition into a disordered fluid state, as shown in Figure 3(b). This disordered region percolates intermittently from the boundaries to the core region of the system, although most of the particles remain crystallized.

When the bumpiness is reduced to a very small value,  $d_w/d = 1/3$ , the ordering throughout the system is almost entirely lost, as revealed in Figure 3(c). Under the same imposed pressure, the system becomes significantly less dense (exhibiting a larger flow height), leading to a further reduction in macroscopic friction (Figure 2).

The striking result, at least for the case of frictionless particles, is that the overall shear resistance diminishes by a factor of four as the boundaries become smoother, i.e., less bumpy, as a consequence of a sort of disordering effect generated by reducing the bumpiness. An exception is the case with bumpiness 0.5 where the measured macroscopic friction is larger than in the cases with  $d_w/d = 5/8$  and  $3/4$ , despite the most of the particles are not crystallized. Future work will focus on consolidating the  $\mu$ - $d_w/d$  curve around  $1/2$  and identifying the location of its local maximum. We point out that zero bumpiness, i.e. perfectly smooth non-bumpy walls, would generate no moving systems since, being the particles frictionless, no energy could be transmitted to the particles by the walls.

## 4 Conclusions

We have performed discrete element simulations of identical, frictionless, inelastic spheres sheared, in the absence of gravity, between two parallel, bumpy planes, under a constant load high enough to induce crystallization. The bumpiness of the planes was due to a monolayer of identical spheres glued together and arranged in a regular,

hexagonal lattice. We have probed the effect of the bumpiness of the boundaries on the self-assembly process and the resulting macroscopic friction of the system, the latter representing a measure of the shear resistance, and being a key quantity to test the capability of the granular material to act (or not) as a lubricant between the moving boundaries.

Our study demonstrates that, in the absence of particle friction, boundary roughness dominates the crystallization process, facilitating a transition of some particles into a fluid-like phase, and leading to a significant reduction in shear resistance as bumpiness decreases. The complete absence of wall roughness would make the motion of granular material impossible due to the lack of friction. Therefore, identifying the optimal roughness value that ensures steady motion while minimizing energy dissipation is a highly relevant objective. These findings underscore the potential of granular materials as effective lubricants, with implications for industrial applications.

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