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Structural templates of disordered granular media

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ABSTRACT

Granular materials, in common with many complex systems, exhibit a range of self-organization processes that control their mechanical performance. Many of these processes directly manifest in the evolution of the contact network as the material responds to applied stresses and strains. Yet the connections between the topology, structure and dynamics of this evolving contact network remain poorly understood. Here we demonstrate that dense granular systems under a variety of loading conditions exhibit preferred structural ordering reminiscent of a superfamily classification. In particular, two distinct superfamilies are discovered: the first is typically exhibited by materials in the pre-failure regime, while the second manifests in the unstable or failure regime. We demonstrate the robustness of these findings with respect to a range of packing fractions in experimental sand and photoelastic disk assemblies subject to compression and shear, as well as in a series of discrete element simulations of compression tests. We show that the superfamily classification of small connected subgraphs in a granular material can be used to map boundaries in a so-called jamming phase diagram and, consequently, offers a key opportunity to bridge the mechanics and physics perspectives on the constitutive behavior of granular systems.

1. Introduction

The development of predictive continuum models for granular materials has a long history. A missing ingredient in this effort in the period preceding the introduction of high-resolution or grain-scale measurements, is knowledge of the *evolving internal structure* in the course of deformation of the material. Despite recent collection of grain-scale measurements, explicit information on the dominant structures, their most pervasive topologies or fabric, and their dynamics are surprisingly lacking. We know of only one system where this information has been comprehensively established and this is based on data from a physical experiment in two dimensions (Tordesillas et al., 2012).

Here we combine the concepts of network motifs pioneered by Milo et al. (2002) and the superfamily phenomenon of Xu et al. (2008) to study the defining fabric of dense granular materials. We study a total of nine tests from simulations and experiments involving two-dimensional and three-dimensional granular materials subjected to different loading tests. The two-dimensional data sets from simulations comprise two biaxial compression tests subject to constant volume boundary conditions (see, for example, Tordesillas, 2007). In three-dimensions, the data from simulations include a compression test of an assembly of polyellipsoidal particles (Peters et al., 2009); a sample of spheres constrained to follow a proportional strain loading path to induce diffuse failure (Sibille et al., 2009); and a sample of spheres subject to shear to study permeability within dilatant shear bands (Sun et al., 2013). Three experimental three-dimensional triaxial tests are considered where μ-CT X-ray methods allow identification of grains and their contacts. Two sand types, Caicos ooid and Hostun, are examined using data from Andò et al. (2013). A third sand type, Ottawa, is examined using data from Druckrey and Alshibli (2014). Some of the samples fail by strain localization, while others exhibit diffuse failure. In addition to these, we also characterize a unique series of

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90 experimental runs that were conceived to explore a recently postulated phase diagram where photoelastic disk assemblies across a range of packing fractions were sheared until they become shear-jammed, i.e., there is a percolating strong network in both spatial directions (Bi et al., 2011). The question we seek to address is: *With respect to structure and structural evolution, is there an unambiguous structural property common to these systems despite the difference in dimensionality, loading condition, material or failure mode?*

To place this effort more precisely with respect to the state of knowledge, not just in the physics and mechanics of granular materials, but also the mathematics and statistics of complex systems, we briefly review some pertinent advances across these disciplines. Broadly, our strategy is to characterize the structure and functionality of each system by mapping material properties to a complex network (Walker and Tordesillas, 2010). By far the most studied is the contact network, although other complex networks based on kinematics and other properties besides the contacts also prove useful. The study of the complex network properties permits the quantitative characterization of structural evolution in an entirely multiscale framework. In many cases, the structure can be characterized using macroscopic quantities which are typically global averages of local microscopic quantities across the entire network (Walker and Tordesillas, 2010). That said, the functionality that is critical to macroscopic granular behavior manifests itself, not at the grain-scale, but at the mesoscale where emergent patterns (e.g., force chains, vortices etc.) and instabilities are the norm. Thus, in the past, much effort has been devoted to the intermediate mesoscopic scale: here structural properties of networks have been investigated, including the prevalence of contact cycles of a given length scale (Tordesillas et al., 2010; Arévalo et al., 2010), the population and transition dynamics of small subgraphs (Tordesillas et al., 2012), assortativity patterns of pore connectivity (Russell et al., submitted for publication), the characteristic length scales of network communities (Tordesillas et al., 2013), to name a few. Recently, Matsushima and Blumenfeld (2014) have uncovered some universal emergent structural properties of 2D granular packings seemingly independent of some material properties within their quadron formulation.

In this study, we are interested in the topology of mesoscopic structures in the contact network which consist of the set of connected subgraphs with four vertices and associated edges (see, Fig. 1 where the subgraphs are itemized by A, B, C, D, E and F). We consider four rather than three vertex subgraphs because in an undirected network there are only two such three vertex subgraphs, namely, a closed and an open triangle; on the other hand, five or higher number vertex subgraphs are challenging to enumerate and their identification in a general network remain a difficult problem. Although it is a challenge to identify the exact number of all six possible four vertex subgraphs in a network, algorithms do exist for determining these tetrad structures (e.g., Kashani et al., 2009).

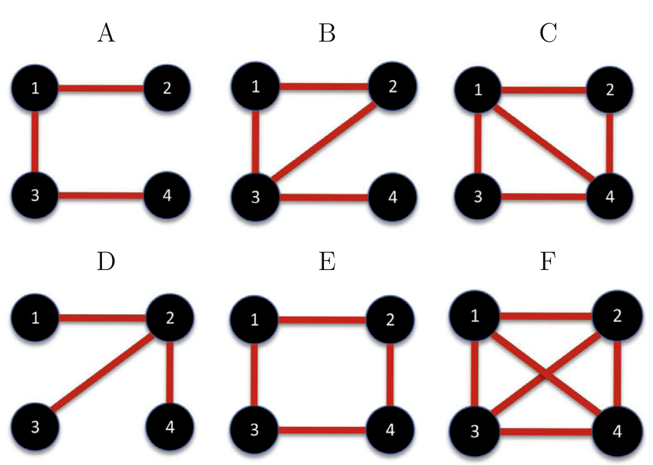

Fig. 1. The six different undirected subgraphs of size four, i.e., four connected vertices.

An important question in understanding the connection between structure and functionality of complex systems (e.g., neurological networks, cellular structure, food webs, electronic circuits, social networks) has been whether or not the structure of a given n-vertex subgraph can be referred to as a motif (Milo et al., 2002, 2004). Motifs are generally defined as recurring small connected subgraphs in a graph whose abundance is greater than would be expected compared to their abundance within an equivalent random graph (Milo et al., 2002, 2004). Knowledge and understanding of motifs is becoming important as they are basic functional building blocks combining and interacting to form larger-scale functions. For example, small-motifs within biological transcription networks been shown to be crucial to regulation of living cells (Mangan and Alon, 2003; Yeger-Lotem et al., 2004). Vázquez et al. (2004) have also demonstrated in cellular networks (i.e., transcription, metabolic, protein interaction) the abundance and aggregation of small subgraphs helps to define a network's large-scale organization. Since networks are constructed to summarize the structural or functional roles of an observed system, network subgraphs identified as motifs are thought to be important building blocks of the network and the system. For example, in a granular materials context, the closed three vertex subgraph, or triangle structure, can be identified as a motif in the contact network of a two-dimensional granular material. These triangles play an important structural and functional role in the physics of granular media (Tordesillas et al., 2010, 2012; Arévalo et al., 2010). In Milo et al. (2004), subgraphs can be identified as motifs by calculating a significance profile score, based on their prevalence in a given network, compared to their prevalence in a distribution of equivalent random networks.

As important as identifying whether a subgraph is a motif or not is the abundance ranking of the population of a subgraph in a network compared to other subgraphs in the same class. For example, for the six four vertex connected subgraphs whether one, or many, are technically motifs is not as relevant as whether one subgraph appears more frequently than another. Perhaps the best example of this is the superfamily phenomenon arising from the relative ranking of four vertex subgraphs in networks constructed from time series data. In Xu et al. (2008) it was shown that the rank-ordering of the population of four vertex subgraphs in so-called phase space networks could provide a broad classification of the underlying dynamical system responsible for the observed time series. That is, networks arising from chaotic time series data exhibited a different superfamily classification to networks arising from periodic time series data. The structure of each four vertex subgraph in these phase space networks also possess a physical interpretation of the geometry of reconstructed phase space and phase space trajectories. Moreover, this superfamily classification was also shown to be robust against moderate levels of observational noise on the time series (Xiang et al., 2012). For the networks we study here — structural contact networks of a granular material — *each of the six four vertex subgraphs have a physical and functional interpretation.* In two dimensions, only three of the subgraphs — those with cycles B, C and E — are technically motifs with respect to the significance profile score in Milo et al. (2004). The subgraph F — four triangles arranged in a three-dimensional tetrahedral-like configuration — arises less rarely in two-dimensional contact networks requiring a wide range of polydispersity to exist. We are thus interested in identifying the relative abundance, or