'Flow & Jam' of frictional athermal systems under shear stress

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Abstract

We report recent results of molecular dynamics simulations of frictional athermal particles at constant volume fraction and constant applied shear stress, focusing on a range of control parameters where the system first flows, but then jams after a time t_{jam}. On decreasing the volume fraction, the mean jamming time diverges, while its sample fluctuations become so large that the jamming time probability distribution $P(t_{jam})$ becomes a power-law. We obtain an insight on the origin of this phenomenology focusing on the flowing regime, which is characterized by the presence of a clear correlation between the shear velocity and the mean number of contacts per particles Z, whereby small velocities occur when Z acquires higher values.

1 Introduction

The non-equilibrium transition from a fluid–like state to a disordered solid–like state, known as jamming transition, occurs in a wide variety of physical systems, such as colloidal suspensions and molecular fluids. Its widespread occurrence suggested to introduce a 'jamming phase diagram', with axes

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temperature, density and shear stress [1, 2, 3, 4], able to describe the jamming transition of all of these systems. In this framework, jamming occurs at small temperature, high density, and small external shear stress. Frictionless athermal systems [1] can be described by the zero temperature plane of the jamming diagram: a transition line is expected to separate a jammed phase, which consists in non–ordinary solid [5, 6], and a flowing phase, where only steady states are observed [7, 8]. Such a simple picture becomes more involved in the presence of friction, which must be taken into account in order to properly describe granular (macroscopic) materials [9, 10, 11, 12, 13, 14, 15, 16].

We have recently investigated the effect of friction on the jamming phenomenology performing Molecular Dynamics (MD) simulations of a frictional granular system at constant volume fraction and constant applied shear stress [15, 16]. In this set–up the jamming phenomenology is very rich, due to the occurrence of four possible *phases*, 'Flow', 'Flow & Jam', 'Slip & Jam' and 'Jam' (as found on increasing the density or decreasing the applied shear stress). In the 'Flow & Jam' and in the 'Slip & Jam' phase, the system reaches an apparently steady flowing state before jamming, or jams after a tiny displacement, respectively. In this paper, we present recent results regarding the 'Flow & Jam' regime, where the system jams after flowing for a time t_{jam}. We describe both dynamical properties of the system, such as the jamming time, as well as structural ones, such as the evolution of mean contact number. Connections and correlations between static and dynamics quantities suggest which is the physical mechanisms responsible of the 'Flow & Jam' phenomenology.

2 The investigated system

We perform MD simulations of the system considered in [15, 16]. Monodisperse spherical grains of mass M and diameter D are enclosed in a box of dimension $l_x = l_y = 16D$, and $l_z = 8D$. Periodic boundary conditions are used along x and y, while the size of the vertical dimension is fixed and chosen to be comparable to that of recent experiments [17, 18, 19]. The upper and lower boundary surfaces of the box consist in rough "virtual" plates: each plate is made by a collection of particles that move as a rigid object. The bottom plate has an infinite mass, and is therefore fix, while the top one has a mass equal to the sum of the masses of its particles (roughly $l_x l_y$). The top plate is subject to a shear stress σ_{xz} ($\sigma_{xz} = \sigma$ from now on).

Grains interact via the standar linear spring-dashpot model. Two particles i and j, in positions $\mathbf{r}_i$ and $\mathbf{r}_j$, with linear velocities $\mathbf{v}_i$ and $\mathbf{v}_j$, and angular velocities ω_i and ω_j , interact if in contact, i.e., if the quantity $\delta_{ij} = D - |\mathbf{r}_{ij}|$ is positive. δ_{ij} is called the penetration lenght, and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the distance between the center of the particles i and j. The interaction force has a normal component $\mathbf{F}_{n_{ij}}$ and a tangential one $\mathbf{F}_{t_{ij}}$, the both having an elastic and a dissipative component:

$$\mathbf{F}_{n_{ij}} = -k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_n m_{eff} \mathbf{v}_{\mathbf{n}_{ij}} \tag{1}$$

$$\mathbf{F}_{t_{ij}} = -k_t \mathbf{u}_{t_{ij}} - \gamma_t m_{eff} \mathbf{v}_{t_{ij}} \tag{2}$$

where k_n and k_t are elastic moduli, while γ_n and γ_t account for dissipative caharacter of the normal and tangential component rispectively. $\mathbf{n}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$, $\mathbf{v}_{n_{ij}} = [(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n_{ij}}]\mathbf{n}_{ij}$, $\mathbf{v}_{\mathbf{t}_{ij}} = \mathbf{v}_{ij} - \mathbf{v}_{\mathbf{n}_{ij}}$ and m_{eff} is the effective mass. $\mathbf{u_{t_{ij}}}$, set to zero at the beginning of a contact, measures the shear displacement during the lifetime of a contact. Its time evolution is fixed by $\mathbf{v}_{\mathbf{t}_{ij}}$ and ω_i and ω_j, as described in Ref. [20]. The presence of tangential forces implies the presence of torques, $\tau_{ij} = -1/2\mathbf{r}_{ij} \times \mathbf{F}_{ij}$. The shear displacement is set to zero both when a contact finish ($\delta_{ij} < 0$), where μ is the coefficient of static friction. We use the value of the parameters of [20]: $k_n = 2\ 10^5$, $k_t/k_n = 2/7$, $\gamma_n = 50$, $\gamma_t/\gamma_n = 0$. Lenght, masses and times are expressed in units of D, m and $\sqrt{m/k_n}$.

The volume fraction φ represents the volume occupied by the grains divided by the volume of the container, i.e. $\varphi = N v_0/V_0 + \Delta\phi$, where $V_0 = l_x l_y l_z$ is the volume of the system and $v_0 = 1/6\pi D^3$ is the volume occupied by a single grain and $\Delta\phi = 0.021$ is a corrective a term which takes into account the effect of the rough plates protruding into the system. By changing the number of particles we vary the volume fraction.

The initial state is prepared setting to zero the friction coefficient [21], randomly placing the particles and then inflating them until the desired volume fraction is obtained; such a protocol is a short-cut of experimental procedures with which it is possible to generate very dense disordered states of frictional systems, such as oscillations of high frequency and small amplitude [22]. After preparing the system we 'switch on' friction, and follow the time evolution of the system under the action of the constant shear stress . We investigate the evolution of the system focusing on a value of Coulomb friction coefficient equal to $\mu = 0.1$ while φ and σ are the variable control parameter. All the data shown here refers to points (φ, σ) falling in the 'Flow & Jam' region of the Jamming–phase–diagram [16]. For each point we perform 50–100 different runs, starting from different initial conditions. In the 'Flow & Jam' region, the steady state last a long time at small volume fractions, where the time t_{jam} the system flows before jamming is large. This is the

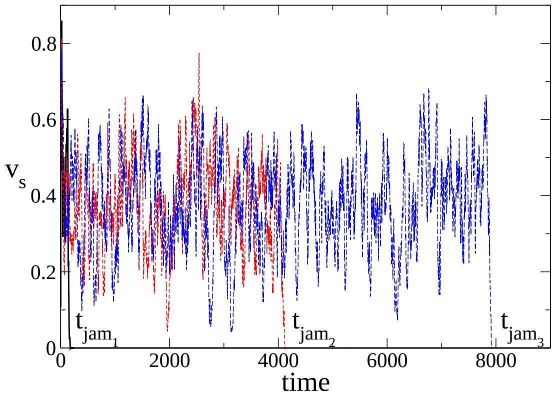

Figure 1: (Color online) Velocity of the upper plate v_s as a function of time for three simulations at $\phi \simeq 0.627$ and $\sigma = 2\ 10^{-3}$. We marked the values of the jamming times, t_{jam}, which differ by more than three decades.

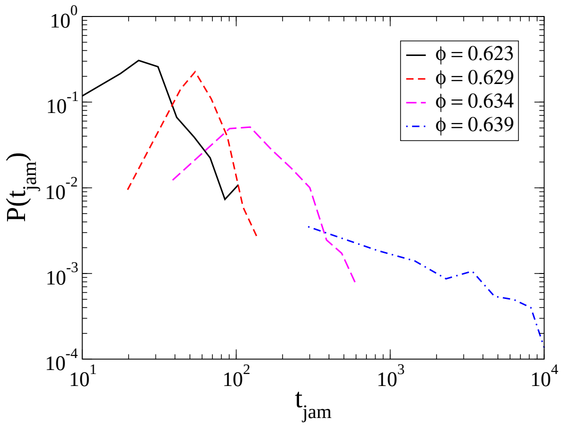

Figure 2: (Color online) Probability distribution $P(t_{jam})$ of the jamming time for $\sigma = 2\ 10^{-3}$ and different values of the volume fraction, as indicated.

region where the 'Flow & Jam' is more surprising, we have investigated in detail performing simulations lasting up to a time $T = 5\ 10^4$. At higher volume fraction t_{jam} is small, and the identification of the steady state becomes more difficult.

3 Flow and Jam region

3.1 Jamming times

In the 'Flow & Jam' phase of sheared granular systems [16], the system first flows with a constant velocity as in a steady flowing phase, but then suddenly jams after a time t_{jam}. Such a phenomenology is shown in Fig. 1, where we report the velocity $v_s(t)$ of the upper plate as a function of time for three simulations at $\phi = 0.627$ and $\sigma = 2\ 10^{-3}$. The average jamming time $\langle t_{jam} \rangle$ depends on the volume fraction. It diverges as a power law on decreasing the volume fraction, at a critical volume fraction $\phi_{j1}(\sigma, \phi)$, and vanishes on increasing the volume fraction, at a critical value $\phi_{j2}(\sigma, \phi)$. The lines $\phi_{j1}(\sigma, \phi)$ and $\phi_{j2}(\sigma, \phi)$ define the boundary of the 'Flow & Jam' phase in the volume fraction, shear stress and friction jamming phase diagram for frictional particles [16] .

However, the jamming time is subject to large fluctuations. For instance, the three simulations shown in Fig. 1 jam at very different times, even though they differ only in the initial configuration. Such an observation suggested to study the sample fluctuations of the jamming time, which we show in Fig. 2 for $\sigma = 2\ 10^{-3}$ and three different values of the volume fraction. While at high volume fractions $P(t_{jam})$ is peaked, meaning that the jamming time is well defined, on decreasing the volume fraction the distribution moves to larger times, and at the same times changes shape, becoming well described by a power law.

In order to understand the origin of the 'Flow & Jam' phenomenology and of the large fluctuations of the jamming time, which are not described by current rheological models such as those based on the inertial number [23] or on rate and state equations [24, 25], we have analyzed the evolution of the micro-structure of the system in the flowing regime and the micro-mechanics of the jamming process, as described below.

3.2 Fluctuations of the micro-structure of the system

Fig. 3 illustrates the time evolution of the mean number of contacts per grain, $Z(t)$, for the same simulations considered in Fig. 1. At the beginning of the simulations, as a consequence of the considered preparation protocol, $Z(t = 0) = 0$. $Z(t)$ rapidly increases as the system start flowing, and then fluctuates around a constant value in the following steady flowing phase. A comparison between Fig. 1 and Fig. 3 suggests the presence of a correlation between the shear velocity $v_s(t)$ and the mean contact number $Z(t)$, whereby large values of Z occurs when the shear velocity is small, and conversely.

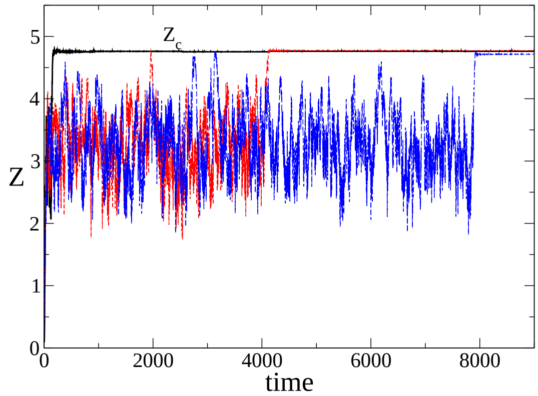

Figure 3: (Color online) Mean number of contacts per grain Z as a function of time, for the simulations shown in Fig.1. The system jams when Z reaches a critical value Z_c.

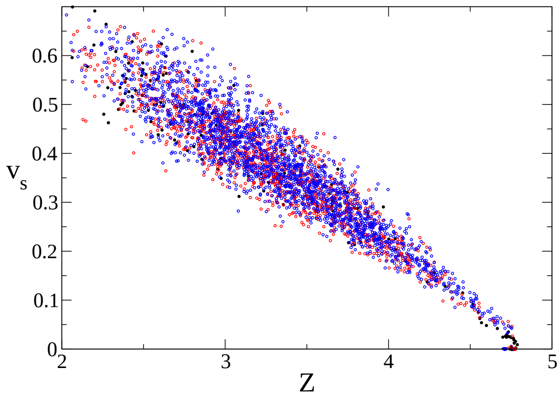

Figure 4: (Color online) Parametric plot of the velocity of the top plate versus the mean number of contacts, obtained from the data shown in Fig.s 1 and 3. The collapse indicates the existence of a correlation between Z and v_s: the higher Z, the slower the system.

Fig. 4 shows a parametric plot of $v_s(t)$ versus $Z(t)$. In such a representation, the data from simulations characterized by very different values of the jamming time display a correlate behaviour.

Note that the fluctuations of the shear velocity decreases as the mean number of contacts increases, suggesting the presence of a well defined critical mean number of contacts Z_c at which jamming occurs, in agreement with the results of Fig. 3. We plot in Fig. 5 the averaged shear velocity as a function of the mean number of contacts, $\langle v_s(Z) \rangle$,The normal component is given by

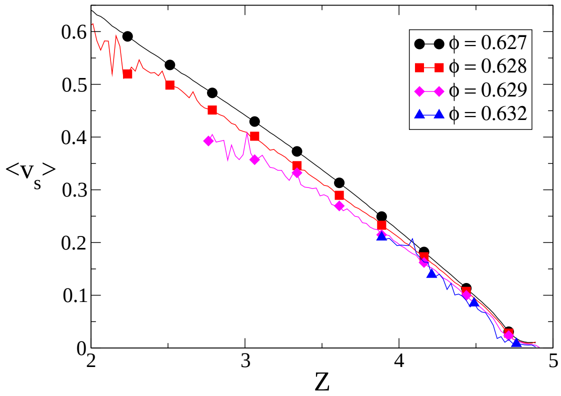

Figure 5: (Color online) Dependence of the average shear velocity $\langle v_s \rangle$ as a function of the mean number of contacts per grain at $\sigma = 2\ 10^{-3}$, for the indicated values of the volume fraction.

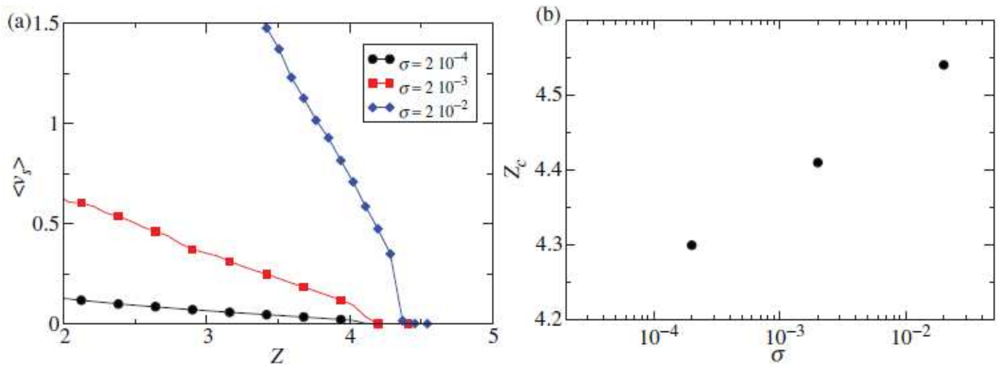

Figure 6: (Color online) At $\phi = 0.629$, **a)** average shear velocity $\langle v_s \rangle$ versus mean number of contacts per grain for the indicated values of the shear stress, and **b)** jamming critical mean contact number Z_c as a function of the applied shear stress.

for the indicated values of the volume fraction. The figure suggests that Z_c is almost independent on the volume fraction, consistently with the existence of a volume fraction range where granular systems with equal mechanical properties can be prepared [16]. On the contrary, as shown in Fig.s 6a,b Z_c increases with the applied shear stress. Considering that the shear modulus is expected to increase with the mean contact number [3], this result suggests that the shear modulus of a jammed system does not simply depend on its volume fraction, but also on the applied stresses which caused jamming, or more generally on the preparation procedure.

4 Jamming mechanism

Here we propose a qualitative mechanism to explain the origin of the 'Flow & Jam' phenomenology, based on the behavior of the shear velocity $\langle v_s(t)\rangle$ and of the mean contact number $Z(t)$, as well as on the dependence of t_{jam} and Z_c on the control parameters. The starting point is the well known dilatancy phenomenon observed in granular systems [27, 28, 29], which is the tendency of flowing particulate systems to dilate. At constant pressure and constant shear strain rate a dilation is actually observed, the larger the greater the shear velocity [30]. At constant volume, which is the case considered here, dilation is obviously forbidden. This leads to a impeded dilatancy which may explain the observed phenomenology.

While flowing, the system visits different microscopic configurations, each one having a typical mean number of contact Z. When Z is small, particles exert a small resistance to the applied stress, the shear rate increases and the system tries to dilate. This leads to a configuration with a larger mean number of contacts, exerting a larger resistance, which causes the system to decelerate. The existence of such a feedback mechanism is suggested by the correlations between Z and v_s illustrated in Fig. 4. The impeded dilatancy appears therefore responsible for the fluctuations of the mean number of contacts. The flowing system jams as a result of a large fluctuation of the mean number of contacts Z, which reaches the critical value Z_c corresponding to configurations able to sustain the applied stress. How frequent are these fluctuations? We expect these fluctuations to be more rare when the volume fraction is small, simply because there are fewer configurations able to sustain the applied stress (i.e. with $Z = Z_c$): this explains why the jamming time increases as the volume fraction decreases. Also, one expects that when the volume fraction is smaller than a threshold value, there are no configurations with $Z = Z_c$, which explains why the jamming time diverges decreasing the volume fraction.

5 Conclusions

In this manuscript, we focused on a region of the control parameters where frictional granular systems jam after flowing with a constant velocity, and described a possible mechanism able to explain the observed behavior, The mechanism is based on the notion of impeded dilatancy and on the presence of correlations between structure and dynamics of the system in the flowing regime. An open question ahead is the explanation of the power-law like distribution of the jamming times at small volume fractions, an indication of the presence of correlations in the dynamics of sheared systems, which needs to be clarified.

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