The jamming transition is a k-core percolation transition

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We explain the structural origin of the jamming transition in jammed matter as the sudden appearance of k-cores at precise coordination numbers which are related not to the isostatic point, but to the sudden emergence of the 3- and 4-cores as given by k-core percolation theory. At the transition, the k-core variables freeze and the k-core dominates the appearance of rigidity. Surprisingly, the 3-D simulation results can be explained with the result of mean-field k-core percolation in the Erdős-Rényi network. That is, the finite-dimensional transition seems to be explained by the infinite-dimensional k-core, implying that the structure of the jammed pack is compatible with a fully random network.

The jamming transition occurs when granular materials reach a certain density such that particle motion is prevented \[^1\]. At this point, the system jams into a disordered packing state that can sustain a non-zero shear stress. The jamming transition is a ubiquitous phenomenon that occurs not only with grains but also with other soft materials like emulsions, colloids, and glasses. Finding the maximum density at which materials can pack in such a disordered state is a problem with ramifications in optimization theory as well, since the jammed state can be thought of as a set of solutions to a large class of constraint satisfaction problems \[^2\]. Thus, any insight into the nature of the jamming transition will have implications for a large number of problems in disciplines ranging from physics to computer science and mathematics.

Due to these broad implications, a large number of studies have been devoted to understanding the underlying nature of the jamming transition. Early work noted that the transition is driven by the coordination number, or the average number of contacts of the particles in the contact network \[^1\]. The transition has been identified with the isostatic point at which all particles in the packing begin to satisfy force-balanced equations. Further theoretical refinements have been developed, including approaches inspired by the theory of spin-glasses applied to hard-sphere glasses \[^3\], and statistical mechanical ensembles of equally-weighted jammed configurations \[^2,4\].

Here we show that there is a simpler topological reason underlying the jamming transition: the transition is dominated by the sudden emergence of the giant k-core in the network of contacts. The k-core is a topological invariant of the contact network defined as the unique largest subgraph with a minimum degree (i.e., coordination number) of at least k. The concept of the k-core was introduced in the field of social sciences \[^5\] to quantify social network cohesion and has since been found to have a large number of applications to network science in general. For instance, it can help to explain how influential spreaders of information viralize information in a social network \[^6\]; the robustness of random networks \[^7\]; the structure of the internet \[^8,9\]; the large-scale structure of the brain \[^10\]; and the collapse of ecosystems \[^11\].

Related to the concept of the k-core, k-core percolation is a well-known mathematical problem \[^2\] that studies the sudden emergence of giant k-cores (a k-connected subgraph) as the network goes through a series of discontinuous transitions of mixed nature with first- and second-order features, when one increases the number of links in the network. For a random Erdős-Rényi (ER) network \[^12\], this problem has been analytically solved by Wormied and collaborators \[^13\]. It was shown that subsequent k-cores appear at well-defined average degrees (average coordination numbers in the contact network). The giant 2-core, corresponding to the giant component studied in percolation, appears gradually at an average degree \(c_2 = 1\) as shown by the classic result of Erdős and Rényi \[^14\]. However, it was shown that for \(k \geq 3\), the subsequent giant k-cores appear suddenly through first-order transitions where the size of the corresponding k-core jumps from zero to a finite value, usually quite large compared to the total size of the network. These transitions occur at sharply defined values of the average degree. For instance, the 3-core appears suddenly at \(c_3 \approx 3.35\) where the 3-core jumps from zero to an occupancy (the number of nodes in the network belonging to the k-core divided by the total number of nodes) of \(p_3 \approx 0.27\). Subsequently, the 4-core appears at \(c_4 \approx 5.14\) with occupancy \(p_4 \approx 0.43\), while the 5-core appears at \(c_5 \approx 6.81\) with occupancy \(p_5 \approx 0.55\). Notice that none of these transitions coincide with the isostatic transitions at \(c = 2d\) (frictionless) or \(c = d + 1\) (frictional) for a jammed system in \(d\) dimensions. The predictions of k-core percolation are valid in an ER network, which is an ensemble of nodes in random networks that is effectively defined in infinite dimensions and ignores all correlations between contacts. That is, the dimensionality of the problem does not appear in the ER formulation and the resulting network is fully random; therefore, it is a solution obtained in the mean-field approximation, as it is called in the physics literature.

Here we employ a quasi-static shear protocol to numerically study the jamming transition of a 3d packing of frictional spheres when the coordination number increases as the system jams under shear. We construct
the network of contact points and study the emergence of the giant k-cores in turn. We find that as the shear strain is increased, the contact networks develop giant k-cores in succession exactly at the precise values \(c_k\) predicted by k-core percolation theory in an ER network as obtained in [15]. In particular, the precursor of the jamming transition occurs at \(c_3 \approx 3.35\) (and not at the isostatic point \(c = 4\)) with the appearance of the giant 3-core.

The solution of Wormald [13] captures very precisely the location of the average coordination number at which each k-core appears in the shear jamming numerical data. This result is surprising since the ER solution is valid in infinite dimensions for a fully randomized network where the correlations introduced by the finite size of the particles in 3d are ignored. The agreement between an infinite-dimensional result and a finite-dimensional 3d simulation indicates that correlations introduced by the particles’ constraints are irrelevant. Thus, the jamming transition may be a more simple constraint satisfaction problem than previously thought. Our results show the close relation to the k-core problem which was extensively studied in the mathematical literature and fully solved.

We use the jammed packings already obtained in [15] where an athermal quasi-static shear protocol has been used to produce a series of packings at different volume fractions that jam under shear at different values of the shear strain. The system is monodisperse and composed of \(N = 2000\) spheres subjected to athermal quasi-static shear (AQS) deformation. Particles interact via a repulsive harmonic potential. We perform athermal quasi-static protocol to obtain sheared configurations at different densities. To implement shear, we first do an affine transformation of particle coordinates in small steps of \(\Delta \Gamma = 5 \times 10^{-5}\), followed by energy minimization using a conjugate gradient method and periodic Lees-Edwards boundary condition at a shear strain \(\gamma = \frac{\Delta \Gamma}{3}\). The initial configurations at different densities (\(\phi = 0.56 - 0.627\)) for shearing are produced by starting from an initial equilibrated hard sphere fluid at \(\phi = 0.45\); a fast initial compression is effected using a Monte Carlo simulation until the desired density is reached for the initial configurations.

The contact network which we generate using shear deformation of mono-disperse soft spheres using the AQS protocol, is then used as input to solve for force and torque balance conditions in compact form as \(M \mid F = 0\), where \(M\) is a \((\frac{D(D+1)}{2})N \times DC\) matrix, \(C\) is the number of contacts and \(F\) is a vector of size \(DC \times 1\), with 3 for \(D = 3\), force components \((f^x, f^y, f^\theta)\) for each contact. The matrix \(M\) is constructed from the unit vectors between spheres in contact. Using the matrix \(M\), we construct an energy function \(E = \langle F \mid M^T M \mid F \rangle\) which we minimize to obtain force balance solutions [15]. We minimize the energy function by imposing positivity of normal contact forces, since we treat systems with repulsive interactions only. The force scale is set by the magnitude of the initial guess.

The results obtained in [13] can be summarized in Fig. 1. For all packings examined, a discontinuous jump is seen in the inset of the figure, in the \(xz\)-plane shear stress \(\sigma_{xz}\) around \(\sigma_{xz} = 5 \times 10^{-5}\) (indicated by the horizontal dashed line in both the figure and the inset), at a certain value of the coordination number \(c\) between \(c = 3\) and \(c = 4\). The jamming transition occurs near the vertical line in Fig. 1 marked ”\(c_{iso} = 4\)” close to the isostatic transition for a 3-dimensional jammed system of frictional particles. This value is approximately independent of the packing’s volume fraction \(\phi\); indeed, the data for all packings collapse roughly to a single curve for different \(\phi\). Although it is close to the expected finding of a discontinuous jump at \(c = d + 1\), or \(c = 4\), this transition appears to have a precursor, with the onset of the shear stress increase apparent below the isostatic value of \(c\). The inset shows \(\sigma_{xz}\) as a function of the strain \(\gamma\). Again, we see a discontinuous jump in the shear stress at the jamming transition, occurring at values of \(\gamma\) which are density-dependent and thus unique to each of the particle configurations examined here.

The inset shows the uncollapsed data when plotted as a function of the shear strain.

We analyze these packings to test the idea that k-core percolation is underlying the sudden transition that is observed in Fig. 1. In fact, the similarities between k-core percolation and the jamming transition have prompted previous works to propose the conjecture of a close relation between the two problems [17].

Figure 2 defines the k-core of the network: the maximal subgraph consisting of nodes having degree at least \(k\) [3, 5]. This subgraph is unique but not necessarily
connected, thus the k-cores might be formed by small clusters spread around the contact network. An algorithm to extract the k-core is linear in the system size and consists of iteratively pruning nodes with degree less than $k$, until the k-core is obtained. By definition, the k-cores are nested, that is, the k-core contains the k+1-cores. For instance, the 1-core contains the 2-core, the 2-core contains the 3-core, and so on. Each k-core is composed of two structures: the nodes at the periphery called the k-shell and labeled $k_s$, and the remaining k+1-core. The periphery of the k-core is defined as the subgraph induced by nodes and links in the k-core and not in the k+1-core. The 1-core corresponds to the full network, and its connected component is the so-called giant connected component in percolation. The 1-shell is a forest, i.e., a collection of trees. This forest can be removed from the network and the resulting 2-core is also the same as the giant component in percolation in a statistical sense. For $k \geq 3$, the k-cores are not related to the giant component and appear suddenly when we add more links to the network. The value $k_{\text{core}}^\text{max}$ of the largest order k-core, which coincides with the largest value of the k-shell index $k_s$, is called the k-core number of the network and corresponds to the innermost core of the network. It is a topological invariant of the network, meaning that it does not depend on how the nodes are labelled or the network portrayed, i.e., it is invariant under homeomorphisms.

We find not only that $k_{\text{core}}^\text{max}$ increases with increasing coordination number $c$ (i.e., those contact networks with higher coordination numbers have a greater number of k-shells), but also that there is a rapid transition in the occupancy of $k_{\text{core}}^\text{max}$ when a new k-core emerges. As can be seen in Fig. [3] upon the emergence of a new k-core, the occupancy of the shell that was previously the innermost rapidly falls to a minimum, while the occupancy of the new innermost shell—the new core—sharply increases. Furthermore, plotted across all of the networks under consideration here, these occupancies collapse to a single curve, with the transition happening at roughly the same point for each packing network regardless of the packing’s volume fraction.

For our analysis, we examine the set of particle configurations with volume fraction $\phi$; associated with each configuration is a set of packings with varying coordination numbers $c$ which capture the state of the configuration before, during, and after the jamming transition. We begin by constructing an adjacency matrix for each packing, wherein a value of 1 indicates a contact between two particles and a value of 0 indicates no contact. A k-shell decomposition [3] is then performed on each matrix, following the algorithm described above, to determine both the maximum number of k-shells $k_{\text{core}}^\text{max}$ and the occupancy in each shell from $k = 1$ (the outermost shell) to $k = k_{\text{core}}^\text{max}$ (the innermost shell, or core).

The points at which the new k-cores emerge in the networks of the packings correspond closely to values theoretically determined via k-core percolation in random Erdős-Rényi networks by Wormald [13]. These transition points are indicated in Fig. [1] by the vertical lines at $c_3 = 3.35$, $c_4 = 5.14$ and $c_5 = 6.81$ (for the emergence of the 3-core, 4-core and 5-core, respectively) and also clearly indicated in Fig. [3]. Furthermore, these data over all packings collapse to a single curve, regardless of the volume fraction. Notice also that the percolation transition at $c_2 = 1$ where the giant component (the 2-core) appears is irrelevant for the jamming transition, since it appears way before the larger cores that provide rigidity to the packing. Indeed, jamming is described by the appearance of the giant 3-core and not the giant connected component, which is a tree at the transition point, as opposed to the 3-core which is a well-connected structure and appears suddenly rather than continuously like the giant component. This core does not appear by nucleation, though. Rather, it appears suddenly, jumping from zero to a finite fraction of nodes given by $p_3$. This sudden appearance is due to the fact that jamming requires a global condition of force balance that is satisfied in all the packing, and cannot be satisfied by nucleation of specific regions in the packing. This global feature of jamming might explain the surprising result of why the physics of jamming is captured by a simple mean-field infinite-dimensional fully-random non-perturbative k-core solution even when the packing is three-dimensional. This result may not be directly relevant for the glass transition due to the existence of finite clusters in finite dimensions. In the jamming zero-temperature description, finite clusters in finite dimensions violate force balance and then the jamming transition must appear as a giant core.

When we fully randomized the links in the packings while keeping the original degree distribution (or coordination number) $c$, we arrive at a null model—the Erdős-Rényi network for this particular $c$ and number of particles. Even when the correlations are removed in this manner, it can be seen in Fig. [3] by the solid lines that the transitions occur at very similar values of $c$ between the real networks and their fully randomized counterparts. We use a set of Erdős-Rényi networks with the same

![FIG. 2: Definition of k-core, k-shells and maximum k-core.](image-url)
number of nodes as the packings \((N = 2000)\) and average degree equal to coordination number \(c\), for \(c = 0.5\) to \(c = 7.0\) in steps of 0.1. Following the procedure as before, we perform a k-shell decomposition of each network and find both the occupancy of every shell in the network, and the network’s value of \(k_{\text{max}}\). For each value of \(c\), 1000 ER networks are generated, and the values for \(k_{\text{max}}\) and shell occupancy are averaged over the generated networks. These results, shown in Fig. 3, as the solid curves in black; blue; red; green; and cyan, correspond, respectively, to 1- through 5-cores. At theoretically-predicted coordination numbers \(c_k\) and fractional k-shell occupancies \(p_k\), denoted in Fig. 3 by the dotted lines, the system undergoes transitions wherein a \(k + 1\)-core (i.e., a new value of \(k_{\text{max}}\)) emerges. As before, for \(k > 2\)-cores the occupancy of the former innermost core falls sharply and discontinuously to a minimum while the occupancy of the new core sharply and discontinuously increases. It can be seen that the points at which new cores emerge in the packings match the points at which the new cores emerge in the generated ER networks, despite the occupancies of the cores being slightly larger in the packings; this could be the only effect of the correlations between the particles. The strong similarity between the emergence of new cores in both packings and generated ER networks thus implies that underlying the jamming transition of the packing is the emergence of a k-core via k-core percolation.

Beyond the jamming transition, the phenomenon of k-core percolation pertains to other systems whose components (the nodes) require a minimum number of \(k\) connections to other nodes to participate in the dominant cluster. Since the k-core sets a constraint on the minimum number of neighboring nodes, the physics of k-core percolation describes also the onset of arrested transitions for other systems with nontrivial constraints, such as spin glasses, glass-forming liquids, and constraint satisfaction problems (CSP). For instance, a prototypical model of spin glass systems, known as the \(p \geq 3\)-spin glass model, exhibits a critical transition with the same exponents as k-core percolation, at least at the mean field level.

In the physics of the glass transition, a way to model glassy dynamics is via kinetically constrained spin lattice models, where down spins denote regions of low mobility of the liquid, and up spins denote regions of high mobility. In addition, a small negative magnetic field is applied to favor down spins and thus the formation of clusters of low mobility. When the temperature of the system is lowered, more and more clusters of low mobility are formed, eventually leading to dynamical arrest of the liquid. The kinetic constraint on the motion of the spins is such that a spin can flip only if the number of neighboring up spins is equal to or greater than some integer \(k\), which models the trapping of particles by cages made up of their neighbors. Given that up/down spins can be mapped to present/removed nodes, this kinetic constraint maps to the k-core condition, and the emergence of a giant cluster of low mobility regions maps to the k-core percolation.

Another important case is that of constraint satisfaction problems, where variables must take values which satisfy a number of constraints. The random K-XORSAT is an example of such CPS. In this case, the percolation of a 2-core separates the Easy-SAT and Hard-SAT phase. In the Easy-SAT phase there is no core, so that solutions can be found in linear time. In the Hard-SAT phase there exists a large 2-core, and no algorithm is known that finds a solution in linear time. This is due to the existence of ‘frozen’ variables inside the core (more precisely in the backbone, which includes the core and all nodes in a corona surrounding the core), which are fixed in all possible solutions. Similarly, in the coloring of random graphs, frozen variables appear if and only if the \(q\)-core of the graph is extensive, where \(q\) is the number of colors.

Our results suggest that the onset of jamming in packings can be understood by the emergence of a 3-core of frozen variables, analogously to these constraint optimization problems. Thus, a large part of the physics of the jamming transition can be explained by this simple structural picture of the emergence of the 3-core at the analogous Easy-SAT to Hard-SAT transition. This is indeed a rigidity transition when frozen variables appear in the dominating clusters. After the 3-core has emerged, there is still a hard region in the coordination number that can be described by following the phenomenology of more sophisticated spin glass type models such as the CSP above.

In conclusion, the picture emerging from this study is that the onset of jamming is not related to the isostatic point nor to regular percolation but to the sudden emergence of the k-core and that the structure of the jammed packing is completely random. That is, the correlations are minimal and the transition is captured well by an ER network—an infinitely dimensional network with no correlations.
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