Constitutive law of dense granular matter

Takahiro Hatano
Earthquake Research Institute, University of Tokyo, 1-1-1 Yayoi, Bunkyo, Tokyo 113-0032, Japan
E-mail: hatano@eri.u-tokyo.ac.jp

Abstract. The frictional properties of dense granular matter under steady shear flow are investigated using numerical simulation. Shear flow tends to localize near the driving boundary unless the coefficient of restitution is close to zero and the driving velocity is small. The bulk friction coefficient is independent of shear rate in dense and slow flow, whereas it is an increasing function of shear rate in rapid flow. The coefficient of restitution affects the friction coefficient only in such rapid flow. Contrastingly, in dense and slow regime, the friction coefficient is independent of the coefficient of restitution and mainly determined by the elementary friction coefficient and the rotation of grains. It is found that the mismatch between the vorticity of flow and the angular frequency of grains plays a key role to the frictional properties of sheared granular matter.

1. Introduction
Granular flow is ubiquitous in solid earth sciences and engineering: e.g. avalanches, landslides, debris flow, silo flow, etc. These phenomena are essentially dominated by the frictional properties of granular matter. Thus, to find a law that describes the behavior of friction coefficient (ratio of the shear stress to the normal stress) of granular matter is an essential problem [1].

The mechanical properties of granular matter generally depend on many ingredients: density, shear rate, pressure, temperature, humidity, interstitial fluid, etc. These ingredients must be carefully controlled in investigating the frictional properties, as they affect the result in unexpected ways. Because such potentially important ingredients are not known a priori, despite extensive experimental efforts, the frictional properties of dense granular matter are still not clear.

In order to rule out chemical processes that potentially affect the frictional properties, numerical simulation plays an important role. Through extensive simulations [2,3], it turns out that the behavior of friction coefficient of dry granular matter is well described by a nondimensional number, \( I = \dot{\gamma} \sqrt{m/Pd} \), where \( \dot{\gamma} \) denotes shear rate, \( m \) is the mass of a grain, \( P \) is the normal pressure, and \( d \) is the grain diameter. This nondimensional number is referred to as the inertial number, which seems to be successful in stating a constitutive law for fast granular flow [4].

To clarify a constitutive law for slow granular flow, da Cruz et al. performed an extensive simulation on a two dimensional system in a wide range of the inertial number: \( 6 \times 10^{-4} \leq I \leq 0.3 \). They find a friction law that reads \( \mu = \mu_0 + aI \), where \( \mu \) is the kinetic friction coefficient, and \( \mu_0 \) and \( a \) are positive constants. However, in three dimensional systems, somewhat different friction law is found, where the inertial-number dependence of friction coefficient is described.
by a power law, which is of the same form as the Herschel-Bulkley model; i.e., $\mu = \mu_0 + s^\phi \omega$, where $s$ is a positive constant and $\phi \simeq 0.3$ [5,6]. This power law behavior is confirmed in a numerical simulation of a certain class of granular matter: particularly smooth (frictionless) beads. However, the validity of this power-law friction in a wide class of granular materials, as well as the theoretical understanding and derivation, are still open. In addition, before theoretical consideration, some questions regarding phenomenology are still open: How do the coefficient of restitution, rolling resistance, and other material properties affect the frictional properties of granular matter? In this paper, these questions shall be answered.

2. Model

2.1. force model

Here each grain is assumed to be sphere. The interaction between grains is described by the discrete element method (DEM) [7], which is the standard model used in powder engineering and soil mechanics. Consider a grain $i$ of radius $R_i$ located at $\mathbf{r}_i$ with the translational velocity $\mathbf{v}_i$ and the angular velocity $\Omega_i$. This grain interacts with another grain $j$ whenever they are in contact; i.e., $|\mathbf{r}_{ij}| < R_i + R_j$, where $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$. The force acting on two particles is decomposed into two direction: normal and transverse to $\mathbf{r}_{ij}$. Introducing the normal unit vector $\mathbf{n}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$, the normal force $\mathbf{F}_{ij}$ is given by $[kh_{ij} - \zeta \mathbf{n}_{ij} \cdot \mathbf{r}_{ij}]\mathbf{n}_{ij}$, where $h_{ij} = R_i + R_j - |\mathbf{r}_{ij}|$ and $k$ is a constant. The coefficient of restitution, $e$, can be calculated using the relation

$$e = \exp \left[ -\frac{\pi}{\sqrt{4mk/\zeta - 1}} \right],$$

where $\bar{m} = m_i m_j/(m_i + m_j)$. In order to define the transverse force, we define the relative tangential velocity as

$$\Xi_{ij} = \dot{\mathbf{r}}_{ij} - \mathbf{n}_{ij} \cdot \dot{\mathbf{r}}_{ij} + \frac{R_i \Omega_i + R_j \Omega_j}{R_i + R_j} \times \mathbf{r}_{ij}$$

and introduce the relative tangential displacement vector $\Theta$ as $\int_{roll} ds \Xi(s)$. The subscript of the integral indicates that the integral is performed only when the contact is rolling; i.e., $k_t |\Theta_{ij}| < \mu_c |\mathbf{F}_{ij}|$ or $\Xi_{ij} \cdot \Theta_{ij} < 0$. Otherwise, the contact is said to be sliding. The magnitude of the tangential force depends on the state of the contact: $\mu_c |\mathbf{F}_{ij}|$ for sliding contact and $k_t |\Theta_{ij}|$ for rolling contact.

2.2. configuration

The particles are bidisperse: the diameters are 0.8$d$ and 1.0$d$, respectively. The number of each particle is the same. For simplicity, the mass of the grains is set to be the same, which is denoted by $m$.

The dimensions of the system are $L \times L \times H$, where we use periodic boundary conditions along the $x$ and the $y$ axes. In the $z$ direction, there exist two rigid walls that consist of the larger particles. One of the walls is displaced along the $x$ axis at constant velocity $V$ to realize plain shear flow, where the velocity gradient is formed in the $z$ direction. The grains that constitute walls interact with the bulk grains via the force described above. This wall is also allowed to move along the $z$ axis so that the pressure is kept constant at $P$, while it is immobile along the $y$ axis. Namely, the $z$ dimension of the system, denoted by $H$, depends on the velocity of the wall. Here we define that $H_0$ is the layer thickness at $V = 0$. Here the dimensions are set to be $H_0 = 12d$ and $L = 10d$, in which approximately 2,000 particles are intervened between the walls. See Fig. 1 for schematic of the computational system. The equation of motion of the wall along the $z$ axis is given as $M \ddot{H} = F_z - PL^2$, where $M$ denotes the mass of the wall and $F_z$ is the repulsive force given by the grains. The mass of the wall, $M$, is set to be $M = 100m$. It should be remarked that the gravity is not taken into account, because the pressure $P$ shall be chosen to be large enough.
2.3. parameters
The transverse spring coefficient is set to be $k_t = k/5$ throughout this study. This relation is empirically known to reproduce experimental results. The other parameters, $\mu_e$ and $\zeta$, generally depends on the material of grains. It is thus important to investigate how these parameters affect the frictional properties of granular matter. The pressure $P$ is kept fixed as $Pd/k = 8.6 \times 10^{-4}$. For de-dimensionalization, we set $d = 1$, $k = 1$, and $m = 1$. Here we estimate the material constants based on the sound velocity and the Young’s modulus, which roughly corresponds to $d\sqrt{k/m}$ and $k/d$, respectively. (Here the numerical factors are neglected.) Note also that any length scale in the simulation is scaled with the grain diameter, $d$. Thus, the unit velocity and the unit pressure in DEM are of the order of kilometer per second and several tens of Gigapascal, respectively. The pressure applied to the system is thus on the order of 10 MPa. In this paper, we limit ourselves to the frictional property of steady states. The steady state is realized after certain strain, which can be confirmed by observing the friction coefficient and the height of the wall, $H$. Here the computational data is taken only after the system is subject to 100 % strain. The traction acting on the moving wall is monitored, which is denoted by $F_x$, so that the bulk friction coefficient of the system is defined as $F_x/PL^2$.

3. Velocity profile
In a certain class of systems including granular matter, the uniform shear deformation can be unstable and deformation tends to localize within a narrow band. This spontaneous structure formation is referred to as shear-banding. Although it is speculated that some healing processes (or thixotropy, velocity-weakening friction, etc) may play a certain role in shear-banding [8], the general mechanism for shear banding is still not clear.

Thus, the internal flow structure (velocity profile) should be measured before discussing the frictional properties. In order to exclude the fluctuation, the instantaneous flow velocity is averaged over a certain strain (100 %). Fig. 2 shows the averaged flow velocity as a function of the depth. Although any healing mechanism is not modeled in the present computational system, the behavior that is similar to shear-banding is observed. Indeed, shear flow tends to localize near one of the wall. It is found that the flow localization is more apparent for systems with larger coefficient of restitution (i.e., with smaller damping coefficient $\zeta$.)

The flow localization is also affected by the driving velocity of the wall. In the right panel of Fig. 2, where the effect of damping is significant ($\zeta = 1$), the shear flow is uniform except for the highest velocity case, $V = 10^{-1}$. Thus, flow localization is more likely to occur at larger
driving velocity of the wall.

It should be remarked that the localization near the wall is also observed in a two dimensional system [9], where the localization is more frequently observed in a system at lower pressure. This tendency is also observed in the present three-dimensional system.

4. Behavior of the bulk friction coefficient

4.1. general description

Shear stress $\sigma$ in steady shear flow is determined by the balance between power input and the dissipation rate $D$.

$$\dot{\gamma} \sigma = D$$

where $\dot{\gamma}$ denotes shear rate. Thus, the nature of shear stress (and thus friction coefficient) involves the mechanism of dissipation. Note that the present computational model has two different sources of dissipation at the particle level: damping in the normal force and friction in the tangential force. The former is proportional to the damping coefficient $\zeta$ and the latter is proportional to the elementary friction coefficient $\mu_e$. Therefore, the dependence of friction coefficient on each parameter may be a key to the understanding the dissipation mechanism in sheared granular matter.

4.2. shear rate dependence

First, the shear rate dependence of the friction coefficient is discussed focusing the effect of the damping coefficient $\zeta$. Fig. 3 shows the bulk friction coefficient as a function of the inertial number $I$ (i.e., nondimensional shear rate) with several values of $\zeta$. Here three cases are investigated: $\zeta = 10^{-2}, 10^{-1}, 1$, whereas the elementary friction coefficient is fixed at 0.6. In terms of the coefficient of restitution $e$, these values of correspond to $e = 0.80, 0.49, \text{and} 0.043$, respectively. (Note Eq. (1)). The bulk friction coefficient is insensitive to shear rate and to the damping coefficient in the lower I regime $I \leq 10^{-2}$. This indicates that the collision in the normal direction is irrelevant to the bulk friction coefficient in dense and slow granular flow. Note also that it is much less than the elementary friction coefficient.

The bulk friction coefficient then sharply increases around $I \sim 10^{-1}$. In such high I region, the friction coefficient apparently depends on the coefficient of restitution: it increases as the coefficient of restitution decreases. (For example, at $I = 0.28, \mu = 0.44$ for $e = 0.80, \mu = 0.50$)
Figure 3. The friction coefficient as a function of the inertial number defined by Eq. (1). The legends denote the coefficient of restitution. The solid and dotted lines are empirical constitutive laws, Eq. (3), where $\phi = 0.5$ for the solid line and $\phi = 1.0$ for the dotted line.

for $e = 0.49$, and $\mu = 0.57$ for $e = 0.043$.) This implies that the dissipation due to normal collision is dominant in the rapid flow region where $I \geq 10^{-1}$. The shear rate dependence can be empirically described by the Hershel-Bulkley model,

$$\mu = \mu_0 + sI^\phi$$

Here the exponent $\phi$ ranges from 0.5 to 1.0. (See Fig. 3). It should be remarked that these values are larger than previously estimated [5,6], where $0.3 \leq \phi \leq 0.4$. The difference may be due to the elementary friction coefficient. In the previous studies [5,6], the elementary friction coefficient is set to be zero or 0.2, while it is 0.6 here. Thus, the exponent $\phi$ depends on the elementary friction coefficient. Although $\mu_e = 0.6$ case is also investigated in Ref. [5], the data are insufficient for the estimate of the exponent.

4.3. effect of elementary friction coefficient

In dense and slow granular flow, the elementary friction coefficient between grains, $\mu_e$, is more important parameter than the coefficient of restitution. Fig. 4 shows how the bulk friction coefficient of a slowly-sheared system ($I = 2.8 \times 10^{-5}$) depends on elementary friction coefficient. The bulk friction coefficient increases as the elementary friction coefficient increases at smaller $\mu_e$, but then becomes independent of $\mu_e$. (There is a maximum value around 0.35). It should be noted that this insensitivity of the bulk friction coefficient to the elementary friction coefficient is also found in two dimensional granular systems [3].

5. Rotation of grains

As shown in Figs. 3 and 4, in dense and slow flow, the extent of dissipation in normal interaction (i.e., the coefficient of restitution) is irrelevant to the bulk friction coefficient but sliding friction between grains plays an important role. Now let us estimate the bulk friction coefficient in the low $I$ regime taking the sliding friction between grains into account.

For simplicity, we consider the two dimensional case. Neglecting the fluctuation in the translational velocity of each particle, the sliding velocity at the contact of two particles is approximately

$$d (\dot{\gamma} \cos \theta_{ij} - (\Omega_i + \Omega_j)/2)$$

(4)
Figure 4. The bulk friction coefficient taken at \( I = 2.8 \times 10^{-5} \) (the slowest data in Fig. 3) as a function of the elementary friction coefficient.

Figure 5. (Left) Schematic of grain rotation and shear flow. (Right) The frustration parameter as a function of shear rate. Here \( \zeta = 1.0 \) and \( \mu_e = 0.6 \).

where \( \cos \theta_{ij} = \mathbf{n}_{ij} \cdot \mathbf{n}_z \). (See the left panel of Fig. 5). Note that \( \theta_{ij} \leq 0 \) without the loss of generality. For simplicity, the diameter is assumed to be the same for all particles. Using the average normal force, \( P n_b d \), where \( n_b \) is the number of contacts in unit volume, the frictional force acting between particles \( i \) and \( j \) is \( \mu_e P / n_b d \). Then the energy dissipation rate per contact reads

\[
\mu_e P n_b^{-1} |\dot{\gamma} \cos \theta_{ij} - (\Omega_i + \Omega_j)/2| \tag{5}
\]

Using the power balance Eq. (2), the bulk friction coefficient is estimated as

\[
\mu = \mu_e \left\langle \cos \theta_{ij} - \frac{\Omega_i + \Omega_j}{2 \dot{\gamma}} \right\rangle, \tag{6}
\]

where the bracket denotes the average over the contacts. Equation (6) indicates that the friction coefficient vanishes if the grains have their neighbors only in the velocity gradient direction (thus \( \cos \theta_{ij} = 1 \)) and \( \Omega_i = \dot{\gamma} \). Similarly, the friction coefficient can also vanish if the grains have their neighbors only in the flow direction (thus \( \cos \theta_{ij} = 0 \)) and \( \Omega_i = \Omega_j \). However, the orientations
of contacts in granular matter are of course random. This is a reminiscence of spin-glasses; the interaction in the flow direction is antiferromagnetic and the one in the gradient direction is ferromagnetic. In addition, there are intermediate interactions and these interactions are coupled to translational velocity.

As the problem is very complicated, let us make further simplification that the angular frequency of particles are the same, i.e., $\Omega_i = \omega$ and $\cos \theta_{ij}$ is replaced by unity. Then Eq. (6) becomes

$$\mu \sim \mu_e \left\langle \left| 1 - \frac{\omega}{\dot{\gamma}} \right| \right\rangle$$  \hspace{1cm} (7)

The quantity $1 - \omega/\dot{\gamma}$, which we shall refer to as the frustration parameter, is thus important to the nature of friction in dense and slow granular flow. The right panel of Fig. 5 shows the typical behavior of the frustration parameter $c$ as a function of shear rate. In slow and dense flow regime, the frustration parameter takes the value around 0.5. This means $\mu \approx 0.5 \mu_e$, which is not a very bad prediction for $\mu_e = 0.6$ case, where $\mu \simeq 0.35$. (See Fig. 4). Note that the value of frustration parameter may depend on $\mu_e$. At this point, we do not know how this quantity is determined from the contact network of grains.

In order to test the validity of Eq. (7), one can consider a model in which the grains do not rotate at all. This leads to $\omega = 0$ so that it is expected from Eq. (7) that $\mu \approx \mu_e$. Fig. 6 shows the bulk friction coefficient of this model, which increases as the elementary friction coefficient increases up to 1.0. This behavior makes a quite contrast to that of the previous model with the particle rotation.

6. Conclusions
The friction coefficient of dense granular matter is an increasing function of shear rate. The coefficient of restitution affects the friction coefficient only in rapid flow. Contrastingly, in dense and slow regime, the friction coefficient is mainly determined by the elementary friction coefficient and the rotation of grains. Mismatch between the vorticity of flow and the angular frequency of grains plays a key role to the friction coefficient.

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