Clustering and phase separation in dense shear granular flow

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Abstract. We investigate various regimes of steady dense Couette flow of inelastically colliding hard disks in the absence of gravity. The two governing parameters in this two-dimensional system are the inelasticity of particle collisions and the average density of particles. The simplest steady state is the uniform shear flow (USF), where the temperature and the density profiles are homogeneous over the system and the velocity of the flow changes linearly between the two moving walls. The USF becomes unstable when the inelasticity of particle collisions exceeds a certain threshold, which depends on the average density of particles. Then the USF gives a way to a "plug flow" regime, where a solid-like cluster coexists with one or two fluid layers. These regimes are investigated using equations of granular hydrodynamics with constitutive relations that interpolate between low and high densities. The results are tested in event-driven molecular dynamics (MD) simulations, and a good agreement is observed.

1. Introduction
Granular materials (materials composed of many macroscopic particles) are ubiquitous in nature and industry. We can find them in the kitchen (sugar, salt) and on the beach (sand), in geophysics (gravel) and astrophysics (interstellar dust). The industrial applications are very wide: from coal mining to food and pharmaceutical industry. Although the founders of the field of granular mechanics were famous physicists like Coulomb and Faraday, for the most part of the 20th century granular mechanics was regarded as a branch of engineering: civil, mechanical, or chemical, depending on the particular application. This era in the development of the field saw a considerable progress in understanding the phenomenology of granular materials. In the last two decades, this field has taken the center stage of condensed matter physics and statistical physics, with the realization that granular materials pose fundamental problems in the behavior of disordered systems, with strong links to subjects such as glasses, chaos and pattern formation, critical phenomena and other areas.

Granular materials are of a great scientific interest [1]-[4]. They exhibit a lot of fascinating phenomena like avalanches [5] and "Brazil Nut" effect [6], surface waves [7] and oscillons [8]. In the middle of the 1980-s, a hydrodynamic description of granular flow was developed by Haff [9] and Jenkins and Richman [10]. Working along the lines of Enskog theory [11, 12], they started from the "microscopic" dynamics of inelastic hard sphere model and kinetic theory of gases and arrived at a granular hydrodynamics in the form of the continuity, momentum and energy equations. However, since the discovery of the clustering instability [13], the validity of these hydrodynamic equations (and, actually, of any continuum theory) became questionable [2]. Granular clustering results from energy losses in inelastic collisions. It was first observed in
A freely "cooling" granular gas in a pioneering work by Goldhirsch and Zanetti [13]. It was found that at large inelasticities, the size of clusters can be of the order of few particle diameters. It is clear that no coarse grained theory is able to describe effects on the particle scale. Quoting from the Review of Modern Physics by Kadanoff (1999): this "might invalidate any hydrodynamic-style theory of the granular material" and "we cannot be at all sure that hydrodynamic equations describe the behavior of granular materials in any general way" [2].

Nevertheless, granular hydrodynamics is expected to be valid in the limit of nearly elastic collisions we will consider throughout the paper. In this limit, the mean free path of the particles is usually much less than any length scale (and the inverse collision rate much less than any time scale) described hydrodynamically. Many different types of macroscopic granular flow has been investigated in past years both in experiments and in molecular dynamics (MD) simulations or theoretically, using the equations of granular hydrodynamics (see Ref. [14] for reviews). One can mention experimental works on Poiseuille flow [15] and Rayleigh-Taylor flow [16]. A lot of work was done on Couette flows [17].

A variety of symmetry-breaking instabilities in fluidized granular media were investigated employing granular hydrodynamics and molecular dynamics simulations. These include phase-separation instability [18] - [23], which is analogous, in many respects, to the spinodal decomposition of the gas-liquid transition of the van der Waals model [23], oscillatory instability [24], thermal granular convection [25], which resembles the Rayleigh-Benard convection, a famous example of pattern formation outside of equilibrium. Exciting clustering instabilities were investigated in a system consisting of array of two (or more) identical compartments, connected by slits in the walls between neighboring compartments [26].

Due to inelastic collisions between particles, one needs to continuously drive the system either by vibration or by shear in order to maintain the particles motion. As a result, a driven granular system can achieve a steady state, where an energy pumped into the system is dissipated by inelastic collisions. Therefore, driven granular media is intrinsically far from equilibrium [4, 27]. In this paper, we consider dense shear granular flow, which has recently attracted significant attention [17]. Different regimes of dense flows were investigated experimentally, theoretically, and using molecular dynamics (MD) simulations. The most widely studied shear flow regime in experiments is the regime of slow dense granular flow. Here particles in the bulk are not fluidized. Therefore, this regime can not be described by granular hydrodynamics. Moreover, even the model of inelastic hard spheres is not valid in this case, since particles collisions are not instantaneous, and multiples particle contacts become very important. In this study, we will focus on rapid (but dense) granular flow, where the granular media is fluidized, and the concept of granular temperature (introduced in granular hydrodynamics) is meaningful.

The most challenging and intriguing flow regime is the "plug flow" [28], where a solid-like cluster of particles coexists with (one or two) fluid-like layers [29] - [32]. Here the solid-like cluster is at rest or moves as a whole with some constant velocity. Figure 1 shows an example of such solid-fluid coexistence, as observed in molecular dynamics simulations. In this work, we investigate different regimes of a dense fluidized granular flow and theoretically describe the "plug flow" regime using both molecular dynamics (MD) simulations [33] and Navier-Stokes granular hydrodynamics [14].

2. The model of fluidized granular media
Let us consider the simplest model of fluidized granular matter [27]. We address here an idealized model that captures only one basic feature of macroscopic grains: inelastic collisions. The grains are assumed to be inelastic hard spheres (or disks in 2D) that interact with each other via a hard-sphere potential. During a collision between two particles, $i$ and $j$, momentum is conserved, and some energy lost. Let us denote the component of the velocity perpendicular to the line connecting the centers of the two disks by $v_{i\perp}$ and the parallel component by $v_{i\parallel}$. Let us denote
Figure 1. Snapshot of the two-phase flow for \( r = 0.992, N = 6480, \) and \( \langle n \rangle = 0.7244 \) \((< \nu > = 0.657)\) [32]. A large stripe-like cluster near the wall moves as a whole, showing solid-like behavior. The corresponding density, temperature, and velocity profiles are shown in Fig. 4. The granulate is fluidized everywhere including inside the cluster: the density is smaller than that of close packing, and the granular temperature is larger than zero. However, since \( n_\eta < n \), the horizontal flow velocity does not vary across the cluster.

the velocities after the collisions by primes. The energy loss in binary collisions is characterized by the coefficient of normal restitution \( 0 < r \leq 1 \). This single parameter distinguishes our idealized granular fluid, \( r < 1 \), from the idealized “normal” fluid, \( r = 1 \). By momentum conservation \( v_{i\perp}' = v_{i\perp} \) and \( v_{j\perp}' = v_{j\perp} \). The perpendicular velocities after the collision are given by

\[
\begin{pmatrix}
    v_{i\parallel}' \\
v_{j\parallel}'
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
    1 - r & 1 + r \\
    1 + r & 1 - r
\end{pmatrix} \begin{pmatrix}
    v_{i\parallel} \\
v_{j\parallel}
\end{pmatrix}
\] (1)

One can easily derive from these relations that the energy loss in each collision is proportional to \( 1 - r^2 \):

\[
\Delta E = \frac{1 - r^2}{4} (v_{i\perp} - v_{j\perp})^2 .
\] (2)

We assume the limit of nearly elastic collisions throughout this study, \( 1 - r^2 \ll 1 \).

Let us consider the dynamics of a system of \( N \) inelastically colliding hard disks of unit mass and diameter \( d \) driven by two opposite walls at no gravity. The ”upper” wall is located at \( y = H/2 \), the ”lower” wall is located at \( y = -H/2 \), see Fig. 1. The two walls move in the \( x \)-direction with opposite velocities, \( u_0 \) and \( -u_0 \) respectively. Typically, the initial conditions are the following: particles have random velocities and are distributed homogeneously over the system. Boundary conditions in the \( x \) direction are periodic. Boundary conditions in the \( y \) direction can be chosen in different ways. One can choose the moving walls to be thermal, which would correspond to constant temperature boundary conditions in hydrodynamic description. Another option is to ensure that there is no heat flux through the walls. This can be implemented in the following way [32]: upon a collision with one of the driving walls, the normal particle velocity switches sign, while the tangential particle velocity is completely ”forgotten”. The new tangential velocity component is taken from Maxwell-Boltzmann distribution. The mean
velocity of this distribution equals the wall velocity, and the variance corresponds to the instant temperature of the layer next to the wall.

3. Granular hydrodynamics and constitutive relations
The Navier-Stokes granular hydrodynamics operates with coarse grained quantities: number density of grains, \( n(r,t) \), granular temperature \( T(r,t) \), and mean flow velocity \( v(r,t) \) [9, 10]:

\[
\begin{align*}
\frac{dn}{dt} + n \nabla \cdot v &= 0, \\
n \frac{dv}{dt} &= \nabla \cdot P, \\
n \frac{dT}{dt} &= -\nabla \cdot Q + P : \nabla v - \Gamma
\end{align*}
\]

Here \( P \) is the stress tensor, \( Q \) is the heat flux, and \( \Gamma \) is inelastic heat losses. The stress tensor \( P \) is given by \( P = [-p(n,T) + \mu(n,T) \text{tr}(D)] I + 2\eta(n,T) D \), where \( D = (1/2) [\nabla v + (\nabla v)^T] \) is the rate of deformation tensor, \( \dot{D} = D - \frac{1}{2} \text{tr}(D) I \) is the deviatoric part of \( D \), and \( I \) is the identity tensor, \( \eta(n,T) \) and \( \mu(n,T) \) are the shear and bulk viscosities. The heat flux \( Q \) is given by \( Q = -\kappa(n,T) \nabla T \), where \( \kappa(n,T) \) is the coefficient of thermal conductivity. In the limit of nearly elastic collisions, \( 1 - r^2 \ll 1 \), an additional term in the expression for the heat flux, which is proportional to the density gradient [34], can be neglected. We also neglect inelastic corrections to transport coefficients [34] and replace \( 1 - r^2 \) factor in the inelastic heat losses term by \( 2/(1 - r) \).

For dilute and moderately dense flows, the Enskog-like shear viscosity, \( \eta_E(n,T) \), the thermal conductivity \( \kappa_E(n,T) \), the inelastic heat losses \( \Gamma_E(n,T) \), and the equation of state \( P_E \) are given by

\[
\begin{align*}
\eta_E &= \frac{4\nu T^{1/2} G_E}{\pi^{3/2} d} \left[ 1 + \frac{\pi}{8} \left( 1 + \frac{1}{G_E} \right)^2 \right], \\
\kappa_E &= \frac{8\nu T^{1/2} G_E}{\pi^{3/2} d} \left[ 1 + \frac{9\pi}{16} \left( 1 + \frac{2}{3 G_E} \right)^2 \right], \\
\Gamma_E &= \frac{8(1-r) n T^{3/2} G_E}{\pi^{1/2} d}, \\
P_E &= n T (1 + 2 G_E).
\end{align*}
\]

Here \( G_E = \nu(1 - 7\nu/16)/(1 - \nu)^2 \), \( \nu = n (\pi d^2/4) \) is the solid fraction, and index \( E \) stays for "Enskog".

In order to describe dense flow regimes, one needs to construct constitutive relations which are valid up to very high densities. Several attempts of extending granular hydrodynamics of inelastic hard sphere fluids to high densities have recently been performed [35, 36, 37]. Grossman et al. [35] investigated a two-dimensional system of inelastic hard disks driven by a thermal wall. The authors pioneered a practical approach, suggesting formulas for equation of state, granular heat conductivity and inelastic energy loss rate which interpolated between the dilute limit and the close vicinity of the hexagonal close packing, \( n_{max} = 2/(\sqrt{3}d^2) \), where free-volume arguments are available [35, 38]. Meerson et al. [36] have taken the same approach, describing the "levitating cluster" in a similar system in the presence of gravity. In these two works only static steady states (with no mean velocity) were considered [35, 36]. The next step was done by Bocquet and coauthors [37], who investigated granular shear flow with the density approaching the random close packing density. In this case, the mean flow velocity is not
zero, so the coefficient of shear viscosity needs to be specified in addition to other constitutive relations. The authors [37] proposed that the shear viscosity coefficient diverges at random close packing density, but with a larger exponent: \( \eta \sim (n_{rcp} - n)^{-\beta} \), \( \beta > 1 \). Khain and Meerson [29] have recently suggested a different approach, incorporating a recent finding [39] that the shear viscosity coefficient diverges like \((n_{\eta} - n)^{-1}\) at a density \( n_{\eta} < n_{max} \), where \( n_{max} = 2/(\sqrt{3} d^2) \) is the density of crystalline close packing.

Therefore, while inelastic heat losses, thermal conductivity, and pressure diverge at the close packing density \( n_{max} \), the shear viscosity diverges at a lower density [39], which may result in coexistence of fluid and solid phases [29, 30, 32]. In a recent work [30], the interpolation of constitutive relations between the dilute and dense limits was proposed (see also Refs. [39, 40]) and tested in a series of MD simulations; a viscosity divergence was also taken into account. The modified constitutive relations are:

\[
\begin{align*}
p & = nT(1 + 2G), \\
\Gamma & = \frac{8(1 - r)nT^{3/2}G}{\pi^{1/2}d}, \\
\kappa & = \kappa_0 \left(1 + 0.1\nu - 10\nu^{10} + \frac{0.11}{\nu_{max} - \nu} - \frac{0.11}{\nu_{max}}\right), \\
\eta & = \eta_0 [1 + a_0(\nu/\nu_0)]((\nu_0 - \nu)],
\end{align*}
\]  

(5)

where \( G = G_0 + \theta [\nu_{max}/(\nu_{max} - \nu) - G_0] \). Here, \( \theta \) is the interpolation function, given by \( \theta = [1 + \exp((\nu_c - \nu)/m_0)]^{-1} \) with \( \nu_c = 0.70, m_0 = 0.0111, \nu_0 = 0.71, a_0 = 0.037 \), and \( \nu_{max} = \pi/(2\sqrt{3}) \) [39, 40]. In the next section we employ the resulting hydrodynamic equations to description of the phase separation between the fluid-like and solid-like regions in dense shear granular flow.

4. The plug flow

The plug in dense shear granular flow was first observed in MD simulations [28]. The basic physics of this regime relies on the fact that the shear viscosity of hard-disks-fluid diverges not at the density of crystalline close packing \( n_{max} = 2/(\sqrt{3} d^2) \) (where pressure, inelastic heat losses and thermal conductivity diverge), but at a smaller density, \( n_{\eta} < n_{max} \). Consider the simplest steady Couette flow: uniform shear flow. Here the density (along with temperature and velocity gradient) is constant over the system. It is well known that the uniform shear flow can become unstable [41], which leads to density inhomogeneities in the system: some regions become more dense, other become more dilute. If the mean density in the system is high, then the density in denser regions can become more than the density of viscosity divergence: \( n > n_{\eta} \). This region then starts behaving like a solid cluster: the velocity can not vary across the cluster since \( n_{\eta} < n \). Interestingly, the density and temperature do vary (since \( n < n_{max} \)), and the particles are fluidized. Other regions behave like fluids, since \( n < n_{\eta} \). This explains the fluid-solid coexistence, shown in Fig. 1. Figure 1 presents the results of MD simulations of \( N = 6480 \) inelastic hard disks. The initial state was homogeneous, but after a transient the system arrived at the state with broken symmetry with the solid plug next to the ”upper” wall at \( y = H/2 \), moving as a whole with the velocity, which approximately equals the velocity of the wall. Obviously, the state with the cluster next to the ”lower” wall at \( y = -H/2 \) is equally probable. To make sure that the system reached the steady state, we analyzed the time dependence of \( y \)-component of center of mass of the system. Figure 2 shows another example of steady plug-flow (the snapshot is taken at time \( t = 1.4 \times 10^6 \)), while Figure 3 shows the dynamics of \( y_{cm} \). After a transient, \( y_{cm} \) reaches a plateau and does not change anymore. Note that the characteristic time of transient dynamics significantly depends on initial conditions. If the initial conditions are symmetric, the system needs to wait for a long time for a large
fluctuation in order to decide what the final steady state should be and whether the solid plug should be near the upper or lower wall. One can make the transient time much smaller, starting with asymmetric conditions, see Fig. 3. These asymmetric conditions can be achieved, for example, by adding a small vertical component to all particles velocities.

![Figure 2. Snapshot of the two-phase flow for](image)

Figure 2. Snapshot of the two-phase flow for $r = 0.986, N = 2600$, and $< n >= 0.591 (< \nu >= 0.536)$. A large stripe-like plug near the wall moves as a whole.

![Figure 3. $Y$—component of center of mass of the system versus time.](image)

Figure 3. $Y$—component of center of mass of the system versus time. After a transient, $Y_{cm}$ reaches a plateau, which corresponds to the steady state flow. The two curves correspond to symmetric initial conditions ($Y_{cm}$ starts from zero) and asymmetric initial conditions ($Y_{cm}$ starts from some nonzero value). The transient dynamics is much faster if the initial conditions are asymmetric (see text). The parameters are the same as in Fig. 2.

Interestingly, the region inside the plug in Fig. 2 is crystallized; the particles form an ordered layer structure. The same ordered structure was observed in other dense granular clusters [36, 42]. An important difference between the steady states is that the states in Refs. [36, 42] are static, while the cluster shown in Fig. 2 moves as a block to the right with velocity, almost equal to the wall velocity. In both cases, the density inside the cluster is smaller than that of the maximal dense crystalline packing, $n_{max}$; the granulate is fluidized, the particles are not at rest, and the granular temperature is larger than zero.

Let us now describe hydrodynamically the possible steady states ($\partial/\partial t = 0$) of Eqs. (3), assuming flow in $x$—direction, zero vertical velocity and $\partial/\partial x = 0$. The coordinate $y$ will be measured in units of the system “height” $H$ (the distance between the two moving walls), the horizontal velocity $u$ will be measured in units of the wall velocity $u_0$, the temperature $T$ in units of $u_0^2$, the density $n$ in units of $n_{max}$, and the pressure $P$ in units of $n_{max} u_0^3$. Eqs. (3) can be written now in the following form

$$
\frac{d}{dy} \left( f_2 T^{1/2} \frac{du}{dy} \right) = 0,
$$

$$
\frac{d}{dy} \left( f_1 T^{1/2} \frac{dT}{dy} \right) + \frac{f_2 T^{1/2}}{4} \left( \frac{du}{dy} \right)^2 - R f_3 T^{3/2} = 0,
$$

$$
f_4 T = \text{const.}
$$

(6)
Figure 4. The density (a), temperature (b), and velocity (c) profiles of the two-phase flow for $R = 259.07$ and $< n > = 0.7244$ ($< \nu > = 0.657$) from Ref. [32]. The results of MD simulations are shown by circles; solid lines denote the theoretical curves obtained from numerical solution of Eqs. (6). The corresponding snapshot of the system is shown in Fig. 1.

Here $R = (16/\pi) (1 - r) (H/d)^2$ is the hydrodynamic heat loss parameter, and the functions $f_i$ are the density-dependent parts of the constitutive relations [Eqs. (5)]:

$$f_1 = \kappa (\sqrt{\pi d}/2)T^{-1/2},$$
$$f_2 = \eta (2d\sqrt{\pi})T^{-1/2},$$
$$f_3 = \nu G,$$
$$f_4 = n(1+2G).$$

The total number of particles is conserved $\int_{-1/2}^{1/2} n(y) dy = < \nu > / \nu_{max}$ and no-flux and no-slip boundary conditions are assumed: $dT/dy(y = -1/2) = T/dy(y = 1/2) = 0$, $u(y = -1/2) = -1$, $u(y = 1/2) = 1$.

Figure 4 shows the profiles of density (the left panel), temperature (the middle panel), and horizontal velocity (the right panel). The hydrodynamic profiles (solid lines) are computed from Eqs. (6). Details of the numerical procedure are given in Ref. [32]. MD simulations support the hydrodynamic predictions, Fig. 4 (circles). The corresponding snapshot of the system is shown in Fig. 1.

Figure 5. Snapshot of the two-phase flow for the same parameters as in Fig. 2, but with much higher aspect ratio: $L_x/H = 4.62$, the number of particles is $N = 19500$. A slight signature of a two-dimensional wavy structure can be seen.

The structures shown in Figs. 1 and 2 are essentially one-dimensional: the density, temperature, and velocity profiles depend only on the "vertical" coordinate $y$ and do not depend on the coordinate $x$, along the flow direction. What happens in case of a wider system? Here, the layered structures may give way to wavy patterns [43]. A snapshot shown in Fig. 5 corresponds
to the same parameters as in Fig. 2, except for the much larger aspect ratio $L_x/H$. Probably, there is some signature of two-dimensional structure in Fig. 5, but a more detailed analysis, both theoretical and using MD simulations is needed. If the moving boundaries are taken to be thermal walls, the wavy patterns occur in the middle of the system, like in Ref. [43]. For moderate densities, some of these structures were explained theoretically [44], while for higher densities the viscosity divergence should be taken into account.

For the fixed aspect ratio of the system, the steady flow regimes are governed by two parameters: the hydrodynamic heat loss parameter $R = (16/\pi) (1 - r) (H/d)^2$ and the average area fraction $<\nu>$. In different regions of the phase diagram ($R, <\nu>$), either uniform shear flow or the plug-flow can be found in MD simulations. Hydrodynamic analysis shows additional nonlinear steady flow regimes, which seem to be unstable [29, 30, 32]. Interestingly, in a certain region of the phase diagram both the uniform shear flow and the plug-flow are stable, and hysteretic behavior can be observed. The reader is referred to Ref. [32] for more details.

5. Summary and discussion
This study focuses on a dense fluidized granular flows in Couette geometry in the framework of the simplest model of fluidized granular media: inelastic hard sphere model. An intriguing plug-flow regime is investigated both theoretically by using Navier-Stokes granular hydrodynamics, and in event-driven molecular dynamics simulations. The plug is formed due to the nontrivial dependence of the coefficient of shear viscosity on density: the shear viscosity diverges at the density smaller than the density of crystalline close packing $n_\eta < n_{\eta_{\text{max}}}$. This explains the observed solid-fluid coexistence: the density in the solid-like plug is above $n_\eta$, while in the fluid-like regions it is below $n_\eta$. Interestingly, the particles inside the cluster form an ordered crystalline structure (though the density is smaller than $n_{\eta_{\text{max}}}$). Does this happen since the density of viscosity divergence $n_\eta$ is very close to the density of the melting point? Or may be the crystallization is a unique feature of inelastically colliding hard disks, since it is observed in systems without any shear as well? Further studies are needed to address these questions.

6. References
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