Rheology of a granular gas under a plane shear

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The rheology of a two-dimensional granular gas under a plane shear is investigated. From the comparison among the discrete element method, the simulation of a set of hydrodynamic equation, and the analytic solution of the steady equation of the hydrodynamic equations, it is confirmed that the fluid equations derived from the kinetic theory give us accurate results even in relatively high density cases.

I. INTRODUCTION

Granular materials consist of macroscopic dissipative particles. In some cases the granular material behaves as an unusual fluid. Although to understand the rheology of the granular fluid is practically important, our understanding on the rheology is not enough. There are several reasons to have poor understanding on the rheology of granular flows: (i) The separation of the length scale between particles and the fluid motion is not enough, (ii) there are some cases that the fluid region coexists with the solid-like region, and (iii) most of experiments are strongly affected by boundary conditions and the external field. Nevertheless, it is believed that rapid granular flows for relatively dilute granular gases can be described by a set of hydrodynamic equations at Navier-Stokes order whose transport coefficients can be calculated by the kinetic theory.

To maintain a granular gas we need to add an external field. The simplest steady situation of the granular fluid is achieved by the balance between an external shear and inelastic collisions between particles. This system is appropriate to investigate what the constitutive equation for the granular fluid is. The kinetic theory may suggest that the stress-strain relation can be described by that at Navier-Stokes order, though the transport coefficients can be functions of the position.

About 50 years ago, Bagnold\cite{5} suggested that the granular fluid is characterized by \( \tau \propto \dot{\gamma}^2 \) where \( \tau \) and \( \dot{\gamma} \) are the shear stress and the shear rate (the strain), respectively. This stress-strain relation is known as Bagnold’s scaling and is different from the conventional Newtonian relation which is \( \tau \propto \dot{\gamma} \). Recently, Pouliquen\cite{6} and Silbert et al.\cite{7} have reconfirmed the quantitative relevancy of Bagnold’s scaling in granular flows on inclined slopes. Mitarai and Nakanishi\cite{8} have demonstrated that the kinetic theory can be compatible with Bagnold’s scaling, when they assume that the the temperature is a slaving variable of the velocity and the density. Santos et al.\cite{9} also indicate that Bagnold’s scaling is valid for steady dilute granular gases without the influence of the gravity in the uniform shear flow (USF), though the transport coefficients such as the viscosity and the heat conductivity are different from those in homogeneous cooling state\cite{10}. However, we still do not know whether Bagnold’s scaling is relevant in other situations.

We should recall that it is difficult to keep granular gases in experimentally relevant situations because of the existence of gravity. Recently, to remove the effects of gravity, the rheology of dense granular flows under the plane shear with a constant pressure has been studied and a new scaling has been reported\cite{10,11}. These studies are important but particles are not in a gas state, \textit{i.e.} each particle is in contact with many other particles simultaneously. The analysis of such process is challenging but we do not have any good tool to analyze it at present. Here, we focus on the granular shear flows without multi-body contacts in a constant volume container to discuss quantitative relevancy of the kinetic theory.

The purpose of this paper is to know the relevancy of the kinetic theory for a granular gas with moderate density under the plane shear with a constant pressure has been studied and a new scaling has been reported. These studies are important but particles are not in a gas state, \textit{i.e.} each particle is in contact with many other particles simultaneously. The analysis of such process is challenging but we do not have any good tool to analyze it at present. Here, we focus on the granular shear flows without multi-body contacts in a constant volume container to discuss quantitative relevancy of the kinetic theory.

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To investigate the above problem, we use the discrete element method (DEM) for particles’ simulation in a plane shear problem of dense granular gases in which particles are confined in a constant volume box (Section II). We adopt the
constitutive equation of hydrodynamics derived by Jenkins and Richman[12] for non-rotational particles in Section III. In Section IV we solve a set of hydrodynamic equations with the above constitutive equation numerically and compare the result with the result of DEM. We also check the renormalization theory of the restitution coefficient developed by Yoon and Jenkins[13]. In Section V we obtain the analytic solution of the steady hydrodynamic equations to verify the quantitative relevancy of the constitutive equation. In section VI we discuss our result and the relevancy of Bagnold’s scaling. In Section VII, we conclude our results. In Appendix, we briefly explain the method to determine the tangential restitution constant as a function of the incident angle.

II. DEM SIMULATION

A. DEM model

The discrete element method (DEM) is one of the standard methods to simulate granular motions.[14] DEM is applicable to most of situations of granular dynamics even when particles are almost motionless and contact with many other particles. We adopt DEM to simulate a granular fluid to check (i) the validity of kinetic theory based on the reliable model, and (ii) the effects of rotation of particles for the granular fluid.

In this paper, we focus on a two-dimensional motion of granular particles under a plane shear. We adopt the linear spring model for the repulsion with the normal stiffness \( k_n \) and the tangential stiffness \( k_t \), and the normal and the tangential viscous coefficients \( \eta_n \) and \( \eta_t \), respectively.

Let us consider a colliding pair of two disks \( i \) and \( j \) of the diameter \( \sigma \) and the mass \( m \) at the position \( \mathbf{x}_k \) with the velocity \( \mathbf{c}_k \equiv \dot{\mathbf{x}}_k \) and the angular velocity \( \omega_k \) for \( k = i \) or \( j \). If the particles are in contact, the overlap distance

\[
\Delta_{ij} \equiv 2\sigma - |\mathbf{x}_i - \mathbf{x}_j|
\]

must be positive. The relative velocity at the contact point is

\[
\mathbf{c}_{ij} = \mathbf{c}_i - \mathbf{c}_j + \frac{\sigma}{2} \mathbf{n}_{ij} \times (\mathbf{\omega}_i + \mathbf{\omega}_j)
\]

with the normal unit vector \( \mathbf{n}_{ij} \equiv (\mathbf{x}_i - \mathbf{x}_j)/|\mathbf{x}_i - \mathbf{x}_j| \). Introducing the normal velocity \( \mathbf{c}_{ij}^\perp = \mathbf{n}_{ij} \cdot \mathbf{c}_{ij} \), the tangential velocity \( \mathbf{c}_{ij}^\parallel = \mathbf{t}_{ij} \cdot \mathbf{c}_{ij} \), the tangential displacement \( \mathbf{w}_{ij}^\parallel = \int_{t_0}^t ds \mathbf{c}_{ij}^\parallel(s) \) with the tangential unit vector \( \mathbf{t}_{ij} \) satisfying \( \mathbf{t}_{ij} \cdot \mathbf{n}_{ij} = 0 \), the normal and the tangential forces \( F_{ij}^n \) and \( F_{ij}^\parallel \) are respectively given by

\[
F_{ij}^n = mk_n \Delta_{ij} - m\eta_n \mathbf{v}_{ij}^\perp \quad \text{for} \quad \Delta_{ij} > 0,
\]

\[
F_{ij}^\parallel = \min(h_t, \mu|F_{ij}^n|) \text{sign}(h_{ij}^\parallel),
\]

where \( h_{ij}^\parallel \equiv -mk_t \mathbf{w}_{ij} - m\eta_t \mathbf{c}_{ij}^\parallel \) with Coulomb friction constant \( \mu \), \( \min(a, b) \) is the function to select the smaller one between \( a \) and \( b \), and \( \text{sign}(x) = 1 \) for \( x > 0 \) and \( \text{sign}(x) = -1 \) for \( x < 0 \). The total repulsive force at the contact can be represented as \( \mathbf{F}_{ij} = F_{ij}^n \mathbf{n}_{ij} + F_{ij}^\parallel \mathbf{t}_{ij} \).

Thus, the equation of motion of particle \( i \) is described by

\[
m \ddot{\mathbf{c}}_i = \sum_{j \neq i} F_{ij},
\]

\[
I \ddot{\mathbf{\omega}}_i = \frac{\sigma}{2} \sum_{j \neq i} \mathbf{n}_{ij} \times \mathbf{t}_{ij} F_{ij}^\parallel,
\]

where \( I = m\sigma^2/8 \) is the moment of inertia. We integrate [15] and [16] in terms of the second order Adams-Bashforth with the time interval \( \delta t = 4.0 \times 10^{-4}(2\sigma/U) \).

Through the paper we adopt the following parameters as \( k_n = 3.0 \times 10^3(U/\sigma)^2 \), \( k_t = k_n/4 \), \( \eta_n = 3.0(U/\sigma) \), \( \eta_t = \eta_n/2 \) and \( \mu = 0.20 \), where \( U \) is the shear speed at the boundary. These parameters lead to the normal restitution constant \( \bar{\epsilon} = 0.85 \) and the tangential restitution \( \beta \simeq -1 + 1.12442 \cot \gamma \) for \( \gamma \leq \gamma_c \) and \( \beta = \bar{\beta}_0 \simeq 0.769235 \) for \( \gamma > \gamma_c \), where \( \gamma \) is the incident angle of two colliding disks and the critical angle \( \gamma_c \) is given by \( \cot \gamma_c \simeq 1.56734 \) (see eq. (A4) in Appendix). As shown in Appendix, the tangential restitution constant \( \beta \) can be approximated by [15]

\[
\beta \simeq \begin{cases} 
-1 + \mu(1 + \bar{\epsilon}) \cot \gamma \left( 1 + \frac{m\sigma^2}{4\mu} \right) (\gamma \geq \gamma_c) \\
\bar{\beta}_0 (\gamma \leq \gamma_c).
\end{cases}
\]

We also note that the realistic value of Coulomb friction constant in both disks and spheres is \( \mu \leq 0.2 \)[16][17][18]. Thus, the renormalization theory of the restitution constant may be applicable to many realistic situations.
Simulations of granular particles under the plane shear have been performed by many researchers, but many of them [19, 20, 21] assume Lees-Edwards boundary condition [22] which may not be adequate to consider the effects of physical boundary. On the other hand, Babic [23], Popken and Cleary [24] have simulated sheared granular flows confined in frictional flat boundaries, but their simulations are restricted to the cases for small systems and almost elastic particles. Kim [25] has indicated that the density of particles near the boundary is higher than that in the bulk region for his simulation of a small system with the flat frictional boundary, while particles are accumulated in the center region for a larger system. Louge [26] has simulated a three dimensional shear flow on the flat frictional boundary to examine the boundary condition proposed by Jenkins [27], but Louge is mainly interested in the behavior of flux, the stress ratio as the functions of volume fraction and the restitution constant. Recent papers by Xu et al. for an experiment [28] and a simulation [29] examine the validity of three dimensional kinetic theory by Jenkins and Richman [30] under asymmetric shears in the presence of a streamwise body force, where they obtain reasonable agreements between the theory and the observations in both the experiment and the simulation.

As long as our knowledge, we do not know papers to discuss the validity of kinetic theory in a transient dynamics and a symmetric shear without a streamwise body force with an enough large system. Thus, we adopt the following setup of our DEM simulation shown in Fig. 1. The system is confined in a two-dimensional container. Without including the effects of the air and the gravity we add a symmetric shear with the shear speed $U$ as shown in Fig. 1. The parameters are fixed as the number of particles $N = 5000$, the linear dimension of the system in $y$ direction $\Delta = 180\sigma$ and the mean area fraction $\bar{\nu} = 0.121$. The boundary condition of $x-$direction is periodic. We non-dimensionalize all quantities by the diameter $\sigma$ for the length scale, $m$ for the mass, and the inverse of the shear rate $2\sigma/U$ for the time scale.

We introduce some fixed particles on the wall to reproduce the bumpy boundary. The reason why we adopt the bumpy boundary is to avoid the large amount of slips on the wall under a physical situation. In our simulation we start from an initial condition without the shear. Then, the wall at $y = \Delta/2$ obeys the equation of motion in $x$ direction

$$M_w \frac{dc_w}{dt} = -m\gamma_w(c_w - Ue_x/2) + F_{ex},$$

where $c_w$ and $e_x$ are respectively the actual wall velocity and the unit vector along $x-$direction. $M_w$, $\gamma_w$ and $F_{ex}$ are the mass of wall $M_w = 5.0 \times 10^6 m$, the relaxation rate $\gamma_w = 10U/(2\sigma)$, and the force acting on the wall by the collision between mobile particles and the wall, respectively.
C. Simulation

![Image of particle configurations](a) (b)

**FIG. 2:** The time evolution of the particles’ configurations from (a) to (b) for \( \bar{\nu} = 0.121 \).

The initial condition is prepared as that the configuration of particles is at random and the velocity distribution function obeys Maxwellian. Figure 2 is the time evolution of particles’ configuration for \( \bar{\nu} = 0.121 \). Two shallow clusters appear near the wall, and move to the center region of the container. Then, the two clusters merge to form a big cluster. A similar behavior can be observed in the simulation under the Lees-Edwards boundary condition.[21]

![Image of energy evolution](a)

**FIG. 3:** The time evolution of the kinetic energy, where the units of time and the energy are \( 2\sigma/U \) and \( mU^2/2 \), respectively.

The time evolution of the total kinetic energy \( E \) in a typical situation is shown in Fig. 3, where the energy is defined by

\[
E(t) = \frac{1}{2} \sum_i (mc_i^2 + I\omega_i^2).
\]  

In this figure, the initial energy is larger than the steady value, but we have checked that the qualitatively similar results can be obtained even when we start from the smaller energy about \( E(0) = 1200 \) in the dimensionless unit. It is characteristics that the total kinetic energy is relaxed to be almost a constant value quickly, but there is the slow evolution of hydrodynamic fields.

The hydrodynamic variables are the local area fraction \( \nu(r, t) \equiv \pi\sigma^2 n(r, t)/4 \) with the number density \( n(r, t) \), the
velocity field \( v(r, t) \) and the granular temperature \( T(r, t) \) which is defined by

\[
T(r, t) = \frac{1}{2n} \int d\mathbf{c}(\mathbf{c} - v)^2 f(r, \mathbf{c}, t).
\]

(10)

In our simulation we divide the system into square cells with the linear dimension \( \sigma \). Then, we can check to what cell each particle belongs. Thus, the measured area fraction in our simulation is given by \( \nu(r, t) \equiv \sum_{i \in C} \pi \sigma^2 / A \) where the summation is taken over the center of particle \( i \) existing in the cell \( C \) at \( r \) with the area \( A = \sigma^2 \). Similarly, the velocity field \( v(r, t) \equiv \sum_{i \in C} \mathbf{c}_i \) is the local average of the velocity of particles. The temperature field is also calculated by

\[
T(r, t) = \frac{1}{2n} \sum_{i \in C} (\mathbf{c}_i - v)^2.
\]

(11)

![Graph](image)

FIG. 4: The time evolution of dimensionless \( u_y \) with (a) at \( t = 60 \) and (b) at \( t = 380 \), where the units of the time and \( u_y \) are \((2\sigma/U)\) and \( U/2 \), respectively.

The time evolution of hydrodynamic variables can be summarized as follows. Corresponding to Fig.2, the local area fraction becomes large near the boundary at the initial stage, and the shallow clusters move to the central region of the container with growing the peak density. Finally, the two clusters merge to form a compact cluster at the center \( y = 0 \).

The interesting behavior can be observed in the velocity field and the granular temperature. The \( x \)-component of the velocity field is almost zero between two clusters during the time evolution, and such plug region is narrower as the distance of two clusters is closer. Even in the steady state, the velocity gradient in the central region is smaller than that near the boundary. The behavior of \( y \)-component of the dimensionless velocity field \( u_y \) is also characteristic, because this quantity shows the tendency to move to the central region and is relaxed to be zero in the steady state (Fig.4). Similarly, the temperature field in the central region is smaller than that near the boundary. However, the minimum value of temperature decreases with time and reaches almost zero in the central region in the steady stage. The results of our DEM simulation except for \( u_y = 2v_y/U \) will be shown in Sections IV and V through the comparison of DEM with hydrodynamic simulations or the theoretical results in the steady state.

The result of our simulation may give us suspicious impression of the validity of kinetic theory for this system, because (i) the density in the cluster is near the closest packing \( \pi/\sqrt{3} \approx 0.907 \) in the steady state, (ii) the particles are almost motionless in the clusters or between clusters. Our result is contrast to the result by Xu et al. [28, 29] where there is no definite motionless clusters because of the existence of a streamwise body force. In their case, the mean density is much higher than that in our case, and the temperature is a nearly constant. Nevertheless, as will be shown, our system can be described by the hydrodynamic equation derived from the kinetic theory.

## III. HYDRODYNAMIC EQUATIONS

The purpose of this paper is to verify the validity of the granular hydrodynamic equation derived from the kinetic theory. Although there are two standard methods, Chapman-Enskog method [3, 4, 31] and Grad expansions [32], most
of established results are limited to low density cases in the derivation of hydrodynamic equations. However, as shown in the previous section, we have to adopt the kinetic theory for dense granular gases. The Chapman-Enskog method by Grazó and Dufty and Lutsko predicts transport coefficients in dense granular gases. On the other hand, Jenkins and Richman derive hydrodynamic equations based on Grad expansion and give transport coefficients. Although the treatment by Jenkins and Richman does not take into account the contraction of the phase space volume in each collision, the theory is suitable for our purpose because it gives us explicit expressions of the transport coefficients in the two-dimensional dense granular gases.

Jenkins and Richman, and Lun derive sets of hydrodynamic equations which include the angular velocity, the spin temperature as well as the density, the translational velocity and the granular temperature. The equations include the couple stress and the collisional loss of spin energy. These sets of hydrodynamic equations are categorized as the micropolar fluid mechanics which was originally proposed by Cosserat and Cosserat for the description of the elastic materials. Application of the concept of micropolar fluid mechanics to atomic gases are developed by Babic, Hayakawa, and Mitarai et al. The micropolar fluid mechanics is applied to granular flows by Kanatani, Lun, Babic, Hayakawa, Hayakawa, and Mitarai et al. The importance of the excitation of the spin on the boundary is indicated by Jenkins, but the effects of the spin can be decoupled with the translational velocity in the bulk region. In particular, Babic indicated that the coupled stress induced by the collisions between circular particles is canceled. Therefore, we believe that the effect of spins can be absorbed in the boundary condition and the renormalized restitution constant.

Recently, Jenkins and Zhang have proposed a scheme of the renormalized restitution constant as the result of the absorption of the rotation of particles. Yoon and Jenkins have extend the scheme to two-dimensional flows as

\[ e \simeq \tilde{e} - \mu + 2\mu^2(1 + \tilde{e}). \]  

(12)

The validity of three dimensional theory has been tested by Xu et al. and Jenkins and Zhang. The latter is consistent with Lun and Bent in part. However, the quantitative validity of Yoon and Jenkins has not been confirmed yet. In addition, some recent papers suggest that the spin effects are relevant in granular flows. For instance, Goldhirsch et al. have indicated that the equipartition between spin energy and the translational energy is violated in a recent paper, and Gefen and Alam discuss the linear stability of sheared micropolar fluid. Therefore, we need to judge whether the concept of micropolar fluid is necessary for the description of granular fluids.

In this paper, we adopt the renormalization procedure of the restitution constant proposed by Yoon and Jenkins to verify the validity of their scheme. Thus, the restitution constant \( e \) appears in hydrodynamic equations is different from \( \tilde{e} \) of DEM, where the relation between two restitution constants is given in eq. (12). Namely, \( \tilde{e} = 0.85 \) in DEM corresponds to \( e = 0.798 \) for \( \mu = 0.20 \) in hydrodynamic equations.

The advantage to adopt the renormalization is that hydrodynamic equations can be simplified as

\[ D_t \rho = -\rho \nabla \cdot \mathbf{v}, \]

\[ \rho D_t \mathbf{v} = -\nabla P, \]

\[ \rho D_t T = -P : (\nabla \mathbf{v}) - \nabla \cdot \mathbf{q} - \chi, \]

(13)-(15)

where \( \rho = nm \) is the mass density and \( D_t = \partial_t + \mathbf{v} \cdot \nabla \). Here \((i, j)\) component \( P_{ij} \) of the pressure tensor \( P \) is expressed as the function of the bulk viscosity \( \xi \) and the shear viscosity \( \eta \)

\[ P_{ij} = [p - \xi(\nabla \cdot \mathbf{v})] \delta_{ij} - \eta \tilde{D}_{ij} \]

(16)

at the Navier-Stokes order, where \( \delta_{ij} = 1 \) for \( i = j \) and 0 for otherwise, \( \tilde{D}_{ij} = (\nabla_i v_j + \nabla_j v_i)/2 \). Here \( \mathbf{q} \) represents the heat flux which can be expanded as

\[ \mathbf{q} = -\kappa \nabla T - \lambda \nabla \rho, \]

(17)

where \( \kappa \) is the heat conductivity and the transport coefficient \( \lambda \) disappear at \( e = 1 \). The collisional loss rate of the energy \( \chi \) can be represented by

\[ \chi = \frac{1 - e^2}{4\sigma \rho_p \sqrt{\pi}} \rho^2 g(\nu) T^{1/2} [8T - 3\sqrt{\pi} \sigma T^{1/2} (\nabla \cdot \mathbf{v})], \]

(18)

where \( \rho_p = 4m/(\pi \sigma^2) \) is the mass density of a particle.

Let us non-dimensionalize the time, the position, the velocity and the temperature as

\[ t = \frac{2\sigma}{U} \tau^*, \quad x = \sigma x^*, \quad v = \frac{U}{2} u, \quad T = \frac{U^2}{8} \theta \]

(19)
TABLE I: The dimensionless transport coefficient by Jenkins and Richman

\[ p(\nu) = \frac{1}{2} \nu [1 + (1 + e) \nu g(\nu)] \]

\[ \xi(\nu) = \frac{1}{\sqrt{2\pi}} (1 + e) \nu^2 g(\nu) \]

\[ \eta(\nu) = \sqrt{\frac{\pi}{2}} \frac{1}{7 - 3e} g(\nu)^{-1} + \frac{(1 + e)(3e + 1)}{4(7 - 3e)} \nu + \frac{(1 + e)(3e - 1)}{8(7 - 3e)} + \frac{1}{\pi} (1 + e) \nu^2 g(\nu) \]

\[ \kappa(\nu) = \sqrt{2\pi} \frac{1}{(1 + e)(19 - 15e)} g(\nu)^{-1} + \frac{3(2e^2 + e + 1)}{8(19 - 15e)} \nu + \frac{9(1 + e)(2e - 1)}{32(19 - 15e)} + \frac{1}{2\pi} (1 + e) \nu^2 g(\nu) \]

\[ \lambda(\nu) = -\frac{\sqrt{\pi}}{2} \frac{3e(1 - e)}{16(19 - 15e)} [4g(\nu)^{-1} + 3(1 + e) \nu] \frac{1}{\nu} \frac{d(\nu^2 g(\nu))}{d\nu} \]

Thus, the non-dimensional pressure tensor, the heat flux and the collisional loss rate of energy are respectively given by

\[ P_{ij} = \frac{\rho_p U^2}{4} P^*_{ij}, \quad q = \frac{\rho_p U^3}{8} q^*, \quad \chi = \frac{\rho_p U^3}{8\sigma} \chi^*. \quad (20) \]

Here the dimensionless quantities are written as

\[ P^*_{ij} = [p(\nu) \theta - \xi(\nu) \theta^{1/2} (\nabla^* \cdot u)] \delta_{ij} - \eta(\nu) \theta^{1/2} \hat{D}_{ij}^*, \]

\[ q^* = -\kappa(\nu) \theta^{1/2} \nabla^* \cdot \theta - \lambda(\nu) \theta^{3/2} \nabla^* \nu, \]

\[ \chi^* = \frac{1 - e^2}{4\sqrt{2\pi}} \nu^2 g(\nu) \theta^{1/2} [4\theta - 3 \sqrt{\frac{\pi}{2}} \theta^{1/2} (\nabla^* \cdot u)]. \]

The explicit expressions of \( p(\nu) \), \( \xi(\nu) \), \( \eta(\nu) \), \( \kappa(\nu) \) and \( \lambda(\nu) \) obtained by Jenkins and Richman \( [12] \) are summarized in table II with the radial distribution function \( [46] \)

\[ g(\nu) = g_c(\nu) + \frac{g_f(\nu) - g_c(\nu)}{1 + \exp [-\nu/(\nu_0 - 1)]}. \quad (24) \]

where \( g_c(\nu) = (1 - 7\nu/16)/(1 - \nu)^2 \) and \( g_f(\nu) = [(1 + e) \nu (\nu/\nu_0 - 1)]^{-1} \) with \( \nu_c = 0.82 \), \( \nu_0 = 0.7006 \) and \( m_0 = 0.0111 \). The choice of \( g(\nu) \) is not unique. For example, we expect that a similar result can be obtained by using the radial distribution function in ref. \( [47] \). Thus, the dimensionless hydrodynamic equations are reduced to

\[ D_1 \nu = -\nu \nabla \cdot u, \]

\[ \nu D_1 u = -\nabla \cdot P, \]

\[ \frac{1}{2} \nu D_2 \theta = -P_{ij} (\nabla_i u_j) - \nabla \cdot q - \chi. \quad (27) \]

From here, the mark * to represent dimensionless quantities is eliminated.

IV. SIMULATION OF HYDRODYNAMIC EQUATIONS

A. The outline of our simulation

To verify the accuracy of a set of hydrodynamic equations \( [23] - [27] \) derived from the kinetic theory by Jenkins and Richman \( [12] \), we simulate hydrodynamic equations. Since the separation of particles’ scale and the hydrodynamic scale
is not enough, each grid in two-dimensional space cannot contain enough number of particles to define hydrodynamic variables. Therefore, we focus on the field equations which have translational symmetry in $x$-direction. Thus, all quantities only depend on $y$ and $t$. However, we should note that we keep $x$-component of velocity. The second purpose of the simulation of hydrodynamic equations is to obtain a reduced set of equations to recover the qualitative accurate results to describe the metastable dynamics after the total energy is relaxed to a constant value.

The method of the discretization of continuous variables is based on the standard procedure. We adopt the classical Runge-Kutta scheme for the time derivative with $\delta t = 0.01$ and the second order accuracy of the spatial derivative of a hydrodynamic variable $\Psi$ as

$$\frac{\partial \Psi}{\partial y} = \frac{\Psi_{j+1} - \Psi_{j-1}}{2h}, \quad \frac{\partial^2 \Psi}{\partial y^2} = \frac{\Psi_{j+1} - 2\Psi_j + \Psi_{j-1}}{h^2},$$

(28)

where $h$ is the grid displacement with $h/\Delta = 1/180$ and $y = jh$ with $j = 0, \pm 1, \pm 2, \cdots$. It should be noted that we do not have to solve Poisson equation for the pressure because the fluid is compressible and the pressure is completely determined by the equation of state.

B. The boundary condition

We adopt the boundary condition proposed by Johnson and Jackson[48]. We define the slip velocity on the boundary as $u_{sl} = u - u_w$, where $u_w = \pm e_x$ at $y = \pm \Delta/(2\sigma)$. Let $t$ and $n$ be the tangential unit vector and the normal unit vector to the wall, respectively. Thus, the conservation of the linear momentum on the wall is given by

$$-n \cdot P \cdot t = \frac{\pi}{4} \phi \Omega(\nu, \theta)|u_{sl}|,$$

(29)

where $\pi/4$ is originated from $m = \pi \rho_p \sigma^2/4$. Here, $\phi$ is the roughness parameter and $\Omega(\nu, \theta)$ is the collisional frequency between the wall and the particles. The expression $\Omega$ is assumed to be

$$\Omega(\nu, \theta) = \nu g(\nu) \theta^{1/2},$$

(30)

where the prefactor is absorbed in the roughness parameter. On the other hand, the energy balance on the wall can be expressed by

$$n \cdot q = -u_{sl} \cdot P \cdot n - \Gamma(\nu, \theta)$$

(31)

where $\Gamma(\nu, \theta)$ is the energy loss rate in terms of the inelastic collisions between particles and the wall, which may be represented as

$$\Gamma(\nu, \theta) = \frac{\pi}{4} \Phi \Omega(\nu, \theta) \theta = \frac{\pi}{4} \Phi \nu g(\nu) \theta^{3/2},$$

(32)

where $\Phi$ is the hardness parameter of the wall. In our simulation we adopt $\phi = 0.20$ and $\Phi = 0.24$ as fitting parameters.

The reason why we adopt the boundary condition by Johnson and Jackson[48] is that their condition is simple. The more precise treatment for the boundary condition can be seen in ref.[49]. When we adopt Jenkins’ boundary condition, the number of fitting parameters may be reduced.

When we represent these boundary conditions as

$$F_{b1}(\Psi, \partial_y \Psi) = 0$$

(33)

and the formal solution of this discrete equation can be formally solved as

$$\Psi_N = F_{b2}(\Psi_{N-1}, \Psi_{N-2}),$$

(34)

where $N = \Delta/2\sigma$ is the grid number on the boundary with symbolic functions $F_{b1}$ and $F_{b2}$. From the consideration of the symmetry in $y$-direction, we have $\nu(y) = \nu(-y)$, $\theta(y) = \theta(-y)$, and $u(y) = -u(-y)$. Thus, it is enough to discuss the boundary condition at $y = \Delta/2$. From (24) we may obtain the $x$-component of the velocity field

$$u_{x;N} = \frac{u_{x;N-2} + 4\phi h\nu_{N-1} g(\nu_{N-1})/\eta(\nu_{N-1})}{1 + 4\phi h\nu_{N-1} g(\nu_{N-1})\eta(\nu_{N-1})},$$

(35)

where the area fraction $\nu_N$ on the boundary is assumed to be

$$\nu_N = 2\nu_{N-1} + \nu_{N-2}$$

(36)
FIG. 5: The initial conditions of hydrodynamic equations (solid lines) and the corresponding data of DEM (open circles) at \( t = 20 \). The solid lines for \( \nu \) and \( \theta \) are the polynomials of even powers of \( y \) until \( y^6 \), while the lines for \( u_x \) and \( u_y \) are the polynomials of the odd powers of \( y \) until \( y^5 \).

It is obvious that \( y \) component of the velocity field satisfies
\[
(38)
\]
\[ u_{y;N} = 0. \]

C. The result of numerical simulation for the complete set of hydrodynamic equations

For the initial condition to simulate hydrodynamic equations we fit the data of DEM at \( t = 20 \) in the dimensionless unit. Each fitting curve is approximated by a polynomial of \( y \) (Fig.5). The reason why we adopt the initial condition at \( t = 20 \) instead of \( t = 0 \), we are interested in the slow evolution of hydrodynamic variables after the total kinetic energy is relaxed to be a constant.

As shown in Figs. 6 and 7 the results of the simulation of hydrodynamic equations well agree with those of DEM. Once we rescale the time, the evolution of hydrodynamic variables in the simulation of hydrodynamic equations is almost equivalent to that of DEM. This agreement between hydrodynamic equations and DEM means that the renormalization procedure by Yoon and Jenkins [13] gives us the accurate results. Amongst hydrodynamic variables the \( y \)–component of the velocity field in the simulation of hydrodynamic equations has much larger than that of DEM though the profile itself is similar with each other, but the other variables in hydrodynamic simulation are almost the same as those in DEM (Fig.7).
FIG. 6: The comparison of the data for the area fraction for $\nu = 0.121$ obtained by DEM (open circles) at $t = 20$ (the label 1), 60 (the label 3) and 380 (the label 5), and the result of hydrodynamic equations (solid lines).

FIG. 7: The time evolution of the granular temperature (a), the velocity fields $u_x$ (b) and $u_y$ (c) in hydrodynamic simulations shown in solid lines, where the data in (a) and (b) are obtained by DEM. The numbers 1,3,5 in these figures correspond to results at $t = 20, 60$ and 380, respectively. The DEM data with the solid squares and open circles correspond to the result at $t = 20$ and 60, respectively. Note that comparison of the theory and DEM in the steady values of $\theta$ and $u_x$ will be shown in the next section, while we do not include DEM data for $u_y$ because of the disagreement in the scale (see Fig.4).

It should be noted that the transient dynamics of a granular shear flow has been discussed by Babic but his system is relaxed to be an USF because of the small system size and inelasticity. On the other hand, ours will not reach USF, and the time evolution of hydrodynamic variables contains a pattern formation.

D. Simulation of a simplified set of equations

To understand the qualitative behavior of phase separations, we need to reduce the degree of freedom of hydrodynamic equations. It is reasonable to deduce the terms proportional to the bulk viscosity is not important. In addition, the advection term $\mathbf{u} \cdot \nabla \mathbf{u}$ in hydrodynamic equations may not play important roles because we are interested in the slow dynamics in the domain growth. The coupling between the spatial gradient and the terms proportional to $1 - e^2$ because the kinetic theory can be applied to cases for small inelasticity.
Thus, we may reduce the set of hydrodynamic equations to be

\begin{align}
\partial_t \nu &= -\partial_y (\nu u_y), \\
\partial_t u_x &= \partial_y \left[ \frac{\eta(\nu)}{2} \theta^{1/2} \partial_y u_x \right], \\
\partial_t u_y &= \partial_y [\eta(\nu) \theta^{1/2} \partial_y u_y - p(\nu)], \\
\partial_t \theta &= -u_y \partial_y \theta - \nu^{-1} \eta(\nu) \theta^{1/2} (\partial_y u_y)^2 + 2 \nu^{-1} \eta(\nu) \theta^{1/2} (\partial_y u_y)^2 - 2 \nu^{-1} \partial_y (\kappa(\nu) \theta^{1/2} \partial_y \theta)
\end{align}

(39-42)

For further simplification, we may assume that the temperature \( \theta \) is a fast variable to slave other slow variables. Thus, we may omit the time derivative in eq. (42), but such simplification does not lead to a simplified treatment to solve hydrodynamic equations. Although \( u_y \) becomes zero in the steady state, it plays an important role for the time evolution of density. Thus, we believe that the set of equations \( (39)-(42) \) is the simplest set of hydrodynamic equations to describe phase separations.

Figure 8 shows the growth of hydrodynamic variables based on \( (39)-(42) \). Although the quantitative behavior is a little deviated from the result of DEM or the full set of hydrodynamic equations \( (25)-(27) \) in particular for \( u_x \), qualitative behavior of this simplified model is similar to those in more accurate treatments. In the steady state both hydrodynamic models reduce to equivalent results.

![Figure 8](image1.png)

**FIG. 8**: The time evolution of the the area fraction (a) granular temperature (b), the velocity fields \( u_x \) (c) and \( u_y \) (d) in the simulation of a simplified model \( (42) \) of hydrodynamic equations. The numbers 1,3,5 in these figures correspond to the data at \( t = 20, 60 \) and 380, respectively.
V. THEORETICAL DESCRIPTION OF THE STEADY STATE

In the steady state, the hydrodynamic variables depend only on \( y \). Thus, the variables are
\[
\nu = \nu(y), \quad u_x = u_x(y), \quad u_y = 0, \quad \theta = \theta(y). \tag{43}
\]

It is obvious that any hydrodynamic variable \( \Psi \) satisfies \( D_t \Psi = \partial \Psi = 0 \). Thus, the equation of mass conservation is automatically satisfied. The remain equations of motion become
\[
0 = \frac{d}{dy} P_{xy}, \tag{44}
\]
\[
0 = \frac{d}{dy} P_{yy}, \tag{45}
\]
\[
0 = P_{yx} \frac{d}{dy} u_x + \frac{d}{dy} q_y + \chi. \tag{46}
\]

Thus, the normal stress and the shear stress are uniform
\[
p \equiv P_{yy} = \text{const.} \quad \tau \equiv P_{yx} = \text{const.} \tag{47}
\]

From the definition of the pressure tensor we obtain
\[
\tau = -\frac{\eta(\nu)}{2} \frac{d}{dy} u_x, \tag{48}
\]
\[
p = \frac{1}{2} \nu [1 + (1 + e) \nu g(\nu)] \theta. \tag{49}
\]

Thus, we obtain the expressions for \( \theta \) and \( du_x/dy \) as functions of \( p, \tau \) and \( \nu \). Substituting them into the last equation of (46) we obtain
\[
\frac{d}{dy} [F(\nu) \frac{d\nu}{dy}] = G(\nu), \tag{50}
\]
where
\[
F(\nu) = \frac{1}{\alpha(\nu)^{3/2}} \left[ \frac{1}{2} + \frac{r}{\alpha(\nu)} \frac{\nu^2 g(\nu)}{\alpha(\nu)} - \lambda(\nu) \right], \tag{51}
\]
\[
G(\nu) = \frac{2 \alpha(\nu)^{1/2}}{\eta(\nu)} - (1 - e) \frac{\xi(\nu)}{\alpha(\nu)^{3/2}} \tag{52}
\]

with \( e = (\tau/p)^2 \) and \( \alpha(\nu) = 2/(\nu[1 + (1 + e) \nu g(\nu)]) \).

It is well established to solve the second order ordinary differential equation such as (50). Introducing \( H(\nu) \) as \( dH(\nu)/d\nu = F(\nu) \) and the multiplying \( dH/dy \) in both sides of (50), and thus integrate the equation from \( y = 0 \) to \( y \) we obtain
\[
\frac{1}{2} \left( \frac{dH}{dy} \right)^2 = \int_{\nu(0)}^{\nu(y)} d\nu F(\nu) G(\nu), \tag{53}
\]
where we use the symmetric condition \( d\nu/dy = dH/dy = 0 \) at \( y = 0 \).
\[
\pm \int_{\nu(0)}^{\nu(y)} \frac{F(\nu)}{\sqrt{2 \int_{\nu(0)}^{\nu(\nu)} F(\nu') G(\nu') d\nu'}} d\nu = y. \tag{54}
\]

Thus, we obtain the equation of \( y \) as the function of \( \nu \).

To draw the actual profile of \( \nu \), we start from a trial \( \nu_1(0) \) to integrate (54) and calculate \( I_1 = \int_{-\Delta/2}^{\Delta/2} \nu_1(y) dy \), where the suffix 1 represents the first trial function. Then we replace \( \nu_1(0) \) by \( \nu_2(0) \) to reduce the deviation between \( I_1 \) and \( \bar{\nu} \). We repeat this relaxation procedure to obtain the converged result \( I_M \rightarrow \bar{\nu} \) until \( M \) th trial. Once we obtain \( \nu \), we can determine \( \theta \) and \( du_x/dy \) by eq. (48).
FIG. 9: The comparison between theory (solid lines) and DEM simulation without the tangential interaction (open circles) for area fraction (a), granular temperature (b) and $u_x$ (c). The mean area fraction is $\bar{\nu} = 0.121$.

FIG. 10: The comparison between theory (solid lines) and DEM simulation with the tangential interaction (open circles) for area fraction (a), granular temperature (b) and $u_x$ (c). Here we use $\gamma = 0.798$ and the mean area fraction $\bar{\nu} = 0.121$.

To compare $\nu$ and $du_x/dy$ with the result of DEM we use a fitting parameter $\epsilon = (\tau/p)^2$, while we need two fitting parameters ($\tau = -0.0017$ and $p = 0.1$ for non-rotational cases and $\tau = -0.0017$ and $p = 0.06$ for rotational cases) to determine $u_x$ and $\theta$. It should be noted that $p$ and $\tau$ are determined by the boundary condition, but the boundary condition in eqs. (29) and (31) with (32) contains two unidentified parameters. Thus, $p$ and $\tau$ cannot be determined within our theory. Figure 9 is the comparison of our theoretical result with the result of DEM without the tangential contact force in the interaction between particles for $\bar{\nu} = 0.121$. The agreement between the theory and DEM is good. Figure 10 is the comparison of our theoretical result with the result of DEM including the tangential interaction taking into account the renormalization of the restitution constant for $\bar{\nu} = 0.121$. We again obtain a fairly good agreement between the theory and the simulation.

The reason why we can use the kinetic theory is that collisions between particles are almost binary even in the dense cluster. Actually, we find that contacted particles are about 1.014% of all particles at an instant, and only 2.4% of contacts are multi-body contacts among all contacts for $\bar{\nu} = 0.121$. Therefore, the kinetic theory can be used even in the dense cluster in which particles are almost motionless.

In principle, we can measure both the normal stress and the shear stress from the data of DEM. However, we only obtain the results with large errors. It seems that there is a tendency to have too small $p$ in the direct measurement, though observed $\tau$ is similar to the fitting value.

Thus, we confirm that (i) the kinetic theory by Jenkins and Richman[12] can reproduce the profiles of hydrodynamic variables to describe the steady state of the granular fluid though the fitting values of the stresses are included, and (ii) the renormalization scheme proposed by Yoon and Jenkins[13] is accurate. Although the setup of our simulation seems to be similar to that by Xu et al.[29], our result for hydrodynamic variables is much heterogeneous than that by Xu et al. in the presence of a streamwise flow. In fact, our system is separated into two regions which are a compact cluster and the very dilute region. The particles within the cluster is motionless, but the particles in the dilute region have large kinetic energy. On the other hand, the steady state obtained by Xu et al. is similar to USF. Thus, the result strongly depends on whether there is a stream flow.

VI. DISCUSSION

Let us discuss our results in this section. To clarify the points we discuss three important points; the linear stability analysis of USF, the validity of the truncation at Navier-Stokes order and the effects of external fields.
A. The linear stability analysis

Our analysis presented here suggests that USF of granular fluid is unstable. To verify such suggestion, we need to discuss the linear stability of USF.

The stability of sheared granular flows has been discussed by many researchers.\[51, 52, 53, 54, 55, 56, 57, 58, 59\] Many of them assume that the granular fluid is confined in an infinitely large system, but Alam et al.\[51\] discuss the bifurcation of the steady solution as a function of the system size. We should note that the stability of granular flows on an inclined slope has also been discussed by some researchers.\[60, 61\]

Here, we have also checked the linear stability of the uniform sheared state assuming Lees-Edwards sheared boundary condition. Since the result is almost equivalent to that by Alam and Nott\[53\], we only summarize the outline of our linear stability analysis. Our result indicates that USF is always unstable for enough large systems, but can be stable if the system size is enough small near $e = 1$. This result is consistent with the results by Babic\[23\] and Popken and Cleary\[24\]. The details of our linear stability analysis will be reported elsewhere.

As indicated in Section I, Bagnold’s scaling can be used if the system is uniform and the heat conduction is negligible. However, the granular gas under the plane shear is not the case that we can assume Bagnold’s scaling. The heat conduction plays an important role and USF cannot be maintained even when we adopt Lees-Edwards boundary condition.

B. The validity of the approximation at Navier-Stokes order

In this paper, we use the set of hydrodynamic equations at Navier-Stokes order. It should be noted that the set of hydrodynamic equations at Navier-Stokes order does not mean Newtonian. Actually, our granular system exhibits non-Newtonian behavior i.e. non-uniform velocity gradient as in Figs.9 (c) and 10(c) in spite of the uniform shear stress in the steady state.

From our analysis, the effects from the contraction of phase volume in collisions in the inelastic Boltzmann-Enskog equation are also small. The effects of tangential contact force and the rotation of particles are also not important in the bulk behavior of hydrodynamics. Therefore, the kinetic theory by Jenkins and Richman\[12\] gives us sufficient accurate results to describe the hydrodynamics.

Santos et al.\[9\] and Tij et al.\[62\] indicate that the transport coefficients in Couette flow depend on the dimensionless shear rate. However, in our system the shear rate only determines the time scale and thus the qualitative behavior should not depend on the shear rate. There is room for discussion on the role of the shear rate in granular gases as an open problem.

Some persons suggest the relevant role of terms at Burnett or super-Burnett order terms\[58, 63, 64\], but our analysis indicate that the contribution from higher order terms should be small. It is known that hydrodynamic equations at Burnett order derived from the classical gas kinetics is unstable for perturbation, i.e. some solutions will blow up when a perturbation is applied to the system.\[65, 66\] Therefore, we may need to be careful to use hydrodynamic equations at Burnett order or super-Burnett order to describe granular fluids.

C. The effects of external fields

Our system does not contain the external force except for the driving force of the boundary plates. In physical situations, it is difficult to remove the effect of gravity and collisions among particles may not be regarded as binary. As indicated in Introduction, recent papers and cited therein\[10, 11\] of sheared granular materials under a constant pressure produce a state of ‘granular liquid’ in which particles are multiple contacts with each other. In these cases, the square root of stiffness of grains becomes a characteristic frequency. Thus, the behavior should depend on the shear rate.

If we are interested in jamming transition or related phenomena of granular materials, we need to apply an external field to the system. Such subject will be important even in practical sense.

VII. CONCLUSION

In this paper, we have confirmed the validity of hydrodynamic equations derived from the kinetic theory by Jenkins and Richman.\[12\] We also confirm the relevancy of the renormalization method of the restitution constant by Yoon and Jenkins.\[13\] This result may be surprised because the system includes a dense cluster whose packing fraction is
close to the maximum value, and the particles in the cluster are almost motionless. Since USF is unstable, we cannot use Bagnold’s scaling to characterize the granular fluid in this case.

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APPENDIX A: THE DERIVATION OF WALTON’S $\beta_0$

In this Appendix, we demonstrate how to derive $\beta_0$ in Walton’s expression in eq. (7) for the tangential restitution coefficient. Although the theory by Maw et al. has been used to evaluate $\beta$, their expression is complicated and has an implicit form. Therefore, an explicit expression for Walton’s $\beta_0$ and the critical angle $\gamma_c$ is useful.

Let us consider a collision between identical disks. Following the notation in Section II (without suffices $i$ and $j$ for colliding particles), the equation of motion for the tangential direction is described by

$$\ddot{w}_t + 2(\eta_t \dot{w}_t + k_t w_t) = 0,$$

when there is no slip during the collision. The factor 2 appears because the reduced mass is the half of mass of each particle. The solution of eq. (A1) is easily obtained as

$$w_t = w_t(0) e^{-\eta_t t} \sin(bt), \quad \dot{w}_t(t) = w_t(0) e^{-\eta_t t} (\cos(bt) - \eta_t b \sin(bt))$$

for $\eta_t^2 < 2k_t$, where $b = \sqrt{2k_t - \eta_t^2}$.

Since we choose large $k_t$ and small $\eta_t$, the relation $\eta_t^2 < 2k_t$ should be satisfied. Similarly, the equation of motion in the normal direction is also described by an equation for a damped oscillation. Thus, the duration time $t_d$ at which $w_n = 0$ is satisfied and the normal restitution constant are respectively given by

$$t_d = \frac{2\pi}{\sqrt{2k_n - \eta_n^2}}, \quad \bar{e} = \exp\left[-\frac{\pi \eta_n}{\sqrt{2k_n - \eta_n^2}}\right].$$

On the other hand, the restitution constant $\beta_0$ for the tangential contact is thus given by

$$\beta_0 = \frac{-\dot{w}_t(t_d)}{w_t(0)}$$

$$= \exp\left(-\frac{\pi A \eta_t}{\eta_n \sqrt{2R - 1}}\right) \left[\frac{1}{\sqrt{2Q/A - 1}} \sin\left(\frac{\pi A \eta_t \sqrt{2Q/A - 1}}{\eta_n \sqrt{2R - 1}}\right) - \cos\left(\frac{\pi A \eta_t \sqrt{2Q/A - 1}}{\eta_n \sqrt{2R - 1}}\right)\right],$$

where

$$A = 1 + \frac{m\sigma^2}{4I}, \quad R = \frac{\pi k_n}{4\eta_n^2}, \quad Q = \frac{\pi k_t}{4\eta_t^2}.$$  

If we substitute the values $k_n = 3.0 \times 10^3$, $k_t = k_n/4$, $\eta_n = 3.0$ and $\eta_t = \eta_n/2$ used in DEM simulation, we obtain $\beta_0 \approx 0.769235$. The comparison between the theory (7) with (A3) and DEM is shown in Fig. 11. Without the introduction of any fitting parameters, agreement between the theory and DEM is fairly good. Here the critical angle $\cot \gamma_c = (1 + \beta_0)\mu(1 + \bar{e}) \approx 1.56734$.

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FIG. 11: The comparison of eq. 7 with (A4) (solid line) and the data obtained from DEM with $\mu = 0.2$ (open circles).

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