Numerical simulation of two-dimensional granular shearing flows and the friction force of a moving slab on the granular media*

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This paper studies some interesting features of two-dimensional granular shearing flow by using molecular dynamic approach for a specific granular system. The obtained results show that the probability distribution function of velocities of particles is Gaussian at the central part, but diverts from Gaussian distribution nearby the wall. The macroscopic stress along the vertical direction has large fluctuation around a constant value, the non-zero average velocity occurs mainly near the moving wall, which forms a shearing zone. In the shearing movement, the volume of the granular material behaves in a random manner. The equivalent friction coefficient between moving slab and granular material correlates with the moving speed at low velocity, and approaches constant as the velocity is large enough.

Keywords: granular shearing flow, friction, molecular dynamics modeling

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1. Introduction

Granular flows exhibit many interesting phenomena, which are quite different from the behaviours of classical fluid and solid materials. Using experiments, researchers investigated the mixing and segregation of particles with different sizes,[1−6] density waves in the outflow through hoppers,[7] spontaneous heap,[8] arching effect,[9] two different kinds of avalanches on an inclined plate,[10,11] granular jets,[12,13] dilute-to-dense transition,[14−16] etc., several theories have been established in order to explain part of those phenomena.[17−21] So far, no universal theory, like Navier–Stokes equation in fluid mechanics, has been found to account for all those fantastic behaviours.[22]

Due to the difficulties in both analytical treatments and experiments, the most commonly used method to study granular materials is numerical simulation. By building the interaction models between particles, the movement of every particle can be traced by integrating classical Newton's law. Usually, the interaction models include a lot of uncertainties, many parameters are difficult to be defined. But from the large amount of works on simulations of different researchers, it is found that the macroscopic statistical results do not depend largely on the microscopic detail of the model, just like different fluids can hold the same governing equation although their microcosmic interactions are quite distinctive. Hence, we believe that the results are reasonable at a macroscopic scale.

This paper studies two-dimensional granular shearing flow using molecular dynamic simulations. Shearing flow is one of the most basic flows in classical fluid dynamics, which has been the source of Newton's friction law. In the study of granular dynamics, the shearing flow is in the highest light also because the shearing behaviour is one of the basic phenomena in granular flows. Many research works have presented about shearing flows.[23,24] For dense flow, a constitutive law has been established based on the inertial number. A monotone relation between the friction coefficient and the inertial number is found for dense flow case.[25,26] More results are included in the review articles Refs. [22] and [27].

In the present paper, a numerical model employed is introduced in Section 2, research results are listed in Section 3, and brief conclusions are given in Section 4.

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2. The model of interaction between particles and numerical method

The forces on every particle include the gravitational force and the interaction force between particles. Consider a particle i (disc in two dimensions), whose position is $\boldsymbol{r}_i$, angular velocity is $\boldsymbol{\omega}_i$, mass is m_i, radius is R_i. And $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$ denotes the relative position of particle j to i, $\boldsymbol{n}$ is unit vector in this direction (normal direction), tangential direction $\boldsymbol{\tau}$ is orthogonal to $\boldsymbol{n}$, which has same direction with the velocity component in tangential plane. The $\boldsymbol{F}_{ij}$ is the force imposed on particle i by j. Then the movement equations of motion of particle i is

$$m_i\ddot{\boldsymbol{r}}_i = \sum_{j\neq i} \boldsymbol{F}_{ij} + m_i g\hat{\boldsymbol{g}}, \tag{1}$$

$$I_i\dot{\boldsymbol{\omega}}_i = \frac{1}{2}\sum_{j\neq i} \boldsymbol{r}_{ij}\times\boldsymbol{F}_{ij}, \tag{2}$$

where $\hat{\boldsymbol{g}}$ is unit vector in vertical downward direction and I_i is moment of inertia of particle i, and $I_i = \frac{2}{5}m_iR_i^2$ for three-dimensional (3D) sphere but $I_i = \frac{1}{2}m_iR_i^2$ for two-dimensional (2D) disc. The force between two particles is nonzero only when they come in contact, i.e., $\boldsymbol{F}_{ij} = 0$ when $|r_{ij}| > R_i + R_j$. When two particles overlap, the normal contact force consists of two parts, $\boldsymbol{F}_{ij}^n = \boldsymbol{F}_{ij}^{\rm rest} + \boldsymbol{F}_{ij}^{\rm diss}$, where

$$\boldsymbol{F}_{ij}^{\rm rest} = -Ym_{\rm e}(R_i + R_j - |r_{ij}|)\boldsymbol{n} \tag{3}$$

is elastic restoration force, Y is Young modulus, $m_{\rm e} = m_im_j/(m_i + m_j)$ is effective mass. Another part of normal force

$$\boldsymbol{F}_{ij}^{\rm diss} = \gamma_n m_{\rm e}\boldsymbol{v}_{ij}^n \tag{4}$$

is dissipation force due to the inelasticity of the collision, where γ_n is the dissipation coefficient, $\boldsymbol{v}_{ij}^n$ is the projection of the relative velocity $\boldsymbol{v}_{ij} = \boldsymbol{v}_j - \boldsymbol{v}_i$ at the contact point in the normal direction. Obviously, this force will change direction in the whole collision process, but the direction of the first part is always from particle j to i. The linear relationships (3) and (4) enables us to obtain an analytic solution of collision time

$$T_{\rm col} = \pi\left(Y - \frac{1}{4}\gamma_n^2\right)^{-1/2}, \tag{5}$$

the time step Δt in the simulation should be about 1/50 of the collision time. The whole collision process will be finished in about 50 steps in order to keep a good accuracy of integration.[28]

The tangential force is caused by friction in a very complicated manner to dissipate the energy, however, various complicated laws with complicated parameters give the same qualitative result. Hence, the simple dissipation laws are usually used in simulations.[29] The simplest one is

$$\boldsymbol{F}_{ij}^{\rm shear} = \gamma_{\rm s}m_{\rm e}\boldsymbol{v}_{ij}^t, \tag{6}$$

which is similar to the dissipation force F_{ij}^n. And $\gamma_{\rm s}$ is shearing dissipation coefficient, $\boldsymbol{v}_{ij}^t$ is tangential component of relative velocity. In many cases, such as arching, heap formation and avalanche, it is important to consider real static friction force instead of Eq. (6).[29] The direct Coulomb law of friction, in which friction is proportional to the normal force F_n and the proportional constant is the friction coefficient μ

$$\boldsymbol{F}_{ij}^{\rm fric} = \mu|F_n|\boldsymbol{\tau}. \tag{7}$$

Sometimes, $F_{ij}^{\rm diss}$ may be larger than $F_{ij}^{\rm rest}$, and if they have different signs, it means that the force between two particles is attractive force. Thus the friction force of Eq. (7) is illogical. To avoid this from happening, the F_n in Eq. (7) is only the restoration force in our simulation. Equations (6) and (7) can be combined to give a tangential force as

$$\boldsymbol{F}_{ij}^t = \min(\gamma_{\rm s}m_{\rm e}|\boldsymbol{v}_{ij}^t|, \mu|F_n|)\boldsymbol{\tau}. \tag{8}$$

In the 3D case, note that the tangential velocity $\boldsymbol{v}_{ij}^t$ can be written as $\boldsymbol{n}\times(\boldsymbol{v}_{ij}\times\boldsymbol{n})$. In Eq. (8), only dynamic friction is considered. If only tangential dissipation force (6) is considered, then the restitution coefficient r, which is defined as the ratio of relative speeds after and before collision, can be determined as[30]

$$r = \sqrt{(r_n^2 + 2r_{\rm s}^2)/3}, \tag{9}$$

where

$$r_n = \exp\left(-\frac{\pi}{\sqrt{\omega^2/\eta^2 - 1}}\right),$$
$$r_{\rm s} = r_n^{2\gamma_{\rm s}/\gamma_n}, \quad \omega = \sqrt{Y}, \quad \eta = \gamma_n/2.$$

These similar force models have been used in many papers.[29–33]

The static friction is taken into account as follows:[34,35] when two particles first contact each other, we put a "virtual" spring between the contact

points of the two particles. Let δs be the total shearing displacement of this spring during the contact and $k_{\rm s}\delta s$ the restoring friction force (static friction). The maximum value of the restoring force is then, according to Coulomb's criterion, proportional to the normal force F_n and the proportional constant is the static friction coefficient $\mu_{\rm s}$. Casted into a formula this gives a friction force

$$\boldsymbol{F}_{ij}^{\rm fric} = {\rm sign}(\delta s){\rm min}(k_{\rm s}|\delta s|, \gamma_{\rm s} m_{\rm e}|\boldsymbol{v}_{ij}^t|, \mu_{\rm s}|F_n|)\boldsymbol{\tau}. \quad (10)$$

We require $\delta s < s_{\max}$ to make sure that the force of spring can be released quickly in dense collision case.[35] In our simulation, we choose $s_{\max} = \mu F_n/k_{\rm s}$, which means that the δs will not increase after static friction criteria is reached.

Note that the velocity difference $\boldsymbol{v}_{ij}$ is defined at the edge of the particle. If we use vector $\boldsymbol{r}$ to denote the interactive position of particles i and j, then

$$\boldsymbol{r} = \frac{1}{R_i + R_j}\left(R_j\boldsymbol{r}_i + R_i\boldsymbol{r}_j\right).$$

At this position, the velocities of these two particles are

$$\begin{aligned}\boldsymbol{v}_i' &= \boldsymbol{v}_i + \boldsymbol{\omega}_i \times (\boldsymbol{r} - \boldsymbol{r}_i)\\ &= \boldsymbol{v}_i + \frac{R_i}{R_i + R_j} * \boldsymbol{\omega}_i \times (\boldsymbol{r}_j - \boldsymbol{r}_i), \quad (11)\\ \boldsymbol{v}_j' &= \boldsymbol{v}_j + \boldsymbol{\omega}_j \times (\boldsymbol{r} - \boldsymbol{r}_j)\\ &= \boldsymbol{v}_j - \frac{R_j}{R_i + R_j} * \boldsymbol{\omega}_j \times (\boldsymbol{r}_j - \boldsymbol{r}_i). \quad (12)\end{aligned}$$

Then we have

$$\begin{aligned}\boldsymbol{v}_{ij} &= \boldsymbol{v}_j' - \boldsymbol{v}_i' = \boldsymbol{v}_j - \boldsymbol{v}_i - \frac{1}{R_i + R_j}\\ &\quad * (R_i\boldsymbol{\omega}_i + R_j\boldsymbol{\omega}_j) \times \boldsymbol{r}_{ij}. \quad (13)\end{aligned}$$

If particle i collides with a plate whose velocity is $\boldsymbol{v}_p$, we treat the plate as an infinite particle. In this way, the contact point is vector $\boldsymbol{r}_j$, and $R_j = 0$, $m_j = \infty$, then the above formulas are still valid.

Usually, only the tangential force $\boldsymbol{F}_{ij}^t$ generates the torque to the particles, and causes the conjunctional rotation of two interaction particles.

Once the force is known, the integration of Eq. (1) can be achieved by a widely used method in molecular dynamics (MD) simulation, the Verlet's method

$$\boldsymbol{r}^{n+1} = 2\boldsymbol{r}^n - \boldsymbol{r}^{n-1} + \frac{{\rm d}^2\boldsymbol{r}}{{\rm d}t^2}\Delta t^2 + O(\Delta t^2), \quad (14)$$

where the second order derivative term can be replaced by the force. To estimate velocities, second order upwind scheme can be used

$$\begin{aligned}\boldsymbol{v}^{n+1} &= \frac{\boldsymbol{r}^{n-1} - 4\boldsymbol{r}^n + 3\boldsymbol{r}^{n+1}}{2\Delta t}\\ &= \frac{3\Delta\boldsymbol{r}^n - \Delta\boldsymbol{r}^{n-1}}{2\Delta t}, \quad (15)\end{aligned}$$

where $\Delta\boldsymbol{r}^n = \boldsymbol{r}^{n+1} - \boldsymbol{r}^n$. The integration process of Eq. (2) is the same only as the extra angular displacement.

3. Simulation of shearing flow and results

In order to understand the dynamics in granular media, it is better to start from the simplest flows. That is the reason we focus on the shearing flow. In granular study, the characteristic quantities should include particle mass m, diameter $d = 2R$ and gravitational acceleration g, such that we can have the basic physical characteristic quantities: length scale d; force mg; time $(d/g)^{1/2}$; velocity $(dg)^{1/2}$ and momentum $m(gd)^{1/2}$. All these will be used as dimensionless quantities. In our simulation, we chose $\gamma_n = 100$, $\gamma_{\rm s} = 10$, $Y = 20000$, $\mu_d = 0.1$, $\mu_{\rm s} = 0.1$, $k_{\rm s} = 5000$, $d = 2$, $m = 1$, $g = 10$, such that the restitution coefficient $r = 0.1$ according to Eq. (9). Figure 1 is the schematic map of our computation domain. Due to the effect of shearing expansion, the top object must have the vertical degree of freedom. Initially, the moving slab with the mass $M = 1830.58$ is set free on the static granular material with $V_x^{\rm top} = 10/(dg)^{1/2}$ and keeps the speed all the time. This powers the whole system in the moving state. Eventually, a quasi-steady state is achieved.

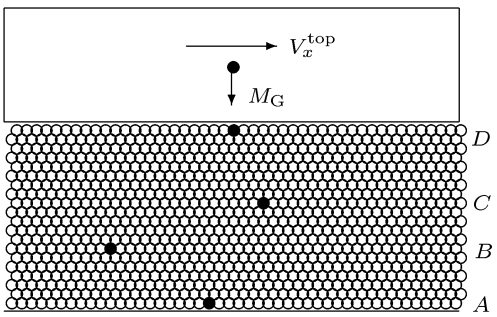


Fig. 1. The sketch map of two-dimensional computation, the horizontal (x) line is periodic boundary, the top is pressed by a heavy object with mass M. It can move up and down in vertical (y) direction. And it moves with an imposed velocity $V_x^{\rm top}$ in x direction. The four black dots • are the particles whose whole moving histories will be followed, and are labeled as A, B, C and D from bottom to top. In our simulation, there are 3170 particles in total, 65 particles fixed on the bottom line, another 65 particles on the top line with velocities specified (not shown in the figure). In between, there are 38 lines, 80 particles per line.

Figure 2 shows the histories of x-velocity v_x of the four selected particles. It is easy to know that, only the particle D which is near the top driven slab has significant velocity, but it still turns negative sometimes because of large fluctuation.

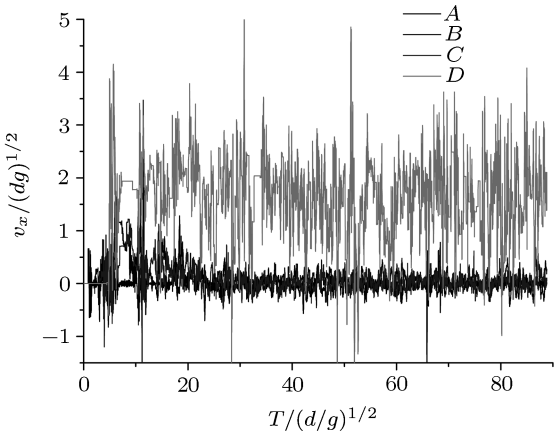


Fig. 2. The velocity v_x of four different particles at four different positions, we can see the large fluctuation, especially for the particle D on the top position.

Figures 3 and 4 are normalized probability distribution functions (PDFs) of v_x and v_y for selected particles. We can see that the particles in the middle area (far from boundary) have near normal Gaussian distributions. And the average velocity are almost zero when the particle is far from the driven slab according to their average values $\overline{v}_x$ and $\overline{v}_y$ or the root mean square σ. This means that there is a shearing zone near the moving slab.

Figure 5 shows the movements of the top slab, it moves down first, then bounces back. Later, it will oscillate slightly all the time because of granular shearing flow. The oscillation is not periodic, and the amplitude changes all the time.

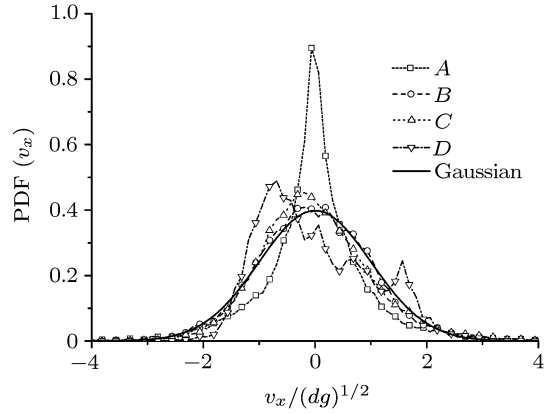


Fig. 3. The PDF of velocity v_x. Curve A: $\overline{v}_x = 0.001, \sigma = 0.086$; curve B: $\overline{v}_x = 0.032, \sigma = 0.141$; curve C: $\overline{v}_x = 0.050$, $\sigma = 0.141$; curve D: $\overline{v}_x = 0.754$, $\sigma = 0.894$. The solid line is normal distribution.

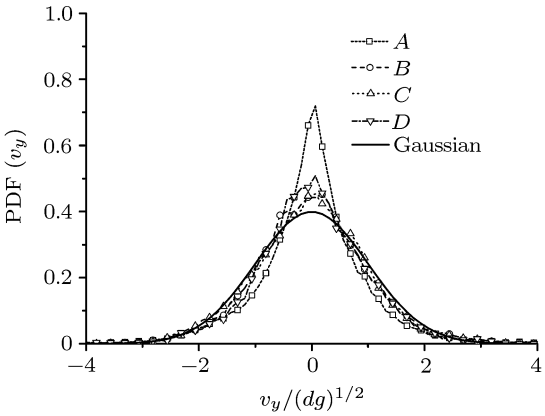


Fig. 4. The PDF of velocity v_y. Curve A: $\overline{v}_y = -0.001$, $\sigma = 0.076$; curve B: $\overline{v}_y = 0.005$, $\sigma = 0.168$; curve C: $\overline{v}_y = 0.003$, $\sigma = 0.209$; curve D: $\overline{v}_y = -0.013$, $\sigma = 0.513$. The solid line is normal distribution.

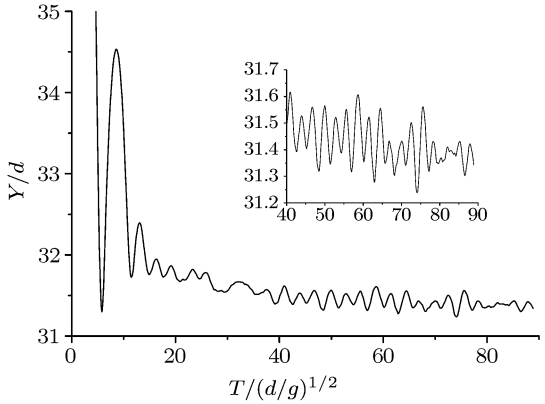


Fig. 5. The height of top line, it moves down first, then bounces back, at last it will oscillate all the time. The inset shows that there is no periodic property as that in Ref. [23].

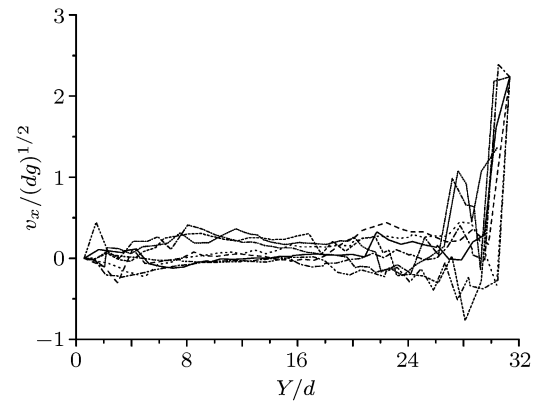


Fig. 6. The instantaneous v_x distributions at different x positions which are distributed equally.

The instantaneous v_x distributions at several different x positions are shown in Fig. 6. Although oscillation exists everywhere, the movements are mainly

in the shearing zone near the top slab. In our simulation, the left and right boundary are periodic (See Fig. 1), such that we can make average along x lines, and the average v_x should be the function of y only. Figure 7 is average v_x distribution at different time, which again shows that the movements are near top slab. The average velocity in the "deep" region is very small in comparison with that in the shearing zone.

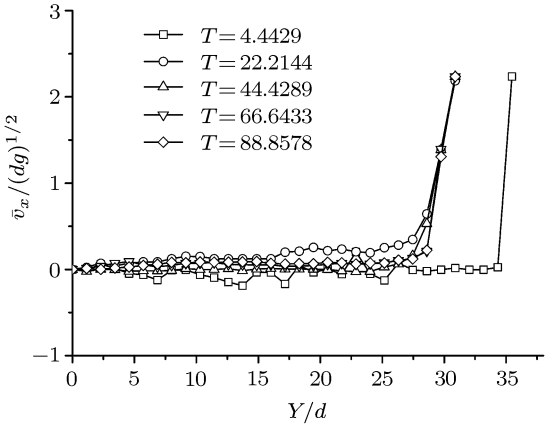


Fig. 7. The $\bar{v}_x$ distribution at different times. Time is scaled using $(d/g)^{1/2}$.

According to the theories of statistical physics, we can gain the stress tensor by

$$\tau_{\alpha\beta} = m\sum_{i}^{N} v_{i\alpha}v_{i\beta} + \frac{1}{2}\sum_{i\neq j}^{N} r_{ij\beta}F_{ij\alpha}, \qquad (16)$$

where subindexes α and β are x or y, $v_{i\alpha}$ is the velocity of particle i in α direction, $r_{ij\beta}$ is the β component of vector $\boldsymbol{r}_{ij}$ which is from particle i to j, and $F_{ij\alpha}$ is the α component of force on particle i by particle j. It is obvious that the most important component of this stress tensor is τ_{xy}. Figure 8 shows the average stress distribution at different times. Although there is large fluctuation, nothing special is noticed near the shearing zone, which is quite different from the distribution of velocity shown in Fig. 7. In the view of continuum, it is natural to consider the stress τ_{xy} to be proportional to the gradient of velocity $\partial u/\partial y$. And the coefficient ν is called viscosity coefficient. For Newtonian fluid, ν is constant, and is considered as a physical property of the fluid. From Fig. 8 we know that there is no such parameter for granular flow, or we can say that its viscosity coefficient is dependent on the specific flow.

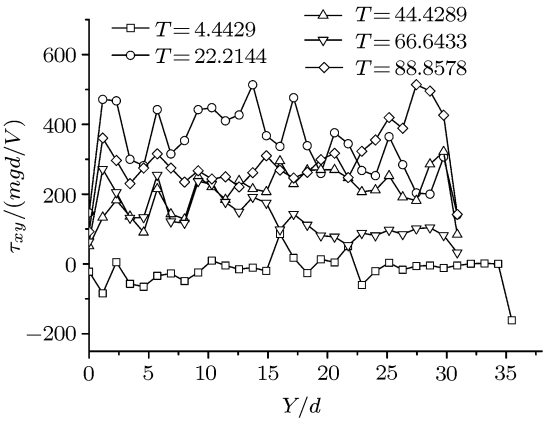


Fig. 8. The distribution of the average stress τ_{xy} at different times. The stress is scaled by mgd/V, V is unit volume.

Friction property between the top slab and particles is examined in particular. We account for friction interaction between the moving top slab and the granular system below. And as shown in Fig. 9, the friction varies with the velocity of the top slab which is set to grow from 10 to 2000 with step 10. And we find that the friction neither remains constant nor fluctuates around a constant value. It keeps relatively small when the velocity is slow, and with velocity coming to a certain value it makes a sudden growth which turns out to be the peak in our plot. Our simulations have been repeated with different initial conditions and yet the peak remains, just at different velocity values. After the peak, the plot is in process towards a flat line which means that the friction becomes a constant in respect to the growing velocity. This discovery is amazing because the interaction model between top object and particles and between particles is rather simple, and uses Newton's law in this work, yet nonlinearity is observed. This could be attributed to the complexity of the granular system.

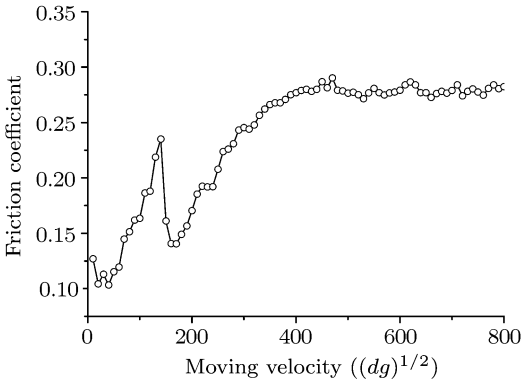


Fig. 9. Equivalent friction coefficient between top slab and the particles.

4. Conclusions

Massive phenomena have been observed in granular flows, it is very difficult to establish a universal continuum model to account for them. However, the simulation work for granular flow is not hard because the interaction model between particles is easy to gain and is insensitive to the system behaviours of the whole system. Our simulation on shearing flow shows that the movement is mainly in the shearing zone, and the velocity PDF varies at different heights. Only far from the boundary, they follows Gaussian distributions. The stress τ_{xy} has large fluctuation even after averaging. It can be considered as uniform along y direction according to the amplitude of both average value and fluctuation. The equivalent friction coefficient between moving slab and granular material depends on the moving speed at low velocity, and approaches constant as the velocity is large enough.

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