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The jamming transition is a k-core percolation transition

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HIGHLIGHTS

- Jamming has precursor in emergence of giant 3- and 4-cores in same-size ER networks.
- Shear stress begins to increase near giant 3-core emergence in ER networks.
- Shear stress has density-independent discontinuous jump at isostatic point.
- ER networks' 3- and 4-cores jump in size around same coord. numbers as packings.
- Applications include constraint satisfaction, computer science, math, soft materials.

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ABSTRACT

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 emergence of the giant 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 Erdös–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, preventing particle motion [1]. The system then 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 has ramifications in optimization theory also; 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 has implications for many problems in disciplines ranging from physics to computer science and mathematics.

A large number of studies have therefore been devoted to understanding the underlying nature of the jamming transition. Early work noted that the transition is driven by the coordination number, or 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 [3–7]. Further theoretical refinements have been developed, including approaches inspired by spin-glass theory applied to hard-sphere glasses [8], and statistical mechanical ensembles of equally-weighted jammed configurations [2,9].

Here we show that there is a simpler topological reason underlying the jamming transition: it is dominated by the sudden emergence of the giant k-core in the contact network. The k-core, a topological invariant of the contact network defined as

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the unique largest subgraph with minimum degree (i.e., coordination number) of at least k, was introduced in the field of social sciences [10] to quantify social network cohesion. It has since been applied broadly to network science in general: it can help to explain how influential spreaders viralize information in a social network [11]; robustness of random networks [12]; structure of the internet [13,14]; large-scale structure of the brain [15]; and collapse of ecosystems [16].

Related to the concept of the k-core, k-core percolation is a well-known mathematical problem [12,17] that studies the sudden emergence of giant k-cores (k-connected subgraphs) 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 Erdös–Rényi (ER) network [18], an ensemble of nodes in random networks effectively defined in infinite dimensions which ignores all correlations between contacts, this problem has been analytically solved by Wormald and collaborators [17]. It was shown that subsequent k-cores appear at well-defined average degrees (average coordination numbers in the contact network). The giant 2-core, or giant component studied in percolation, appears gradually at average degree $c_2 = 1$ as shown by the classic result of Erdös and Rényi [19]. However, it was shown that for $k \geq 3$, the subsequent giant k-cores appear suddenly through first-order transitions at sharply defined values of the average degree 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. For instance, the 3-core appears suddenly at $c_3 \approx 3.35$, jumping from zero to an occupancy (number of nodes in the k-core divided by 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. The dimensionality of the problem does not appear in the ER formulation and the resulting network is fully random; it is a solution obtained in the mean-field approximation.

We employ a quasi-static shear protocol to numerically study the jamming transition of a 3-D packing of frictional spheres with increasing coordination number as the system jams under shear. We construct the network of contact points and study the emergence of the giant k-cores in turn. As the shear strain is increased, the contact networks develop giant k-cores in succession exactly at the precise values c_k predicted by theory for an ER network [17]. In particular, the precursor of the jamming transition occurs at $c_3 \approx 3.35$ (rather than the isostatic point $c = 4$) with the appearance of the giant 3-core.

The similarity between k-core percolation and the jamming transition have been shown in previous works by Schwarz et al. [20]. The critical exponents defining the jamming transition, including $\beta = 1/2$, $\gamma = 1/2$, and $\nu = 1/4$, which measure the dependence of the coordination number, the vanishing of the shear modulus, and the diverging length scale, respectively, with the volume fraction near the jamming transition, have been calculated numerically [3–7,20]. The values c_k mentioned above are not discussed in [20]. As the coordination number c is lowered from above to the value at which jamming occurs, it depends on the exponent β as $\langle c\rangle = c_{jam} + c_0(\phi - \phi_{jam})^\beta$ for volume fraction ϕ, with subscripts *jam* and 0 denoting the value where jamming occurs and the starting value, respectively; the shear modulus, or ratio of shear stress to shear strain, disappears as the exponent γ goes to 1/2; and the exponent ν describes the divergence of the length scale [20]. They agree with those predicted by k-core percolation [20]; therefore, these results further stress the analogy between jamming and the k-core.

The solution of Wormald [17] captures very precisely the location of the average coordination number at which each k-core appears in the shear jamming 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 3-D are ignored. The agreement between an infinite-dimensional result and a finite-dimensional 3-D simulation indicates that correlations introduced by the particles' constraints are irrelevant—the jamming transition may be a simpler constraint satisfaction problem than previously thought.

We use the jammed packings already obtained in [21] where a series of packings at different volume fractions that jam under shear at different values of the shear strain were produced using an athermal quasi-static shear protocol. The system is monodisperse and composed of $N = 2000$ spheres interacting via repulsive harmonic potential, subjected to athermal quasi-static shear deformation. To implement shear, we first do an affine transformation on a system of frictionless particles in small steps, followed by energy minimization using a conjugate gradient method and periodic Lees–Edwards boundary condition at shear strain γ. Initial configurations at different volume fractions ($\phi = 0.56 - 0.627$) for shearing are produced by starting from an 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.

The obtained contact network is then used as input to solve for force and torque balance conditions as described below, allowing for both normal and tangential forces, corresponding to friction. Past work [22] has demonstrated that sheared frictionless spheres evolve contact geometries that can support finite stresses if frictional forces are also present [22]. We estimate the normal and the tangential force components independently, *i.e.,* in the limit of infinite friction: for a given contact network, we write the force and torque balance conditions in compact form as $M\,|F\rangle = 0$, where M is a $((\frac{D(D+1)}{2})N \times DC)$ matrix, C is the number of contacts and $|F\rangle$ is a vector of size $DC \times 1$, with 3 for $D = 3$, force components (f^n, f^θ, f^ϕ) for each contact. The matrix M is constructed from unit vectors between spheres in contact. Using M, we construct an energy function $E = \langle F \mid M^T M \mid F\rangle$ which we minimize to obtain force balance solutions. We minimize the energy function by imposing positivity of normal contact forces, since we treat systems with repulsive interactions only.

The results obtained in [21] are replotted in Fig. 1 as a function of the coordination number. For all packings examined, a discontinuous jump is seen in the inset of the figure, in the *xz*-plane shear stress (σ_{xz}) around $\sigma_{xz} = 5 \times 10^{-9}$ (indicated by the horizontal dashed line in both the figure and the inset). The jamming transition occurs at the isostatic point, given

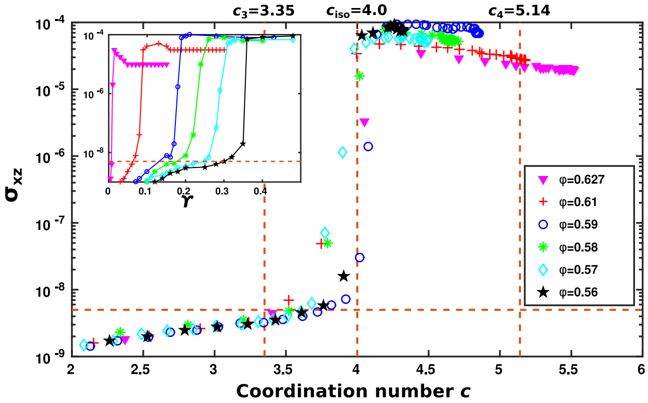

Fig. 1. Jamming transition. Shear stress versus coordination number collapse into a single curve for all volume fractions. Inset shows the uncollapsed data when plotted as a function of the shear strain.

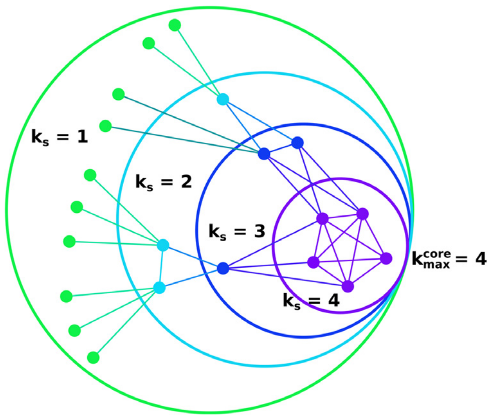

Fig. 2. Definition of k-core, k-shells and maximum k-core.

by the vertical line in Fig. 1 marked "$c_{\text{iso}} = 4$", for a 3-dimensional jammed system of frictional particles. This value is approximately independent of the packing's volume fraction ϕ; indeed, the data for all packings collapse to a single curve for different ϕ. This isostatic transition appears to have a precursor where shear stress starts to increase. The inset shows σ_{xz} as a function of the strain γ. Again, we see a discontinuous jump in the shear stress at the jamming transition, occurring at density-dependent values of γ unique to each particle configuration examined.

We analyze these packings to test the idea that k-core percolation is a precursor to the sudden transition observed in Fig. 1. Fig. 2 defines the k-core of the network: the maximal subgraph consisting of nodes having degree at least k [10,12]. This subgraph is unique but not necessarily connected; 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, 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 (the k-shell, labeled k_s) and the remaining k+1-core. The periphery 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, which can be removed from the network. The resulting 2-core is statistically the same as the giant component in percolation. For $k \geq 3$, the k-cores are not related to the giant component, appearing 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, independent of how the nodes are labeled or the network portrayed, i.e., it is invariant under homeomorphisms.

We examine the set of particle configurations with volume fraction ϕ; 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 contact between two particles and a value of 0 indicates no contact. A k-shell decomposition [11] is then performed on each matrix, following the above algorithm, to determine 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).

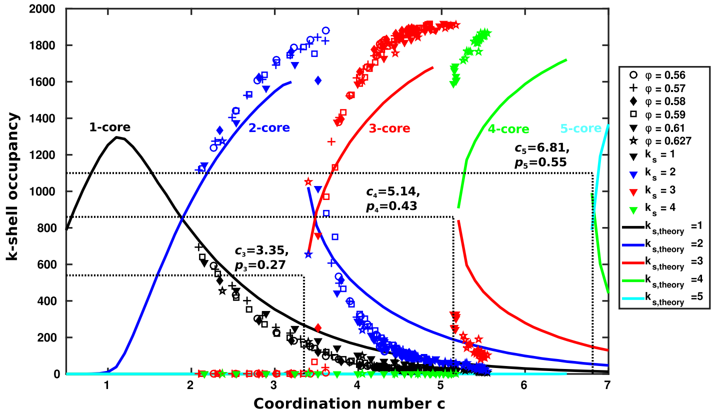

Fig. 3. The jamming transition is described by the successive appearance of giant k-cores at coordination numbers predicted by random ER theory [17]. The solid lines represent the theoretical predictions for the emergence of k-cores on an ER network, while the discrete points represent our data. Data plotted in black; blue; red; green; and cyan represent the populations of the 1- through 5-cores, respectively, while each shape represents a different volume fraction.

We find not only an increase in $k_{\text{core}}^{\text{max}}$ with increasing coordination number c (i.e., contact networks with higher coordination numbers have more k-shells), but also 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 $k_{\text{core}}^{\text{max}}$, the occupancy of the previous $k_{\text{core}}^{\text{max}}$ rapidly falls to a minimum, while the occupancy of the new $k_{\text{core}}^{\text{max}}$ 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 volume fraction.

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 Erdös–Rényi networks by Wormald [17]. These transition points are indicated in Fig. 1 by vertical lines at $c_3 = 3.35$ and $c_4 = 5.14$ (for the 3-core and 4-core, respectively) and also clearly indicated in Fig. 3. 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 preceded by the appearance of the giant 3-core and not the giant connected component, which is a tree at the transition point whereas the 3-core is a well-connected structure. It appears suddenly rather than continuously (like the giant component) or by nucleation, jumping from zero to a finite fraction of nodes given by p_3. The sudden appearance arises from jamming requiring a global condition of force balance to be satisfied throughout the packing, which cannot be satisfied by nucleation of specific regions. 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. Our result may not be directly relevant for the glass transition due to the existence of finite clusters in finite dimensions. These violate force balance in the jamming zero-temperature description; the jamming transition must then appear as a giant core.

We arrive at a null model—the Erdös–Rényi network for this particular c and number of particles—by fully randomizing the links in the packing while keeping the degree distribution (coordination number) c. Even removing the correlations in this manner, the transitions occur at very similar values of c between the real networks and their fully randomized counterparts (the solid lines in Fig. 3). We use a set of Erdös–Rényi networks with the same 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. We then perform a k-shell decomposition of each network, finding both the occupancy of every shell in the network, and the network's value of $k_{\text{core}}^{\text{max}}$. For each value of c, 1000 ER networks are generated, and the values for $k_{\text{core}}^{\text{max}}$ and shell occupancy are averaged over these. The 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 $k_{\text{core}}^{\text{max}}$) emerges [17]. 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. 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 jamming, the phenomenon of k-core percolation pertains to other systems whose components (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) [23]. 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. Such a model is at the basis of the infinite-dimensional jammed sphere model in [6].

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. A small negative magnetic field is applied to favor down spins and thus the formation of low-mobility clusters. When the temperature of the system is lowered, more and more of such clusters 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 [23]. 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.

Furthermore, our results support the hypothesis that certain features of the k-core percolation transition in the mean field carry over to three dimensions. The discontinuities in the occupancies of the 3- and 4-cores in Fig. 3 suggest this. Whether this phenomenon is a true transition that survives in the thermodynamical limit will require further theoretical developments, i.e., analytical solutions valid for infinite system size that could avoid the finite size effect inherent in our simulations. In turn, we note that the shear stress does not show any particular behavior for the specific coordination values at which the different k-cores appear as expected by the k-core analysis. However, the appearance of the discontinuity in the shear stress is clearly happening at the isostatic point. In this regard, we can associate the sudden appearance of the 3-core at c_3 with the onset of the discontinuity in the shear stress. While it is difficult to define clearly this onset in terms of the behavior of the shear stress, from Fig. 1 we can see that the shear stress starts to deviate around c_3, ultimately ending in the jump at the isostatic point.

In conclusion, the picture emerging from this study is that the onset of jamming is related to the sudden emergence of the k-core and that the structure of the jammed packing is completely random. That is, correlations are minimal and the transition is captured well by an ER network—an infinitely dimensional network with no correlations.

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