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Self-organization in the localised failure regime: metastable attractors and their implications on force chain functionality

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Abstract. In transitive metastable chaotic dynamical systems, there are no invariant neighbourhoods in the phase space. The best that one can do is look for metastable or almost-invariant (AI) regions as a means to decompose the system into its basic self-organising building blocks. Here we study the metastable dynamics of a dense granular material embodying strain localization in 3D from the perspective of its conformational landscape: the state space of all observed conformations as defined by the local topology of individual grains relative to their first ring of contacting neighbors. We determine the metastable AI sets that divide this conformational landscape, such that grain rearrangements from one conformation to another conformation in the same AI set occurs with high probability: by contrast, grain rearrangements involving conformational transitions between AI sets are unlikely. The great majority of conformational transitions are identity transitions: grains rearrange and exchange contacts to preserve those topological properties with the greatest influence on cluster stability, namely, the number of contacts and 3-cycles. Force chains show a clear preference for that AI set with the most number of accessible and highly connected conformations. Here force chains continually explore the conformational landscape, wandering from one rarely inhabited conformation to another. As force chains become overloaded and buckle, the energy released enables member grains to overcome the high dynamical barriers that separate metastable regions and subsequently escape one region to enter another in the conformational landscape. Thus, compared to grains locked in stable force chains, those in buckling force chains, confined to the shear band, show a greater propensity for not only non-identity transitions within each metastable region but also inter-transitions between metastable regions.

1 Introduction

Grain rearrangements around force chains are indispensable for effective force transmission. Unlike their counterparts in architectural structures, columnar force chains are far from static. Grain motions in and around force chains continually occur, enabling force chains to explore a range of mutating conformations in a rich conformational and stability landscape [1–3]. Emerging evidence suggests that this landscape, populated by hills and valleys of varying depths and widths, shapes the rich ordered patterns of interaction in granular systems that emerge in the lead up to and during failure [1–4]. Here we focus on this process of self-organization in the localized failure regime and explore the organization of this landscape. We search for metastable attractor regions in this landscape to understand persistent or frequently occurring local grain arrangements and rearrangements in a dense granular dynamical system embodying shear bands in three dimensions. To understand force chain formation and evolution in this context, we go beyond ‘static’ information and determine the structure and dynamics underlying *conformational transitions* of member grains in force chains, as the system evolves from one equilibrium state to the next.

Specifically, building on [1, 2], we investigate the presence of metastable attractors which facilitate the creation and persistence of force chains in 3D frictional materials. The role of conformational transitions in force chains has been explored in 2D experiments on synthetic (photoelastic), as well as virtual, granular materials [1]. In these studies, the conformations are characterized by the topological configurations inhabited by a grain relative to its first ring of contacting neighbors. All such conformations observed in the system during loading define a conformational state space. This state space is then divided into regions, known as almost-invariant metastable sets, between which conformational transitions are unlikely: that is, there is a high probability that a grain undergoes a rearrangement from one conformation to another in the same metastable AI set. As to which of these sets force chains prefer to inhabit is crucial for the formulation of robust constitutive stress-strain relations for granular media [5, 6]. Equally important, especially for control of the underlying self-organization process, is the transition pathway followed by force chains in this conformational landscape under varying loading conditions. Such an exploration into 3D systems is challenging given the scarcity of data from physical experiments on interparticle contact forces for many

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Table 1. DEM model parameters and material properties.

Parameter	Value
Applied strain rate $\dot{\epsilon}_{yy}$	-5×10^{-2} s^{-1}
Confining pressure P	494.91 k N m^{-2}
Particles n	55100
Particle radii R	$(0.76 - 1.52) \times 10^{-3}$ m
Particle density ρ	2650 kg m^{-3}
Modulus of elasticity E_c	91.86 M Pa
Poisson's ratio ν_c	0.5
Rolling stiffness coefficient β	1.0
Inter-particle friction angle μ	0.7
Rolling coefficient $\eta = \mu^r$	0.02
Wall friction angle μ_{wall}	0.0 – 0.7

stages of a single test [2]. This challenge was recently overcome for near-frictionless hydrogel spheres [2]. However, transitions in the conformational landscape of 3D frictional systems representative of common real granular materials (e.g. sand) have not been explored and is the focus of this study. Given the absence of requisite data on interparticle contact forces in real granular systems, we use data from discrete element simulations.

Our analysis proceeds in two phases. In Phase 1, we establish the conformational landscape, a state space in which all observed conformations reside. In Phase 2, we divide this state space into the metastable AI sets. With attention paid to force chains, our objective here is to find the conformations and conformational transitions at the opposite extremes of the frequency spectrum: the most prevalent *intra*-transitions *within*, and the rare *inter*-transitions *between*, AI sets. A comprehensive analysis of the conformational landscape of dense granular systems in the limit state is reported in [4].

2 Data

The data set used here is from a DEM simulation of various assemblies of frictional 3D spherical particles submitted to triaxial compression under constant confining pressure. The simulation uses the YADE package [7]. Here we focus on a three-dimensional analogue of a well-studied two-dimensional system [3, 4, 8]. The same simulation and material properties are used as the two-dimensional system where possible to enable direct comparison with previously published results. A summary of the simulation and material parameters is provided in Table 1. Figure 1 (inset) shows the stress-strain response that is typical of densely packed granular systems [9].

3 Method

Analysis proceeds in two phases. In Phase 1, we establish the conformational state space for the triaxial test sample as it evolves from one equilibrium state to another in the failure or "persistent shear band" (PSB) regime where the underlying dynamics is assumed to be stationary. This begins with the contact network, in which the grains and their contacts are represented by nodes and links in a network [1, 2]. For the entire series of equilibrium states in the PSB regime, we enumerate all observed conformations of every node in the contact network and its local connectivity, d^t_s: d is the node degree (number of links), t is the number of 3-cycles, and s is the number of shared edges between the 3-cycles. For example, in the physical space of the sample, conformation 3^1_0 corresponds to a grain with three contacting neighbors and a single rotationally frustrated 3-cycle [3, 10].

In Phase 2, we partition the conformational state space into their almost-invariant sets, following the method in [11]. To do this, we perform a spectral analysis of the Markov transition matrix P that is constructed from the information gained in Phase 1. The conformations correspond to a collection of $S = \{1, \ldots, n\}$ states, where n is the total number of unique conformations observed in the PSB regime. We also track all the grain rearrangements between all consecutive pairs of equilibrium strain states and map these into P as a transition from conformation state i to conformation state j. This leads to the row-stochastic $n \times n$ transition matrix P, such that P_{ij} denotes the conditional probability of transitioning from state i to state j in one strain interval. The aim is to partition the collection of states S into subsets $A_k \subset S$, $k = 1, \ldots, K$, with $\bigcup_{k=1} A_k = S$ and $A_k \cap A_\ell = \emptyset$, $k \neq \ell$. The eigenvectors of P are used to partition the conformational state space S into metastable regions A_k known as almost-invariant (AI) sets, between which conformational transitions are unlikely. The elements A_k are then partitioned as follows: for each $k = 1, \ldots, K$, the probability that A_k at time t transitions to A_k at time $t+1$ is as large as possible, while for $k \neq \ell$ the probability that A_k at time t transitions to A_ℓ at time $t+1$ is as small as possible. Such a partition $\{A_k\}^K_{k=1}$ is called *almost-invariant* because each partition element acts approximately as its own dynamical process and is almost disconnected dynamically from the other partition elements.

4 Results

A total of 363 unique grain conformations are observed in the persistent shear band (PSB) regime, which leads to a stochastic transition matrix P of dimensions 363×363. However, the leading unit eigenvector of P is not unique. We correct this by interpreting P as an adjacency matrix of a graph G, and retaining the edges associated with the largest connected component of the graph G. This removes 17 rare conformations, corresponding to those with no information about their next transition: that is, transitions which when entered cannot be left, and isolated small components of G. This leads to a corrected stochastic transition matrix $\tilde{P}$ of size 346×346. From the leading unit eigenvector of $\tilde{P}$, we obtain the probability density distribution that quantifies the frequency that a given conformation is inhabited during the PSB regime (Figure 1). We found five metastable regions, AI sets $A - E$ (overlaid symbols in Figure 1), with the proportions of grains inhabiting

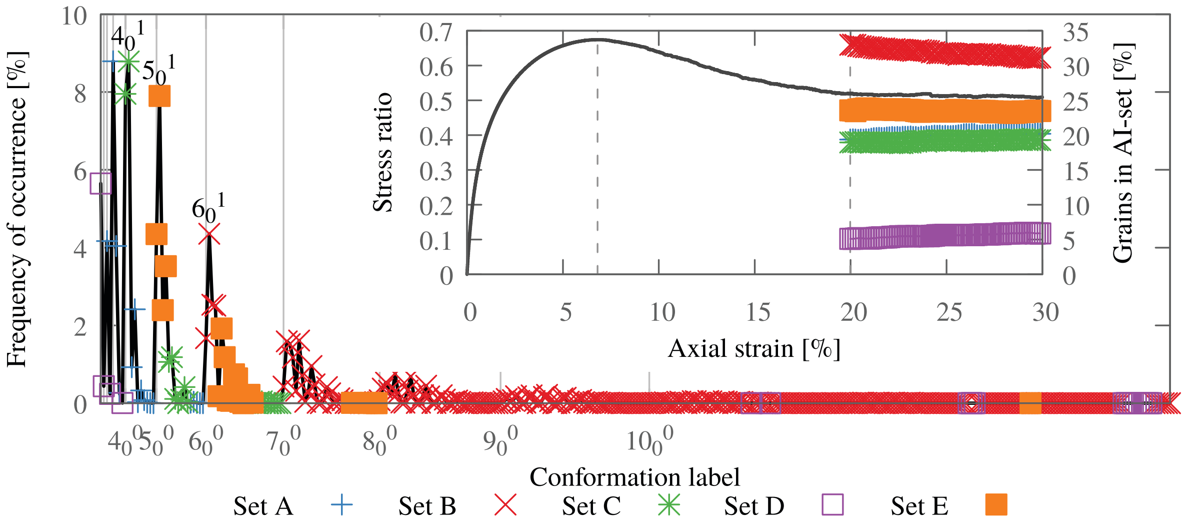

Figure 1. Frequency of occurrence of each conformation (black curve); overlaid is the classification of each conformation into one of the five almost-invariant set $A - E$ (symbols). (inset) Stress ratio and percentage of grains in each almost-invariant set.

each metastable region across the PSB regime shown in the inset. The near-invariant strain evolution of the population of grains in each region provides corroborating evidence to support past observations that the PSB regime exhibits stationary dynamics.

Prevalent conformations: We observe several prominent peaks in the probability density distribution, suggesting the presence of *preferred* self-assembled mesostructures. The top five peaks corresponding to the most preferred conformations, in decreasing order of occurrence, are: 4^1_0 (set C), 3^0_0 (set A), 5^1_0 (set E), 4^0_0 (set C) and 0^0_0 (i.e. a rattler, set D). Outside these peaks are infrequently inhabited grain conformations. As shown in Figure 1(inset), the majority of these are in set B, the most populated region with the largest number of accessible conformations that are densely connected (i.e. $d \geq 6$ and $s \geq 1$) yet rarely visited. The least populated region in the conformation state space is D, which consists of rattlers and poorly supported conformations (e.g. 0^0_0, 1^0_0 and 2^1_0).

Prevalent conformational transitions: Identity transitions comprise around 90% of all grain transitions (i.e. no change in local topology with respect to degree and 3-cycle membership and arrangement). The five most frequently occurring non-identity transitions are $3^0_0 \rightarrow 4^1_0$ (i.e. gain of a 3-cycle), $4^1_0 \rightarrow 3^0_0$ (i.e. loss of a 3-cycle), $3^0_0 \rightarrow 4^0_0$ (i.e. gain of a contact), $4^0_0 \rightarrow 3^0_0$ (i.e. loss of a contact), and $2^0_0 \rightarrow 3^0_0$. These preferred transitions are cyclic (e.g. Figure 2) and are characteristic of the underlying dynamics in the shear band where grain rearrangements are greatest.

Local arrangements around force chains: Grains found in force chains, classified according to their almost-invariant set membership, show a distinct preference for the densely connected conformations in set B and spend considerably less time visiting metastable regions with poorly supported conformations: A 6%, C 11%, $D < 1$%, E 24% versus B 58% (Figure 3(a)). Set B distinguishes itself from the other four regions of the conformational

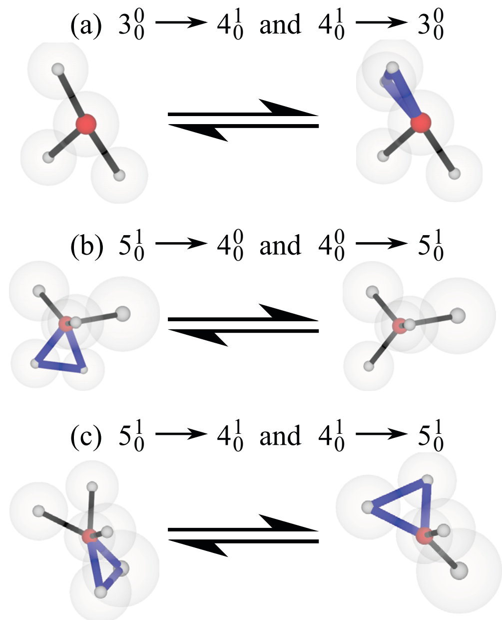

Figure 2. Top three most prevalent cyclic transitions involving a 3-cycle and their corresponding AI set (focal grain in red, 3-cycle in blue).

landscape by having the most number of accessible yet infrequently visited conformations. As the conformations in B have high d, resident grain clusters have more degrees of freedom to explore accessible sites in this region of the conformational state space. The prevalence of conformations with 3-cycles (increasing t and s) that frustrate grain rotations and provide truss-like support to force chains make B an ideal breeding ground for force chains [10].

Local rearrangements in and around force chains: Rearrangements around force chains typically preserve structural stability, with 90% of conformational transi-

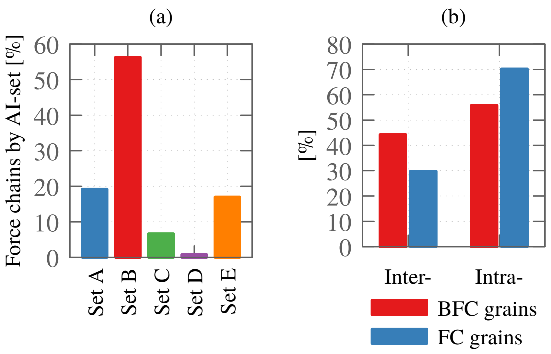

Figure 3. (a) Force chain grain conformations classified by their respective AI set. (b) Proportion of inter- and intra- transitions for grains found in and around force chains (FCs) and buckling force chains (BFCs).

tions maintaining the same number of contacts and 3-cycle topology (i.e. identity transitions). In stark contrast, BFCs are far more unstable, with only 56% of rearrangements being identity transitions. The non-identity transitions can be classed into two categories: intra-transitions and inter-transitions (Figure 3(b)). Compared to force chains which are locked in more stable configurations, grains in unstable BFCs are more likely to overcome the dynamical barriers that separate the metastable regions in the conformational landscape. Indeed, around 30% (44%) of grains in force chains (BFCs) undergo inter-transitions. Overcoming the dynamical barriers that separate the metastable regions in the conformational landscape requires an expenditure of energy. In this context, the propensity for BFCs to traverse a dynamical barrier, escaping a metastable region to inhabit another, is entirely consistent with past findings that showed these failure events are accompanied by bursts in kinetic energy, dissipation and mesoscale nonaffine deformation [1, 3, 4, 6, 8, 12].

5 Conclusion

We study the process of self-organization, on the scale of a grain and its first ring of contacting neighbors, during localised failure of a dense granular material submitted to triaxial compression. Attention is paid to those equilibrium states when the sample deforms in the presence of a fully developed persistent shear zone. The conformational landscape of the system embodies five metastable attractor regions, in each of which there is a high (very low) probability that a grain undergoes a rearrangement from one conformation to another in the same (different) region, across a single strain interval in the persistent shear band regime. The great majority of conformational transitions are identity transitions, implying that grains rearrange and exchange contacts to preserve the topological properties with the greatest influence on cluster stability: degree and the number of 3-cycles. Of the five metastable regions, force chains show a clear preference for that region with the most number of accessible and highly connected conformations. Here force chains continually explore state space, wandering from one rarely inhabited conformation to another. Force chain failure by buckling, confined to the shear band, involves grains that show a greater propensity to follow trajectories that involve non-identity transitions either within each metastable region or inter-transitions between metastable regions. The latter suggests that the stored energy released in force chains during buckling enables member grains to overcome the dynamical barriers that separate metastable regions and subsequently escape one region to enter another in the conformational landscape.

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References

[1] A. Tordesillas, D.M. Walker, G. Froyland, J. Zhang, R.P. Behringer, Physical Review E **86** (2012)
[2] D.M. Walker, A. Tordesillas, N. Brodu, J.A. Dijksman, R.P. Behringer, G. Froyland, Soft Matter **11**, 2157 (2015)
[3] A. Tordesillas, Q. Lin, J. Zhang, R. Behringer, J. Shi, Journal of the Mechanics and Physics of Solids **59**, 265 (2011)
[4] S. Pucilowski, A. Tordesillas, G. Froyland, Powder Technology (2016), in preparation
[5] A. Tordesillas, M. Muthuswamy, Journal of the Mechanics and Physics of Solids **57**, 706 (2009)
[6] A. Tordesillas, S. Pucilowski, Q. Lin, J.F. Peters, R.P. Behringer, Journal of the Mechanics and Physics of Solids **90**, 215 (2016)
[7] V. Smilauer, E. Catalano, B. Chareyre, S. Dorofeenko, J. Duriez, N. Dyck, J. Elias, B. Er, A. Eulitz, A. Gladky et al., *Yade documentation 2nd ed* (2015)
[8] A. Tordesillas, Philosophical Magazine **87**, 4987 (2007)
[9] J. Kozicki, J. Tejchman, H.B. Mühlhaus, International Journal for Numerical and Analytical Methods in Geomechanics **38**, 1923 (2014)
[10] A. Tordesillas, D.M. Walker, Q. Lin, Physical Review E **81**, 011302 (2010)
[11] G. Froyland, Physica D: Nonlinear Phenomena **200**, 205 (2005)
[12] H. Zhu, G. Veylon, F. Nicot, F. Darve, European Journal of Environmental and Civil Engineering pp. 1–24 (2016)