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Similarity Networks of the Functional Evolution of Cycles in Structural Networks

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Abstract—We construct networks summarizing similarity of local mesoscopic cycle evolution within structural contact networks of quasistatically deforming dense granular materials. In essence, at each stage of the deformation, a contact network is created and a minimal cycle basis is calculated. For each grain we compare its local mesoscopic cycle topology across a specified strain (or temporal) interval and summarize this evolution in a similarity network. We propose a prescription for finding a suitably sized strain interval. Concentrating on times when stick-slip or jamming-unjamming behaviour is evident we relate properties of the similarity networks (e.g., community structures) to areas of failure throughout the material.

1. Introduction

Granular materials span a broad spectrum of important substances (e.g. minerals, soil, chemical powders and pills, food grains etc.). When subjected to different stresses they exhibit properties in common with other forms of matter (e.g. foams, colloids, and glasses) and complex behaviour (e.g. self-organized pattern formation, scale invariance and co-existing multiphase behaviour). It is therefore important to develop methods in order to characterize, understand, model and perhaps control the behaviour. As such many experiments and simulations have been devised to probe the rheological response of granular materials to different stresses [1, 2, 3, 4]. These tests have the potential to generate vast quantities of data across different spatial and temporal scales. The techniques of complex network theory have recently been shown to be of use in analyzing such data and a purpose of this paper is to introduce a novel way of using similarity networks to study the functional role grains play in the structural and rheological evolution of a dense granular material.

The properties of complex networks have been used in the past to study granular rheology. The majority of work has concentrated on characterizing the topology of structural contact and contact force networks at different stages of loading and force thresholds (e.g. [5, 6, 7]). More recently, efforts have been made to construct more functional networks of granular properties using kinematical measurements over short strain intervals [8] and even longer temporal behaviour of grain structures [12]. Here, we propose

a method whereby the rheology of a dense granular material can be studied which examines the evolution of the local topology of structural contact networks. The role of each grain plays within such evolution is summarized in a similarity network from which communities of grains with similar functional evolution can more easily be identified. More broadly, the method allows the dynamical evolution of complex networks to be studied by tracking how a node's local motif (cycle) topology evolves.

2. Compression Test System

We consider a sample of 5098 grains in a Discrete Element Method (DEM) simulation of biaxial compression subject to constant confining pressure from the lateral boundaries [9]. The grains are poly-disperse spheres constrained to move in the plane and so the DEM simulation is effectively two-dimensional. The contact laws for two interacting particles are a combination of springs, dashpots and sliders [4]. A coefficient of rolling friction is introduced to a contact moment to better model the effects of particle shape seen in real sand experiments [10]. This sample exhibits multiphase behaviour and a crossover from a solid-like to a liquid-like response regime through the formation of a persistent shear band extending from the lower left corner of the sample to the upper right corner. This transition of behaviour is seen in the marked drop from peak shear stress with increasing strain as shown in Figure 1. The prevailing kinematics at the scales of interacting grains, mesoscopic clusters of grains and the bulk sample are as follows: throughout the entire loading history quasi-linear chains of particles bearing the majority of the load are present. These are the so-called force chains. The force chains are laterally supported by weaker neighbours with local topologies taking the form of different length cyclic structures. From the onset of loading we see an almost linear increase in macroscopic shear stress ratio, possible because force chains have enough support to bear more and more load. As this increase in shear stress ratio begins to slow down, within the material grain rearrangements continually occur including so-called local microbanding. Eventually, somewhere in the body of the sample the lateral support to a force chain weakens, most likely due to dilative rearrangements, and the force chain can no longer

support the increased load. At this point failure is triggered through the mechanism of force chain buckling and load gets redistributed onto existing force chains and newly formed force chains. The region of the material where this occurs is (strain) localized in what becomes the persistent shear band. As the load increases towards peak shear stress the rate of force chain failure reaches the point where we see collective buckling of force chains in a fully formed shear band. The material can no longer support a significant load and the prevailing dynamics is one of birth and death of force chains in the high strain region manifest as oscillations in the shear stress ratio reflecting the localized stick-slip or jamming-unjamming kinematics. Simultaneously we also see intermittent vortex-like structures across short strain intervals within the shear band. Throughout the entire loading, so-called rattlers are present. These are grains that for a given observed strain state have zero or one contact and no surrounding lateral support. Our interest in this paper is to track the contact topology evolution of each grain across strain intervals spanning stick-slip (jamming-unjamming) motion and in particular the initial failure drop from peak shear stress.

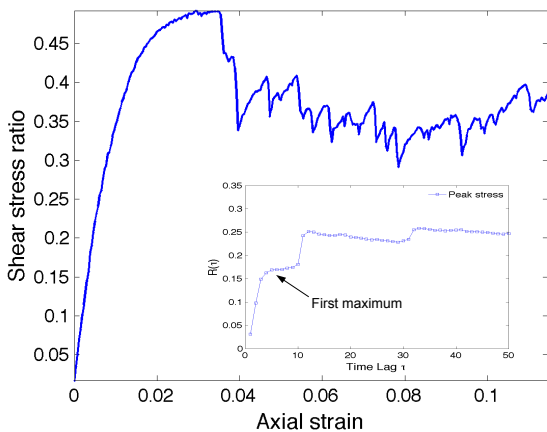


Figure 1: The evolution of the shear stress ratio with respect to increasing axial strain. *Inset:* The change in $R(\tau)$ from peak shear stress ratio. The first maximum occurs for a $\tau = 5$ and so we use this strain interval (time scale) to construct the mesoscale cycle similarity network.

3. Contact Network and Minimal Cycle Basis

The rheology of dense granular materials including the compression test described above has previously been analyzed and characterized using network measures of the evolving structural contact network [5, 6]. The contact network of an assembly of grains is constructed by representing each grain as a node and a link connects two nodes if the grains are in physical contact with each other. The rheological response of the material is captured by the changing network properties of the evolving contact net-

works (e.g. degree, clustering coefficient, centrality measures etc.). The change in the population of network motifs is also revealing of the grain rearrangement and deformation apparent in the material. In particular the membership of a minimal cycle basis of the contact networks, i.e., 3-cycles, 4-cycles and longer length cycles can reveal the onset of dilatation. In addition, the interplay of mesoscopic scale low-order cycles with the load-bearing force chain structures within the material is of relevance to force chain stability and failure of force chains through buckling. Here, we are interested in characterization of the mesoscale evolution of the cycle topology of a grain across a strain interval. For example, consider the arrangement of particles shown in Figure 2 which can be regarded as a mechanism for buckling of a force chain synonymous with slip or unjamming rearrangements. The vertical arrangement of the three central particles represent a force chain which buckles. The local cycle topology of the central particle consists of six 3-cycles which rearrange after an increase of strain to a local cycle topology consisting of one 3-cycle, one 5-cycle and, for the sake of argument, two 6-cycles. Clearly a suitable network and resulting network property capable of measuring such deviation is of great interest. Likewise, a measure capable of capturing the reverse rearrangement of jamming is also of use. A purpose of this paper is to search for such a property within similarity networks to enable the study of the whole system.

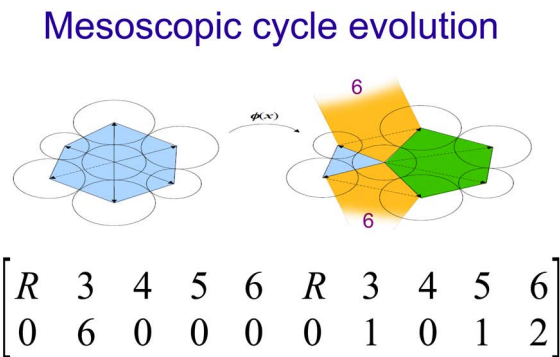


Figure 2: The evolution of the local mesoscopic cycle topology of a grains rearrangement in a possible force chain buckling event and its representation as a row vector.

4. Similarity networks

We modify the role-similarity network construction technique for directed networks to examine the mesoscopic scale deformation of cycles in an evolving contact network [11]. The idea is to construct a set of coordinates which represents a node's role within a network. For directed networks this can be based on the number of shortest in and out paths of a given length associated with a node. A

row vector for each node is constructed by augmenting this “in” and “out” information. The pairwise distance between all of these row vectors can be calculated to produce a matrix which can be considered as a network weight matrix. Using appropriate thresholding we can convert this weight matrix to an adjacency matrix to form a complex network. Properties of this network such as community structure assignment can reveal relationships between nodes based on their role with respect to shortest path lengths and directions in the original directed network.

In our case we do not have directed networks, however, we do have different contact networks for increasing strain. Increasing strain gives a (temporal) direction and so we propose to create a coordinate vector for each node which represents its local mesoscopic cycle evolution. That is, we consider a grains cycle membership at two equilibrium strain states to construct a similarity matrix \mathbf{C} where each row corresponds to a particle and the first n columns list the number of 3, 4, 5, . . . , n -cycles the grain is a part of at strain state t . The remaining n columns list the number of 3, 4, 5, . . . , n -cycles the grain is a part of in the contact network at strain state $t + \tau$. For grain i , a row of X takes the form

$$\mathbf{C}^i = [C_t^i | C_{t+\tau}^i] \quad (1)$$

where C_t^i represents a count of the cycles in the contact topology of grain i at strain t . We observe that it is possible for a grain to not be a part of any cycle at a given strain state (e.g., a rattler) and after a strain interval τ may remain a rattler. In this case \mathbf{C}^i would be a zero-vector. Since the distance function we will be using is cosine distance a zero vector causes problems. Thus we append C_t^i with an extra entry which is equal to one if the grain has no cycles and is equal to zero otherwise.

Consider the central particle in Figure 2 where we follow the topological evolution of a possible force chain buckling failure event. At time t we see that the particle is a part of six 3-cycles and so, for cycles up to length 6, we have

$$\mathbf{C}_t^i = [R \#3 \#4 \#5 \#6] = [0 \ 6 \ 0 \ 0 \ 0] \quad (2)$$

and at time $t + \tau$ we have

$$\mathbf{C}_{t+\tau}^i = [R \#3 \#4 \#5 \#6] = [0 \ 1 \ 0 \ 1 \ 2] \quad (3)$$

where we have assumed the “open” cycles are of length six for exposition. Thus

$$\mathbf{C}^i = [0 \ 6 \ 0 \ 0 \ 0 \ | \ 0 \ 1 \ 0 \ 1 \ 2]. \quad (4)$$

A (weighted) similarity network W is constructed by calculating the pairwise distance between each \mathbf{C}^i . We use the *cosine similarity* for distance defined as

$$d_C(x, y) = 1 - \frac{x \cdot y^T}{\|x\| \|y\|}. \quad (5)$$

A distance threshold can be applied to convert W to the form of an adjacency matrix of a complex network. The

properties of this network, including degree distribution, clustering coefficients, etc. can be calculated to characterize the functional role of grains in the evolving contact networks. Furthermore these properties can be mapped back to the physical domain so that the spatial effect of these temporal changes can be examined.

A method for selecting a connection threshold which we have had some success with in the past when analyzing the rheology of sand specimens using functional kinematical networks is to connect each grain to its k -closest grains with respect to the distance metric [8, 12]. The value of k is chosen to be the minimum integer such that the resulting network forms one connected component. This means that each node is connected to every other node by a finite shortest path length. We will refer to the network produced by applying this method to the weighted similarity network W as the k -similarity network.

At a given strain stage t we can measure the average deviation of the local mesoscopic cycle evolution across a strain interval of length τ . That is, for N_p grains,

$$R(\tau) = \frac{1}{N_p} \sum_{i=1}^{N_p} d_C(C_t^i, C_{t+\tau}^i). \quad (6)$$

Recalling prescriptions for selecting useful lags for time delay embedding (e.g., first minimum of the average mutual information function) we suggest that a useful prescription for selecting a time lag τ is to choose the first local maximum of $R(\tau)$. We find that such a choice appears to be a good balance of suggesting a τ that is large enough for local deformation to have taken place but not too large that important local rearrangements are lost. For example, considering the initial time at peak shear stress, the value of $R(\tau)$ for time lags from 1 to 50 strain steps later is shown in the inset of Figure 1. We see that the first local maximum occurs at $\tau = 5$ suggesting this is a good strain interval to examine local mesoscopic cycle deformation.

5. Spatial Structure of a Stick-Slip Event

We study the major failure process from peak shear stress. In Figure 1 (*Inset*) we showed that a strain interval of length $\tau = 5$ was an appropriate interval to examine. A k -similarity network can be constructed for this strain interval using cycles up to the maximum cycle length of 13. A value of $k = 112$ was the minimum number of neighbours needed to first obtain a single component network. Six community structures using local modularity were found within this network. For each community we can examine the typical change in cycle topology by totalling $C_t - C_{t+\tau}$ for each node. In Figure 3 we show these changes and the inset shows each particle in the assembly coloured by community assignment. The dilatation occurring within the sample is evident from an examination of the larger community populations (dark/light blue and yellow) where we observe loss of 3- and 4-cycles (+ve change) and an increase in

higher cycles (-ve change). The distinction between communities being the length of higher order cycles which are “born” (e.g. yellow particles increase their 5- and 6-cycle membership but dark blue particles see an increase in 8-cycles). We also note that the dark blue particles are predominantly in the area of shear band localization and as such are associated to more higher order cycles. Of interest are the green coloured particles. These show a gain in 4-cycles and a loss of 10-cycles capturing behaviour akin to jamming rearrangements. It is clear that communities of k -similarity networks constructed based on evolving cycle motif topologies are detecting subtle changes within the material. A task for future work is to study how standard rheological measures such as non-affine strain and curvature correlate to structural properties of these networks.

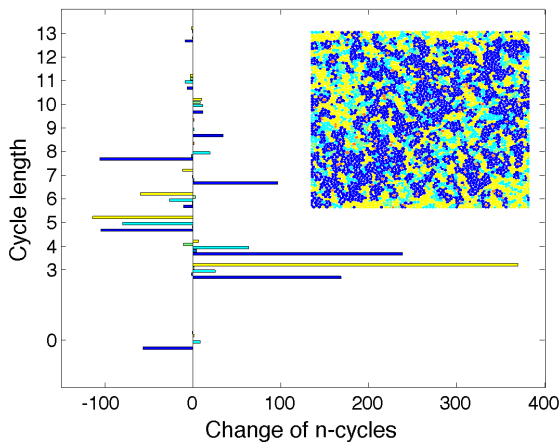


Figure 3: The overall change in cycle numbers for each community. *Inset*: Assembly of particles coloured by community assignment.

6. Summary

We have introduced a novel application of similarity metrics to study the rheology of dense granular materials during important stick-slip (jamming-unjamming) mechanisms. We have constructed a functional similarity network which captures the local evolution of mesoscopic cycle topologies in structural contact networks. Communities and properties of the resulting k -similarity networks reveal the collective role of grains during rearrangement events. We have thus provided a new network tool to further analyze and characterize the rheology of failure in dense granular materials.

Acknowledgments

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