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Structural and Dynamical criteria to Characterize Dynamical Clustering in Granular Gases

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Abstract

Dense granular gases under continuous excitation in microgravity can develop spatial inhomogeneities of the particle number density. The process of dynamical clustering depends upon geometrical and physical parameters such as container geometry, filling fraction and mechanical excitation protocols. We propose dynamical criteria for cluster detection and compare them with established classical ones based on structural aspects, viz. the Kolmogorov–Smirnov test and particle caging analysis. Suitability and reliability of these criteria are tested with frictional spheres in a cuboid container, computed by Discrete Element Method (DEM) simulations. A key finding is that the transition from the homogeneous gas to the clustered state under variation of the system parameters is continuous and a general definition of the state of the ensemble from its dynamical or structural characterization is problematic. Nevertheless, we suggest a procedure that allows to establish a state diagram.

Keywords: Granular gases, Dynamical clustering, Statistical analysis, Machine Learning

1 Introduction

Granular matter is ubiquitous, in cosmic formations like nebulae or protoplanetary disks, in natural structures and phenomena such as sand deserts or landslides, and in everyday life in the form of grains, sugar, or coffee beans [1–3]. These ensembles of large numbers of macroscopic particles can exist in three different states. Dilute systems can form gaseous states where particles interact only by short mutual collisions. When the space filling increases, particles can form a liquid-like phase which is characterized by frequent yet non-permanent contacts. Finally, when the particles form permanent contacts, the system can be considered as solid-like [4, 5]. The grains can undergo transitions between these states, for example, when the energy input changes.

In certain situations, homogeneous granular gases can form local clusters where the number density of particles is increased substantially with respect to the surroundings [6]. The dynamics in such clusters rather resembles that of a liquid than of a gas. The macroscopic behavior of granular gases is primarily determined by the inelastic character of the collisions of the constituents. Continuous excitation is needed to keep such a system in a dynamic state [7] and to avoid the continuous loss of kinetic energy, so-called granular cooling. An experimental realization of three-dimensional (3D) granular gases requires the confinement of the particles in a container (usually box-shaped). Energy input can be implemented mechanically by vibrating container walls [7] or by alternative excitation methods [8]. 3D granular gases are commonly studied under microgravity conditions to avoid accumulation of particles at the bottom of the cell caused by gravity. Possible options include drop towers, sounding rockets, and, within some limitations, also parabolic flights [9, 10].

As observed earlier [6, 11], local inhomogeneities naturally arise in the cooling phase. Dense patterns, called dynamical clusters, can appear when the particle number density in a granular gas system is sufficiently large. Clustering is a central feature of granular gases, for different reasons, both during permanent external excitation and during granular cooling. It is essential in manifold situations from cosmology to natural phenomena and industrial processes. Dynamical clustering (DC) was previously studied in systems of spheres [5, 10, 12, 13], and of prolate cylinders [14]. In these papers, it was demonstrated that a combination of system parameters controls the transition from the gaseous to the cluster regime.

We consider the clustering of ensembles of grains during excitation from external sources. The energy input stops the granular cooling, it can keep the total kinetic energy at a stable level. It is not necessary to excite all particles equally. A common option considered here is to employ vibrating container walls. Statistically, this excitation results in some spatial inhomogeneity, with higher velocity ('hot') particles near the vibrating walls and regions with higher particle number densities roughly halfway between the walls. This reminds one of the granular Leidenfrost effect described by

Eshuis et al. [15]. The transition from the homogeneous gaseous state into a cluster state was studied by Menéndez et al. [16] who established a state diagram with filling fraction and excitation strength as relevant parameters. Sizes, positions and stability of clusters depend on energy input and dissipation. Density inhomogeneities tend to dissolve when the excitation strength is reduced.

Two system parameters have been identified as the most important for the gas-cluster transition, viz. the number of particles in the system (defining the average particle number density), and the excitation strength [10]. A third parameter that was already considered in our earlier investigation is the phase shift between the oscillations of the two opposite vibrating container walls [13, 14].

While clusters can often be detected intuitively by visual inspection, a definition of quantitative criteria for a systematic classification is non-trivial. They should be suitable to classify experimental data, but one can derive and test them with simulated data sets. There are different options to define such criteria.

When one has only positional information in 2D or 3D from the experimental ensemble and no data of the particle dynamics, one may resort to simple criteria that were proposed earlier. We mention two established approaches, viz. the Kolmogorov–Smirnov (KS) test [5] and a caging criterion (CC), both based on the analysis of local packing fractions. A certain weakness of these approaches is that they both disregard dynamical features of the ensemble. In addition, the results of the KS-Test are sensitive to geometric limits and the chosen significance level, which requires careful selection and critical evaluation of the test parameters. In a previous publication [13], we have introduced a numerical simulation technique to create ‘synthetic’ data of the particle ensembles for selected sets of system parameters. It was shown that machine learning can be a promising approach to predict the state of the ensemble from known parameter sets after training.

Alternative approaches to KS and CC tests can be developed based on dynamical aspects like diffusion coefficients of individual particles and their statistical distribution. One can also analyze correlations of the motion of neighboring particles. These methods require more effort than the two classical tests listed above, in particular when applied to experimental data. They require the complex task of not only extracting 3D positions of the particles but also their tracking to retrieve the velocity data. This challenging goal is achieved much easier with simulated data sets where positions and velocities are easily accessible.

The next section introduces the main motivation of our work, followed by a section describing the experimental setup and the DEM based simulation software, and the statistical criteria used to quantify DC. In the fourth section, the results are presented, and the final section contains the conclusions and gives an outlook.

2 Motivation

In the present study, we compare possible structural and dynamical criteria to distinguish homogeneous and clustered states of a driven granular gas and we test their strengths, limits and reliabilities. As a basis of our analysis, numerical simulations are performed with the same software as in Ref. [17]. The geometry of our simulations

is derived from the VIP-Gran (*Vibration-Induced Phenomena in Granular Matter*) experiment setup [7] of the ESA Topical Team SPACE GRAINS [18], and we consider frictional spheres [13]. In our numerical DEM study, we employ a scheme introduced earlier [13] to systematically create ‘synthetic’ datasets that form the basis of the analysis. These data are generated for multiple sets of system parameters. Our final goal, which is beyond the scope of the present paper, shall be to train and evaluate different Machine Learning (ML) methods to detect clustering by using these data in a statistical analysis. The essential prerequisite for a classification with ML methods is the establishment of reliable quantitative criteria for clustering, which is attempted here. We will also examine the nature of the transition between homogeneous and clustered states when the system parameters are varied. This includes the question whether an objective criterion can be defined to distinguish clustered from homogeneous states.

3 Methods

In this section, we first briefly describe the experimental setup, and then give an overview of the DEM based simulation software. We resume the classical tests and suggest alternative criteria to characterize clustering.

3.1 The experimental reference system

Our reference system, the VIP-Gran setup (Fig. 1), consists of a closed cuboid cell containing granular particles that can be excited by two opposing vibrating walls. It is designed for experiments in microgravity, e. g. in a drop tower or on the ISS, and was used before in parabolic flights [7]. Two synchronized cameras allow quantitative stereoscopic measurements including particle tracking (in case of diluted systems) or visual flow and shadow density analysis (in case of dense granular ensembles, see Refs. [10, 19]), to extract packing fraction and mean velocity profiles. In previous experiments, the cameras recorded video footage with a frame rate of 900 frames per second (fps). The same experimental configuration was the basis for several earlier studies [5, 10, 12, 14] and of our previous numerical investigation [13].

The cross section of the container is $30 \times 30 \text{ mm}^2$. The two opposing piston walls with an initial distance of 40 mm are magnetically connected to voice coils that can shift the walls by $\pm 10 \text{ mm}$ against each other. Spherical grains can be placed directly into the cells prior to flight or injected using a special bead feeder during flight. The fill fraction is $\phi = N\pi d^3 / (6V_{\text{container}})$, where d is the diameter of the spheres, N is the number of particles, L_x, L_y, L_z are the container dimensions and $V_{\text{container}} = L_x L_y L_z$ is the averaged container volume.

The positions of the right and left walls along the excitation axis x are given by

$$w_1(t) = L_x/2 + A \sin(\psi(t)), \quad w_2(t) = -L_x/2 + A \sin(\psi(t) + \theta), \quad (1)$$

where $x = 0$ corresponds to the container center, $\psi(t) = 2\pi ft$, f is the excitation frequency, θ is the phase shift of the two pistons, t is the time. The excitation period is $T = 1/f$. In individual runs of the experiment, the excitation parameters as well as the number of particles N can be systematically varied.

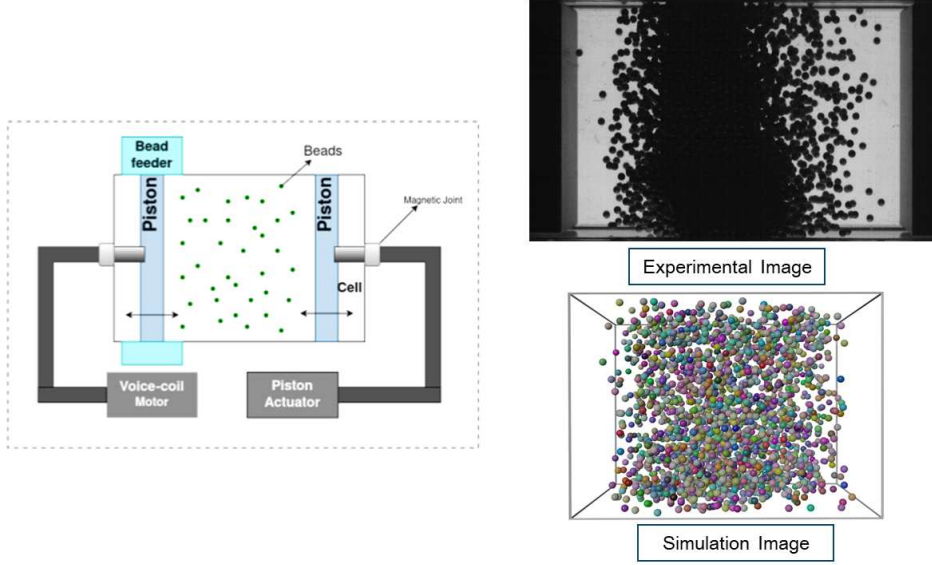


Fig. 1: Left: Cross-sectional view of the of the VIP-Gran experiment with spherical grains. Right: Snapshots from experimental images recorded during a Parabolic Flight Campaign (top) and from CPU-GPU hybrid DEM simulation [17] (bottom). The schematic image and experimental footage were adapted from material kindly provided by the ESA Space Grains topical team [18]. Colors are used for visualization purpose only; all particles are physically identical.

Table 1: Constant parameters used in the simulations, same as in Ref. [13]

Symbol	Parameter Name	Value
ρ	Particle density	8730 kg/m ³
d	Particle diameter	1 mm
m	Particle mass	4.57 mg
Y	Young's modulus	5 MPa
ν	Poisson ratio	0.3
μ	Coefficient of friction	0.4
ε	Coefficient of restitution	0.85
f	vibration frequency	15 Hz

3.2 Numerical simulations

As numerical scheme, we used a hybrid CPU-GPU based Discrete Element Method (DEM) [17, 20], which takes advantage of the parallelism inside GPUs. Very similar to Ref. [13], we simulate the mechanically excited ensemble, and obtain particle positions, velocities and orientations using realistic material parameters.

Table 2: Variable parameters used in the simulations, same as in Ref. [13]

Symbol	Parameter Name	Range
$N(\phi)$	Number of particles (filling fraction)	[1834, 5643] (2.7%, 8.2%)
A	Piston amplitude	[2 mm, 5 mm]
θ	Relative phase shift of pistons	π

The simulation software models particle interactions using spheres with a diameter of $d = 1$ mm and density 8730 kg/m^3 , which corresponds to bronze. Collisions between particles, as well as between particles and the walls, were modeled using the Hertz-Mindlin contact model. The normal Young’s modulus was set to $E = 5$ MPa, the Poisson’s ratio to $\nu = 0.3$, and the normal restitution coefficient to $e_n = 0.85$. For simplicity, the shear modulus was $G = 0.5 E$, and the tangential restitution coefficient was set equal to the normal coefficient ($e_t = e_n$). The friction coefficient between particles and the particles-wall was set to $\mu = \mu_w = 0.4$ [12]. The ranges of all parameters varied in this study are detailed in Tab. 2 and the integration time step was $\delta = 10^{-7} \text{ s}$. Although the used value of Young’s modulus is unrealistically low for metallic spheres, this choice was found appropriate for our purposes [13] and does not affect the simulation results. In all cases, the low characteristic particle speed result in a maximum particle overlap lower than 2.5% in terms of the particle diameter.

The choice of phase shifts between the two wall vibrations was restricted here to anti-phase ($\theta = \pi$) piston movement. This has two consequences. First, the cell volume alternates periodically. Second, the excitation is symmetric, so that the potential central cluster experiences a statistically equal impact from both sides during the entire excitation cycle.

After some initial transients, the ensemble dynamics generally synchronizes with the wall excitation (see [10] for details). For simplicity, we count the duration of the simulations in units of excitation periods. The simulation output was saved for every 10000 iterations. In accordance with the experiment, we will refer to instant snapshots of the granular gas as ‘frames’, corresponding to a rate of 900 frames/second. Each run consisted of 120 excitation periods, where the first 60 periods were discarded in the statistical analysis. Our simulations, along with previous investigations [10, 13, 21] show that this period is long enough for the system to “forget” the initial distribution of particle positions and velocities and to reach a stable dynamical state, dependent only on the system properties and excitation parameters.

3.3 Classical clustering test criteria

Structural clustering criteria require much less evaluation efforts than dynamical ones when applied to the experimental data. The latter require 3D positions of the particles and the reconstructions of the velocity components by particle tracking.

The fundamentals of the Kolmogorov-Smirnov test (KS test) in our system were described in detail in previous publications [5, 10, 13, 22], thus we recollect only briefly its concept: The test quantifies the distance between the actual cumulative distribution

of particles $U(x)$ in the sample and the homogeneous distribution $u(x)$ of an ideal gaseous state as the null hypothesis [22]. The cumulative distribution function $U(x)$ is calculated by counting particles with coordinates along the excitation axis that are smaller than x , normalized by the total number of particles. The supremum distance between the two distributions, $D_{\max} = \sup_{w_1 < x < w_2} |U(x) - u(x)|$, is determined for the full period. When $D_{\max}$ exceeds a given threshold T , the system is classified as clustered. The minimum of the differences $T - D_{\max}$ between across all periods, $\delta_{\min}$, is estimated for a given set of system parameters $\{N, A, \theta\}$ using KS test [13].

Alternatively, clusters can be identified by the caging effect [5], and the application of this criterion to our system was explained in Ref. [13] as well. Particles entering a cluster get caged inside and their kinetic energy is dissipated to a large part in inelastic collisions. The concept of Voronoi tessellations is closely related to this criterion. The maximum value of the ratio between the number of caged particles N_{caged} and N in the system is obtained for each ψ across all phases defines the maximum fraction of caged particles, φ_{caged} . It has been extensively used to study the transition between states of multiparticle systems in previous work [13, 23, 24]. This studies motivated us to investigate Probability Density Functions (PDFs) of local packing fractions in different oscillation phases $\psi(t)$.

Although relatively simple and less demanding, these structural characterization methods do not explicitly capture the dynamical properties of clusters, and thus disregard some essential features associated with the motion of the particles.

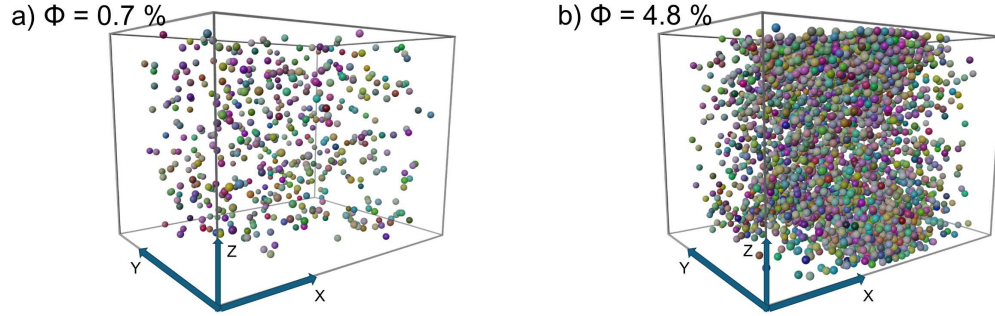


Fig. 2: Snapshots of simulated gaseous (a) and cluster states (b) which contain 500 particles ($\phi = 0.7\%$) (a) and 3357 particles ($\phi = 4.8\%$) (b), respectively. Data were taken from CPU-GPU hybrid DEM simulations [17] of frictional spheres, rendered using the Blender 3D software.

3.4 Dynamical clustering test criteria

The following test criteria focus on the specific particle dynamics in clusters.

In this approach, we consider the displacements of spherical particles in the three spatial directions x , y , and z . The Probability Distribution Functions (PDFs) for these displacements are extracted for different sets of N and A , respectively. The primary reason for choosing these PDFs is that they specify how far the particles are displaced

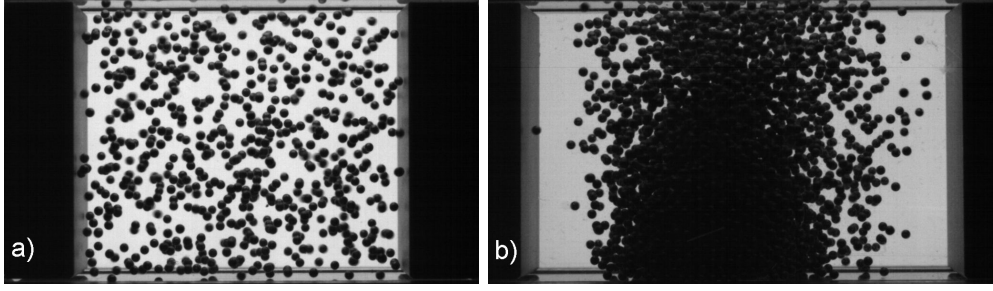


Fig. 3: Snapshots of experimental gaseous (a) and cluster (b) states containing 750 particles ($\phi = 1\%$) (a) and 6500 particles ($\phi = 8.7\%$) (b), respectively. Excitation parameters are $A = 1.8$ mm, $f = 20$ Hz (a) and $A = 4$ mm, $f = 15$ Hz, respectively. The phase shift is $\theta = \pi$. These snapshots were taken during a Parabolic Flight Campaign.

within a specific time period. This feature may help to characterize the state of a given configuration, gaseous or clustered, in particular when the graphs are analyzed in the limits of small displacements. As a simple qualitative feature, one may choose the intersections of the PDF with the ordinate. In a gaseous state, the probability of having near-zero displacements is very small. The particles move freely in each direction within the container, and the case where all three displacement components vanish simultaneously is negligible (cf. the Maxwell-Boltzmann distribution of a molecular gas). When the particles start to cluster, the probability of near-zero displacements increases because of caging. Hence the corresponding PDFs intersect the ordinate axis in reasonable distance from the origin. These PDFs are extracted for various time windows, and their ordinate intersections are taken as important features for given system configurations $\{N, A\}$.

Another sign of clustering is the decrease of the number of free particles interacting with the pistons. The simulation software do not explicitly register such collisions during runtime, due to the frequent CPU-GPU communication would create a severe performance bottleneck. Instead, particle-piston collision were detected a posteriori by combining a velocity-reversal criterion with a wall-proximity threshold: a collision is registered when the x -component of a particle's velocity changes sign with a given magnitude and the particle is located within 1 mm of a piston wall. Because the wall-proximity region is very dilute, it did not impact the further analysis.

One may additionally normalize the number of collisions by the total number of particles and compute the mean particle-wall collision frequency. As is demonstrated later on, it gives an aggregate measure of how intensely the particle ensemble interacts with the driving walls.

Complementarily, we investigate the dynamic behavior via the distribution of the squared speed $v^2 = v_x^2 + v_y^2 + v_z^2$. The PDFs of v^2 is determined for consecutive time intervals and relevant properties of these PDFs are also evaluated.

We also analyze the correlations of motions of neighboring particles. In a homogeneous gas state, there should be little or no such correlation, whereas the velocities in clusters should be correlated to a certain extent. To quantify local velocity correlations,

we evaluate the directional coherence of motion of directly neighboring particles. For each nearest-neighbor pair (i, j) , the cosine of the angle γ_{ij} is given by the normalized scalar product of their instant velocities:

$$\cos \gamma_{ij} = \frac{\mathbf{v}_i \cdot \mathbf{v}_j}{\|\mathbf{v}_i\| \|\mathbf{v}_j\|} \quad (2)$$

We consider all pairs of particles and their nearest neighbors in a given frame (at a given time) and calculate the ensemble averaged first and second Legendre polynomials of $\cos \gamma_{ij}$, S_1 and S_2 . The hypothesis is that a strongly coordinated motion within a cluster should yield significant deviations of these two parameters from zero, whereas uncorrelated motion yields $S_1 = S_2 = 0$. The regions near the piston walls must be excluded, because collisions with these walls naturally generate correlations of the velocities in x direction in all cases.

$S_1(t) = \langle \cos \gamma_{ij} \rangle$, measures directional alignment. It ranges from $S_1 = 1$ for fully parallel motion to $S_1 = 0$ for uncorrelated motion or mirror-symmetric distributions. High values should indicate collective directional migration typical of cohesive clusters. Similarly, $S_2(t) = \langle \frac{3}{2} \cos^2 \gamma_{ij} - \frac{1}{2} \rangle$, measures the velocity alignment regardless of the sense of direction. It ranges from $S_2 = 1$ for strictly parallel or antiparallel motion and $S_2 = 0$ for isotropic motion to $S_2 = -\frac{1}{2}$ for the unrealistic case of mutual strictly perpendicular instant velocities.

The PDFs of displacements, squared speeds and velocity correlations are extracted over 60 consecutive oscillation periods, starting from the 60th oscillation period. The collision statistics are determined for 40 oscillation periods, starting from the 60th oscillation period. All these data can be in principle concatenated so that the complete feature set encodes information on both the structural and dynamical states of the particle ensemble, towards an objective quantitative characterization of the system.

4 Results and Discussion

We restrict our analysis to antiphase excitation ($\theta = \pi$) but the approach is practically the same for other phase shifts. Simulations were performed for a set of filling fractions ϕ , with the number of particles N chosen as 1834 ($\phi = 2.66\%$), 2214 ($\phi = 3.2\%$), 2595 ($\phi = 3.7\%$), 2976 ($\phi = 4.3\%$), 3357 ($\phi = 4.8\%$), 3738 ($\phi = 5.4\%$), 4119 ($\phi = 5.98\%$), 5262 ($\phi = 7.64\%$) and 5643 ($\phi = 8.2\%$) and different excitation amplitudes A between 2 and 5 mm. These combinations of parameters guaranty a representative sampling of the phase space.

4.1 Distributions of Local Packing Fractions

We start with the static, structural features. The distribution of local packing fractions is closely related to the definition of caging. Figure 4 shows the distribution of Voronoi cell volumes and local packing fraction φ_{loc} at $A = 2$ mm.

With increasing N , the fraction of particles that are considered caged (φ_{caged}) (red dashed line) increases. The numerical threshold value $\varphi_{\text{loc}} = 0.285$ was derived geometrically [5], but is in fact more or less arbitrary. Thus, the classification of

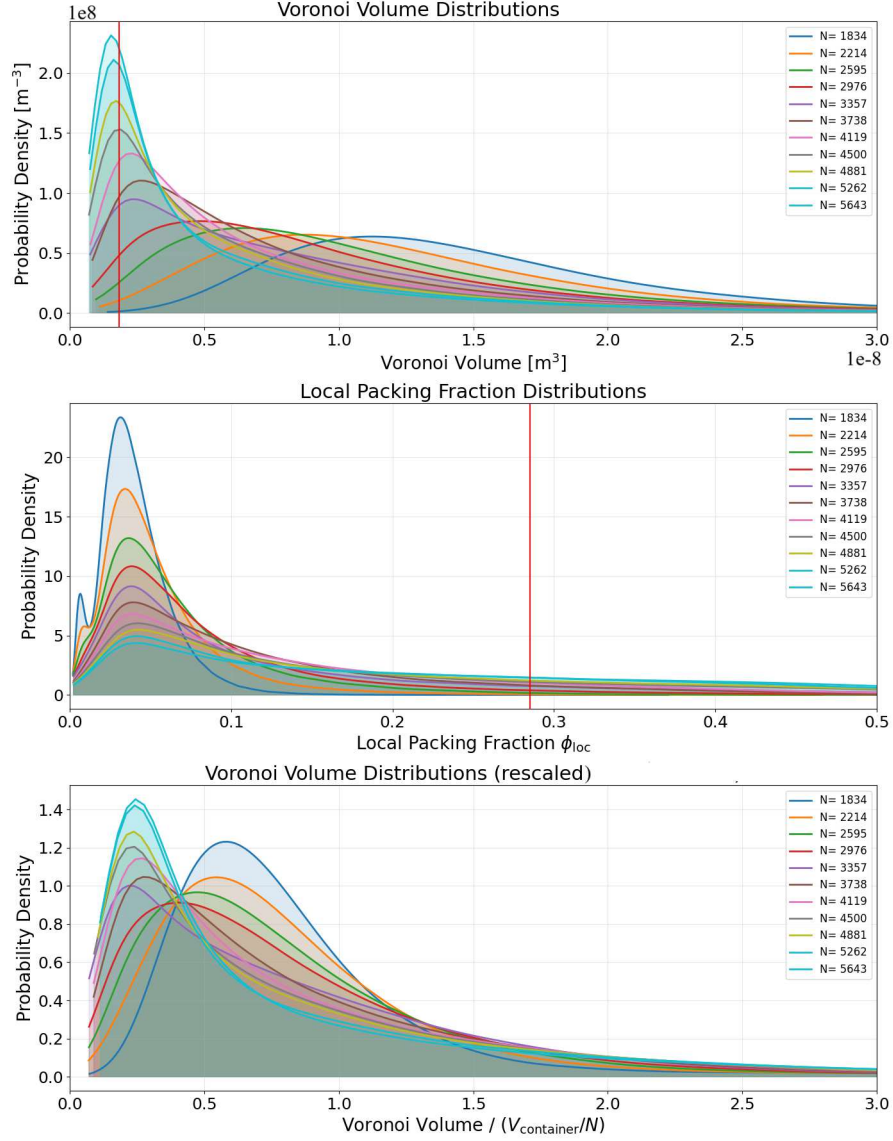


Fig. 4: The first two plots show the Voronoi volume and local packing fraction distributions at $A = 2$ mm for different N . In the first plot, the distributions of the Voronoi cell volumes is shown. The vertical red line marks the critical volume corresponding to the caging threshold ($\phi_{\text{loc}} = 0.285$ as proposed earlier [5]). The second plot gives the distributions of the local packing fraction ϕ_{loc} , with the same threshold indicated by a red line. As N increases, both distributions shift continuously without showing threshold-like signatures. The third plot shows the distribution of Voronoi volumes rescaled with the mean packing fraction (ratio $V_{\text{container}}/N$).

the system as clustered or homogeneous is rather subjective. However, any threshold definition between 0.2 and 0.4 would not qualitatively change the classification. The transition stretches continuously over a broad range of N . When one scales the Voronoi volume distributions by the mean volume per particle $V_{\text{container}}/N$, the distributions show a certain qualitative change at $\phi \approx 4\%$. The distribution maxima shift from values > 0.4 at lower fill fractions to > 0.4 at denser filling.

The plots in figures 5 and 6 show the influence of the excitation amplitude A . In the dilute system, a significant influence of A is seen. The system is much more homogeneous at $A = 2$ mm than at higher excitation, indicating a transition to a more clustered distribution. In the denser system, the differences between the graphs are not significant, the system can be considered clustered for all excitations. The mode (peak position) of the distribution of rescaled Voronoi volumes appears at values $\tilde{\varphi}_{\text{Vor}} > 0.4$ only at the lowest amplitude and the low filling fraction. In all other graphs it is smaller, indicating clustering. This is consistent with the conclusions drawn from Fig. 4.

Summarizing, the Voronoi analysis clearly demonstrates the dependence of the structural factors on packing fractions and amplitudes without providing arguments for the objective definition of a clear threshold, rather indicating a broad region of continuous transition between gas- and liquid-like phases in the parameter space.

4.2 Probability Distribution Functions of dynamical features

We consider now the distributions of displacements of the particles after certain time lags, which reflects an essential feature of the ensemble dynamics. In contrast to the established methods proposed earlier, KS test and caging criterion, this analysis considers the dynamics of clusters: Inside a cluster, the individual particle displacements are hindered. While instant velocities may still be large, the absolute displacements remain small and restricted to the cage, which moves only on long time scales.

4.2.1 Distributions of absolute displacements

Figure 7 shows the distributions $P_d(\Delta s)$ of absolute displacements Δs of the individual particles for time lag of four excitation periods, $\Delta t = 4T$, $A = 2$ mm.

The statistics are obtained over an observation window of excitation periods, starting after 60 excitation periods to exclude transients. With increasing number of particles N , the probability density for very small displacements increases, reflecting caged spheres. As a significant feature, one may evaluate the intersection P_0 with the ordinate, shown in Fig. 8 for different N . P_0 increases monotonically with N . For low filling fractions up to about $\phi = 4\%$ ($N=2700$), the value is close to zero, almost all particles move freely. The probability density of near-zero displacements as a signature for caged particles increases with N , again indicating the smooth transition from the homogeneous to the clustered state.

A second prominent feature of the transition to the clustering regime is that a peak (mode) of P_d is formed at small displacements. For a quantitative comparison, we take the mean distance of particles to their next neighbor $r_n = \Gamma(4/3) \phi^{-1/3} d/2$

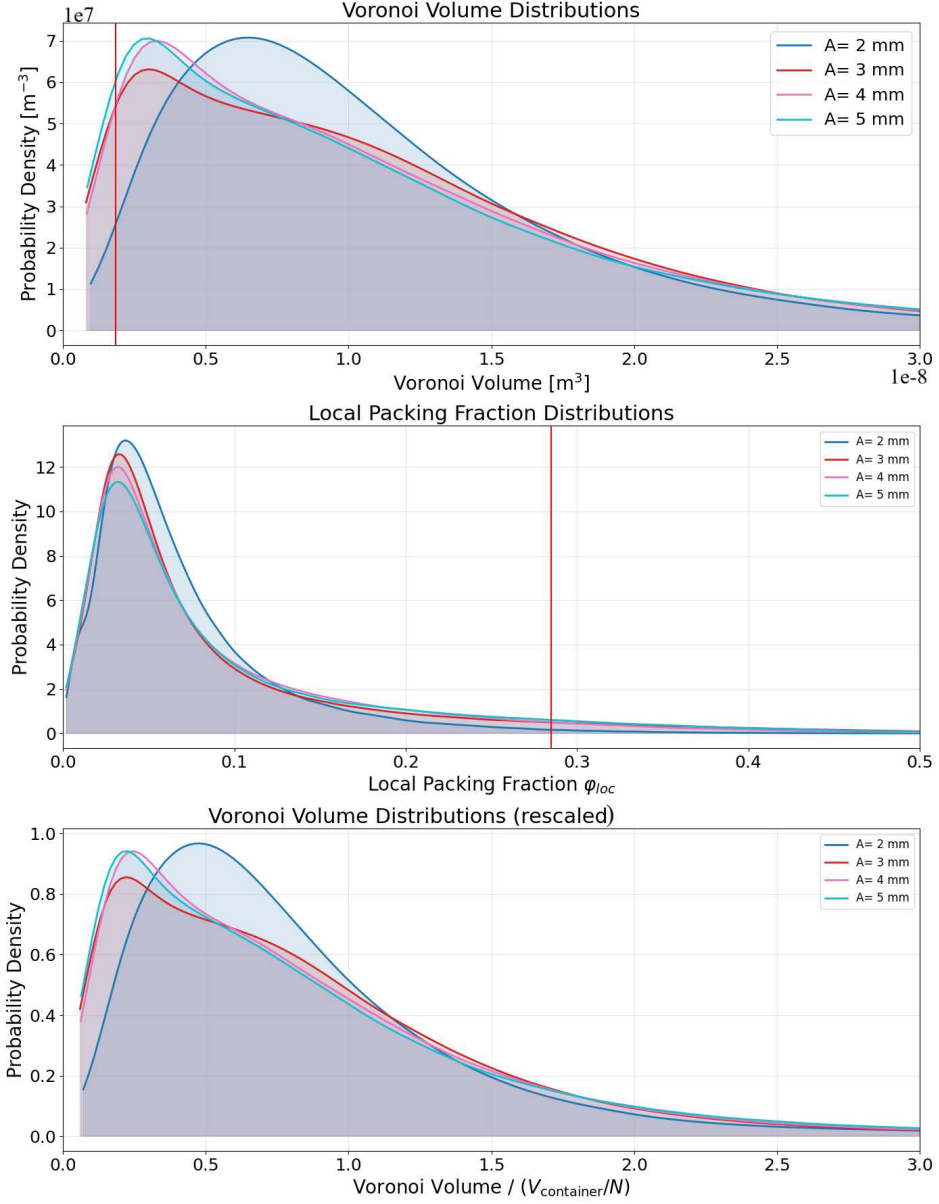


Fig. 5: The first two plots show the Voronoi volume and local packing fraction distributions at a low fill fraction of $N = 2595$ for different amplitudes A . The top plot shows the distributions of the Voronoi cell volumes with the vertical red line marks the Voronoi volume corresponding to ($\phi_{loc} = 0.285$). The second plot shows ϕ_{loc} , with the same threshold indicated by a red line. In the bottom plot, the Voronoi volume were rescaled with $V_{\text{container}}/N$ as above.

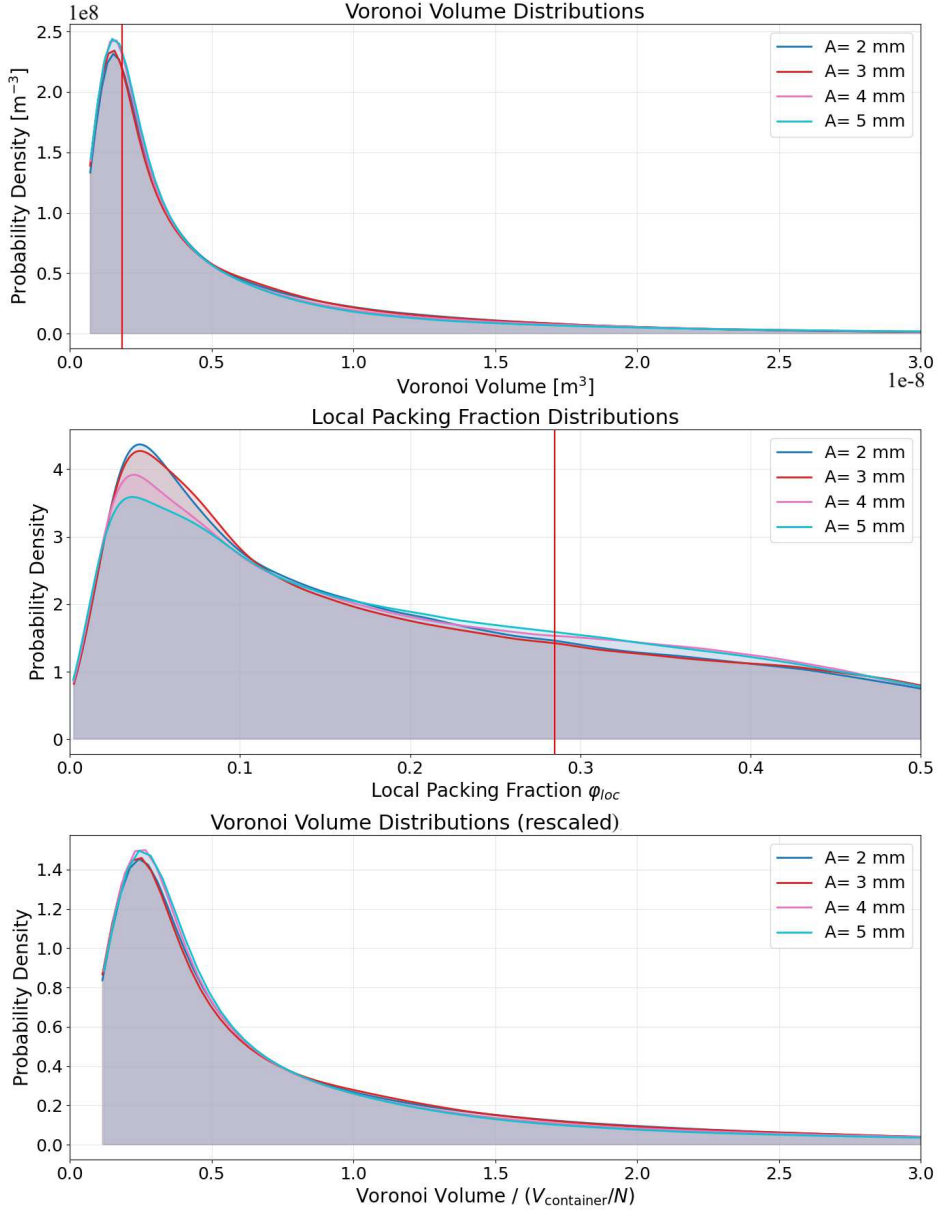


Fig. 6: The top plot shows the distributions of the Voronoi cell volumes at the densest computed ensemble with $N = 5643$ for different A , and the second plot show the distributions of ϕ_{loc} . The red lines have the same meanings as in Fig. 5. In the bottom graph, the Voronoi volumes were rescaled with $V_{\text{container}}/N$. The system is considered clustered for all amplitudes.

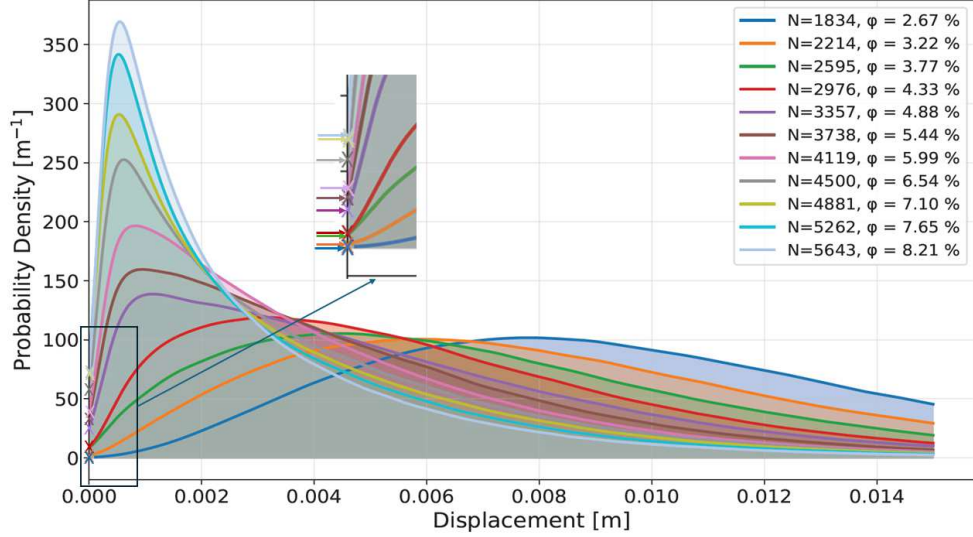


Fig. 7: Distributions $P_d(\Delta s)$ of absolute displacements of spherical particles during a time lag of $\Delta t = 4T$, $A = 2$ mm and $\theta = \pi$. Colored arrows indicate the ordinate intersections marked by crosses.

[25] as a scaling measure ¹. For the range of ϕ considered in our simulations, it yields values between 1.0 (most dense) and 1.5 mm (most dilute). Figure 7 shows that for dilute ensembles ($\phi < 4\%$), the peak of the PDF lies well beyond r_n , while for larger ϕ , the pronounced peak is at smaller distances. This indicates that a large percentage of particles are trapped in clusters.

The role of the excitation amplitude is shown in Figs. 9, 10, and 11. Note that in all three plots, a higher excitation strength is connected with an overall broadening of the distributions, because the mean energy entry is higher and the particles are statistically faster. At a sufficiently low fill level (Fig. 9), the majority of displacements is well beyond r_n for all excitation strengths. A subtle peak is formed at smaller displacements at stronger excitation, indicating that few particles may be trapped in small clusters structures, but the prominent share of particles is still moving unconstrained. At intermediate fill levels (Fig 10), the excitation intensity has a larger influence, but there is no clear transition from the free homogeneous to a clustered state. Rather, it seems that the displacements reflect a quite uniformly distributed state at low excitation ($A = 2$ mm), then stronger excitation forms a dominant peak at small displacements (1 ... 2 mm), indicating the beginning of clustering. High excitation strength ($A > 4$ mm), however, destroys the spatial inhomogeneities again, and the small-displacements peak disappears. For the largest fill level (Fig. 11), the system is in a clustered state at all excitation strengths. The distributions simply broaden because of the higher mean particle velocities when the excitation amplitude is increased.

¹This result is for 3D point clouds, it does not reflect exactly the actual mean distance of spheres

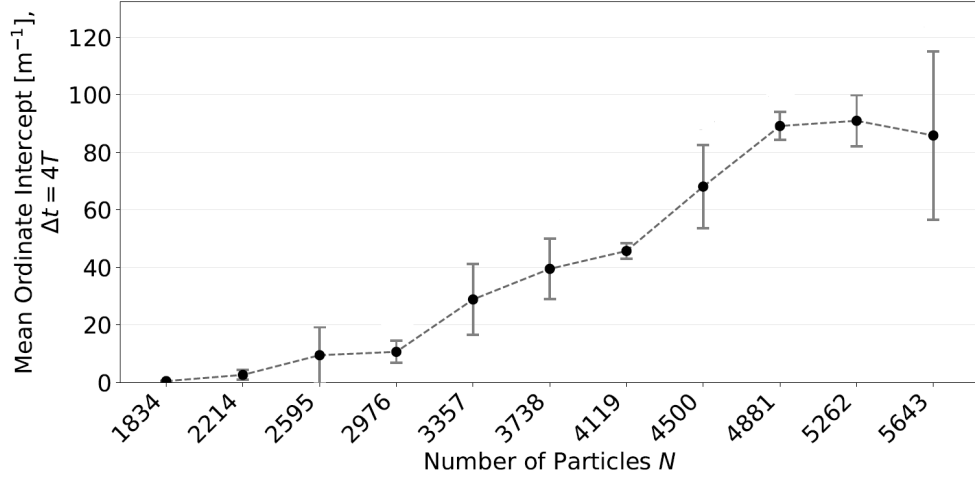


Fig. 8: Variation of the ordinate intersection $P_0 = P_d(0)$ with N , $\Delta t = 4T$, $A = 2$ mm and $\theta = \pi$. Error bars mark deviations between three individual runs of each parameter set.

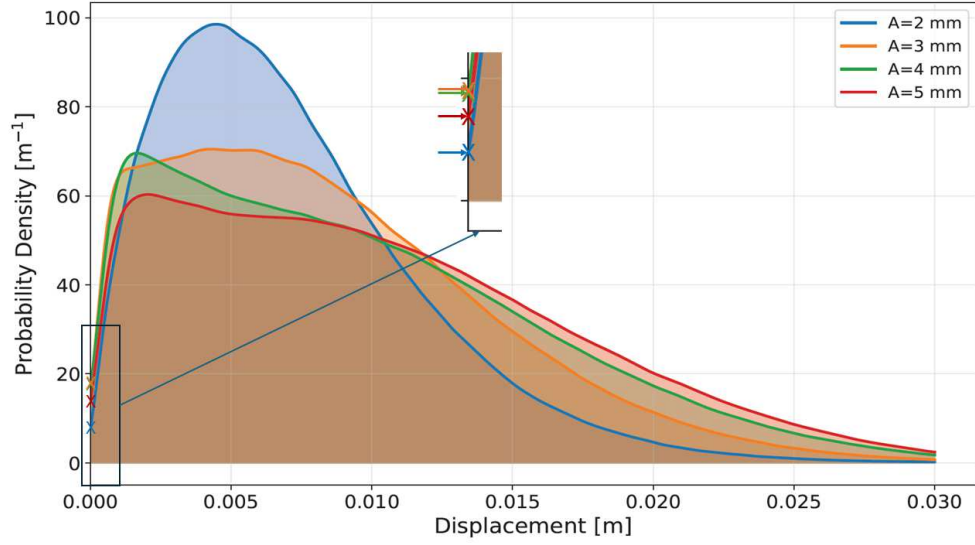


Fig. 9: Distributions $P_d(\Delta s)$ of absolute displacements for time lag $\Delta t = 4T$, $N = 2595$ ($\phi = 3.7\%$) particles and $\theta = \pi$. Crosses indicate ordinate intersections and colored arrows represents corresponding N .

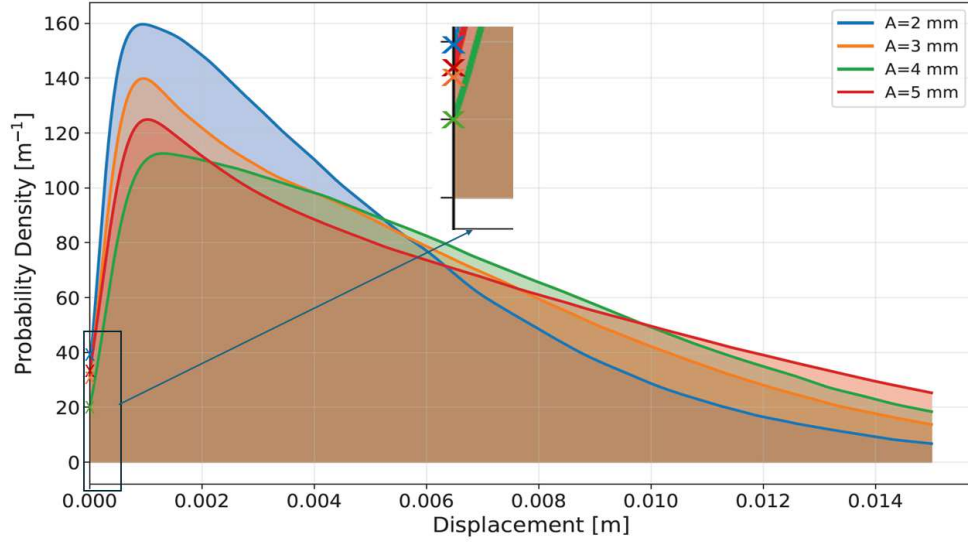


Fig. 10: Distributions $P_d(\Delta s)$ of absolute displacements for $\Delta t = 4T$, $N = 3738$ ($\phi = 5.4\%$) particles and $\theta = \pi$. Crosses mark the ordinate intersections. Colored arrows indicate ordinate intersections (crosses) for the different N .

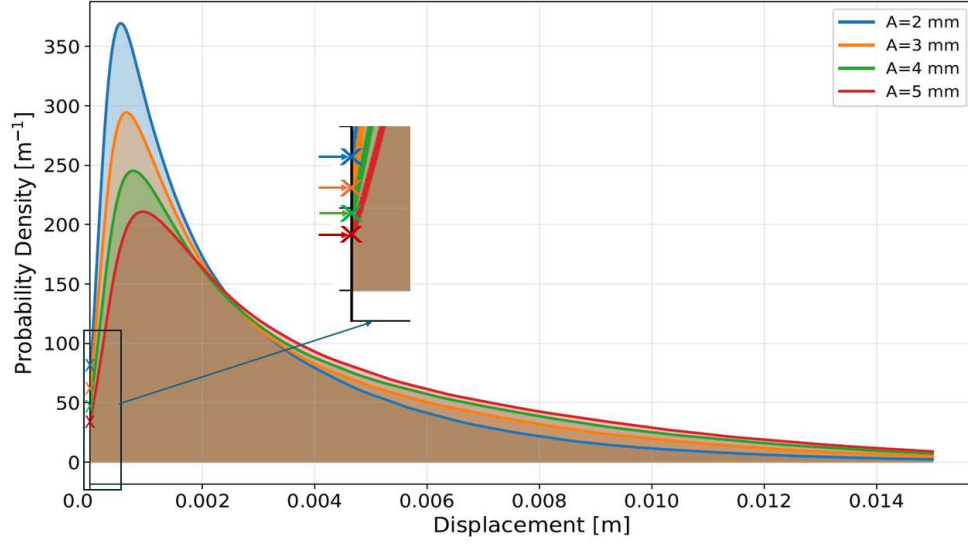


Fig. 11: Distributions $P_d(\Delta s)$ of absolute displacements for $\Delta t = 4T$, $N = 5643$ ($\phi = 8.2\%$) particles and $\theta = \pi$. Crosses mark the ordinate intersections. Crosses indicate ordinate intersections and colored arrows represents corresponding N .

4.2.2 Piston Collision Counts

Another signature of clustering is that the majority of particles assemble far from the moving pistons. Thus, the frequency of collisions of particles with the pistons strongly depends upon the homogeneity of the ensembles. The results of the analysis of this quantity are shown in Fig. 12. There was no statistically significant variation of the collision numbers with the left and right piston walls; thus their sum n_c is shown. We also included results of simulations with more dilute ensembles, $N = \{500, 1000, 1500\}$.

The total collisions-per-particle metric (Fig. 12) increases monotonically from low A , high N to high A , low N . Individual particles collide more frequently at low N and high A . The dependence of the wall collision number on the amplitude A can easily be explained. It is a consequence of the faster dynamics at higher energy entry when N is kept constant, and of the increased volume swept by the moving walls. Because the influence of the excitation amplitude on the homogeneity of the sample is small, stronger excitation causes a higher collision rate in both homogeneous and clustered states.

The influence of the filling fraction is counterintuitive at first glance: The collision frequency per particle decreases monotonically when more particles are in the box. At the same time, the total collision number increases with N in very dilute ensembles but then starts to decrease with N . Two effects are responsible for that. The first one is that there are many more particle-particle collisions in the denser medium since the mean free path length is smaller. The strongest influence, however, has the accumulation of particles in the center of the cell due to cluster formation.

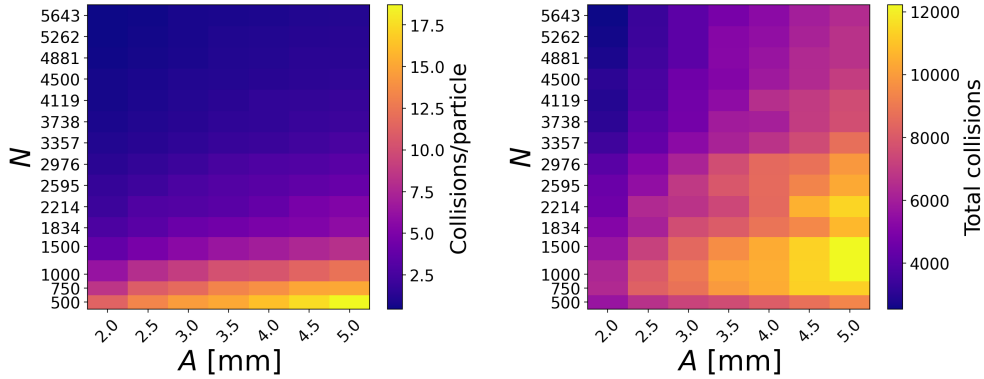


Fig. 12: Variation of collisions per particle (left) and total collisions n_c (right) during 40 periods across all N and A utilized in this work ($\theta = \pi$).

To understand this effect in detail, total number of collisions as a function of N for three fixed amplitudes A is shown in Fig. 13. The roughly linear increase with N in dilute ensembles is directly related to the increasing particle number density in the nearly homogeneous gas. A maximum is reached at $N \approx 1000$ – 1500 , then the collision rate decreases monotonically as clustering sets in near the center of the box. In fact, this feature, the position of the peak as a function of the number of particles, appears

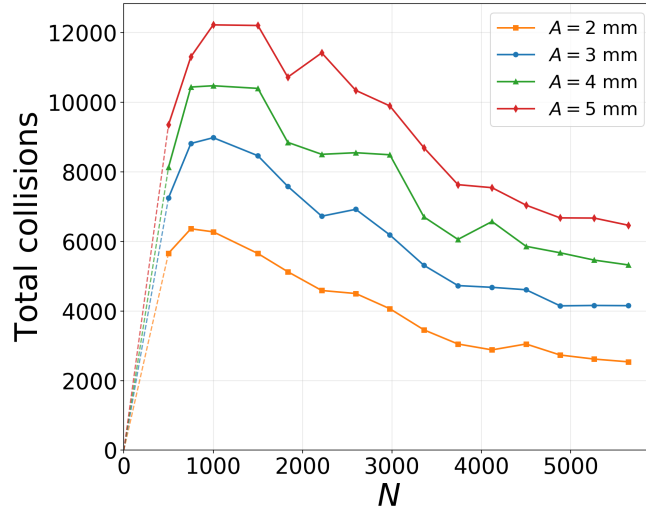


Fig. 13: Variation of total number of collisions n_c with the piston as a function of N , for $A = 2$ mm, $A = 3$ mm, $A = 4$ mm and $A = 5$ mm (including dilute ensembles with $N = \{500, 750, 1000, 1500\}$).

to be a reliable indication of cluster formation at constant excitation amplitudes. We consider it as the most reliable quantitative feature that helps to distinguish the clustered from homogeneous states. The disadvantage is that one needs to analyze the N dependence and one cannot classify individual ensembles. It is not helpful when only different excitation amplitudes are compared.

4.2.3 Distributions of Squared Velocities

As the mobility of particles in clusters should be strongly restricted, and the granular temperature is expected to be lower in the clusters than in the rest of the gas, we tested the distributions of squared velocities for signatures indicating cluster formation. The result is shown in Fig. 14.

The graphs show the distributions of squared velocities. As N is increased in the container, all particles show a significant drop in their mean velocities caused by a higher frequency of inelastic collisions. On the other hand, the shape of the curves remains practically unchanged except for the rescaled velocity scale. The curves are stretched by roughly the inverse of the particle number density (in accordance with the expected average collision rate). The bimodal character of the curves is a consequence of the periodic excitation, the high-energy peak belongs to the phase when the pistons move inward, while the low-energy peak is formed when the pistons move outward.

Figure 15 shows the distributions of squared velocities for varying A and fixed $N = 3738$. Again, the role of increasing A is a broadening of the curves, but there is no noticeable qualitative change in the distributions. As with the dependence on the particle number density, there is no signature of clustering in these curves.

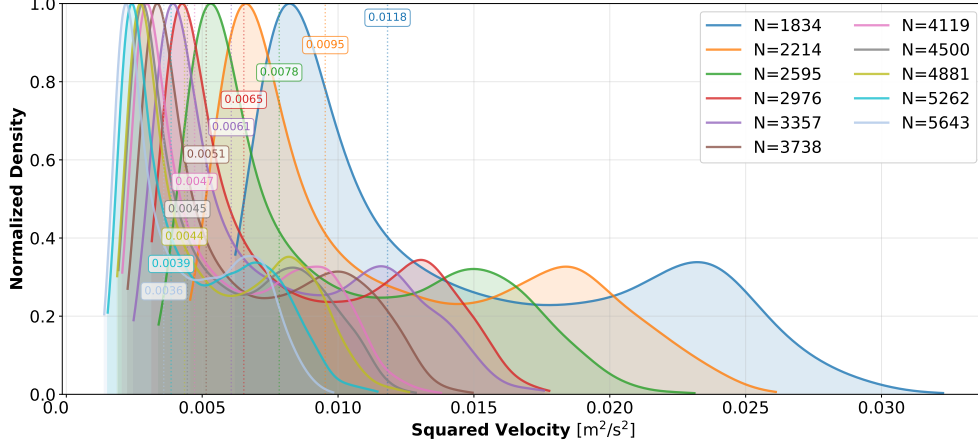


Fig. 14: Distributions of squared velocities for different N , excitation amplitude $A = 2$ mm. The dashed lines represent median velocities in m^2/s^2 .

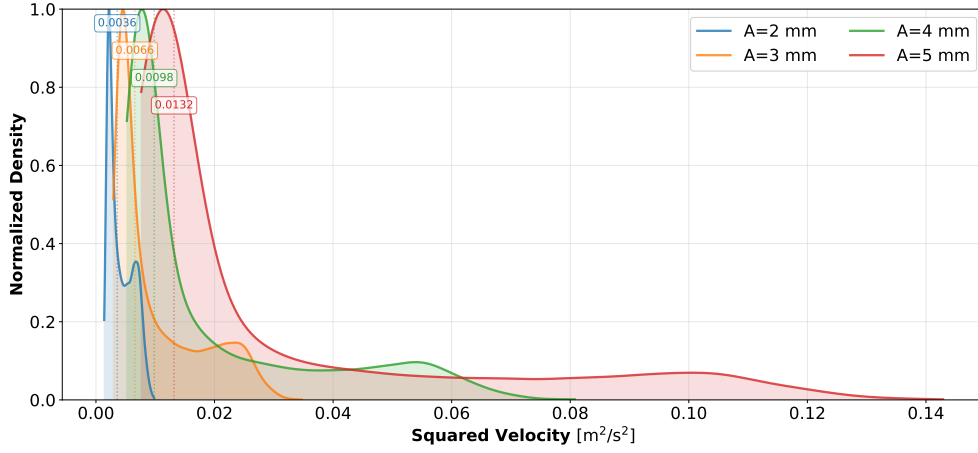


Fig. 15: Distributions of squared velocities for different A , where N and θ are fixed at 5643 particles and π , respectively. The dashed lines represent median velocities in m^2/s^2 .

4.2.4 Distributions of particle velocity alignments

To capture correlated motion of neighboring particles, we computed for each nearest-neighbor pair (i, j) the angle γ_{ij} between their velocity vectors. We evaluated $S_1 = \langle \cos \gamma_{ij} \rangle$ for each simulation frame (frame rate $60/T$), where the average is over all pairs of particle. It was compiled for 60 oscillation periods. This quantity is sensitive to correlated motions. Another characteristic quantity, $S_2 = \langle 3 \cos \gamma_{ij} - 1 \rangle / 2$, is insensitive to the sense of direction. Figure 16 shows the distributions of S_1 for particles

close to the center of the container, sufficiently far from the pistons. This corresponds roughly to the region where clustering takes place. The total average of S_1 increases with N . Since this quantity is independent of absolute velocities, it is a clear signature of collectivity in the motion of neighbors, and thus indicates the degree of clustering. Near the pistons, particles always show correlations in their motion because when they leave the wall, they have a preferential velocity component v_x . S_1 is not useful there for characterizing a correlated cluster motion. Thus, we excluded these regions.

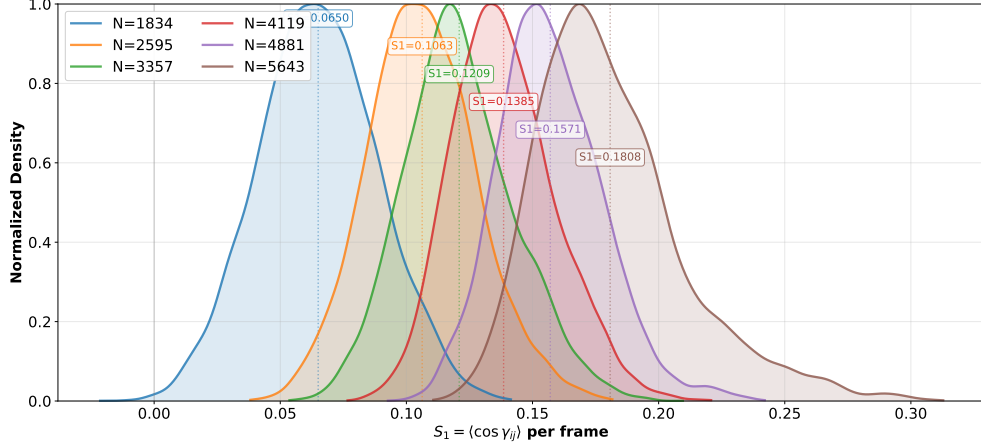


Fig. 16: Distribution of S_1 in the middle region of the cell for varying N with $A = 4$ mm. Each $S_1(t)$ is calculated as the average of $\cos \gamma_{ij}$ over all particles at a given instant (within individual frames).

Figure 17 shows the distribution of S_2 in ensembles with different filling fractions. A clear trend is seen in the dependence on N : At low particle number densities, the distribution is centered around zero, and with increasing N , the distribution shifts to positive values, while its width remains quite constant. This is a signature of clustering, but no threshold behavior is found.

4.2.5 Effect of initial conditions on $\delta_{\min}$ and φ_{caged}

Before we draw the final conclusions of the study, it remains to be tested how different initial conditions of the simulations affect the outcome of the evaluations. We show this by the example of KS and Caging tests for two different filling fractions. To assess the sensitivity of the results to different initial conditions, each configuration was simulated with four different SEED parameters (450, 650, 750 and 850). For each particle number N and phase shift θ , Tables 3 and 4 report the mean ($\bar{\delta}_{\min}$ and $\bar{\varphi}_{\text{caged}}$), the sample standard deviation σ and the coefficient of variation of $\delta_{\min}$ and φ_{caged} , respectively. For the KS test, $\delta_{\min}$ is highly reproducible across seeds: the magnitude of the COE remains below 0.07 for all cases, with the largest variation found for $N = 4119$ and $\theta = 0$ ($|\text{COE}| = 0.0655$). For the caging criterion, $N = 4119$ yields

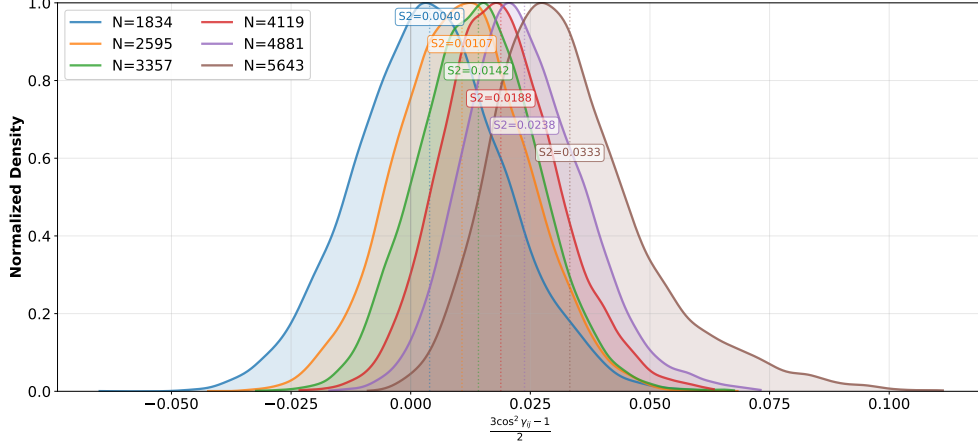


Fig. 17: Distribution of $S_2 = \langle \frac{3}{2} \cos^2 \gamma_{ij} - \frac{1}{2} \rangle$ in the middle region $-10 \text{ mm} < X < 10 \text{ mm}$ for varying N with $A = 4 \text{ mm}$. S_2 is the average of $(3 \cos^2 \gamma_{ij} - 1)/2$ over all particles within individual frames.

a consistent mean caged fraction of $\bar{\varphi}_{\text{caged}} \approx 0.13$ for both $\theta = 0$ and $\theta = 1$, with a COE of approximately 0.12. For $N = 1834$, φ_{caged} is effectively zero for all seeds (at most 3.4×10^{-5}).

Table 3: Statistics of $\delta_{\min}$ (KS test) over four seeds.

N	θ	$\bar{\delta}_{\min}$	$\sigma_{\delta_{\min}}$	COE = $\sigma_{\delta_{\min}}/\bar{\delta}_{\min}$
1834	0	-0.018397	0.000552	-0.0300
1834	π	0.017417	0.000633	0.0363
4119	0	-0.096485	0.006315	-0.0655
4119	π	-0.045458	0.001213	-0.0267

4.3 Influence of N and A on structural and dynamical features

Figure 18 shows the influence of N and A on the evaluated features. The graphs give on first glance a rather inconsistent picture. Within the range of simulation parameters, four of the computed quantities, P_0 , φ_{caged} , S_1 and S_2 , show a monotonically increasing trend with increasing N . The remaining two (wall collisions per particle n_c and scaled Voronoi volumes distribution modes $\bar{V}_{\text{Vor}}$) exhibit the opposite trend. All these quantities reflects a gradual, threshold-less smooth transition from the homogeneous gas to clustering. Since these trends are strongly correlated or anti-correlated, they may serve as a semi-quantitative measure of cluster formation at constant excitation,

Table 4: Statistics of φ_{caged} (caging criterion) over four seeds.

N	θ	$\bar{\varphi}_{\text{caged}}$	$\sigma_{\varphi_{\text{caged}}}$	COE = $\sigma_{\varphi_{\text{caged}}}/\bar{\varphi}_{\text{caged}}$
1834	0	2.556×10^{-5}	1.704×10^{-5}	0.667
1834	π	8.520×10^{-6}	1.704×10^{-5}	2.000
4119	0	0.13494	0.01606	0.119
4119	π	0.12529	0.01474	0.118

where clustering appears to be connected with larger P_0 , φ_{caged} , S_1 and S_2 and smaller wall collision rates and scaled Voronoi volumes. It is understood straightforwardly what causes these trends at constant excitation.

However, the dependence of these features on excitation amplitudes shows a very different picture. Here, we find three features (S_1 , S_2 and φ_{caged}) that show only a very dependence on amplitude A for all N , one feature ($\bar{V}_{\text{Vor}}$ mode) exhibits a stronger increasing trend with A , and the remaining two, P_0 and n_c show a decreasing trend.

Analyzing potential direct influences of excitation strengths on the evaluated features, our explanation is as follows: As explained above, the negative trend seen for P_0 with stronger excitation is caused by the higher overall granular temperature at stronger excitation, which increases not only the dynamics of particles outside the clusters, but also inside, and the motion of the clusters themselves. Thus, the fraction of nearly immobile particles decreases with A even when the cluster size is larger, i. e. when the share of particles trapped in the cluster is higher. This trend is observed after 1, 2, or 4 excitation periods.

The opposite trend of increasing collision frequencies of individual particles can be explained with the higher granular temperature at stronger excitation. Free particles move faster and thus return to the pistons more frequently.

Consequently, the latter two features do not reflect an appropriate measure for cluster formation when the amplitude of excitation is changed. The S_1 , S_2 and φ_{caged} obviously reflect the correct picture that clustering is only weakly sensitive to the excitation strength in the investigated parameter range.

5 Discussion and Summary

We have performed simulations of permanently excited granular ensembles of spheres using the geometry of the VIP-Gran experiment [7], which represents a typical example of granular gases under permanent excitation in microgravity. Based on these simulations, we compared established methods to characterize the clustering state and to detect the transition from a homogeneous to a clustered state by analyzing characteristic features of the ensemble, primarily of dynamical nature. Two system parameters, viz. the fill fraction ϕ (via N) and the excitation strength A , were varied.

The results show that attempts to classify the system in a strict two-state matrix with a well-defined transition based on the structural and dynamical features considered here is not well-substantiated. There are two main reasons for that: First, all the features considered here show a smooth transition from the rather homogeneous gas

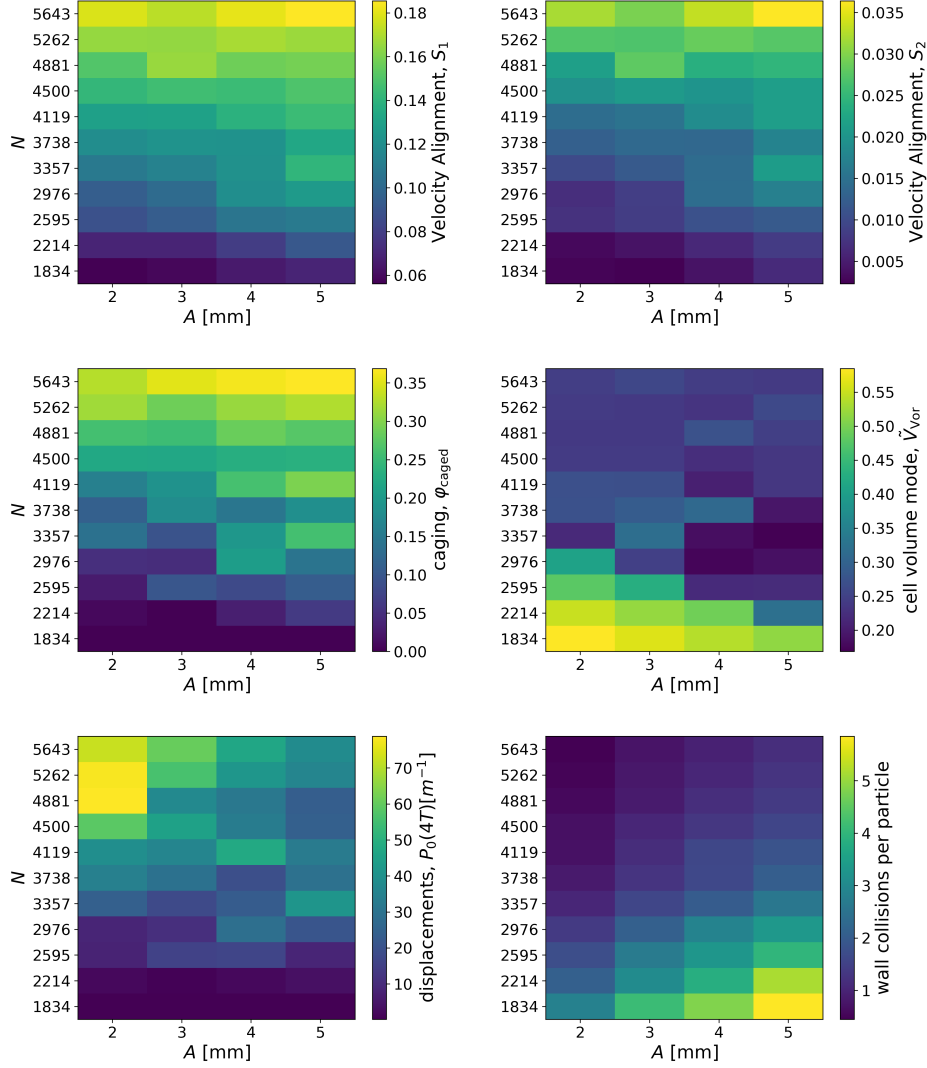


Fig. 18: Influence of N and A on various structural and dynamical features. A consistent trend with particle number density is found for all features. The excitation amplitude dependence is consistent only for the top two rows, the two bottom plots provide an incorrect trend as explained in the main text.

to the spatially inhomogeneous, clustered state. By visual inspection, it is easy to distinguish the two limiting cases, clustering at high particle numbers and homogeneous state for low particle numbers, but the definition of a transition threshold between these states is quite arbitrary.

The second problem is that the features considered here cannot be quantitatively related to one of the two states. The interpretation of the particle displacements, in

particular their extrapolation to near-zero displacements P_0 , is easy when only the number of particles is varied, but when the excitation amplitude is changed, competing effects have to be taken into account: With increasing A , clustering may lead to a larger share of closely packed particles, but mean particle velocities, mean cluster displacements and internal cluster dynamics counteract the effect on the PDFs and on P_0 . Thus, the trend towards lower P_0 with increasing excitation strength is not a signature of lower clustering efficiency but only of a faster dynamics in general.

Similarly, the piston collision frequency per particle naturally increases when the excitation is stronger, since the mean velocity per particle increases (see Fig. 15). This is irrespective of the number of clustered particles since these do neither contribute to the collision rate nor to the mean velocity of the free particles. Thus, the piston collision frequency cannot be regarded a reliable signature of clustering either.

Judging from all these arguments, a reasonable conclusion is that the structural parameters (local packing fraction from Voronoi cell analysis and caging criterion) as well as the velocity correlations S_1 and S_2 between neighbors in the center of the cell are reliable and best suited to characterize the state of clustering of a driven granular gas at given system parameters, at least in the VIP-GRAN experiment. However, they provide no objective threshold criterion.

This said, the results of this study need to be set in the context of earlier experimental and numerical investigations of the VIP-Gran experiment [5, 10, 22, 26] where the clustering was classified. These studies remain valid and very useful in any case. Alternatives to the classical criteria (KS and caging) that have been proposed and tested here do not provide a better characterization of the state of clustering. One of the dynamic alternatives, the velocity correlations in the center of the simulation box, has proved equally efficient as the local packing (Voronoi cell analysis) and caging analysis to provide semi-quantitative measures of the degree of clustering. At the same time, the second dynamic criterion, based on the distribution of particle displacements, is useful to understand the diffusive properties of the system but is too susceptible to overall kinetic energies at changes of the excitation strength.

All features tested in the present study support the scenario of a smooth transition from the homogeneous granular gas to a clustered state under continuous variation of the system parameters (global filling fraction and excitation amplitude). The homogeneity of the ensemble is best for low particle number densities, while the excitation strength has only minor importance.

Finally, we make a suggestion how a state diagram can be established using the features determined in our study, even though they are insufficient to classify individual states. The solution is seen in Fig. 13. If one can measure the rate of collisions of particles with the vibrating walls, n_c , as a function of the number of particles in the container at fixed excitation strength, the curve starts with an almost linear slope. The collision frequency increases nearly proportional to the mean particle number density in the container. We disregard here the minor influences of the particle number density on the velocity distribution which leads to some reduction of the slope. At a certain point, the cluster forms and the particles accumulate in the center, which causes thinning of the particle number density near the piston walls. Then, the $n_c(N)$ curve reaches a plateau and subsequently decays. The peak in this curve can be regarded as

a more or less objective criterion for the onset of clustering. For each different excitation scheme, the procedure must be repeated. From the graphs in Fig. 13, we conclude that at lower amplitudes A , the transition sets in at slightly smaller particle numbers. We should note that in comparison to the other structural and dynamical criteria (e. g. caging), the transition in wall collision rates happens for considerably lower packing fractions. The drawback of this approach is that it is not easily related to other established clustering criteria and to the properties of the particles inside the cluster. At the same time, there is a clear benefit of the wall collision count criterion because it is more or less free from subjective influences. Another important advantage is that the extraction of collision numbers from experimental video footage is a relatively simple and reliable procedure in contrast to the analysis of the complete ensemble.

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Data Availability

The raw DEM simulation files and dataset underlying the figures in this study are available in Zenodo at <https://doi.org/10.5281/zenodo.22999376>. The complete simulation results, due to their size, can be provided for download by the corresponding author on reasonable request.

Code Availability

The custom simulations and analysis code used in this study is available from the corresponding author on reasonable request.

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Author contributions

D.P. conceived the study, S.P.S. performed the simulations, worked on the data analysis, and prepared the manuscript draft. R.C.H. developed the simulation software, D.P., S.P.S. and R.S. analyzed and interpreted the results. All authors edited and reviewed the manuscript.