Letter

Assur graphs, marginally jammed packings, and reconfigurable metamaterials

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Isostatic frames are mechanical networks that are simultaneously rigid and stress-free. Isostaticity itself is a powerful concept in understanding phase transitions in soft matter and designing mechanical metamaterials. We show that the contact network of marginally jammed packings approaches not only isostaticity but minimal isostaticity in the thermodynamic limit. We define in turn this minimal isostaticity and describe how global nonlocal mechanical responses are hallmarks of minimally isostatic graphs (MIGs) known previously as Assur graphs. By using the related concept of Assur decomposition, which we generalize for periodic boundary conditions, we not only assess our claim about jammed packings but we also offer a new design principle for mechanical metamaterials in which motion and stress can propagate in reconfigurable pathways, while rigidity of the entire structure is maintained. We also briefly note an apparent relationship between fully repulsive interactions and the emergence of MIGs at the unjamming point.

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I. INTRODUCTION

The concept of rigidity is central to both soft matter physics (from gelation [1,2], jamming [3], to mechanical transitions in biological tissues [4]) and the design of mechanical metamaterials, where deformation and stress responses are programed via geometry and topology [5,6]. Given the tensorial nature of rigidity (as opposed to connectivity or conductivity, which are scalars), rigidity transitions can take many forms characterized by distinct universality classes. Among them, the special point of "isostaticity," where the numbers of nontrivial zero modes (ZMs, normal modes of zero energy) and states of self-stress (SSSs, force-balanced stress eigenstates) both vanish, characterizes a type of mechanical critical point where the whole system is coordinated in a unique way where all degrees of freedom are marginally constrained [7–9]. It is known that the jamming transition of athermal frictionless repulsive disks (or spheres in three dimensions) occurs at the isostatic point [3,10–12], whereas many other rigidity transitions do not [1,13–22].

Interestingly, it has recently been shown that isostatic networks derived from disk packings close the jamming point not only approach isostaticity, but also exhibit a *global* change in rigidity when arbitrary edges are added or removed [20]. Furthermore, this property was shown to be special to these marginally jammed packings (MJPs) and not common to other disordered isostatic networks.

In this paper, we provide a rigorous characterization of the graph (connectivity) property underlying this observed behavior. We identify this property as "minimal isostaticity" and relate it to the notion of the Assur graphs from the mechanical engineering literature [23,24]. In particular, we generalize the concept of Assur graphs from the case of pinned graphs to graphs embedded on the torus, apply it to MJPs under periodic boundary conditions (PBCs), and reveal that their contact networks approach minimal isostaticity in the thermodynamic limit. We also prove that this is a necessary consequence of purely repulsive interactions in the special case of jamming in circular containers. We see this as an indication that the unique properties of Assur graphs may be relevant to answer the question of how the physical process that assembles MJPs leads to their unique mechanical properties. Furthermore, we propose a design principle based on Assur decomposition for mechanical metamaterials in which the switch of one connection can sharply and remotely control the range of motion and stress propagation. We highlight this practical aspect since we perceive that combinatoric rigidity in general has gone underutilized in metamaterial design.

II. ASSUR DECOMPOSITION AND MINIMAL ISOSTATIC GRAPHS

A. Review of combinatorial rigidity and Assur decomposition in pinned graphs

We start by reviewing the notion of generic (i.e., combinatorial) rigidity. Given a framework that is a collection of rigid bars (or springs), with perfectly flexible hinges joining them, it is natural to ask what conditions must it satisfy to be rigid. This question was addressed by Maxwell [25] back in 1864, and it has seen much development recently. Modern generic rigidity theory comes from the recognition that a framework can be described as a graph G realized in space by giving the vertices positions $\mathbf{X}$ and having the edges as straight lines connecting them, and crucially, that most properties concerning "rigidity" are derivable from just the graph G. A graph G is said to be rigid if it can be realized into a frame $(G, \mathbf{X})$ that is infinitesimally rigid. By infinitesimally

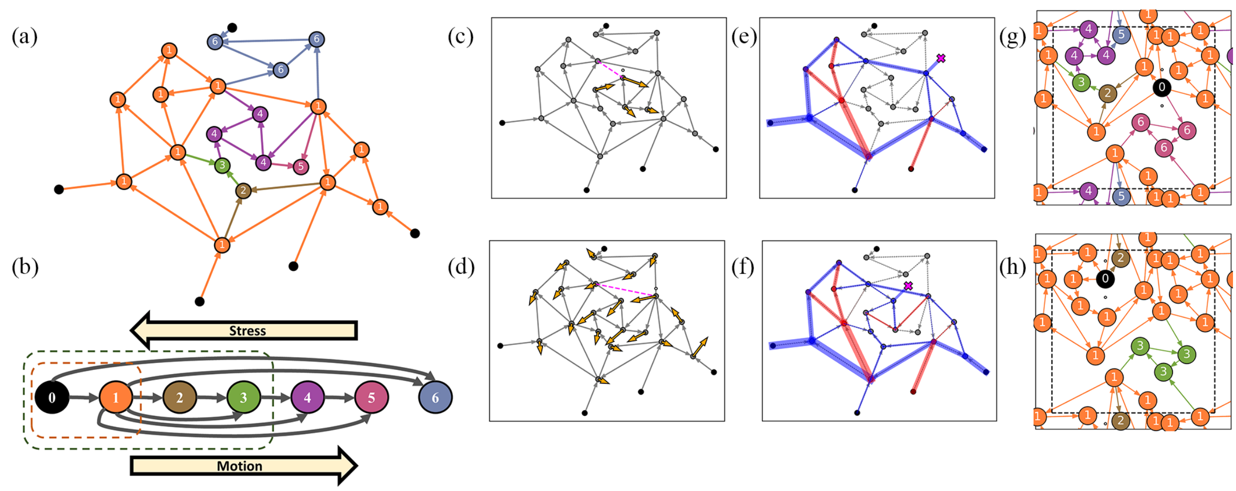

FIG. 1. Assur decomposition for pinned and torus isostatic graphs. (a) A pinned isostatic graph with its six Assur components identified. (b) Partial order of the Assur components of the graph in (a), with two isostatic subgraphs identified with boxes and the directions for the propagation of motion and stress marked. In the following panels, the pruned edges are marked by dashed magenta lines, external forces represented as the addition of a redundant edge to ground (magenta cross). The resulting ZM is plotted in orange arrows (with the displacement amplitude proportional to the length of the line excluding the arrowheads) and the resulting stress in red (tension) and blue (compression). (c) Pruning an edge in component 4 results in a ZM that only moves component 4 and its descendants. (d) Pruning an edge in component 1 results in a full ZM that moves all vertices. (e) External force on component 1 stresses only component 1. (f) External force on a vertex of component 4 stresses component 4 and its ancestors. (g), (h) Assur decompositions of a torus isostatic graph, where different choices of the ground (black "0" vertex with two pebbles) led to different decompositions. PBC boxes are shown as black dashed squares. This ambiguity is avoided in the torus PGA algorithm we use (see SM, S-3 [27]).

rigid we mean that no nontrivial set of infinitesimal vertex displacements leaves edge lengths unchanged to first order. Such sets of displacements are called ZMs, and so one can say a framework is rigid *iff* it has no nontrivial ZMs. Almost all realizations of a rigid graph are infinitesimally rigid [8] and are thus called *generic* (and in our discussions below, when we say something is "generally" true we refer to this notion). The isolated exceptions are called *geometrically singular* or just singular. In general, geometrically singular realizations of rigid graphs will still be rigid to finite displacement [8,26]. The phrase "almost all realizations" may require some clarification. In very precise terms, what this refers to is that the space of all nonrigid realizations of a rigid graph is of lesser dimension than the space of all realizations. This implies that for points taken at random from the space of all realizations, the probability of it being not rigid is infinitesimal.

When a graph has more edges than necessary to ensure rigidity, these edges are called redundant and lead generically to SSSs. An isostatic graph is a rigid graph with no redundant edges.

A minimally isostatic graph (MIG) is an isostatic graph with no proper rigid subgraphs [23,24,28–30]. The removal of any portion of a MIG results in a global loss of rigidity (otherwise the part that remained rigid would be a proper rigid subgraph). Most studies of MIGs are either on pinned or unpinned graphs on the plane. Figure 1(a) shows an example of a pinned isostatic graph, and we orient the graph, assigning a direction to each edge, by using the pebble game algorithm (PGA) for pinned graphs [29] based on Laman's theorem [7]. The PGA and its variants have a long history of use in the soft matter community for the analysis of rigidity percolation problems [13]. For our purposes, the PGA is an algorithm that takes as input an undirected graph and gives as output a fully directed or partially directed graph, as some edges called redundant are left undirected. Crucially, the output of the PGA contains all relevant information about generic rigidity. Different scenarios, such as having pinned vertices or being embedded in d spatial dimensions or on a torus, have different rigidity rules and therefore different variations of the PGA. In general, across the different PGAs d "pebbles" are assigned to each unpinned vertex, representing its inherent degrees of freedom (DOFs), where d is the dimension of the underlying space. The PGA then searches for a "d-in orientation," i.e., an orientation where as many edges as possible are oriented, and each vertex has up to d edges pointing towards it. The number of free pebbles at each vertex s, which is d-in degree (s), represents the number of unconstrained degrees of freedom, i.e., ZMs. Undirected edges, on the other hand, correspond to redundant constraints and therefore imply SSSs. Note that these ZMs and SSSs are generic. Additional pairs of ZMs and SSSs can be generated when the realization of the graph is at a geometric singularity.

Now, consider the framework in Fig. 1. Here all internal vertices have in-degree of 2, representing the two DOFs (pebbles) of that vertex being constrained by the corresponding oriented edges. The ground has in-degree 0 (no inherent DOFs). Here we have used the word "ground" to denote the collection of points with no DOF, so they can be thought of as bolted or fixed to the literal ground. This usage is also very much in analogy to the ground in electrical circuits. Such a result of the PGA where all edges are oriented and all internal vertices have in-degree 2 indicates that all the DOFs are paired with corresponding constraints and there are no redundant edges. The existence of this orientation is sufficient and necessary for pinned isostaticity, and the orientation is unique up to the reversal of cycles [24]. Important information is carried by this 2-in orientation: upon the removal of one edge, the motion of each vertex is determined by its two immediate ancestors (vertices upstream), and this information is then passed to its descendants (vertices downstream), as shown in Figs. 1(c) and 1(d). Conversely, stress (i.e., violation of length constraints from the edges) travels upstream, as shown in Figs. 1(e) and 1(f). One can think of this as adding a prestressed edge. The response to this external force generally results in tension on all edges upstream (ancestors) from the node where the force is applied.

The orientation of a pinned isostatic graph gives a decomposition of this graph into strongly connected components (defined as clusters in which every vertex can be reached from every other vertex along directed edges): the so-called Assur components [24,29]. This decomposition identifies *clusters on the graph where their motion or stress must emerge or disappear in a synchronous way*. Crucially, this decomposition tells us all possible pinned isostatic subgraphs. This is because Assur components of an isostatic graph have a partial order according to the orientation such as depicted in Fig. 1(b). Isostatic subgraphs correspond to subsets of these Assur components such that for every component, all of its ancestors are also in the subset. This procedure of using the pinned pebble game to orient graphs and finding the Assur components has been explained in Ref. [29].

It is worth noting that this discussion can be framed algebraically in terms of the compatibility matrix C (also known as the rigidity matrix or the kinematic matrix), which acts on vertex displacements u and gives the resulting edge elongations e ($e = Cu$), and its transpose the equilibrium matrix Q, which acts on edge tensions t and gives the resulting forces f at the vertices ($f = Qt$) [31]. Thus the null space of C corresponds to ZMs and the null space of Q to SSSs. The Assur decomposition imposes a partial ordering on the vertices and edges. By placing the columns and rows according to the partial ordering, the matrix C is written in lower block triangular form

$$C = \begin{pmatrix} C^{(1)} & 0 & \cdots & 0 \\ C^{(2,1)} & C^{(2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ C^{(m,1)} & C^{(m,2)} & \cdots & C^{(m)} \end{pmatrix}, \tag{1}$$

where each block in the diagonal is square and full rank and identified with one Assur component [24]. The equilibrium matrix $Q = C^T$ is upper block triangular, correspondingly. The previously described mechanical properties of the decomposition can be shown by solving block by block matrix equations $e = Cu$ and $f = Qt$. Thus, when an edge in component i is pruned, the resulting ZM will involve all vertices in components $j \geqslant i$. The addition of any new edge in component i (either between nodes in i or connecting them to the ground which represents external forces) will introduce an SSS that involves all edges in components $j \leqslant i$.

In light of this discussion, we can then characterize pinned isostatic graphs with only one Assur component, which are of special interest to our discussion. For a pinned isostatic graph, it is known that the following statements are equivalent: (i) it contains no proper isostatic subgraphs, (ii) it is indecomposable (i.e., strongly connected for any 2-in directed orientation), (iii) the compatibility matrix has no proper block triangular decomposition, (iv) removal of any edge results in a ZM that moves all vertices, and (v) forces exerted on any vertex stresses all edges. Graphs satisfying these conditions are called Assur graphs or MIGs [23,24].

B. Assur decomposition of graphs on the torus

We next generalize these concepts to frames on the torus, as PBCs are adopted in most studies of jamming. Let us take a step back and review Laman's theorem for frameworks on the plane. In that case, there are always three trivial motions and therefore $2N - 3$ edges are necessary to ensure rigidity. Laman's theorem tells us that in order for a graph to be isostatic on the plane, it must have exactly $2N - 3$ edges, and for all subgraphs with N_b' edges and N' vertices, $N_b' \leqslant 2N' - 3$. This condition is sufficient and necessary. A more succinct way of stating Laman's theorem is that "isostatic graphs on the plane are (2,3)-tight graphs," where (d, k)-tight means that the graph has $dN - k$ edges and all subgraphs have $\leqslant dN' - k$ edges [32]. For frameworks embedded on a flat two-dimensional (2D) torus, rotations are forbidden, which leaves only two trivial translations. One might then expect that being a $(2, 2)$-tight graph would be synonymous with being isostatic on the torus, in analogy to the plane. This is not the case. The nontrivial topology of the underlying space complicates matters, and one must distinguish between contractible and noncontractible loops. Laman's theorem for isostaticity along with an appropriate PGA has been generalized in Ref. [33] such that for a graph of N vertices to be generically isostatic when embedded on the torus ("torus isostatic" for short), it must be both (2,2)-tight, and all (2,2)-tight subgraphs are embedded constructively (i.e., possess noncontractible loops) [33]. More details can be found in the Supplemental Material (SM) [27]. We use the torus PGA algorithm devised in Ref. [33] to obtain orientations of our graphs, and from them Assur decompositions [Figs. 1(g) and 1(h)].

We thereby generalize the definition of MIGs to torus isostatic graphs, along with their unique properties in the following theorem (see the SM [27] for the proof).

Theorem 1. Given a graph G that is isostatic on the torus, the following are equivalent:

(a) G has no proper subgraphs that are isostatic on the torus.

(b) Any orientation of G where the in-degree of all but one vertex is 2 is strongly connected on all but that one vertex.

(c) Removal of any edge results in a generic ZM that moves all vertices relative to each other.

(d) A generic torque on any edge stresses all edges.

(e) Adding one edge introduces an SSS that either stresses all edges or only a nonconstructive subgraph.

In the context of this theorem, it is worth defining the notion of a "minimally (2,2)-tight" graph, a graph that is (2,2)-tight with no proper (2,2)-tight subgraphs. Note the analogy to the definition of a MIG. Such a graph can be realized as a MIG on the torus. In fact it is a necessary condition (as discussed above), a pinned MIG (i.e., an Assur graph), by taking one vertex to be the ground, and as a free frame on the plane with only one SSS (which must be a global SSS), sometimes called a Laman circuit. This is just to highlight further alternative characterizations and curious connections to other structures. We give a brief demonstration of this in the SM, S-3 [27]. We also propose that many of the unique properties presented here can be generalized to minimally (k, k)-tight graphs (see the SM, S-2D [27]), although the physical realization of such structures is not a problem we address here.

III. ASSUR DECOMPOSITION OF MARGINALLY JAMMED PACKINGS

We first prepare jammed packings of soft frictionless disks of one-sided Hertzian repulsion by starting from a random configuration with high volume fraction ($\phi = 0.90$), and we decompress until we have only two excess contacts. At each step the energy is minimized using the FIRE algorithm [34]. For a system of N disks, isostaticity on a torus is reached when the system has $2N - 2$ contacts (leaving the two trivial translations). This exact state is very hard to reach in large systems, so we choose to terminate decompression at two SSSs ($2N$ contacts) and obtain MJPs at various system sizes. We then run the torus PGA [33] on the contact network, which leaves two undirected edges (i.e., the redundant contacts) and two free pebbles (i.e., the two trivial ZMs) on the torus. The directed portion of the contact network, which is now directed, is spanning and torus isostatic.

We then find the Assur components of this spanning isostatic graph, using the aforementioned strongly connected decomposition adapted for graphs on the torus following these steps: Given G isostatic on the torus:

(i) Orient G according to the PGA on the torus.

(ii) Place the remaining two pebbles on one of the ends of the last covered edge, making it the ground s_0. (This happens automatically when the PGA finishes.)

(iii) Partition the vertices into strongly connected components according the PGA orientation.

(iv) Define an Assur component for each strongly connected component except the ground as all the vertices in the strongly connected component along with edges point to these vertices.

(v) Choose a neighbor s_1 of the ground vertex s_0, and assign the ground s_0 to the same Assur component as s_1 is in. This is an induced subgraph of G and also minimally isostatic on the torus.

We present a more detailed explanation and a discussion about whether this decomposition is unique in the SM, S-3 [27]. On this point it is important to note that for our isostatic graphs obtained from jammed packings, the decomposition was always found to be unique. The result of this decomposition for MJP's was in general a first Assur component, a MIG by definition from Theorem 1, covering the entire graph G except a few "diads" (an Assur component of one vertex and two edges), as shown in Fig. 2(a). We perform this analysis at different system sizes, and collect the fraction η of vertices in this MIG [Fig. 2(c)]. We find that $\eta = 1 - O(N^{-1})$ as $N \to \infty$, meaning that the number of vertices in G not belonging to the MIG does not grow with system size. The choice of the ground does not change the Assur decomposition in the case of the MJPs, as we show in the SM, S-3 [27].

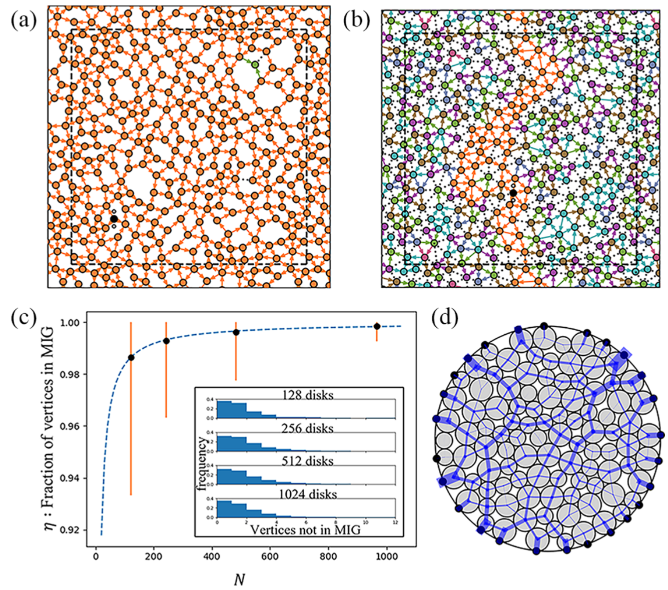

FIG. 2. Torus Assur decomposition of jammed packings. (a) A MJP contains a large MIG with almost all vertices. There are two redundant edges in this contact network (black dashed line). (b) A torus isostatic graph obtained by pruning redundant edges (black dashed lines) from a packing above the jamming transition contains a large number of Assur components. [Same convention for PBC and ground as in Figs. 1(g) and 1(h).] (c) The fraction η of vertices belonging to the MIG, as a function of total number of vertices in the graph. The removal of rattlers led to horizontal error bars, which are too small to be visible. Vertical error bars indicate 2nd and 98th percentile, from the statistics of testing 100 packings at each system size, and different choices of the two undirected edges in each packing. The inset shows the statistics of the number of vertices not in the MIG, which appears independent of system size. (d) A jammed packing (close to marginal) in a circular container, with a full SSS shown.

The fact that almost all nodes belong to the one MIG is a unique property of MJPs. This can be shown by taking other isostatic graphs, e.g., dense packings above the jamming transition and randomly pruning redundant edges in the contact network until isostaticity is reached. This results in a large number of small Assur components [Fig. 2(b)], in direct contrast with the case of the MJPs.

IV. RELATION BETWEEN MINIMAL ISOSTATICITY AND PURELY REPULSIVE INTERACTIONS

It is natural to ask whether the minimal isostaticity of MJPs comes from the fact that the disks assemble under purely repulsive interactions. Interestingly, we have an example in which this is indeed the case. Consider a set of repulsive disks in a hard frictionless circular container [Fig. 2(d)]. Contacts of disks with the wall can be represented as edges to the ground, making the contact network a pinned frame. A system of fully repulsive disks is only stable if there is an SSS that involves all disks and is compressive at all contacts. This condition comes from the study of the rigidity of tensegrities [35] (more on this at the end of this section). It can also be seen from the following intuitive picture: a stable jammed packing of repulsive disks is stressed, and this stress (which must be an SSS) is compressive at all contacts, because the disks cannot carry attraction. At the same time, any packing in a circular container has a ZM that involves all disks: a global rotation. Therefore, any MJP in a circular container has a full SSS and a full ZM. The existence of a realization that satisfies this condition is sufficient and necessary for the graph to be a pinned MIG [36]. Thus, minimal isostaticity emerges as a consequence of the repulsive nature of the interaction in this case. One may conjecture that in the thermodynamic limit, the difference between circular container and torus becomes unimportant, thereby extending the conclusion to the case of PBC. However, we do not have a rigorous proof of this argument.

Let us briefly address the necessity of "SSS that involves all disks and is compressive at all contacts" for stability of the packing. If you consider the packing as a network of all struts, a member that can support only compression, not tension, you have a "tensegrity" structure such as those described by Roth and Whitely [35]. They give conditions for "rigidity" of this structure, which is to say when they are *not* free to move; this is what we meant by "stable" earlier. In doing this, we find a perhaps simpler presentation of some of their results, which starts from the known theorem of the alternative from linear algebra. We find this to be an interesting observation but not the main focus of this work, and so we have added it as SM, S-4 [27].

V. RELATION TO OBSERVATIONS OF GLOBAL RESPONSE IN REF. [20]

Our findings here partially explain the observation that the removal of any contact makes all vertices in the contact network hinges, and the introduction of any new edge stresses all contacts. This closely relates to Theorems 1c and 1e. The key difference is the existence of nonconstructive plane isostatic subgraphs [also known as Laman or $(2,3)$-tight] with the number of vertices $N_{\mathrm{ISG}} > 3$ (the cases of $N_{\mathrm{ISG}} = 2$ or 3 are simply edges and triangles, which do not affect vertices becoming hinges and cannot be stressed by the addition of a new edge). If there were no such subgraphs and the network was a MIG on the torus, observations in Ref. [20] follow. However, if a MIG on the torus had such subgraphs, removal of any edge that is not in such a nonconstructive plane isostatic subgraph would make this subgraph, along with all other vertices, mobile, but internal vertices in this subgraph would not be hinges, and adding one edge to this subgraph would only stress this subgraph. This is a generalization of the minimal isostaticity discussed by Penne [30] in which the graph in question is isostatic on the plane, and the only allowed plane isostatic graphs are single edges. Thus the results in Ref. [20] indicate that it is very rare to find any large plane isostatic subgraphs in MJPs, making these networks akin to Penne's MIGs.

VI. RECONFIGURABLE MECHANICAL METAMATERIALS BASED ON ASSUR GRAPHS

The notion of Assur decomposition depicts the remarkable nonlocality of graph rigidity, where a small change in connectivity can affect rigidity *arbitrarily far away* [13]. This unique property can be powerful in the design of "Maxwell" mechanical metamaterials where the proximity to isostaticity gives rise to rich phenomena in terms of modes, stress, and reconfiguration [37–42].

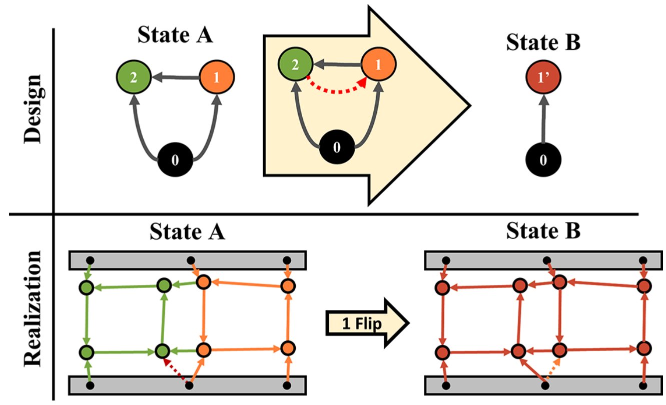

FIG. 3. Assur-decomposition-based design principle for reconfigurable mechanical metamaterials. In the design phase (upper panel), we start from Assur components and their partial ordering, including ground presented as a single node "0." Here each Assur component can represent any number of nodes in the actual graph. On the right, by adding a directed path from component 2 to 1 we create single strongly connected component 1′. We show a realization in the lower panel. Edges at the lower middle pin are the connections that are changed, where a solid (dashed) line represents the present (cut) connection.

Here we propose to utilize Assur graphs to design mechanical metamaterials that reconfigure the spatial distribution of motion and stress, and thus precisely direct actuation. We give a simple example in Fig. 3 that switches between two states: State A, a decomposable pinned isostatic frame, and State B, a MIG. Note that we have divided the figure into two panels. The upper panel represents an abstract design that could be applicable to a range of actual structures, while the lower panel is one such structure. At the design phase, we envision a pinned isostatic frame with two Assur components such that if an external force is exerted on component 1, then only component 1 is stressed, we call this State A. Then, by reversing the orientation of one edge that connects the two components, we make the whole graph strongly connected, which in turn would make the response to an external force propagate to all edges, not just the ones in former component 1; this is State B. This reversal can be achieved by changing just one connection (which is identified using the pinned PGA), and rigidity is always maintained, as shown in the realization in the lower panel. Note that similar to the propagation of stress, the propagation of motion is also dramatically affected as a result of changing the one connection. If the connections to ground on component 2 are taken to be actuators, meaning that an external operator can change their length at will, this will produce motion in the network. In State A only component 2 moves, whereas in State B the whole structure moves. From our simple framework in Fig. 3, a more space-filling version with arbitrarily many vertices can be built, with the same functionality, via the fundamental graph extensions presented in Ref. [43].

VII. CONCLUSIONS AND DISCUSSIONS

Here we examine the substructures of isostatic graphs in a physical system by extending the concept of Assur decomposition to graphs with PBC. We show that MJPs are not only isostatic but minimally isostatic, as well as proposing a design rule for mechanical metamaterials reconfigurable via remote mechanical control. Our results on the minimal isostaticity of MJPs may relate to a broad set of theories for jamming transitions, such as jamming percolation [44], k-core percolation and mixed first- and second-order scenarios for jamming [45], critical scalings of jamming [12], and mixed transitions of rigidity percolation [17,46].

Many intriguing new questions follow from these findings: What is the substructure of rigidity in packings of more complex particles, such as frictional [18], nonspherical particles [15], or packings in three dimensions [3]? How can we optimize this type of mechanical remote control to obtain significant changes in motion and stress propagation in experimental systems with imperfections? How do we obtain networks with mechanical properties that resemble jammed packings without the packing process [47,48]? And more interestingly, can we control isostatic substructures by programming particle properties and protocols, thereby obtaining self-assembled reconfigurable metamaterials? These would be interesting questions for future research.

ACKNOWLEDGMENT

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