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# The dynamical collision network in granular gases.

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We dynamically construct the interaction network in a granular gas, using the sequence of collisions collected in an MD event driven simulation of inelastic hard disks from time 0 till time  $t$ . The network is decomposed into its  $k$ -core structure: particles in a core of index  $k$  have collided at least  $k$  times with other particles in the same core. The difference between cores  $k + 1$  and  $k$  is the so-called  $k$ -shell, and the set of all shells is a complete and non-overlapping decomposition of the system. Because of energy dissipation, the gas cools down: its initial spatially homogeneous dynamics, characterized by the Haff law, i.e. a  $t^{-2}$  energy decay, is unstable towards a strongly inhomogeneous phase with clusters and vortices, where energy decays as  $t^{-1}$ . The clear transition between those two phases appears in the evolution of the  $k$ -shells structure in the collision network. In the homogeneous regime the  $k$ -shell structure evolves as in a growing network with fixed number of vertices and randomly added links: the shell distribution is strongly peaked around the most populated shell, which has an index  $k_{max} \sim 0.9\langle d \rangle$  with  $\langle d \rangle$  the average number of collisions experienced by a particle. During the final non-homogeneous regime a growing fraction of collisions is concentrated in small, almost closed, *communities* of particles:  $k_{max}$  is no more linear in  $\langle d \rangle$  and the distribution of shells becomes extremely large developing a power-law tail  $\sim k^{-3}$  for high shell indexes. We propose the  $k$ -shell decomposition as a quantitative characterization of Molecular Chaos violation.

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## I. INTRODUCTION

The study of dilute granular materials [1], as well as of other many particles systems lacking an equilibrium description (glass forming liquids in their non-equilibrium regime [2], for instance), requires the use of appropriate tools, models and paradigms in order to simplify the picture and gain new insights. The introduction of the free inelastic hard spheres model has been of fundamental relevance for the rigorous foundation of granular kinetic theory and hydrodynamics [3]. The model consists of a gas of  $N$  hard spheres in a volume  $V$ , with inelastic collisions modeling the macroscopic nature of grains: the internal microscopic degrees of freedom are excited during the collision, their energy is then irreversibly dissipated into heat, so that the relative motion between two colliding grains is damped. Such simple generalization of the hard sphere model leads to dramatic consequences: the gas performs a non-stationary dynamics, cooling down and evolving toward a final state of thermal death. Moreover, in large enough systems a homogeneous granular gas is unstable toward the formation of vortices and clusters of closely packed grains.

A satisfying description of the late dynamics of the gas, after the onset of strong inhomogeneity, is still lacking. Coarse-grained descriptions in terms of hydrodynamic fields are made difficult by an apparently general lack of separation between microscopic and macroscopic scales [4, 5]. Velocity or density structure factors, usually difficult to be measured because of rapid temporal evolution, indicate a generic growth of structures but are insufficient to appreciate the rich kinetic behavior at the level of small groups of grains. Analogies with percolation transitions, Burgers models, or 2D turbulence have been proposed, sometimes on the mere basis of phenomenological similitudes.

In front of the openness of this problem, we propose a novel method of analysis, borrowed to the graph's theory, the so-called  $k$ -core analysis [6, 7, 8]: a  $k$ -core is the maximum subgraph containing only nodes with at least  $k$  links in the same subgraph. Very recently, the theory of  $k$ -cores has proved to be useful in defining a possible universality class for the dynamical glass transition, the bootstrap (also called "jamming") percolation [9]. In simple models of glass forming liquids, at finite temperature and above a critical value of the tunable average density, a jammed giant component in the  $k$ -core subset of the contact network (defined in a specific way) percolates the system, marking a breaking of ergodicity. Even if these works have been of some inspiration to us, we stress that our study addresses a different phenomenology and applies the analysis of graphs in a substantially different way. Therefore we do not claim any analogy between the dynamical breaking of the Homogeneous Cooling State of a granular gas and the jamming percolation or any other proposed glass transition scenario.

Our proposal is to dynamically construct a graph by linking two nodes (particles) each time a collision happens: the resulting graph grows with time and the average number of links per node is equal to two times the average number of collisions per particle. The decomposition of the interaction network into a hierarchy of cores of increasing degree

of self-interaction will prove to be a powerful tool to distinguish between particles in the solid-like phase from those in the fluid-like phase. The sequence of collisions in the non-homogeneous regime is in fact dominated by repeated impacts among grains trapped into sorts of self-sustained cages with very small escape probabilities. Such cages can be thought as almost closed *communities* in an interaction network. Strongly dissipating collisions, on the other side, are mostly concentrated outside of those cages, in the periphery of clusters, and involve particles which still have a certain degree of mobility.

More specifically, the  $k$ -core decomposition of the collision network appears as the natural characterization of the violation of Molecular Chaos. In an ideal gas, i.e. a gas satisfying the Molecular Chaos assumption, a grain never collides with another grain that is connected (through collisions) to its own previous history. In terms of graphs, true Molecular Chaos is equivalent to the following statement: the collision network is a tree, and therefore all the cores of index larger than 1 are empty. The minimal mechanism of Molecular Chaos breaking is that of *rings collisions*, which appear as loops in the collision graph, i.e. the simplest structures in cores of index 2. An example of dynamical collision network, with trees and loops, is given in figure 1. Cores of high degrees, i.e. systematic violations of Molecular Chaos, appear naturally in any finite system, even with purely random collisions. We will focus on the difference between pure finite-size correlations and effects really induced by inelasticity.

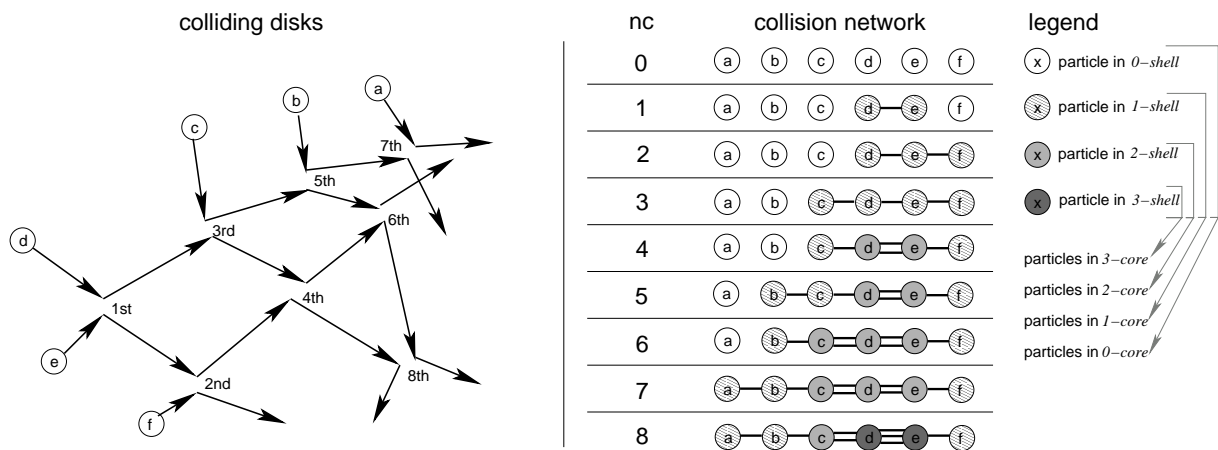


FIG. 1: Evolution of the network of collisions for a system of 6 particles. Left: the ordered sequence of collisions. Right: collision network at each time step, where  $nc$  is the number of realized collisions. All particles are in core of index 0. Particles not appearing in higher cores are also in shell of index 0. In general a  $k$ -core has all the particles with shell index  $\geq k$ .

In section II a description of the model of inelastic hard disks and of his known regimes will be given. The construction of the dynamical collision network will be explained in section III. In section IV we will show numerical results for the homogeneous regime, while the non-homogeneous regime will be discussed in section V. A discussion with conclusions and perspectives will come in section VI.

## II. THE GRANULAR GAS OF INELASTIC HARD SPHERES

One of the simplest models of granular gas is the gas of free inelastic hard objects (rods, disks or spheres, depending on the dimensionality) with constant coefficient of restitution. We restrict the discussion to  $D = 2$  dimensions, considering an assembly of  $N$  inelastic hard disks of diameter 1 and mass 1 in a box of volume  $V = L \times L$  with periodic boundary conditions. Between collisions each particle moves freely. When two particles  $i$  and  $j$  collide their velocities change from  $\mathbf{v}_i, \mathbf{v}_j$  to  $\mathbf{v}'_i, \mathbf{v}'_j$ , using the following rule:

$$\mathbf{v}'_{i(j)} = \mathbf{v}_{i(j)} - \frac{1 + \alpha}{2} [(\mathbf{v}_{i(j)} - \mathbf{v}_{j(i)}) \cdot \hat{\boldsymbol{\sigma}}] \hat{\boldsymbol{\sigma}}, \quad (1)$$

where  $\alpha \in [0, 1]$  is the restitution coefficient, while  $\hat{\boldsymbol{\sigma}}$  is the unity vector joining the centers of the two particles.

This model is widely used in the theoretical work on granular gases, conveying usefulness and simplicity: it reproduces the main features of real dilute granular experiments, allows fast event driven simulations and is prone to analytical formalization, being at the very basis of rigorous kinetic theories [3]. A vast campaign of studies has been devoted, in recent years, to understand the properties of this model during the so-called Homogeneous Cooling Regime (HCS) and the linear departure from it. The system is prepared in a random homogeneous configuration with positions

uniformly distributed in the box and velocities extracted from a Maxwellian with temperature  $T_g(0) \equiv \langle \mathbf{v}_i^2(0) \rangle / 2 = 1$ . A thermalization phase follows, where the system evolves with elastic collisions. Finally the real inelastic evolution begins: all time and collision counters start from this moment. During evolution, the granular temperature decreases since a fraction of kinetic energy is lost after each collision. Nevertheless the initial stage of the cooling remains homogeneous in space, with a decay of the granular temperature given by the Haff law:

$$T_g(t) = \frac{T_g(0)}{(1 + t/t_e)^2} \quad (2)$$

with  $t_e = \tau_e/\gamma$ ,  $\tau_e$  the mean free time between collisions at the beginning of the evolution, and  $\gamma = (1 - \alpha^2)/4$ . During the HCS, the cumulated number of collisions per particle,  $\tau(t)$ , grows logarithmically with time:

$$\tau(t) \propto \log(1 + t/t_e). \quad (3)$$

In figure 2 we show  $T_g$  vs.  $t$  (left frame) as well as  $\tau$  vs.  $t$  (right frame).

Simulations and linear stability analysis of macroscopic (hydrodynamic-like) models [10, 11, 12], have shown that the HCS is unstable when the size of the system  $L$  is larger than a critical size  $L_c$ . For systems large enough, therefore, spatial homogeneity is eventually broken and the formation of vortices and clusters is observed. A sign of this symmetry breaking is the departure from the Haff law: the growth of structures reduces the dissipation, reflected by a slower decay of  $T_g$ . The generally accepted scenario is a two-stages process: initially the density remains homogeneous while a macroscopic velocity field with vortical structures emerges (shear instability); after a while the density field begins to develop clusters (clustering instability). Both kinds of structures seem to obey a coarsening dynamics with characteristic lengths growing as  $\sim t^{1/2}$  [12]. In figure 3 a sequence of snapshots of a granular gas simulation illustrates the breakdown of the Homogeneous Cooling State and the onset of a highly clustered regime.

Recently the evidence of an asymptotic non-homogeneous cooling dynamics has been shown in large ( $N \sim 10^6$ ) event driven 2D and 3D simulations [13, 14, 15, 16]. The observation of this “final” cooling regime has been made possible by implementing a regularization of the dynamics, in order to get rid of the inelastic collapse problem. Inelastic collapse [10] is a singularity of the inelastic hard spheres dynamics which is triggered by rare collisions happening at very low relative velocities and in situations of high density, and it is not related to the shear and clustering instability. Many kinds of regularization have been proposed: in the rest of our paper we will use the one implemented by Ben-Naim et al. [13], the so-called elastic cut-off: all collisions happening at a relative velocity  $|(\mathbf{v}_1 - \mathbf{v}_2) \cdot \hat{\boldsymbol{\sigma}}| < v_e$  are treated as elastic. We (as well as in Ben-Naim’s work) have verified that the statistics behavior (e.g.  $T_g$  and  $\tau$  vs.  $t$ ) does not depend on the choice of  $v_e$ , provided that  $v_e \ll \sqrt{T_g(t)}$ . The percentage of those “fake” elastic collisions remains negligible, but they are enough to prevent the collapse.

The main characterization of the asymptotic regime, independently of the regularization mechanism, is the granular temperature decay,  $T_g \sim t^{-D/2}$  (in  $D \geq 2$  dimensions). The  $t^{-D/2}$  law could be generally explained as the consequence of some kind of diffusion: while this seems true for the velocity field at the beginning of the instability, i.e. still in the presence of a homogeneous density distribution [17], it becomes less evident in the asymptotic, strongly compressible, situation. Ben-Naim and coworkers have conjectured the belonging of this “final” cooling stage to the universality class of the Burgers equation: this is reasonable for a 1D inelastic gas, which is similar to a gas of sticky particles, but it has proven to be uncorrect in higher dimensions [18]. A mode-coupling theory, put forward by Brito and Ernst [16], suggests an asymptotic decay of  $T_g \sim \tau^{-D/2}$ . While in many simulations (see for example the inset of right frame in figure 2) the asymptotic relation between  $\tau$  and  $t$  seems to be linear, this is not true for any value of  $\alpha$ . On the contrary, the temperature decay  $t^{-D/2}$  does not depend upon  $\alpha$ . Isobe [14] has shown the remarkable (and unexplained) similitude between the final cooling regime and two dimensional turbulence in incompressible fluids. Miller and Luding [15] have suggested that the formation of clusters is a sort of percolation process. Meerson and Puglisi [19] have shown that in  $D = 2$  elongated geometries (such that one direction is stable and the other is unstable) the HCS is followed by an intermediated *flow-by-inertia* regime, and finally a coalescence of quasi-singular clusters à la Burgers. An observation that we report here (reserving details in further communications) is the strong narrowing of scale separation between microscopic and macroscopic dynamics, which makes difficult in practice a hydrodynamic description of this final cooling regime [20].

### III. THE NETWORK OF COLLISIONS AND THE K-CORES ANALYSIS

Let us introduce the  $k$ -core decomposition. Given a graph  $G = (V, E)$  of  $|V| = n$  vertices and  $|E| = e$  edges, the definition from [6] of  $k$ -cores is the following

**Definition 1** A subgraph  $H = (C, E|C)$  induced by the set  $C \subseteq V$  is a  $k$ -core or a core of order  $k$  iff  $\forall v \in C$  :  $\text{degree}_H(v) \geq k$ , and  $H$  is the maximum subgraph with this property.

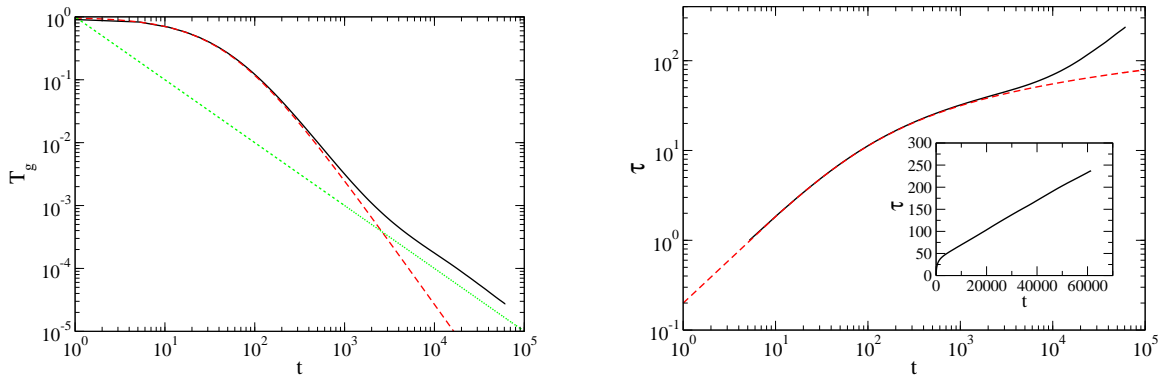


FIG. 2: **Color online:** Left: decay of granular temperature  $T_g$  vs. time  $t$ . The dashed red line marks the Haff law,  $T_g = 1/(1 + t/t_e)^2$  with  $t_e \approx 52$ , the dotted green line is a  $t^{-1}$  decay. Right: cumulated number of collisions per particle  $\tau$  vs. time  $t$ , the dashed red line shows the logarithmic growth of collisions in the Haff phase,  $\tau = a \log(1 + t/t_e)$  with  $a \approx 10$ . In the inset a linear plot of  $\tau$  vs.  $t$  is shown, focusing on the behavior at large times ( $t \gg 10^4$ ). The system is a gas of  $N = 10^6$  inelastic hard disks with restitution coefficient  $\alpha = 0.9$  in a box of size  $3163 \times 3163$  (units of a diameter) with periodic boundary conditions. Averages over 10 different initial conditions have been performed.

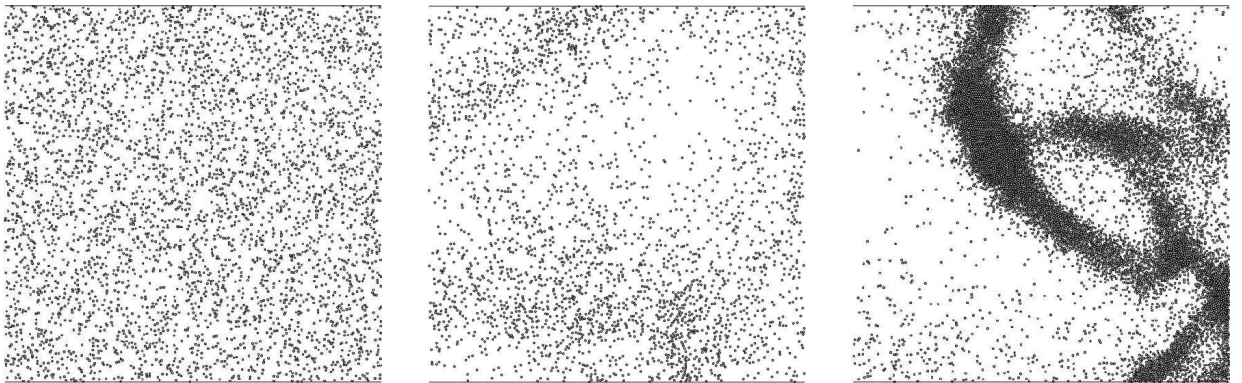


FIG. 3: Three snapshots of a small part of the gas of  $10^6$  inelastic hard disks with restitution coefficient  $\alpha = 0.9$ . In the snapshots is portrayed a square of surface  $200 \times 200$ , in units of a diameter, where the whole system is  $3163 \times 3163$ ; therefore the pictures portray a fraction 0.004 of the total surface. Left: just after thermalization (0 cpp). Center: after 100 cpp (collisions per particle). Right: after 200 cpp.

A  $k$ -core of  $G$  can therefore be obtained by recursively removing all the vertices of degree less than  $k$ , until all vertices in the remaining graph have degree at least  $k$ . It is worth remarking that this process is not equivalent to prune vertices of a certain degree. Indeed, a star-like subgraph with node with a high degree that connect many vertices with degree one and connected only with a single edge to the rest of the graph is going to belong only to the first core no matter how high is the degree of the node. We will also use the following definitions

**Definition 2** A vertex  $i$  has shell index  $k$  if it belongs to the  $k$ -core but not to  $(k + 1)$ -core.

**Definition 3** A component is a connected subgraph, i.e. a path exists between any pair of nodes in the same component.

The  $k$ -core decomposition therefore identifies progressively internal cores and decomposes the network layer by layer, revealing the structure of the different  $k$ -shells from the outmost one to the more internal one (e.g. Fig. 4).

Now, we define a collision network as follows: each particle is a node of the network, and each collision between two particles is represented by a connection between both nodes. This network has the particularity that each node may have multiples connections with other nodes. Technically we say that a collision network is not a graph, but a multigraph, i.e each edge may be multiple.

We have considered two possibilities to build a dynamical collision network at time  $t$ . The first is obtained collecting all collisions from time 0 to time  $t$ : we call it a *complete* network. The second one is built taking only the collisions occurred during a window of time of fixed length (in terms of number of collisions), ending at time  $t$ : this has been

called a *partial* network. Qualitatively the analysis of both networks produce the same results: the distribution of populated shells is narrow in the uncorrelated/homogeneous phase and is very spread in the correlated/inhomogeneous one. The shell distribution in the partial network has the advantage of being concentrated in a fixed range of shells indexes, while the complete network distribution shifts with time toward high shell numbers, since the average number of links per node is growing. On the other side, the complete network offers a better resolution of higher cores, which becomes crucial in the non-homogeneous regime: during this regime, defining a characteristic time scale and choosing the length of the time window for the partial network gets harder and harder. For this reason, in the following, we have focused our attention on the complete network.

It is important to remark that the time complexity to compute the  $k$ -core decomposition is very low. The vertex degree  $d$  is given by the number of nearest neighbors. Given a graph  $G$  represented by its list of vertices, where each vertex has a list of neighbors, the  $k$ -core decomposition can be computed as following:

- Make an ordered array of lists, where each list is composed by the vertices with the same degree. This step takes  $\mathcal{O}(n)$ , where  $n$  is the number of vertices.
- Compute each  $k$ -core, recursively, starting by the minimum degree  $d_{\min}$ , until any vertex remains in the graph. The time complexity of this step is  $\mathcal{O}(e)$ , where  $e$  is the number of edges.

To compute each  $k$ -core, it is enough to cut the vertices, and their corresponding edges, with degree lower than  $k$ . Note that when a node loses a neighbor, its degree is decreased, therefore it changes its degree-list and may possibly fall into a degree-list which is being cut. Then, the final time complexity for a general graph is  $\mathcal{O}(e + n)$ , which is transformed into  $\mathcal{O}(e)$  for a connected graph (where  $e > n - 1$ ).

Using this algorithm, it is very easy to compute the  $k$ -shell. Normally, the algorithm begins from the nodes in the  $k - 1 = d_{\min}$  list. All cut vertices form the  $(k - 1)$ -shell, while the surviving graph is the  $k$ -core. Then at each step, the  $k$ -core and the  $(k - 1)$ -shell are obtained.

It is important to observe that a 1-core has not isolated vertices, and a 2-core has no trees. For example, given a tree  $T$ , computing its 1-core leads to the same tree  $T$ ; if its 2-core is computed, the result is an empty graph. Only a graph with loops gives a non empty 2-core. In general, a graph containing a  $n$ -clique, i.e. a graph with its  $n$  vertices all connected among themselves, has a non empty  $(n - 1)$ -core.

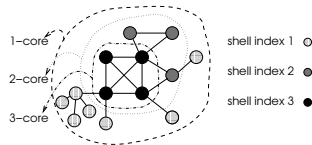


FIG. 4: This figure shows a graph and its decomposition in  $k$ -cores. The *shell index* is the maximum core that a node belongs to, then the 2-core has nodes with shell index 2 and 3.

#### IV. RESULTS: HOMOGENEOUS SYSTEMS.

In this section we present results about the analysis of the collision network in homogeneous systems. In particular we will analyze the dynamical collision network of four different models:

- a “small” system of inelastic hard disks ( $\alpha = 0.9$ ) that cools down staying in the HCS during its whole history;
- an elastic system ( $\alpha = 1$ ) that permanently remains homogeneous in its equilibrium dynamics;
- a system of inelastic hard disks simulated with the so-called homogeneous Direct Simulation Monte Carlo [21] (DSMC). In the homogeneous DSMC each particle can collide with any other particle (spatial coordinates are discarded) and the random choice of colliding couples is performed with a probability proportional to  $(\mathbf{v}_i - \mathbf{v}_j) \cdot \hat{\boldsymbol{\sigma}}$ , in order to reproduce the kernel of the collisional integral in the Boltzmann equation;
- a pure randomly growing network where links (collisions) are added with uniform probability on the set of all possible couples of nodes.

All the four considered systems have  $10^6$  particles (i.e. sites). In the first case, the size of the system is compared to the critical size given by linear stability analysis of the HCS. This analysis [12] shows that a minimum size  $L_c = \frac{2\pi}{k^*}$

is needed to have unstable shear modes, with  $k^* = \frac{\sqrt{1-\alpha^2}\sqrt{3}}{2\lambda}$ , i.e.  $L_c = \frac{4\pi\lambda}{\sqrt{1-\alpha^2}} \approx 29\lambda$ , where  $\lambda = L^2/(\sqrt{2\pi}N\sigma)$  is the mean free path. The small system considered here has a size  $200000 \times 200000$ , corresponding to a density  $\rho = 2.5 \times 10^{-5}$ , an area fraction  $1.96 \times 10^{-5}$  and a mean free path  $\lambda \approx 1.6 \times 10^4$ , so that  $L \sim 12.5\lambda \ll L_c$ . The elastic system instead has the size of the large inelastic system discussed in the next section, i.e.  $3163 \times 3163$  (it is smaller in units of a diameter, but is much larger in units of a mean free path).

In figure 5 we present the evolution of degree distribution  $f(d, \tau)$  of  $d$  edges attached to a node, with time  $\tau$  measured in collisions per particle ( $cpp$ ), for the four different cases. The average number of edges attached to each vertex (i.e. of collisions done by one particle) is linearly growing with the total number of collisions, i.e.  $\langle d \rangle = 2\tau$ . The four systems display almost identical degree distributions. The form of the distribution is close to a Poissonian when  $\langle d \rangle$  is small and becomes a Gaussian at large  $\langle d \rangle$ . Poissonian and Gaussian statistics are the natural expectations for homogeneous systems where no preferential attachment is at work.

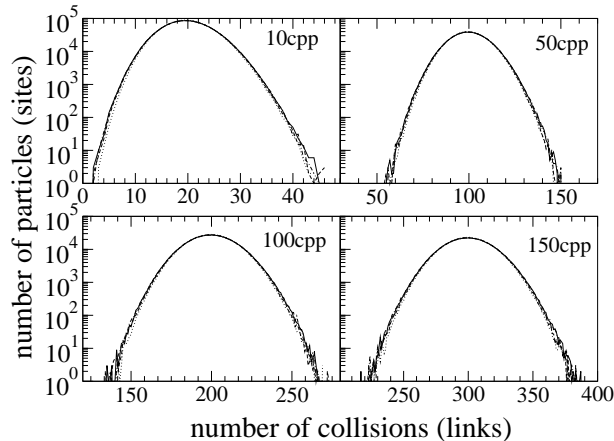


FIG. 5: Distribution of number of links per node (collisions done by each particle) at different times for the four homogeneous cases taken into account: a small inelastic system of hard disks (solid line), a gas of elastic disks (dashed line), a gas of inelastic disks simulated with the DSMC algorithm, and a randomly growing network where each link/collision is done choosing with uniform probability over the set of all possible pair of nodes (dotted line).

In figure 6 results of the  $k$ -shell decomposition are shown for the four different cases. Very similar results are observed for all the cases: a small group of few shells is populated, the shape of the distribution is stationary and is linearly shifting in time towards high shell numbers. A shift in time is expected from the simple fact that  $\langle d \rangle$  is growing. Since the shape of the distribution is conserved, we can track the growth of the average shell number looking at the index of the maximally populated shell,  $k_{max}$ . We observe for all the systems a growth  $k_{max} \sim 1.8\tau \sim 0.9\langle d \rangle$ . To our knowledge, the only calculation of a similar quantity is in [8], in the case of Erdős-Rényi graphs (i.e. random graphs with a Poisson degree distribution with average  $\langle d \rangle$ ) where the largest index of a populated core grows as  $0.78\langle d \rangle$ . Even our random case is different, since we look to a random network with *constant* total number of edges. On the other side, the shape of the shell distribution seems almost identical in all the four homogeneous case and strikingly resembles the shape of Erdős-Rényi graphs depicted in Ref. [8], with an asymmetric distribution and  $k_{max}$  coinciding with the largest index of a populated shell. In particular a nice exponential fit can be applied to the left tail of the distribution with a growth rate that asymptotically (for large  $\tau$ 's) does not depend upon  $\tau$ .

A core of order  $k$  can be, in principle, divided in components, i.e. each of one is a connected subgraph and they are not connected among them. We have verified that in all the four considered cases only one component is present in the graph and in all subgraphs of any core index, consistently with the scenario of the  $k$ -core percolation: the maximum core is therefore a giant fully connected component of the whole graph.

From the results of this section some conclusions can be drawn on the properties of a dynamical collision network in the absence of inhomogeneities. The coincidence of results between an inelastic DSMC gas and a randomly constructed network is not surprising, since the only difference (the bias coming from the collision frequency due to relative velocity) is not a preference on the degree of connection and therefore does not affect the network topology. On the other side, we stress that in gases of hard disks with finite diameter, small spatial correlations in the form of non-flat structure factors are naturally present. This fact, at the level of diluteness we had considered (area fraction smaller than 10%), gives place only to a small correction in the collision frequency, usually taken into account by the so-called Enskog factor in the collisional integral of the Boltzmann equation, with a small  $\alpha$  dependence. In any case those finite diameter correlations do not bias the attachment between nodes after a given total number of collisions. Instead, an interesting observation can be made on the effect of inelasticity: an almost perfect overlap is found between



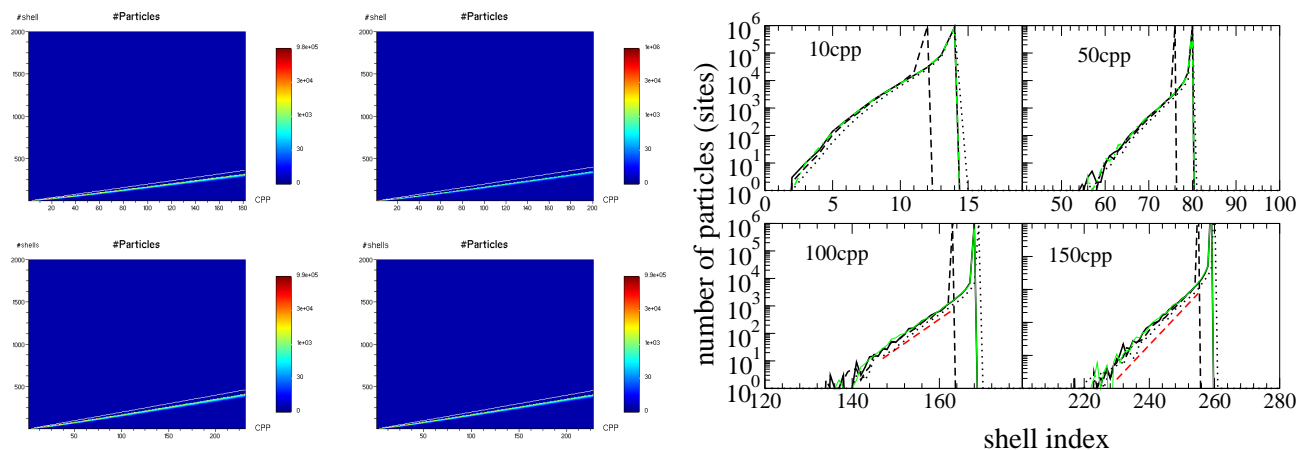


FIG. 6: **Color online:** Distribution of  $k$ -shells for the four homogeneous systems against time  $\tau$  measured in collisions per particle (cpp). Left: time is on the  $x$ -axis, while shell index  $k$  is on the  $y$ -axis. Brightness/color indicates population (number of particles in the shell). The four sub-frames are, starting from the top-left one and going clockwise: the small inelastic MD, the elastic MD, the random network and the DSMC. Right: sections of the left graph at four different times (solid line): the solid line is the small system of inelastic hard disks, the dashed line is the elastic system of hard disks, the (green) dot-dashed represents the system of inelastic hard disks simulated with the DSMC algorithm, the dotted line is the random network. The bold dashed (red) line in the two bottom graphs marks an exponential growth  $\sim \exp(0.24k)$ .

the two inelastic systems (hard disks and DSMC). Inelasticity slightly modifies the distribution of relative velocities which, in turns, modifies the statistics of collisions, and this small effect influences the  $k$ -core distribution both in MD and in DSMC.

Before proceeding, the meaning of “Molecular Chaos” for real finite systems can now be discussed. As mentioned in the introduction, the only realization of a gas satisfying the true Molecular Chaos constraint is a gas where each particle collides with particles that are not connected (via other collisions) with its own previous history: this of course requires infinite particles and gives place to a collision network without cores of index larger than 1, i.e. a tree structure. In finite systems re-collisions are always possible and they are reflected in the percolation of cores of growing indexes, as shown in this section. Anyway, a vast literature teaches us that in all systems discussed here, most of the predictions coming from kinetic equations with the assumption of Molecular Chaos are satisfied. As a matter of fact, the violations of Molecular Chaos described by the presence of cores of growing indexes are negligible for the most of physical observables. We propose, therefore, to use in this case the term “Finite Size Molecular Chaos”. This assumption is analogous to the assumption, typically used in the theory of random graphs, that a graph is “locally a tree”.

A striking deviation from this behavior is observed when spatial homogeneity is broken, as we discuss in the next section.

## V. RESULTS: NON-HOMOGENEOUS COOLING

We consider here a large inelastic system breaking homogeneity (specifically spatial translational invariance). Number of particles is again  $10^6$ . System size is  $3163 \times 3163$ , the density is  $\rho = N/(L^2) = 0.1$ , corresponding to an area fraction of about 7.8% and a mean free path  $\lambda \approx 4$ : in this case  $L \sim 790\lambda \gg L_c$ . This system, after a first stage in the HCS, develops strong and persistent structures in the velocity and density field. Figure 2 clearly illustrates that after  $\sim 40$  cpp (collisions per particle) the HCS is no more a good description of the time evolution of energy and collision frequency. In particular, after  $\sim 70$  cpp, the “final” regime is reached where  $T_g \sim t^{-1}$ . As displayed in figure 3, during the whole “final” regime, a continuous condensation of clusters is at work. Visual inspection of the gas indicates the presence of groups of particles involved in a huge number of collisions dissipating a very small fraction of the energy, while the remnant particles constitute an even more dilute gas and dissipate most of the energy in collisions among themselves or against the clusters.

The analysis of degree distribution of the dynamical network is given in figure 7, compared to the same measure for the elastic system of the same size (which is representative of all homogeneous systems discussed previously). Degree distribution starts to deviate from the Gaussian behavior at  $\sim 40$  cpp, i.e. together with the departure from Haff law. The distribution develops a very fat tail at large values of the number of links per node, representing the contribution



of particles trapped in clusters. No power law tails are observed, but large stretched exponentials.

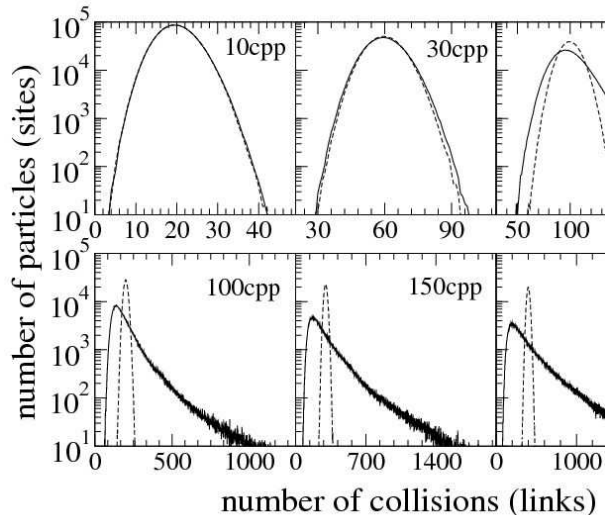


FIG. 7: Histograms of degree distribution  $f(d, \tau)$  for different values of  $\tau$ , i.e. of number of collisions per particle: comparison between the large inelastic system (solid line) and the elastic system (dashed line).

The  $k$ -core analysis of the dynamical collision network is presented, giving results averaged over 10 simulations starting from different random initial conditions, in figure 8. Inspection of left frame of this figure reveals an immediate and striking difference with the corresponding plot for homogeneous systems in Figure 6: at the time of deviation from the HCS ( $\sim 40$  cpp) given by the departure from the Haff law, the narrow distribution of populated  $k$ -shells starts to spread, while the index of the maximally populated shell begins to deviate from the linear law  $k_{max} \sim 1.8\tau$  discussed in the previous section, becoming slower. In the right frame,  $k$ -shell distributions at given times are shown to better illustrate the phenomenon of very large cores contagion. Shells with very high indices are populated by a consistent fraction of particles. The tail at large  $k$ 's of the shell distribution is well fitted by a power law decay with  $\sim k^{-3}$ , while the small and medium  $k$  range resemble a Gaussian function.

The analysis of connected components in the whole graphs (core of index 0) and in the core subgraphs of higher index  $k$ , shown in figure 9 for a given time, teach us that a large component percolates the core, but at high indexes it is accompanied by other few lesser components. A more detailed analysis reveals that the different components are located in different spatial regions, as expected: the disconnected components represent separate clusters.

Finally in figure 10 (left frame) we display some relevant observables as a function of each shell at a given (large) time  $\tau$ . The most remarkable observation concerns the average dissipated energy per collision as a function of the shell index: a strong decay (compatible with an exponential ramp) is visible. This suggests that a typical scale  $k^* \sim 100 \div 150$  (choosing a three orders of magnitude of difference), slightly depending upon  $\tau$ , separates a group of shells where high dissipating collisions occur against a larger group of shells dominated by weakly dissipating collisions. This observation also provides a nice physical interpretation of  $k$ -core decomposition: such decomposition fairly manages to discriminate between the gas-like phase (few strongly dissipating collisions) and the solid-like phase (many weakly dissipating collisions).

Note that, while this separation is clear when the average dissipated energy per collision is regarded, it becomes less evident when looking at the total dissipated energy: collisions in high-index shells dissipate few energy but dominate, in number, the total number of collisions in the gas. We can still say that the most of the total energy of the gas is dissipated in the first group of shells, but we cannot put a clear discriminating mark between “gas” and “solid”.

Another interesting observation concerns the kinetic energy contained in the various shells. Total energy (i.e. summed over all particles in a shell) still reproduces the large peak at small shell indexes followed by a very large tail.

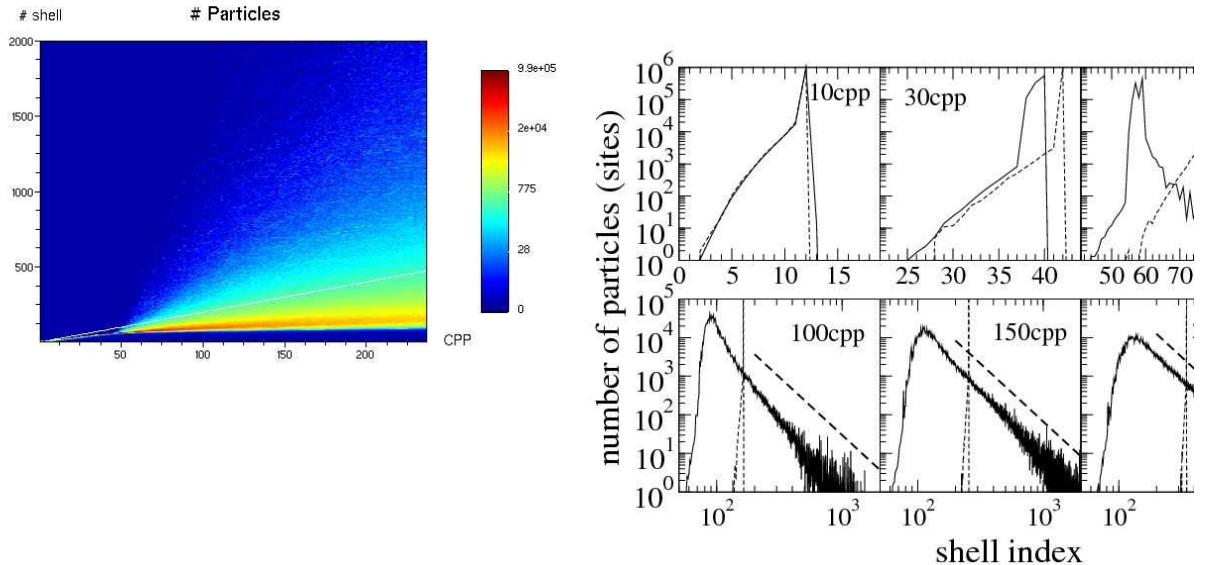


FIG. 8: **Color online:** Distribution of  $k$ -shells in the large inelastic system against time  $\tau$  measured in collisions per particle (cpp). Left: time is on the  $x$ -axis, while shell index  $k$  is on the  $y$ -axis. Brightness/color indicates population (number of particles in the shell). The solid white line marks the  $1.8\tau$  law observed in the homogeneous case. Right: sections of the left graph at six different times (solid line), compared with the elastic system of same size (light dashed lines). The bold dashed line marks a power law decay with  $-3$  exponent.

On the other side the average kinetic energy per particle has much weaker  $k$ -dependence: all shells contain particles with similar kinetic energies, i.e. velocities in absolute value.

The spatial location of grains of a given shell index, given in the right frame of figure 10, confirms the above physical interpretation: particles in the first group of shells (indexes 0-150, at the time chosen) are spread in a low density/high mobility phase, while the rest of the particles constitute compact clusters: in particular, higher shell indexes individuate inner grains whose escape probabilities are smaller and smaller.

Figure 11 shows a synthetic representation of a part of the total collision network after 100 cpp (i.e.  $10^8$  links) for both granular MD simulations, i.e. homogeneous (left) and non homogeneous (right). Only a fraction (20%, i.e.  $2 \times 10^7$ ) of the total number of links is considered in the construction of the picture: this leads to a distributions of shells that differs from the previous analysis (core indexes are much smaller). All particles/nodes are placed in the graph as dots: size, color and position reflect various properties of that node. The color of a dot tells its shell index (following the color scale on the right). The size represents the number of different particles linked to it (following the size scale on the left). The position of each node is able to represent both its core index and the connected component (in its own core) it belongs: each core component is a group of circles with the same center and radii proportional to the core index, while different components have displaced centers, so that they can be distinguished. Small (second order) modifications of this rule are applied to represent also the number of links of the node toward higher shells. In the visualization also a sample (only 1000) of the considered links is displayed, in order to give a flavour of the density of connections in different parts of the network. Looking for example at the right frame, one can clearly see that at low indexes (violet) there is only one component, at high indexes (blue-cyan) there are few different components, while at the highest indexes (red) again only one component is present: all this is consistent with Fig. 9. The reader can find a complete description in [22] and [23]. From this visualization it is possible to immediately evaluate the difference between the homogeneous and inhomogeneous case. In the first case (left of Fig 11) there are very few shells and most of the particles are in the maximum core, while all the cores have a unique connected component, reminding a random graph behavior [7]. On the contrary, in the non homogeneous case (on the right of Fig 11), several components are present, each representing a cluster, while the index of the maximum core is much larger than

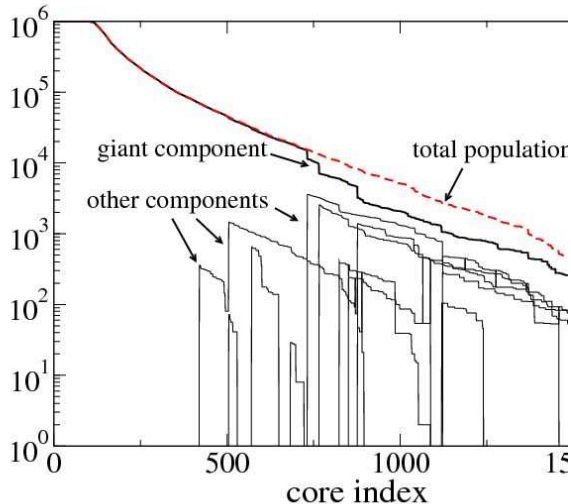


FIG. 9: **Color online:** Plot of the number of particles in disconnected components in each core, as a function of the core index, at time  $\tau = 200$  cpp. At small core indexes, the number of observed disconnected components is 1, then it grows up to  $\sim 6$ .

in the homogeneous case.

## VI. CONCLUSIONS

In this work we have exploited a novel statistical method, originally introduced in the theory of random graphs, to gather information about re-collisions (i.e. collisions among correlated particles) in a cooling granular gas. We constructed a network using the collision sequence up to a given time, then we decomposed it in the  $k$ -core and  $k$ -shell structure. In the homogeneous regime, the finiteness of the system naturally induces a giant component that percolates the core of index  $k_{max} \sim 1.8\tau$  where  $\tau$  is time measured as a number of collisions per particles. When the gas becomes inhomogeneous, because of inelasticity and large size, the system separates into two populations with dramatically different core statistics: a large component percolates the low index  $k$ -cores, while the rest of the gas (a non negligible part) is found in a finite (small) number of disconnected components at very high index  $k$ -cores, corresponding to spatial clusters. The dilute low-core phase is characterized by strongly dissipating collisions, while in the clustered high-core phase the dissipated energy per collision is  $\sim 100$  times smaller.

This is a powerful method to decompose the degree of inter-correlation among particles of a gas, and we believe that an effort should be done to compute its analytical counterpart, in order to gain a theoretical quantitative account of observed results. In principle one should be able to write down a  $k$ -core kinetic equation, of the kind:

$$\partial_t P_k(v, t) = \mathcal{G}_k(v, t) - \mathcal{L}_k(v, t) \quad (4)$$

where  $P_k(v, t)$  is the probability density of finding a particle with velocity  $v$  in the core (or shell)  $k$ , while  $\mathcal{G}$  and  $\mathcal{L}$  are the gain and loss terms respectively, due to collisions with particles of the same or other cores. Nevertheless, we remind that this is not a trivial task, since the evolution of the shell index of a particle is in principle non-local and involves global rearrangements.

On the other hand, this analysis can be easily applied to any “hard core” system, including systems with soft interactions that can be simplified as piecewise hard-like potentials. A natural extension is the study of hard disks and spheres gases at very high packing fractions, with the hope of elucidating the glass transition in off-lattice systems,

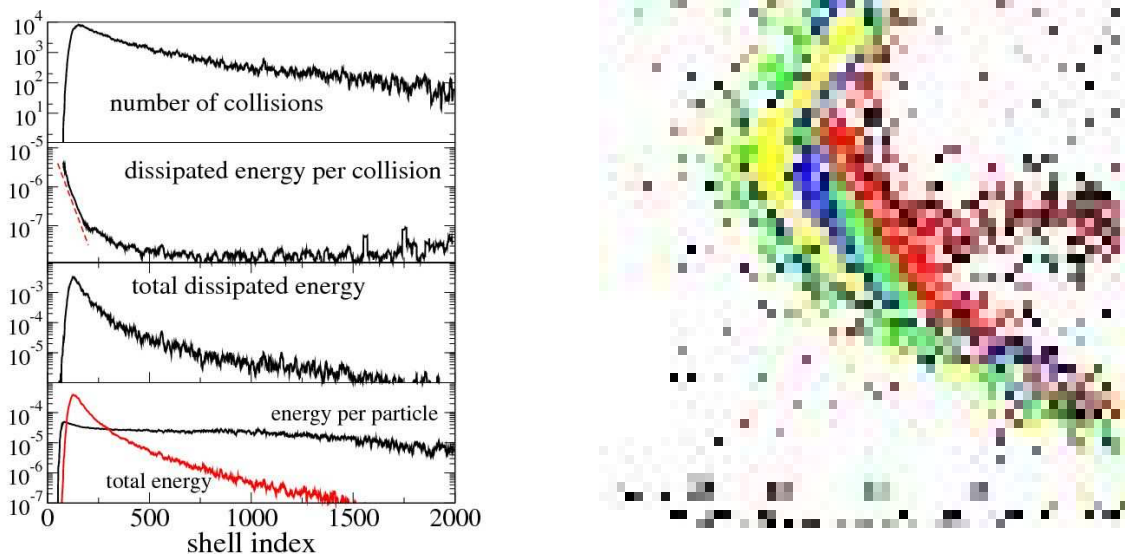


FIG. 10: **Color online.** Left: statistics of physical observables in different shells at a given time ( $\tau = 200$  cpp). Topmost graph: number of collisions performed by particles in a given shell. Second graph from top: dissipated energy per collision, together with an exponential fit of the first decay  $\sim \exp(-0.03k)$ . Third graph: dissipated energy summed over all collisions done by particles in a given shell. Fourth graph: average energy competing to each particle in a given shell and total energy contained in a given shell, rescaled in order to appear on the same scale. Right: a snapshot of the system at  $\tau = 200$  cpp, showing in different colors the shell each grain belongs to.

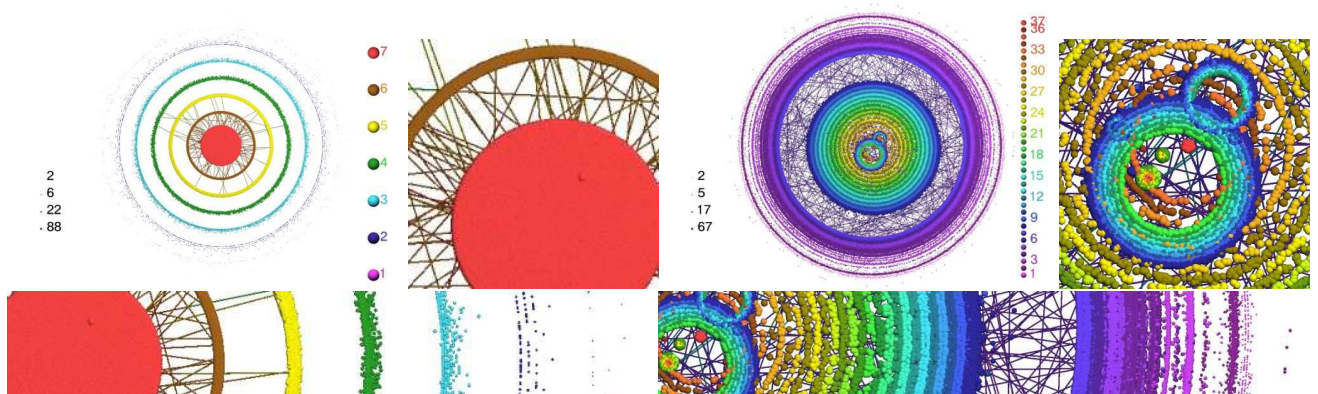


FIG. 11: **Color online.** Visualization of the collision network using LaNet-vi [23]. Left: an homogeneous case, right: non homogeneous case. Both visualizations have been done using a uniformly sampled network because the size of the original one cannot be load into 3GB of RAM memory (only 20% of the collisions have been taken). Each sampled network has the complete visualization (top and left), a zoom of a central part (top right), and an half of a longitudinal cut (bottom).

as well as experimental studies of granular materials, where the use of rapid cameras is today able to collect huge amounts of collisional data.

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