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Dynamical clustering in driven granular gas

E. Opsomer\( (a) \), F. Ludewig and N. Vandewalle

GRASP, Physics Department B5a, University of Liège - B-4000 Liège, Belgium, EU

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Abstract - Driven granular gases present rich dynamical behaviors. Due to inelastic collisions, particles may form dense and slow regions. These clusters emerge naturally during a cooling phenomenon but another dynamical clustering is observed when the system is continuously excited. In this paper, the physical processes that trigger the transition from a granular gas to a dynamical cluster are evidenced through numerical simulations. At the granular scale, the transition is evidenced by the observation of caging effects. At the scale of the system, the transition is emphasized by density fluctuations. Physical arguments, based on relaxation times, provide an analytical prediction for the edge between dynamical regimes.

Our interest goes to the transition from the granular gas to the dynamical cluster that can be triggered by the manipulation of a broad range of parameters. Since microgravity is required for sustaining a granular gas, numerical simulations using DEM-like algorithms are performed. Our work is based on the experimental features of the VIPGRAN [13] device of the European Space Agency.

In this paper, the detection of the dynamical regime in the system is achieved by a statistical adequation test already used in earlier simulations [12,14]. Space-time diagrams of the mean kinetic energy in the system are presented and open new perspectives.

Numerical model. – Our numerical model reproduces the experimental setup of VIPGRAN. Figure 1 gives a brief overview of this system geometry. Inside a cell of dimensions \( 30 \times 30 \times 60 \) mm, two pistons \( \pi_1 \) and \( \pi_2 \) enclose \( N \) spherical particles of radius \( R \). These pistons are oscillating sinusoidally in phase opposition around their respective equilibrium points \( z_1 \) and \( z_2 \) with an amplitude \( A \) and a frequency \( f \). The distance \( L = |z_1 - z_2| \) can be modified in order to change the mean volume for a fixed amplitude. The period of oscillation is noted \( T \).

The simulations are based on the Molecular Dynamics (MD) [15,16] approach. This model is widely used in soft-matter physics and especially in the simulation of granular materials [12] because of its capacity to handle efficiently multiple collisions that are unavoidable in dissipative systems. Normal forces \( F_{nj}^{n} \) are composed by a repulsive \( F_{ij}^{rep} \) and a dissipative \( F_{ij}^{dis} \) component. The repulsive

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\( (a) \)E-mail: eric.opsomer@doct.ulg.ac.be
Fig. 1: (Color online) Sketch of the VIPGRAN cell. Two pistons are oscillating sinusoidally in phase opposition around their respective equilibrium points $z_1$ and $z_2$. The oscillation parameters are the amplitude $A$ and the frequency $f$. The distance $L$ separating $z_1$ and $z_2$ is tunable. Finally, the side length $\ell$ is fixed during each experiment.

The component follows Hooke’s law

$$F_{ij}^{rep} = -k_n \delta_{ij},$$  \hspace{1cm} (1)$$

where $\delta_{ij}$ is the overlap of two adjacent solids $i$ and $j$. The constant $k_n$ is the normal stiffness which is a purely numerical parameter. The stiffness is determine by a maximum particle deformation of $R/100$ for two grains in frontal collisions with relative velocity $2A \omega$, where $\omega = 2 \pi f$. The dissipative component is taken into account by viscous forces according to the following law:

$$F_{ij}^{dis} = -\gamma_n (k_n, \varepsilon) \frac{\partial \delta_{ij}}{\partial t},$$  \hspace{1cm} (2)$$

where the viscous constant $\gamma_n$ \cite{15} is a function of the normal stiffness $k_n$ and the restitution coefficient $\varepsilon$. This restitution coefficient is used for both, grain-grain and grain-wall collisions. Tangent forces $F_{ij}^t$ are bounded and depend on the relative tangent velocities $v_{ij}^t$ between the colliding solids $i$ and $j$. One has

$$F_{ij}^t = -k_t v_{ij}^t \quad \text{and} \quad \|F_{ij}^t\| \leq \mu F_{ij}^n,$$  \hspace{1cm} (3)$$

where $\mu$ is a friction coefficient and $k_t$ a purely numerical constant. For more realistic force models, such as viscoelastic forces, similar results are expected. Further details concerning the MD simulations are given by Taberlet \cite{17}.

Numerical results. – A large number of numerical simulations were realized in order to cover the complete set of tunable parameters. For fixed values of $L$, $A$ and $R$, different dynamical regimes could be observed depending on the number $N$ of grains in the system. A complete description of the investigated parameters is given in table 1. The side length $\ell$ cannot be changed in the VIPGRAN experiment but its influence on the system’s dynamics is numerically investigated. Note that all simulations were realized for fixed values of $\varepsilon = 0.9$ and $f = 10$ Hz.

Indeed, the latter exhibits that the frequency might not be a pertinent parameter for the emergence of the expected phenomenon. Figure 2 presents snapshots of the simulated cell for a typical set of parameters referred as $S$ in table 1. In the dilute case of 1000 grains (nearly one grain layer at rest), particles are homogeneously distributed in the whole volume. Moreover, collisions are rare events and the particle velocities approach $A \omega$. In opposite, for 4000 grains, contacts between particles are frequent events and according to the dissipative character of these collisions, energy is dissipated. When the number of grains increases, one can assist to the formation of dense zones of low grain velocity growing from the corners towards the centre of the cell. These dark gray (blue) clusters, that can be detected by a following caging criteria, are surrounded by a loose gas-like zone. Both phases are coexisting and form a complex dynamical equilibrium. Surface grains are indeed ejected

Table 1: Parameters for the different simulated systems. Symbols are given according to the results presented in figs. 5 and 7. The symbol $S$ stands for a typical set of parameters corresponding to figs. 2, 3, 4 and 6. The symbol $\times$ corresponds to earlier simulations \cite{12}.

<table>
<thead>
<tr>
<th>$A$ (mm)</th>
<th>$L$ (mm)</th>
<th>$\ell$ (mm)</th>
<th>$R$ (mm)</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.0</td>
<td>30.0–47.5</td>
<td>30</td>
<td>0.5</td>
<td>●</td>
</tr>
<tr>
<td>5.0</td>
<td>30.0–47.5</td>
<td>30</td>
<td>0.5</td>
<td>○</td>
</tr>
<tr>
<td>6.0</td>
<td>35.0–47.5</td>
<td>30</td>
<td>0.5</td>
<td>■</td>
</tr>
<tr>
<td>5.0</td>
<td>35.0–47.5</td>
<td>30</td>
<td>0.6</td>
<td>□</td>
</tr>
<tr>
<td>5.0</td>
<td>35.0–47.5</td>
<td>30</td>
<td>0.7</td>
<td>△</td>
</tr>
<tr>
<td>5.0</td>
<td>47.5</td>
<td>30</td>
<td>1.0</td>
<td>▽</td>
</tr>
<tr>
<td>5.0</td>
<td>30.0–47.5</td>
<td>15</td>
<td>0.5</td>
<td>▲</td>
</tr>
<tr>
<td>5.0</td>
<td>40.0</td>
<td>30</td>
<td>0.5</td>
<td>△</td>
</tr>
<tr>
<td>2.5</td>
<td>10.0</td>
<td>10</td>
<td>0.13–0.32</td>
<td>×</td>
</tr>
</tbody>
</table>

Fig. 2: (Color online) Snapshots of the main cell for, respectively, $N = 1000$ and $N = 4000$ grains. One grain layer at rest contains nearly 1000 grains. For small number of grains the system behaves like a gas. When the number of grains increases, dense and slow moving clusters are formed in the corners and grow towards center of the system. These dark gray (blue) clusters are detected by the following caging criteria.
by the cluster, but this loss of matter is recovered by new energetic particles coming from the pistons.

At the scale of grains, the presence of clusters can be linked to some “caging effect”. Indeed, high local densities imply that a grain cannot leave its neighborhood without colliding and losing kinetic energy. Evidence of such caging effect is illustrated in fig. 3 by the tracking of randomly chosen particles during 20 periods. The system is based on the set of parameters \( S \). In order to simplify the visualization a \((y, z)\)-projection is used. The trajectories of three particles are represented by a black, a gray (blue) and a light gray (red) line. For a gas \((N = 1000)\), the trajectories are rather straight lined and of the size of the system. The entire volume is visited, which is expected for a homogenous gas. For a clustered system \((N = 4000)\), trajectories are straight lined in the gas phase near the pistons, but once a grain travels into the central zone, a caging effect is observed. Indeed, the trajectories remain localized. The grains and their energy is dissipated by a succession of inelastic collisions.

The loosest local configuration corresponding to a cage is a grain surrounded by 6 neighbors in a cubic lattice of side length \( \sqrt{6} R \). For this arrangement, the central grain cannot travel beyond its neighborhood without collision. In terms of packing fraction \( \phi = N v_g / V \), where \( v_g \) is the volume of a grain and \( V \) the maximum volume of the cell, a cage is formed above a threshold value \( \phi_c = 0.285 \) that was already observed in earlier work [12]. In order to count the number \( N_c \) of grains that are caged in the system, a local packing fraction \( \phi_{\text{loc}} \) has to be measured. This can be achieved from a Voronoï tessellation. Indeed, for each particle a Voronoï cell of volume \( V_{\ell} \) is obtained. Accordingly, a grain is considered as caged if \( \phi_{\text{loc}} = v_g / V_{\ell} > \phi_c \). For the set of parameters \( S \), fig. 4 describes in gray (blue) the evolution of \( N_c \) for increasing \( N \). The first significant value of \( N_c \) is obtained for \( N = 3525 \). Important dissipative phenomena are then expected.

At the scale of the whole system, the signature of the cluster formation is given by the positions of the grains in the cell volume. Expecting that for low densities the grains will spread homogeneously, a uniform distribution corresponds to a gas-like system. A statistical test is a reliable tool in order to detect the dynamical regime of the system [12]. The two-sample Kolmogorov-Smirnov adequation test (KS test) [18] compares the cumulative distribution function \( F(z) \) of the grain positions along the \( z \)-axis with the cumulative distribution function \( U(z) \) of a uniform law. For a fixed number of grains \( N \), the test value \( T_{KS} \) is given by

\[
T_{KS} = \sqrt{\frac{k}{2}} \sup_{|z| \leq L/2A} |F(z) - U(z)|, \tag{4}
\]

where \( k \) is the number of classes characterizing the distributions. If \( T_{KS} \) exceeds the statistical threshold \( K_\alpha \), depending on \( k \) and on the the level of significance \( \alpha \), the hypothesis of uniformity is refuted and the system is assumed to be in a cluster regime. Figure 4 describes in black, the evolution of \( T_{KS} \) as a function of \( N \) realized for the set of parameters \( S \). The statistical threshold \( K_\alpha \) is represented in light gray (red). Once \( T_{KS} > K_\alpha \), a critical number of grains triggering the transition can be extracted. Moreover, this transition corresponds to the apparition of the first significant number of caged particles and the results of the global test are in perfect agreement with the results of the local detection method.

An automatic detection of the gas-cluster transition curve is introduced. In each simulation, the KS test is used
to detect the dynamical regime of the system. Starting with two initial filling numbers of $N = 500$ and $N = 5000$, a gas and a cluster are respectively detected. Obviously, the transition occurs between those values and can be approached by interpolation. For the obtained number of grains a new simulation is performed and the test is applied again. This dichotomy allows to refine the edge with sufficient precision. Figure 5 presents the gas-cluster transition points depending on the number of grains and on the height $L - 2A$ of the constraint-free zone of the cell. The symbols refer to the different simulation parameters according to table 1. The error bars correspond to the precision of the detection and depend on the number of iterations in the dichotomy procedure.

All transition lines present similar behaviors but for different ranges of the parameters. For a fixed height, as more energy is dissipated, clustering appears when the number of grains increases. Moreover, a cluster appears for a constant grain number by increasing $L - 2A$. This seems counterintuitive since the number density $\eta = N/V$ gets lower. Nevertheless, if the volume increases for constant $N$, less particles are present next to the pistons and less energy is injected in the cell. As only few energetic particles arrive in the central part of the cell, the system cools down, which leads to the formation of a dense region. In order to investigate more deeply this energetic approach of clustering, space-time diagrams were established. Based on the set of parameters $S$, fig. 6 describes the evolution, at different heights $z$, of the mean kinetic energy $E_k$ in the system as a function of the dimensionless time $t/T$. This energy is normalized by the kinetic energy of a single grain moving at speed $A\omega$ and displayed using a linear color scale. In order to improve the statistics, the diagram is averaged over 20 periods.

In the gas state (fig. 6, top) one observes that for $0.4 \leq t/T < 0.8$ a large amount of energy is injected into the system according to the motion of the pistons. Evaluating the slopes of typical trajectories in this diagram leads to an approximative injection velocity $v_0$ that lies between $A\omega$ and $2A\omega$. Despite the average of the collected data, discrete energetic trajectories are visible for $0.8 \leq t/T < 1.4$. This could evidence a periodic behavior of the particles in the cell. Indeed, the energetic branches on the diagram could correspond to the different oscillation modes established in the system. In the cluster case (fig. 6, bottom) one can find a correspondent energy injection near the pistons. However, even if initially the slopes are similar, the energy level is much lower which means that for high $\eta$ less grains are near the pistons. Moreover, one observes a deviation of the trajectories at about $t/T = 0.7$ corresponding to the encounter of the energetic grains with the cluster. Due to multiple collisions, the speed drops and the slope of the trajectories decreases more and more. The discrete trajectories present in the gas are no longer visible and only a few grains are leaving the central zone. At the scale of one period, the injected energy reaching the center of the system is not high enough to break up the clusters and to spread the grains through the system.

**Energetic approach.** – Our numerical results stress the importance of two main processes in the cluster formation mechanism: i) the amount of injected energy
and its propagation; ii) the dissipation of this energy through a series collisions. This last mechanism has been quantified for free cooling systems and follows Haff’s law (5) as long as the system is dilute. One has

$$\langle v(t) \rangle = \frac{v_0}{1 + t/\tau_H},$$  \hspace{1cm} (5)$$

where $v_0$ is the typical injection velocity and the operator $\langle \cdot \rangle$ denotes the average. The Haff time $\tau_H$ is the typical relaxation time [19] for granular gases and is given by

$$\tau_H = \frac{2}{v_0 (1 - \varepsilon^2) \eta \sigma}.$$  \hspace{1cm} (6)$$

where $\sigma$ is the cross-section $\pi(2R)^2$ of the grains. The propagation of the energy through the system is more complex and depends on the mean free path of each particle as well as on the size of the system. The typical length $\delta$ of the system is given by the mean distance that the grains achieve when they pass across the constraint-free zone. Accordingly, $\delta$ corresponds to the average distance separating two points $P_1$ and $P_2$, respectively, in the surfaces $\pi_1$ and $\pi_2$ of the pistons when they are as close as possible.

$$\delta = (|P_1P_2|).$$  \hspace{1cm} (7)$$

The effective volume visited by a grain is then given by $\delta \sigma$ which leads to a number $n = \eta \delta \sigma$ of encountered collisions during its particle motion. At each binary collision, a certain amount of energy is dissipated. This loss can be translated in terms of velocity according to the law $v' = v + \delta$, where $v$ and $v'$ are, respectively, the grains velocities before and after the collision. If one sees the energetic transfer as a dissipative chain reaction through the system, a characteristic propagation time $\tau_P$ can be estimated. One has

$$\tau_P = \frac{\delta}{n} \left( \sum_{i=0}^{n} \frac{1 - v_i v_i}{v_0 v_i} \right),$$  \hspace{1cm} (8)$$

where $\delta/n$ acts as the mean free path. If the energetic impulse coming from the piston has enough time to travel across the system and to spread the particles in the whole volume as is seen in fig. 6 the system is in a gas-like regime. In the opposite, if the system has not enough time to propagate, dense central zones are generated due to cooling. The system dynamics appear as a competition between both time scales. Accordingly, a clustering condition can be given by

$$\tau_H < \tau_P.$$  \hspace{1cm} (9)$$

By simplifying and using the geometric character of the sum in $\tau_P$, the condition (9) can be reformulated as follows:

$$\delta > \frac{\xi}{\sigma \eta}.$$

where $\xi$ depends on $\varepsilon$ according to

$$\xi = - \left( \frac{1 + 2}{\ln \varepsilon} \right) - 1.$$  \hspace{1cm} (11)$$

However, the estimation of $\tau_P$ neither takes into account the size of the grains nor their deviation at impact. Since the interaction between particles depends on a surface-to-surface distance, a corrective term $\pi d^2$, with $0 < r_0 < 2R$ has to be subtracted from the typical length $\delta$. This value $r_0$ is linked to the impact angle $\theta$ and can be determined by considering the repartition of the velocities. Indeed, after each binary collision assuring the energy transmission, both grains continue their movement with different velocities. The transmitted speed corresponds to $\cos \theta$, where $v$ is the velocity of the incident grain before impact. By following after each collision the fastest grain, the deviation in the energy transmission is limited by a critical angle of $\pi/3$ that leads to the estimation

$$r_0 = \frac{3}{\pi} \int_0^{\pi} 2 \cos(\theta) d\theta = 1.654.$$  \hspace{1cm} (12)$$

By reorganizing condition (10) in order to use the packing fraction $\phi = \sigma \eta R^3$, a dimensionless expression can be obtained and the parameters $\phi$ and $\delta/R$ assure the collapse of the gas-cluster transition points presented in fig. 5 along a unique curve of equation

$$f(\phi) = \frac{\xi}{3\phi} \left( \frac{1}{1 - 3(r_0/R)\phi} \right).$$

Figure 7 is a $(\delta/R, \phi)$-phase diagram presenting these transition points by using the symbols of table 1 in black and $f(\phi)$ in light gray (red). Equation (13) captures the transition for all sets of data investigated herein.

In order to confirm the reliability of the presented law, $f(\phi)$ is compared to the empirical frontier between gas and cluster regime of earlier Mini-Texus simulations [12] represented by the gray (blue) crosses in fig. 7. The agreement is excellent. Nevertheless, $f$ departs from the set of points for large values of $\phi$. Indeed, the limits of the model are reached, the hypothesis of strong dilution is not respected and Haff’s law [19] is no longer valid.
Conclusion. – In summary, we characterized and numerically confirmed the transition between a granular gas and a dynamical cluster at the scale of the grains and at the scale of the entire system. Both approaches concord and lead to an efficient cluster detection. A model based on the energy propagation in the system provides a scaling law for the edge between both dynamical regimes. The only fitting parameter \( r_0/R \) of this law is constant for systems of different dimensions and oscillation types.

Our work opens new perspectives. Indeed, our results could help to fix the parameters of the VIPGRAN experiment. Moreover, a model taking cells with several compartments into account could be imagined in order to manipulate or to direct clusters.

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