



# Properties of interaction networks in compressed two and three dimensional particulate systems

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## Abstract

We consider two (2D) and three (3D) dimensional granular systems exposed to compression, and ask what is the influence of the number of physical dimensions on the properties of the interaction networks that spontaneously form as these systems evolve. The study is carried out based on discrete element simulations of frictional disks in 2D and spheres in 3D. Within the constraints of the considered simulation protocols, the main finding is that both the number of physical dimensions and the type of particle-particle interaction significantly influence the properties of interaction networks. These networks play an important role in bridging the microscale (particle size) and macroscale (system size), thus both aspects (the interaction model and dimensionality) are carefully considered. Our work uses a combination of tools and techniques, including percolation study, statistical analysis, as well as algebraic topology-based techniques. In many instances, different techniques and measures provide complementary information that, when combined, allow for gaining better insight into the properties of interaction networks in compressed particulate systems.

**Keywords** Compressed granular matter · Force networks · Topological data analysis · Persistent homology

## 1 Introduction

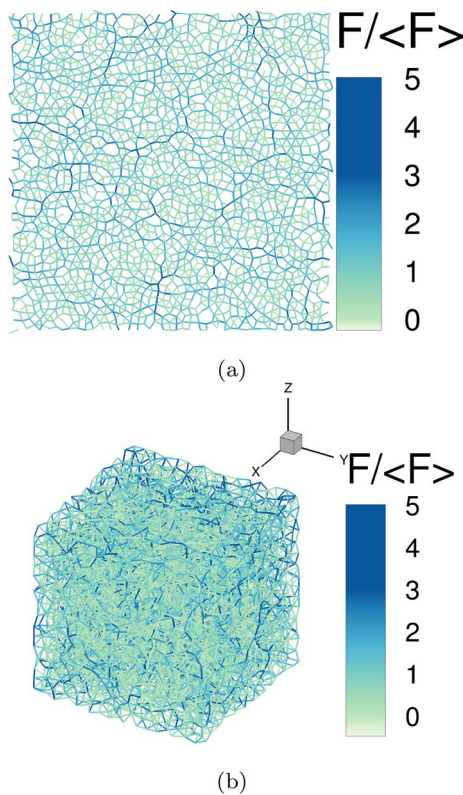
Particulate systems are very common in nature and take different forms ranging from dry or wet granular matter to suspensions. Still, there are many unresolved fundamental questions. In particular, the connection between microscale behavior (on the scale of constitutive granular particles) and macroscale response of granular systems subject to external load, such as compression or shear, is still an open question.

A significant body of work, that has been mostly developed during the last decade, suggests that connecting the micro and macroscale involves interaction networks that spontaneously develop in particulate-based systems. These works involve topology-based studies [1–14], cluster analysis [15–17], community detection schemes [18, 19], force network ensembles [20–22], statistical analysis [23–25] percolation-based approaches [26–29], and discussion of percolation and jamming transitions [29–34].

Most past analysis of interaction networks obtained computationally is carried out in two spatial dimensions (2D) due to reduced computational complexity and simplified interpretation of the results. A significant amount of experimental work focusing on interaction networks has been carried out in 2D as well, mostly using photoelastic particles, see, e.g. [35, 36]. However, most applications focus on three spatial dimensions (3D). In 3D experiments, it is difficult to extract information about particle contacts and, in particular, interaction strength. While there have been recent experimental works in 3D using, e.g., hydrogel [37] rubber [38] particles, or oil droplets [39], the progress has been rather limited. Currently, experimental techniques that could be used to track the force networks for stiff and frictional 3D particles, are just being developed [40], and this field of investigation has to rely mostly on simulation results. 3D simulations are complicated to analyze compared to 2D; as an illustration of this additional complexity, Fig. 1 shows two examples from the simulations we will consider in the present paper. We note that recent approaches that focus on inter-particle forces include measurements of force probability density function [41], as well as various network-based approaches (see [42] for a review). However, it is not obvious how to correlate and compare 3D results to the ones

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**Fig. 1** Examples of interaction networks for the **a** 2D and **b** 3D granular systems.  $\langle F \rangle$  is the average force. Animations of the compression process are available as supplementary material (videos 1 and 2)

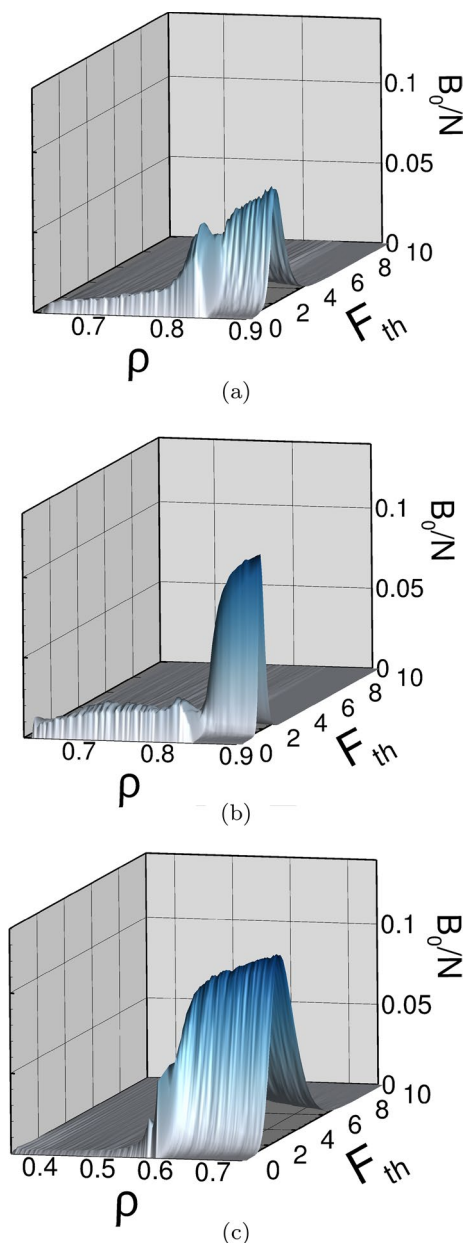
obtained in much more commonly considered 2D geometry. This is the main goal of the present work.

The number of physical dimensions has a complex influence on the properties of interaction networks in particulate systems. First, the interaction networks are built on top of contact networks between the particles, and contact networks are clearly influenced by the number of physical dimensions since the geometry of particle contacts differs in 2D and 3D. Second, the interaction between the particles is influenced by the particle shape—commonly, disks are considered in 2D and spheres in 3D (of course, more complex 2D and 3D shapes could be considered, but we do not discuss these in the present work). Assuming the validity of the standard approach based on the Hertz model, one finds that the (normal) interaction force,  $F$ , between particles should scale as  $F \propto x^\delta$ , where the compression distance,  $x$ , is defined in soft particle simulations as the difference between the sum of particle radii and the distance of their centers, and  $\delta = 1.0, 1.5$  for 2D and 3D, respectively. Thus, there are two obvious aspects of the influence of the number of physical dimensions on particle interactions. It is desirable to separate these two aspects so that one can distinguish between the influence of the number of dimensions on contact geometry and on the force interaction law. In addition,

experiments carried out in 2D in some cases find that particle interaction law deviates from Hertzian theory and that  $\delta \approx 1.4 - 1.5$  [13]. Therefore, motivated both by our desire to separate the aspects influencing particle interactions and by the listed experiments, we consider 2D systems with both  $\delta = 1$  and  $\delta = 1.5$ , in addition to considering 3D systems with  $\delta = 1.5$ .

In this paper, we focus on granular systems; however, we expect that the results will be of interest to other particulate-based systems, such as suspensions, emulsions, or foams, and even to the systems characterized by a more complex interaction between interacting particles, such as gels. We focus on the compression protocol so that we can discuss the evolution of interaction networks as the considered systems evolve through jamming transition. The evolution from small to large volume fractions is driven by slowly converging walls, as discussed in more detail in Sect. 3.

To introduce the results that will be discussed in the rest of this paper, Fig. 2 shows the simplest topological measure, zeroth Betti number,  $B_0$ , that counts the number of connected components (clusters), as a function of imposed force threshold,  $F_{th}$  and packing fraction,  $\rho$ . We will discuss Betti numbers more precisely later in the paper (Sect. 5); for the present purposes, it is sufficient to specify that a cluster consists of all particles such that at least one of their contacts is characterized by the total force magnitude which is larger than  $F_{th}$ . The results shown in Fig. 2 (see also [6] for related results focusing on a 2D system where linear force model is used) illustrate the complexity of the dependence of  $B_0$  on  $F_{th}$  and  $\rho$ . The most interesting part involves large values of  $\rho$ : here, for small values of  $F_{th}$ ,  $B_0$  is close to unity since all particles are connected into a single cluster; for large values of  $F_{th}$ ,  $B_0 \rightarrow 0$  since the number of contacts experiencing forces larger than  $F_{th}$  vanishes as  $F_{th}$  increases. In between of these two extremes, typically for the force thresholds slightly larger than the average contact force, the number of clusters reaches the maximum. The differences between the considered systems considered in Fig. 2 will be discussed extensively in the paper. To put the results in perspective, we note that choosing a threshold,  $F_{th}$ , that corresponds to the average force between the particles would separate the considered networks into ‘strong’ (the contacts involving forces larger than the average), and ‘weak’ (the remaining contacts) [43]. The approach considered in the present work is more general since we vary the considered force thresholds continuously and are therefore in the position to obtain a more complete picture describing the networks. In this paper, we will discuss  $B_0$  introduced above, as well as  $B_1$ , that measures the number of loops in 2D, or tunnels in 3D (sometimes also called ‘cycles’). In 3D we will also discuss  $B_2$ , measuring the number of enclosed voids, but to a much lesser extent. In the second part of the paper, we present the results obtained by implementing more complex measures



**Fig. 2** The number of clusters in the interaction network,  $B_0$ , normalized by the total number of particles,  $N$ , for different values of packing fraction,  $\rho$ , and force threshold,  $F_{th}$  for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. The animations of different views of the panels are available as Supplementary Material (videos 3, 4 and 5)

based on persistent homology. We note that the software for computing Betti numbers, as well as persistence measures discussed later in the paper, is widely available in the public domain [44–46].

Before closing the Introduction, we should also point out the aspects of the considered problem that are addressed only marginally in the present work. First, the main part of the results reported in the manuscript are obtained using

specified domain size for the 2D and 3D systems considered. We carried out a limited set of additional simulations and corresponding data analysis to verify that the results regarding interaction networks remain valid for other system sizes but have not carried out the extensive analysis, leaving such endeavor for future work. We point out to the reader that there is a number of works where the influence of system size has been discussed; for the discussion in the context of interaction networks, we refer the reader to [26, 27] and references therein; carrying out a similar type of analysis with a focus on the detailed properties of interaction networks remains to be done. Second, most of the results that we report in the manuscript are empirical since we are not aware of a well-defined theory or at least a model that could be used for comparison in the context of connectivity and structure of the interaction networks. This being said we attempt where possible to provide at least qualitative arguments rationalizing the physical reasons leading to the observed properties of the interaction networks.

The rest of this paper is organized as follows. The force model describing the interaction between particles is discussed in Sect. 2, and the protocol of the simulations in Sect. 3. Section 4 gives results based on consideration of percolation, jamming, and force distributions. A complementary set of results obtained using topology-based methods is discussed in Sect. 5. Section 6 gives an overview and conclusions.

## 2 Force model

We perform discrete element simulations using a set of circular disks confined to a square domain (2D) or spheres in a cubic domain (3D). The number of particles in 2D is  $\approx 2000$  and  $\approx 4000$  in 3D. The walls are flat and are given the material properties of plexiglass (the choice of the wall material is motivated by recent experiments [37]). The domain length is initially set to  $50 \times 50$  (in 2D) and  $20 \times 20 \times 20$  (in 3D) average particle diameters. To avoid crystallization, the system particles are chosen as bidisperse in all systems, and the ratio of the diameters of the small and large particles is 1:1.4. The ratio of the number of small to large particles is 2:1.

Particles are soft and interact via normal and tangential forces, including static friction and viscous damping. The force model used in the simulations is either linear or non-linear. The linear force model is used only in 2D and arises from the derivation of the Hertz law. The non-linear force is considered for both 2D and 3D. The analysis of the results for the non-linear force model in 2D is motivated by our recent study [13] that showed that using the non-linear force model in 2D is essential for achieving a quantitative match between simulations and experiments.

The general form of the normal force between particles  $i$  and  $j$  is (for more details, see [47])

$$\begin{aligned} \mathbf{F}_{ij}^n &= k_n x^\delta \mathbf{n} - \gamma_n x^\nu \bar{m} \mathbf{v}_{ij}^n \\ &\text{if } ||k_n x^\delta \mathbf{n}|| \geq ||\gamma_n x^\nu \bar{m} \mathbf{v}_{ij}^n|| \\ &= \mathbf{0} \text{ otherwise} \end{aligned} \tag{1}$$

$$r_{ij} = |\mathbf{r}_{ij}|, \quad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \quad \mathbf{n} = \mathbf{r}_{ij}/r_{ij}$$

$$k_n = \frac{2Y}{3(1-\sigma^2)} d_{ave}^{1-\beta},$$

where the expression in the if statement is used to avoid negative forces. Exponents  $\delta = 1$  and  $\nu = 0$  for linear and  $\delta = 1.5$  and  $\nu = 0.5$  for non-linear force model with  $1 + \beta = \delta$ ;  $\mathbf{v}_{ij}^n$  is set to the relative normal velocity and  $Y$  and  $\sigma$  are Young’s modulus and Poisson ratio, respectively. The amount of compression is  $x = d_{ij} - r_{ij}$ , where  $d_{ij} = (d_i + d_j)/2$ ,  $d_i$  and  $d_j$  are the diameters of the particles  $i$  and  $j$ . Note that for simplification we assume that  $d_{ave}$  in the expression for the force constant,  $k_n$ , is the overall average particle diameter of all particles. Also,  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ , where  $\mathbf{r}_i, \mathbf{r}_j$  are the vectors pointing from the centers of particles  $i, j$  towards the point of contact. The value of Young’s modulus  $Y = 23.45$  KPa and Poisson ratio  $\sigma = 0.5$  is set to those of soft hydrogel particles in [48]. Choosing the same values of material parameters for 2D and 3D simplifies the comparison between different systems that we consider; it should also be noted that the choice simply specifies the time scale in the problem; a different choice of (for example) stiffer particles would simply change the relevant time scale without modifying the results in any significant manner.<sup>1</sup>

We implement the commonly used Cundall-Strack model for static friction [49], where a tangential spring is introduced between the particles for each new contact that forms at time  $t = t_0$ . Due to the relative motion of the particles, the spring length,  $\xi$ , evolves as  $\xi = \int_{t_0}^t \mathbf{v}_{ij}^t (t') dt'$ , where  $\mathbf{v}_{ij}^t = \mathbf{v}_i - \mathbf{v}_j - \mathbf{v}_{ij}^n$  and  $\mathbf{v}_{ij}$  is the relative velocity. For long-lasting contacts,  $\xi$  may not remain parallel to the current tangential direction defined by  $\mathbf{t} = \mathbf{v}_{ij}^t / |\mathbf{v}_{ij}^t|$  (see, e.g., [50]); we therefore define the corrected  $\xi' = \xi - \mathbf{n}(\mathbf{n} \cdot \xi)$  and introduce the test force

$$\mathbf{F}^{t*} = -k_t x^\beta \xi' - \gamma_t x^\nu \bar{m} \mathbf{v}_{ij}^t \tag{2}$$

where  $k_t = 6/7k_n$  (close to the value used in [51]) and  $\gamma_t$  is the coefficient of viscous damping in the tangential direction (with  $\gamma_t = \gamma_n$ ). The value of the friction coefficient is set

to  $\mu = 0.5$ . To ensure that the magnitude of the tangential force remains below the Coulomb threshold, we constrain the tangential force as follows

$$\mathbf{F}^t = \min(\mu |\mathbf{F}^n|, |\mathbf{F}^{t*}|) \mathbf{F}^{t*} / |\mathbf{F}^{t*}|. \tag{3}$$

The interaction between a particle and flat wall is given by the same expression as in the case of interaction between two particles except for assuming that the amount of compression  $x = 0.5d_i - r_i$  where  $d_i$  is particle diameter and  $r_i = |\mathbf{r}_i|$  is the vector pointing from the particle center towards the point of contact with the flat wall.

All the results in the rest of the paper are presented using the following length, time, and mass scales. The characteristic length scale is  $d_{ave} = 1.735$  cm, and the average particle mass,  $\bar{m} = 3.0$  g [48], is the mass scale. The binary particle collision time,  $\tau_c$ , is the time scale set to [47]

$$\tau_c = \zeta(\beta)(1 + 0.5\beta)^{\frac{1}{2+\beta}} \left( \bar{m} \frac{3(1-\sigma^2)}{2Yd_{ave}^{(1-\beta)}} \right)^{\frac{1}{2+\beta}} v_0^{-\frac{\beta}{2+\beta}} \tag{4}$$

where  $v_0 = 10^{-2}$  cm/s is a characteristic magnitude of velocity in the system (compression speed); prefactor  $\zeta(\beta)$  is of the form [52]

$$\zeta(\beta) = \frac{\sqrt{\pi} \Gamma(1/(2+\beta))}{(1+\beta/2)\Gamma((4+\beta)/(4+2\beta))}, \tag{5}$$

where  $\Gamma$  denotes the Gamma function. In particular, for the linear force model we have  $\zeta(0) = \pi$  and for the non-linear force model  $\zeta(0.5) = 2.94$ . The damping coefficient  $\gamma_n$  is obtained as reported in [47]. Note that the average particle mass and diameter are the same for 2D and 3D systems; the thickness of the disk particles in 2D is chosen to ensure that this is the case.

We integrate Newton’s equations of motion for the translational and rotational degrees of freedom using a 4th order predictor-corrector method with the time step  $\Delta t = 0.02\tau_c$  and  $\Delta t = 0.005\tau_c$  in 2D and 3D, respectively. A smaller value of time step in 3D is needed to keep the minimum distance between interacting particles sufficiently large for the whole duration of the simulations. The use of smaller time steps in 3D does not influence the results that follow in any visible manner.

### 3 Protocol and methods

The initial condition is produced by placing the particles on a square (2D) or a cubic (3D) grid, and by assigning to each particle a random initial velocity; we verified that the results presented here are not sensitive to the specific distribution from which the velocities are sampled. To ensure the

<sup>1</sup> Minor influence of different material properties of the particles could be due to particle-wall interaction, and, in the case of a non-linear force model, due to weak dependence of the particle collision time on impact speed.

statistical significance of the results, we perform simulations for 20 different initial conditions for each considered system.

The system is compressed by moving the walls inward with the velocity  $v_0$ . Relaxation is interjected after each compression step of  $\Delta\rho = 0.02$ , where  $\rho$  is the packing fraction, defined as the ratio of the total volume of the particles and the domain volume. After each compression step, the kinetic energy dissipates exponentially when the system is relaxed; we continue relaxation until the fluctuation of the kinetic energy drops to 0.1 of the mean, which is computed over  $1.5 \times 10^5$  time steps. We verified that a more strict relaxation condition does not change our conclusions, nor does it change the measured quantities significantly; however, if the threshold for the kinetic energy fluctuations is set to a value  $< 0.1$ , the computational time increases significantly, and the differences in the results are on the level of random fluctuations in each measured quantity. We find that using a protocol for relaxation based on the total magnitude of the kinetic energy does not yield different results either. We have also implemented different relaxation protocols based on tracking the average contact number change and cooling the particles (annealing). The protocol corresponding to the first method verifies that the contact number drops to a near-zero value for unjammed systems and that for jammed systems, the contact number does not change over a large number of time steps. We find that such a protocol does not influence the results presented in this paper, and it turns out to be more computationally expensive. The annealing protocol implements the approach for cooling the particles during relaxation as discussed recently [53]. For the system considered in this work, we find that jamming transition is influenced by cooling rate, even for the smallest cooling rates we could use with available computing resources, and is therefore not suitable for our study.

It is beyond the scope of the present work to discuss why implemented annealing protocol has such an influence in the considered simulations; one possibility is that the differences between implemented protocols vanish in the limit of large system sizes; however, as pointed out already, such an analysis is left for future work.

The reason for this detailed discussion of the implemented protocol is the presence of a relatively small but non-vanishing, number of clusters for packing fractions below jamming in particular for 2D simulations, see Fig. 2, and Figs. 4 and 6 later in the paper. One obvious question is whether these clusters would disappear if a different relaxation protocol were used. Our finding is that these clusters remain present for any of the considered relaxation protocols.

This observation is consistent with the earlier works [54, 55] that found that the cooled unjammed systems always contain clusters of connected particles, at least for the simulation setup and relaxation protocols considered in the present work. One could also ask whether such clusters would

still be present as the system size increases or whether the fraction of the particles participating in such clusters would decay as the system size increases. Such questions should be considered in future work.

*Interaction networks:* We consider the forces between particles and define the interaction network in a granular system by its nodes (particle centers) and weighted edges (inter-particle forces). The interaction networks are analyzed for different values of  $\rho$  and for a range of (dimensionless) force thresholds,  $F_{\text{th}} \in [0.0, 3.0]$ , where only the forces that are larger than  $F_{\text{th}}$  are taken into account. We note that the forces are always rescaled by the average force in an interaction network,  $\langle F \rangle$ , which itself is strongly  $\rho$ -dependent (see [56] for the dependence of the average force, quantified by the pressure, in the simulations following a similar protocol as the present one). For simplicity, in this work, we consider only the total force between the particles (the absolute value of the vector sum of the normal and tangential forces at each contact). We show the results up to the value of  $\rho$  such that the average force does not exceed a maximum,  $F_{\text{max}}$ , defined as follows. We find the average force in an interaction network,  $\langle F \rangle$ , for all  $\rho$ 's (averaged over 20 realizations for 2D linear and non-linear, and for 3D systems), and determine the value  $F'_{\text{max}} = \max\{\langle F \rangle\}$  for each considered system. We define  $F_{\text{max}} = \min\{F'_{\text{max}}\}$  so that for all considered systems, the results are given for the same range of average force thresholds. The maximum packing fractions are found as 0.906, 0.890 and 0.710 for the non-linear 2D system, linear 2D system, and the 3D system, respectively. We note that at the high end of considered packing fractions the distances between the interacting particles may be up to 10% smaller than the sum of the radii.

*Clusters:* In the presentation that follows, we will rely heavily on the concept of a cluster, which we define here; later in Sect. 5 we will discuss in more detail other relevant topological measures. A cluster/connected component, whose number is counted by zeroth Betti number,  $B_0$ , is defined as a collection of particles connected by the contacts whose total force magnitude is above the specified threshold,  $F_{\text{th}}$ . Another quantity of interest is cluster size,  $S$ , which specifies the number of particles in a cluster. We will also consider the average cluster size,  $\langle S \rangle$ , which is the average of  $S$  over all clusters in the computational domain, and also over all realizations.

*Data pre-processing:* During compression, especially for small values of  $\rho$ , the particles collide and often form two-particle clusters. The particles with only one or no contacts are referred to as rattlers. As in the previous experimental and numerical studies [13, 57, 58], we do not consider rattlers in our computations; these clusters are not included in the Betti number results discussed later in the paper.

We note that we have carried out additional simulations using different system sizes:  $25 \times 25$  and  $75 \times 75$  (in 2D)

and  $10 \times 10 \times 10$  and  $30 \times 30 \times 30$  (in 3D) average particle diameters. The finding of relevance for the present paper is that the results reported in the rest of the manuscript remain qualitatively the same for the considered domain sizes. We have also carried out simulations using different friction coefficients (in addition to the value  $\mu = 0.5$  considered in all the reported simulations, we used  $\mu = 0.0$  and  $\mu = 0.03$ ). The only visible difference between systems with different friction values was found in the specific value of  $\rho_j$ , and in the precise values of the various measures describing the interaction networks.

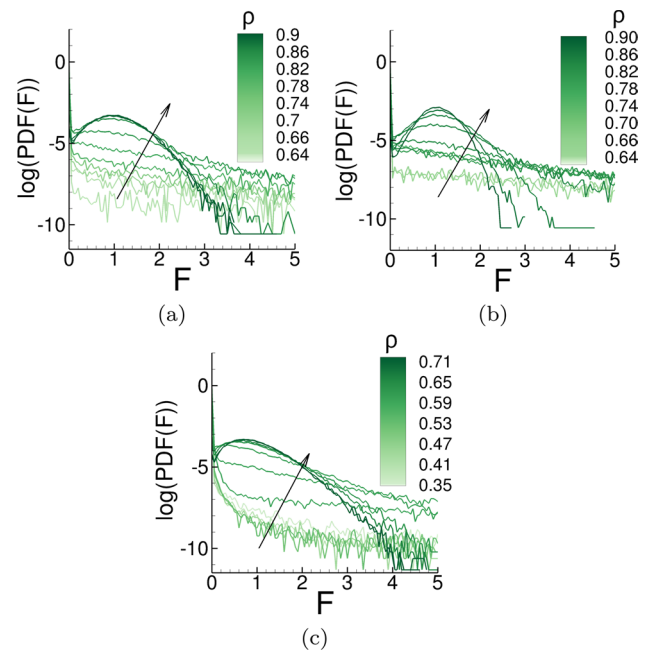
## 4 Force distribution, percolation, and jamming transitions

In this section, we focus on the differences between 2D and 3D systems that undergo jamming and percolation transitions (described below) in terms of the distribution of forces and properties of the interaction networks.

During compression and relaxation, particles come into contact and clusters randomly form and break. Since we include relaxation between compression steps, the compression protocol is quasi-static, and we expect that the percolation and jamming transitions occur at the same packing fraction [30]. Note that both here and in [30], a jamming transition is characterized by a rapid increase of average contact number. More specifically, jamming packing fraction,  $\rho_j$ , is defined here as the point at which  $Z(\rho)$  curve has an inflection point. We refer the reader to recent works that discuss in more detail the current understanding of jamming in granular systems [59, 60]. Percolation transition is defined by  $\rho = \rho_p$  at which a percolating cluster connecting at least two opposite walls of the domain forms. We indeed observe the formation of a stable percolating cluster (that does not disappear even after arbitrarily long relaxation) for any (and only when)  $\rho > \rho_j$ , confirming that  $\rho_p = \rho_j$ . Finding that  $\rho_p = \rho_j$  also suggests that the relaxation protocol that we use is essentially quasi-static, so that the results are not influenced in any meaningful manner by the relaxation protocol, see [30] for further discussion regarding this issue. For future reference, we note that for the systems that we consider, the jamming occurs at  $\rho_j = 0.842$ ,  $0.834$  for the 2D non-linear and linear systems, respectively, and  $\rho_j = 0.57$  for the 3D system (note that exact numerical values may be influenced by the system size).

### 4.1 Force distribution

Figure 3 shows the force distribution,  $\text{PDF}(F)$ , for the three considered systems. We note that the width of the distributions for the largest values  $\rho \approx \rho_{\max}$  differs for the linear and two non-linear systems, with smaller width of  $\text{PDF}(F)$  in the



**Fig. 3** PDF of forces for different values of  $\rho$  for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. The arrows indicate the direction of increased  $\rho$ . For the shown systems, jamming occurs at  $\rho_j = 0.842$ ,  $0.834$ ,  $0.570$  for **a**, **b**, **c**, respectively

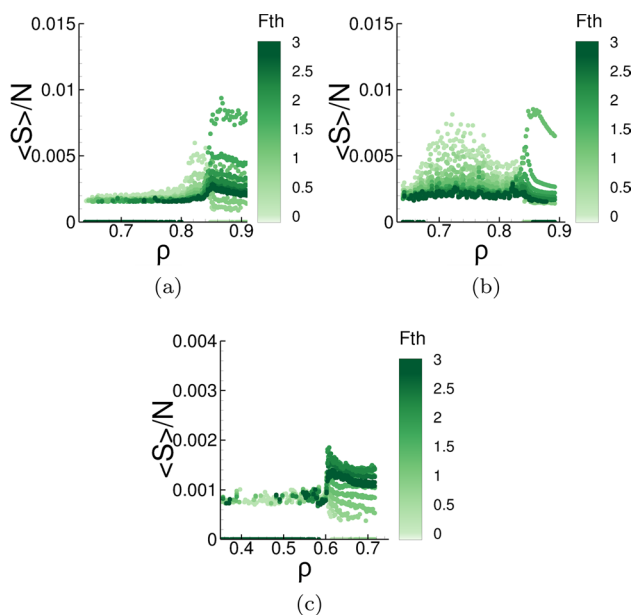
linear system, suggesting a smaller variation of the forces and a more homogeneous interaction network. The systems based on the non-linear force model have wider distribution, and in the 3D system, we observe the largest variation. While the functional form of  $\text{PDF}(F)$  has been widely discussed in the literature [10, 39, 48, 61–65], we are not aware of the precise comparison of these functional forms between the systems characterized by different number of physical dimensions, or by different interaction force model.

In the next section, we will use  $\text{PDF}(F)$  results together with the topological measures that will be introduced to discuss further distinguishing features of the interaction networks as the number of physical dimensions and the force model are varied.

### 4.2 Force cluster analysis: non-percolating clusters

We continue our analysis of the forces between particles by examining the cluster size distribution in the interaction networks. We omit the percolating cluster if it is present in the interaction network. Since percolating cluster has a different characteristic scaling behavior [29] than the average cluster size of the non-percolating clusters [26, 27], we discuss its properties separately.

Figure 4 shows the average cluster size,  $\langle S \rangle$ , rescaled by the total number of particles,  $N$ , for different values of  $F_{\text{th}}$ . In the 2D systems, the largest values of  $\langle S \rangle / N$  are observed



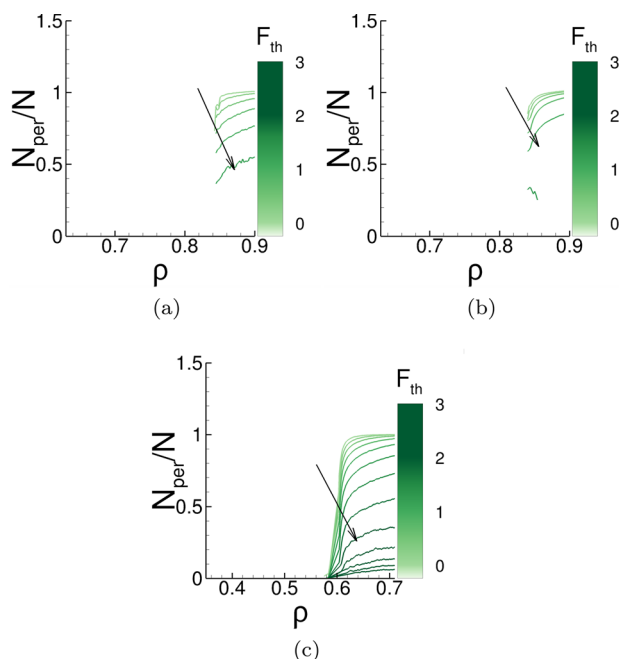
**Fig. 4** Average cluster size,  $\langle S \rangle$ , normalized by the total number of particles,  $N$ , for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. For the shown systems, jamming occurs at  $\rho_j = 0.842, 0.834, 0.570$  for **a, b, c**, respectively. Note that for  $\rho \ll \rho_j$ ,  $\langle S \rangle$  may vanish in the case no clusters are found

for  $F_{th} = 1.25$  and  $F_{th} = 1.5$  for the linear and non-linear systems, respectively. This finding implies that regardless of the force model, the interaction network is dominated by the force clusters composed of forces near the average force in 2D. Force model becomes important in 2D when  $F_{th} \geq 2.0$  and  $\rho > \rho_j$ . Specifically, in the linear case,  $\langle S \rangle/N$  decays faster than in the non-linear one. In other words, the interaction network is more uniform for the linear system, and we expect to observe a smaller variation of forces for  $\rho \rightarrow \rho_{max}$ . Indeed, our discussion of PDFs in the context of Fig. 3 confirms that the PDF( $F$ ) in the linear system follows a more narrow distribution than the PDF( $F$ ) in the non-linear one.

Turning now our attention to the influence of the number of physical dimensions, we compare the panels (a) and (c) of Fig. 4. The most obvious difference between the two is the  $F_{th}$  for which  $\langle S \rangle/N$  attains the maximum for  $\rho > \rho_j$ . In the 3D system, the largest values of  $\langle S \rangle/N$  are observed for  $F_{th} \approx 2.0$ . Therefore, the interaction networks in 3D contain more clusters with large forces - the forces are less concentrated around the mean force. The PDF( $F$ ) for the 3D system shown in Fig. 3 is indeed wider, confirming larger force variation in comparison to 2D.

### 4.3 Force cluster analysis: percolating cluster

Figure 5 shows the average force and the number of particles participating in a percolating cluster,  $N_{per}$ , normalized by the total number of particles,  $N$ . We remind the reader that the

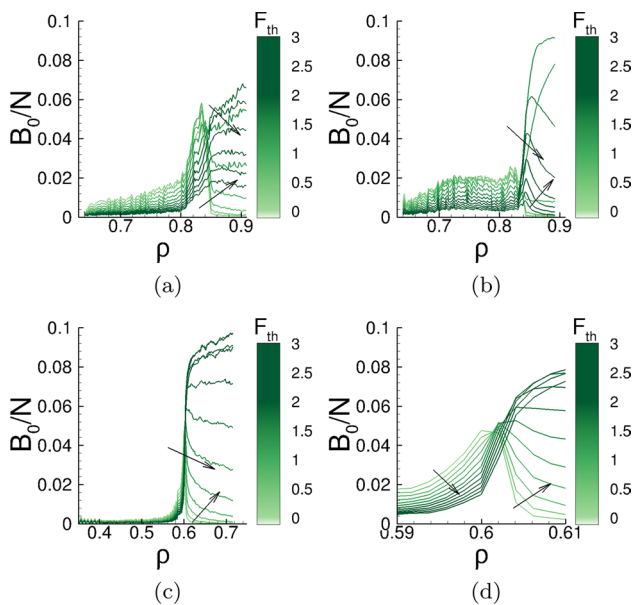


**Fig. 5** Proportion of the particles in a percolating cluster for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system for different values of  $F_{th}$ . The arrows indicate the direction of increased  $F_{th}$

results are averaged over 20 realizations for each system; here, we only show the results if at least 50% of the realizations contain a percolating cluster. Recall that percolation is observed only when the system jams, consistently with our previous findings [30]. We note that when we take into account all the contacts, i.e. when  $F_{th} \approx 0.0$ , the percolating cluster in the 2D systems contains almost all the particles. However, in the 3D case, in particular, for  $\rho \approx \rho_j$ , the percolating cluster contains only a very small number of particles, as it can be seen in Fig. 5.

The reason why fewer particles are needed for percolation in 3D is purely geometrical and is discussed next. We consider the interaction networks at  $F_{th} = 0.0$  first and represent them as random networks with particles as vertices and contacts represented by edges. We also define the mean degree of a random network,  $\langle k \rangle$  as the mean number of edges per vertex (in the context of granular systems  $\langle k \rangle$  is equivalent to the average contact number,  $Z$ ). Let us now assume that a given random network has  $N$  vertices and a mean degree  $\langle k \rangle$  and ask what is the maximum number of vertices we can randomly remove and still have a percolating cluster. From the theory of random networks [66, 67], a critical occupation probability is estimated by

$$\phi_c = \frac{\langle k \rangle}{\langle k^2 \rangle - \langle k \rangle}. \tag{6}$$



**Fig. 6** Average number of clusters/components,  $B_0$ , rescaled by the total number of particles,  $N$ , for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. The panel **d** is a closeup of the 3D granular system showing a clear peak in  $B_0/N$  for small  $F_{th}$ . In **a–c** the arrows pointing up show an (increasing) trend of the curves from the smallest  $F_{th}$  and then the arrows pointing down show a (decreasing) trend when  $F_{th} \rightarrow \max\{F_{th}\}$

( $\phi_c$  is the smallest ratio of the vertices present in a random network leading to a percolating cluster). Note that  $\phi_c$  provides a lower bound for  $N_{per}/N$ . We can now use Eq. (6) to estimate  $\phi_c$  in 2D and 3D. In our simulations close to jamming, we find that, as expected,  $\langle k \rangle \approx 3$  and  $\langle k \rangle \approx 6$  in 2D and 3D, respectively. Note that the exact value of  $\langle k \rangle$  depends on the friction between particles [68–71] and is estimated by  $\langle k \rangle \approx d + 1 + (2N_m/d)$  where  $N_m$  is the mean number of contacts that have tangential forces equal to the Coulomb threshold [42, 68, 70, 72]. If we assume that  $\langle k^2 \rangle \approx \langle k \rangle^2$  (this assumption would be exactly satisfied if each particle had the same number of contacts), we find  $\phi_c \approx 0.5$  in 2D and  $\phi_c \approx 0.2$  in 3D at  $\rho_j$ . This estimate provides an intuitive (even if only approximate) explanation of why we observe smaller (relative to the total number of particles) percolating clusters in 3D compared to 2D systems when  $\rho \approx \rho_j$ . Note that this argument is purely geometrical and does not depend on simulation protocol, particle properties (other than friction that plays a role in the  $\langle k \rangle$  estimate), or the system size.

Our results show that the differences in  $N_{per}/N$  extend to the non-zero force thresholds and  $\rho > \rho_j$ . Specifically, we find that whenever percolating cluster exists for the 2D systems, it is composed of a significant number of particles. In 3D, on the other hand, we can find a percolating cluster composed of a very small percentage of particles, particularly when  $F_{th} > 2.0$  or when  $\rho \approx \rho_j$ . Let us also reiterate that

the presented results are robust with respect to the details of the relaxation period, at least within the range that we could consider using available computational resources.

## 5 Topology of interaction networks

We now continue with the study of topological properties of interaction networks. We focus on the number of components/clusters in the interaction network, the number of loops and voids (to be defined below), and on the measures emerging from persistent homology [7]. The general motivation is that Betti numbers and persistence analysis can be used to compare the geometries of the force distributions [8] and find their characteristic behavior during the jamming transition [9]. We will see in what follows that this type of analysis indeed allows for quantifying significant differences between the topology of interaction networks in 2D and 3D systems, as well as in 2D systems characterized by different interaction force models. To start with, we discuss the simplest topological measure, Betti numbers.

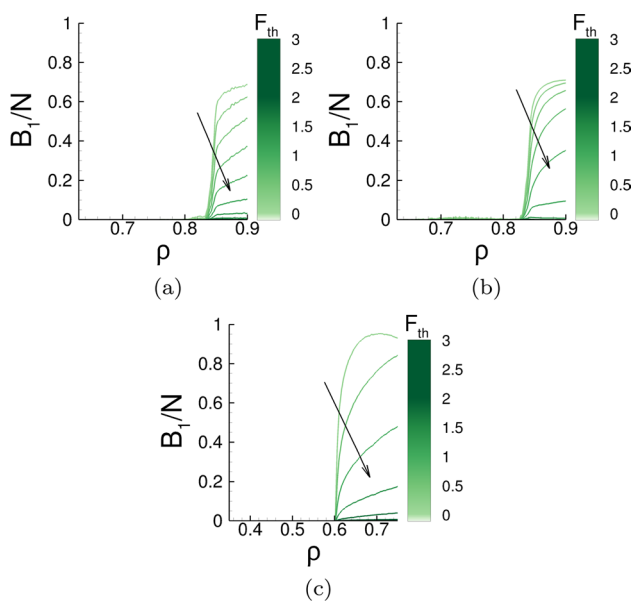
### 5.1 Betti numbers

Zeroth Betti numbers,  $B_0$ , denotes the number of components (clusters), and  $B_1$  denotes the number of loops in a force network (a loop in an interaction network is a collection of connected edges forming a closed cycle). The next Betti number,  $B_2$ , relevant to 3D geometry, counts the number of cavities. Note that  $B_0$  provides different (but related) information than the average cluster size,  $\langle S \rangle$ , discussed in Sect. 4.2;  $B_0$  provides the information about the number of clusters, independently of their size.

When analyzing Betti numbers,  $B_1$  in particular, one has to make a choice of whether to consider the loops made out of three particles in contact, sometimes referred to as 3-cycles in the studies of interaction networks in granular systems [16]. It is known that such loops play a role in the stability of interaction networks in granular systems [5, 16]. However, since 3-cycles are prevalent and not unique to a specific set of physical parameters or the number of physical dimensions, we ignore them in the present analysis and focus on the loops involving at least four particles, similarly as it was done in our earlier studies [6–9].

Let us begin by examining the number of clusters,  $B_0$ , forming in the interaction network during compression. For a complete representation of the interaction network evolution, a range of force thresholds is considered for each packing fraction. Figure 6, which shows a set of cross-sections of the introductory Fig. 2, plots  $B_0$  rescaled by the total number of particles,  $N$ . When considering Betti numbers, the inclusion of the percolation cluster is





**Fig. 7** The evolution of the number of loops,  $B_1$ , normalized by the total number of particles,  $N$ , during compression for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. The arrows indicate the direction of increased  $F_{th}$

not relevant, since it modifies  $B_0$  only by unity; for simplicity, we include it in the Betti number count.

Figure 6a, c shows that for small values of  $F_{th} < 0.5$ , the systems based on the non-linear force model develop a pronounced peak near the respective jamming packing fractions,  $\rho_j$  (see in particular Fig. 6d, which is a zoom-in of Fig. 6c).

The observations made based on Fig. 4 suggest that there are important structural differences between the linear and non-linear systems. For the non-linear force model, we find that for  $F_{th} < 0.5$  and  $\rho \approx \rho_j$  the clusters are more numerous compared to the ones found for  $\rho > \rho_j$  (leading to the peaks visible in Fig. 6a, c, d). In contrast, for the linear force model the peak in  $B_0/N$  is rather insignificant.

Figure 7 shows, perhaps surprisingly, that  $B_1/N$  results follow the same trend for all systems considered. The  $B_1/N$  evolution is generic during compression: for small  $\rho$  below jamming, we do not observe any loops forming, and only beyond jamming,  $B_1/N$  starts to rise and then plateaus for  $\rho$  close to  $\rho_{max}$ . The only visible difference between 2D and 3D systems is the larger magnitude of  $B_1/N$  for the 3D case.

The evolution of the next Betti number,  $B_2/N$ , is not analyzed here in detail since  $B_2$  is not defined in 2D. We only briefly mention that in 3D,  $B_2$  vanishes for  $\rho < \rho_j$  and grows in a monotonous fashion as  $\rho$  increases beyond  $\rho_j$ .

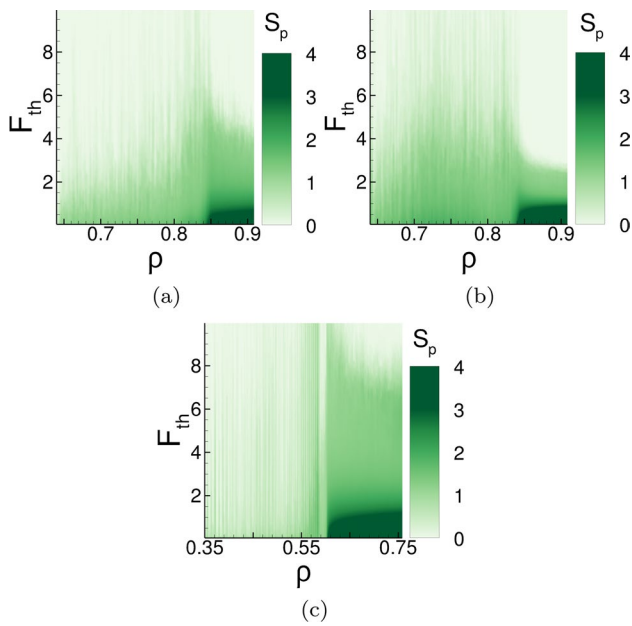
### 5.2 Shape of the clusters

The Betti numbers provide only the count of the clusters and loops in the interaction network and do not provide any information about the cluster shape; based on Betti numbers, we do not know whether the clusters are isotropic, chain-like, or of some other form. To explore the cluster shape, we introduce a shape parameter,  $S_p$ , defined as the number of edges in the clusters divided by the number of participating particles, averaged over all realizations. The motivation behind such a measure is the following. If the particles that participate in a cluster all have one or two contacts, the cluster forms either an open or closed path, defined as a sequence of vertices (here particles). Note that a closed path is a loop and contributes to  $B_1$  count. Let us assume that the number of particles in such a path is  $N_L$ . Then, the number of inter-particle contacts forming an open path is  $N_L - 1$  and the resulting shape parameter for such a path is  $\bar{S}_p = (N_L - 1)/N_L \in [0.5, 1.0]$ . For any loop, we have  $\bar{S}_p = 1.0$ . For more complex shape structures (not simple paths), we expect that  $\bar{S}_p \in (1.0, 4.0]$  in 2D and  $\bar{S}_p \in (1.0, 7.0]$  in 3D. (To avoid any confusion, we refer by  $S_p$  to the measure averaged over all clusters and realizations and by  $\bar{S}_p$  to the measure describing the shape of an individual cluster, or to the measure describing the clusters of an individual realization). The upper values of  $\bar{S}_p$  are estimated from the maximum average contact number for the 2D and 3D systems. For the purpose of simplifying the discussion below, we refer to the clusters with more than (on average) two contacts per particle as complex clusters; the clusters that are not complex are simple.

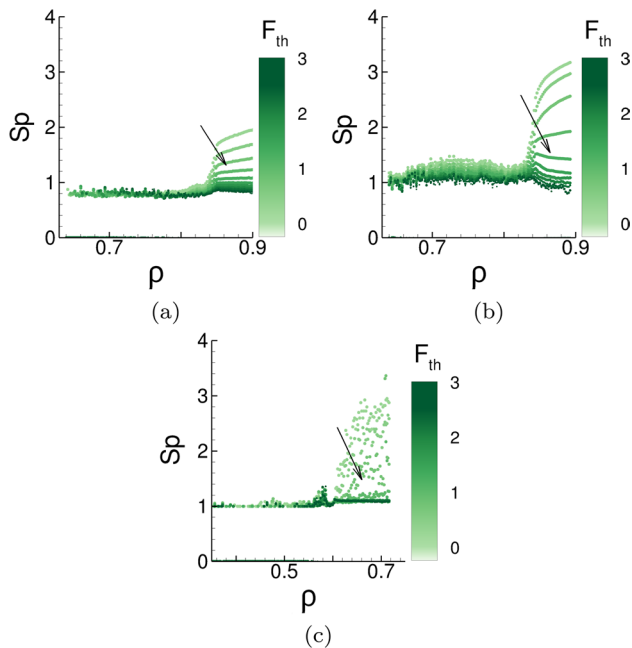
Figure 8 shows  $S_p$  for all systems and for all values of  $F_{th}$  and for varying packing fraction,  $\rho$ ; Fig. 9 shows cross-sections of  $S_p$  for selected values of  $F_{th}$ . Note that we put  $S_p = 0$  whenever  $\bar{S}_p = 0$  for at least half of the realizations. Otherwise, the values are averaged only over the realizations such that  $\bar{S}_p \neq 0$ .

In discussing the results shown on Figs. 8 and 9, we focus first on the 2D systems, and small packing fractions,  $\rho < \rho_j$ . We observe that for both systems  $S_p \approx 1$ . Further insight is obtained by relating this result to the ones for  $B_1/N$  shown in Fig. 7. Figure 7 shows that there are no loops present for  $\rho < \rho_j$ , and therefore the interaction network must be composed of open paths for such values of  $\rho$ . Although the results for the considered 2D systems and  $\rho < \rho_j$  are similar, we still observe that  $S_p$  is consistently larger for the linear system compared to the non-linear one, in particular for smaller values of  $F_{th}$  (compare Fig. 9a and b).

Still considering the 2D systems, but for  $\rho > \rho_j$ , we observe that for large  $F_{th}$ ,  $S_p$  approaches 1.0 for both systems, and we can again use the observations from Fig. 7 to conclude that the interaction network is composed of open paths, since  $B_1/N$  is small. The differences between linear



**Fig. 8** Shape parameter,  $S_p$ , as a function of  $\rho$  for all values of  $F_{th}$  for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. See also Fig. 9 that illustrates in more detail the differences between the considered systems



**Fig. 9** Shape parameter,  $S_p$ , as a function of  $\rho$  for the chosen values of  $F_{th}$  for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system. The arrows indicate the direction of increased  $F_{th}$

and non-linear systems appear when smaller values of  $F_{th}$  are considered: here we find that the values of  $S_p$  are significantly larger for the linear compared to the non-linear

system. The main finding here is that for a significant range of force thresholds around the average force, the clusters are significantly more complex for the systems based on linear compared to nonlinear force model.

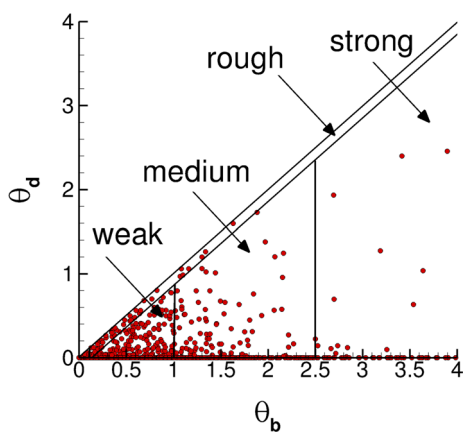
Let us now consider the 3D system, shown in Figs. 8c and 9c. First of all, note that the data are noisier in 3D, particularly for small  $F_{th}$ . The reason for the noisiness is two-fold: first, there are only few clusters when  $F < 1.0$  at large  $\rho$ , so the statistics is not very good; second, there are also more possible cluster shapes in 3D compared to 2D; a quick intuitive explanation comes from considering a lattice in 2D and 3D and counting the number of possible cluster shapes with a fixed number of particles. Despite the restrictions imposed by noise, one can still conclude that the clusters are more complex in 3D compared to the 2D (non-linear) system, although the difference between the two is not as significant as expected based on geometry considerations (note that the upper limit of  $S_p$  is 7 and 4 for 3D and 2D geometry, respectively). For  $F_{th} > 2.0$ , we find  $S_p \approx 1.0$ . We use again the results shown in Fig. 7 to conclude that the interaction network in this regime consists mainly of open paths.

To summarize, we find that for small or average force thresholds (less than twice the average force) regardless of the number of physical dimensions, the non-linear systems contain clusters with less complex structure compared to the linear system, suggesting that the force model plays a crucial role in determining the cluster shape. For large force thresholds (considering forces larger than twice the average force), the force networks are typically composed of open paths for all systems considered, independently of the force model and of the number of physical dimensions.

### 5.3 Persistence diagrams

In Sect. 5.1, we analyzed  $B_0$ 's for a set of force thresholds,  $F_{th}$ . Zeroth Betti number however, provides only information about the number of clusters and not about how they are connected. This information can be obtained by analyzing persistence diagrams, which allow us to capture information about the force clusters for all force thresholds at once, including their persistence as a considered force threshold, is changed. We explain the use of the persistence diagrams in interaction network analysis further by considering an example below; the reader is referred to [8] for the in-depth discussion of persistent homology in the context of interaction networks for particulate systems and to [7, 9, 56] for less technical descriptions that also include multiple examples helping to interpret the results of persistent analysis. We note that multiple software packages and libraries can be used to compute persistence diagrams [44–46]. We used JavaPlex [44] to obtain the results discussed in this section.

When the force threshold,  $F_{th}$ , changes, the clusters that are formed in the force network composed of forces above

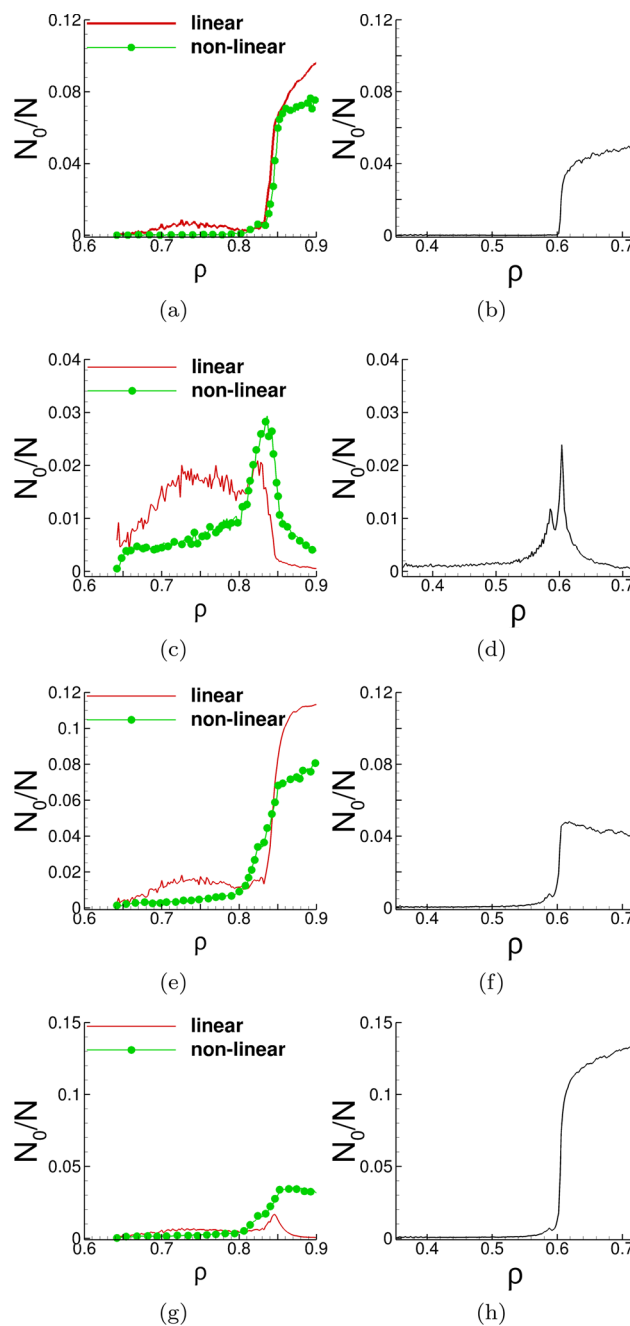


**Fig. 10** An example of a  $B_0$  persistence diagram for 2D non-linear force model. This example shows a separation of the persistence diagram into the following categories: rough, strong, medium, and weak as discussed in the text

$F_{th}$  either appear or disappear: note that a cluster disappears when it merges with another one. We indicate a birth,  $\theta_b$  ( $F_{th}$  at which a cluster appears), on the  $x$ -axis and death,  $\theta_d$  ( $F_{th}$  when a cluster disappears), on the  $y$ -axis. The set of points constructed in this way forms a persistence diagram (PD); we construct a PD for each  $\rho$ . Note that for a given  $\rho$ , a persistence diagram contains the information about particle connectivity for all force thresholds at once. Betti numbers, for example, could be easily computed directly from the persistence diagrams. However, the opposite is not true since the amount of information contained in persistence diagrams is significantly larger. For the present purposes, we also define the lifespan of a cluster as the difference  $\theta_b - \theta_d$ . The relevance of lifespan in describing the interaction networks is discussed further below.

Figure 10 shows an example of a PD (2D non-linear system is used here). One approach to analyzing persistence diagrams is to split them into bins: rough, strong, medium, and weak, similarly as in [7]. A point on a persistence diagram belongs to the rough category if  $\theta_b - \theta_d \leq 0.1$ . Such points indicate clusters that have a short lifespan (after birth, clusters in the rough region disappear after only a slight change in  $F_{th}$ ) and can be thought of as noise. The points that have a lifespan larger than 0.1 are divided into the following bins: weak when  $0.1 \leq \theta_b < 1.0$ , medium when  $1.0 \leq \theta_b < 2.5$ , and large when  $2.5 \leq \theta_b$ . This binning of the forces is, in spirit, similar to the separation of interaction networks into ‘strong’ and ‘weak’ categories, commonly used in the granular literature. We use the binning approach to develop a better understanding of the differences between the granular systems considered so far. Specifically, we will discuss the origins of the  $B_0/N$  ridge in Fig. 2.

Figure 11 shows the average point count in all persistence bins for the 2D and 3D systems;  $N_0$  denotes the average



**Fig. 11** Average number of points,  $N_0$ , in different parts of persistence diagrams, normalized by the total number of particles,  $N$ . 1. rough: **a** 2D and **b** 3D; 2. weak: **c** 2D and **d** 3D; 3. medium: **e** 2D and **f** 3D, and 4 strong: **g** 2D and **h** 3D

number of persistence points found in the specified category (recall that the results are averaged over 20 realizations), and  $N$  is the total number of particles.

To start the discussion of Fig. 11, we first comment on the results relevant to the bins for which the differences between considered systems are minor: rough and medium. Regarding the rough regime, Fig. 11a–b, we

observe that the roughness of the force network is very similar near jamming for all the systems. For the medium bin, see Fig. 11e–f, we observe a sudden increase of the curves beyond jamming. For both rough and medium bins, we note a smaller number of points for the considered non-linear systems; we comment on this result in the case of medium bins further below.

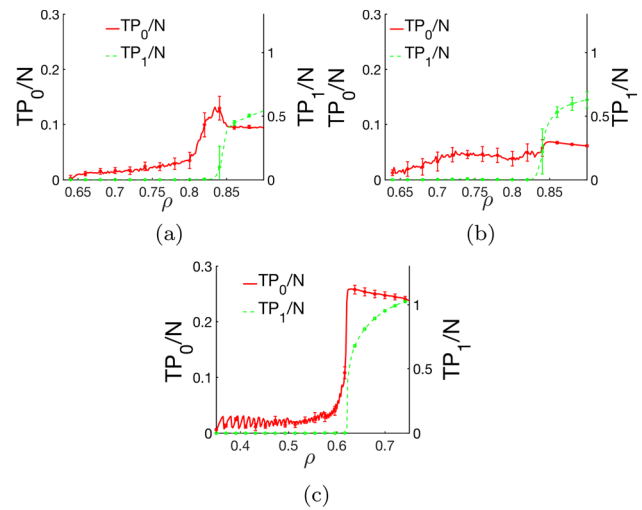
The most significant differences between the systems based on different force models can be observed for strong, Fig. 11g–h and weak, Fig. 11c–d bins. Considering first the strong bin, we note that the 2D system based on the linear force model develops a peak of  $N_0/N$  during jamming, while for the non-linear systems, such a peak is lacking, since these systems show large values of  $N_0/N$  beyond jamming as well. Such a peak during jamming can be explained by strong collisions of the particles that form relevant clusters. For the system based on the linear force model, for  $\rho > \rho_j$ , the majority of the clusters remain in the medium bin; see Fig. 11e (note that a similar behavior was observed for the 2D systems in continuously compressed systems [7]). However, for the non-linear force model, the clusters formed by strong collisions remain in the strong bin as  $\rho$  increases. The softness of the non-linear interaction potential plays an important role and strongly influences the properties of the interaction networks as a system is compressed beyond jamming. One consequence of this difference between linear and non-linear systems is the larger force spread for the non-linear systems for  $\rho > \rho_j$ . Consistently, as already observed in Fig. 3, for  $\rho > \rho_j$ , the PDFs of the non-linear systems are wider compared to the linear case.

In contrast, Fig. 11c–d shows a pronounced peak in the weak force bin around jamming for the systems based on the non-linear interaction model but not for the linear one. Recalling formation of the ridge in  $B_0$  (viz. Figure 6) for similar packing fractions, we conjecture that the ridge is formed by weak interactions that dominate the interaction network for  $\rho \approx \rho_j$ .

Another measure based on the persistence diagrams is total persistence [7] of a PD, defined as

$$TP(PD) = \sum_{(\theta_b, \theta_d) \in PD} (\theta_b - \theta_d)$$

where the sum ranges over all  $(\theta_b, \theta_d)$  pairs corresponding to the points in the  $B_0$  and  $B_1$  persistence diagrams. For simplicity of notation, we refer to the total persistence for the clusters by  $TP_0$ , and for the loops by  $TP_1$ . The physical interpretation of these quantities could be best described by a landscape analogy: if we think of an interaction network as a landscape, then large  $TP_0$  implies a landscape containing a large number of prominent peaks and valleys, and large  $TP_1$  suggests well developed connectivity between the peaks



**Fig. 12** Total persistence in the 2D systems for **a** 2D non-linear force model, **b** 2D linear force model and **c** 3D system;  $N$  is the total number of particles

(leading to loops). Note that the concept of force threshold is not relevant anymore here since total persistence includes the information about all force thresholds at once.

Next, we discuss briefly  $TP_0$  and  $TP_1$  for the considered systems. A detailed discussion regarding  $TP_2$  is omitted since this measure is defined only in 3D. It suffices to mention that  $TP_2 \approx 0$  for  $\rho < \rho_j$  and increases monotonously for  $\rho > \rho_j$ .

Figure 12 shows  $TP_0$  and  $TP_1$  for the considered 2D and 3D systems. The most obvious finding that is relevant to both  $TP_0$  and  $TP_1$  is a significantly more prominent increase of these measures close to  $\rho_j$  for the 3D system, compared to the 2D ones. This result suggests that additional physical dimension leads to an increasingly complex force landscape with many prominent peaks and valleys. To understand this landscape more precisely, one needs to consider the relevant persistence diagrams in more detail. Such in-depth analysis is left for future work.

To reiterate the findings discussed in this section, we find that both the number of physical dimensions and the force model play a role in determining the topology of interaction networks. The number of physical dimensions influences the behavior of the percolating cluster in the interaction network and the  $B_0$  results show that the force model is important when we consider small forces in our computations of interaction network properties. We also find that the properties of the interaction networks during jamming transition can be quantified by persistence diagrams and derived quantities, such as total persistence.

## 6 Conclusions

In this work, we analyze the properties of interaction networks with a focus on the influence of the number of physical dimensions and of the force model (linear vs. non-linear) describing particle interactions. The comparison of the force distribution reveals differences between the considered systems for a large range of packing fractions,  $\rho$ . Specifically, the force distributions are found to be significantly different between 2D and 3D systems in the case of small  $\rho$ 's, despite consistent preparation and relaxation protocols. Beyond jamming, we find that the distribution of forces is wider for the non-linear systems regardless of the number of physical dimensions. This being said, we emphasize that our results were obtained mainly for one system size; while the general features of the results were found to hold as the system size was varied, no systematic analysis of the influence of system size on our results has been carried out so far.

The analysis of the percolating cluster and its size as the force threshold,  $F_{th}$ , is varied for  $\rho \geq \rho_j$  shows that a percolating cluster is composed of a significant number of particles in 2D (often at least half of the total number of particles) at any time percolation occurs. On the other hand, in 3D, we find percolating clusters composed of a very small number of particles for the granular system close to jamming or when  $F_{th}$  is large, typically for  $F_{th} > 2.0$ . For small force thresholds, we explain this finding based solely on the number of physical dimensions.

Our force distribution and percolation analysis results suggest important structural and topological differences between the 2D and 3D systems, as well as between the systems that are based on different force models. This motivates the analysis of the average cluster size,  $\langle S \rangle / N$ , shape,  $S_p$ , and the first two Betti numbers,  $B_0$  and  $B_1$ .

The average cluster size,  $\langle S \rangle / N$ , in an interaction network (not including the percolating cluster), shows a peak formation for small  $F_{th} \approx 0$  close to jamming transition. Such a peak occurs only for the granular systems based on non-linear interactions. The differences between 2D and 3D systems arise beyond jamming; for 3D there are larger clusters characterized by a larger interaction force (when normalized by the average force) compared to 2D.

One of the prominent results of this study is the formation of a pronounced ridge in the number of clusters at  $\rho \approx \rho_j$  for the non-linear force models. This ridge's formation and properties, which become visible when considering a weak interaction network, have been carefully analyzed using topological measures. We conjecture that the softness of the non-linear interaction model plays a significant role in determining the properties of the interaction networks as the systems go through jamming. The

consequence is that close to jamming, one could expect significantly different behavior of the systems involving particles interacting by different interaction laws.

In conclusion, based on a well-defined set of measures, we provide a precise and objective comparison of the interaction networks in finite-size compressed granular systems in this work. The main finding is that both the nature of the interactions between the constitutive particles, and the number of physical dimensions, play a significant role in determining the interaction networks' properties. In contrast, the interaction networks are found to be only weakly influenced by friction between the particles. To what degree these findings extend to more complex systems exposed to shear or other types of external influences remains to be seen.

**Supplementary Information** The online version contains supplementary material available at <https://doi.org/10.1007/s10035-023-01379-y>.

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## Declarations

**Conflict of interest** The authors declare no conflict of interest.

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