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K. Karapiperis, J.E. Andrade

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Nonlocality in Granular Complex Networks: Linking Topology, Kinematics and Forces

K. Karapiperis, J. E. Andrade

Abstract

Dry granular systems respond to shear by a process of self-organization that is nonlocal in nature. This study reveals the interplay between the topological, kinematical and force signature of this process during shear banding in an sample of angular sand. Using Level-Set Discrete Element simulations of an in-situ triaxial compression experiment, and complex networks techniques, we identify communities of similar topology (cycles), kinematics (vortex clusters) and kinetics (force chains), and study their cooperative evolution. We conclude by discussing the implications of our observations for continuum modeling, including the identification of mesoscale order parameters, and the development of nonaffine kinematics models.

Keywords: granular materials, complex networks, nonlocality

1. Introduction

The study of nonlocality in granular materials can be traced back to the pioneering experiments of Roscoe [1] and, later, Mühlhaus and Vardoulakis [2], establishing the characteristic width of a shear band in sand at 8-10 particle diameters. Further evidence of nonlocality has been identified in the dynamic flow regime [3] for example in the form of nozzle jamming in silos [4] and thickness-dependent repose angles in surface flows [5, 6]. Later, advances in experimental techniques [7–9] as well as discrete element (DEM) [10] and contact dynamics (CD) [11] simulations inspired grain-scale studies in an effort to explain these emergent phenomena. Most notably, photoelastic experiments and particle simulations helped identify the heterogeneous nature of force transmission in an assembly in the form of force chains [12–14]. Subsequent experiments conjectured force chain buckling [8] as a mechanism for shear localization, which was later investigated through structural stability analyses enabled by DEM [15, 16]. Measurements of force correlations were used in [17] to quantify the heterogeneous nature of force networks under shear, yielding a consistent correlation length of about 10 particle diameters. Similarly, the study of velocity correlations has revealed the nonaffine nature of granular kinematics, termed granulence [18, 19]. As a
signature of these correlations, vortices of characteristic sizes emerge [20–22], accompanied by intense particle rotations [23–27], eventually leading to the development of a shear band [28–31]. Finally, the use of complex networks techniques [28, 32–38] has contributed to the identification of stable [35] and unstable [39] mesoscale features and communities [40] and their topological transformations.

Alongside these micromechanical studies, it was recognized that standard continuum theories failed to capture nonlocal effects [41, 42]. As a result, two major families of theories have emerged: enhanced continua [43] and nonlocal theories [44]. Enhanced (or weakly nonlocal [45]) continua depart from the standard Cauchy assumption of affine deformation, by introducing higher-order kinematics and their conjugate kinetics. Most notably, the micropolar theory [46, 47], which equips the material point with rotational degrees of freedom, has successfully captured several aspects of shear bands in sands [2, 48]. On the other hand, (strongly) nonlocal theories introduce an additional field that represents the (solid-like or fluid-like) state of the material locally [44, 49]. Characteristic examples include the Landau-type [50] order parameter formulation termed partial fluidization theory [49], gradient plasticity [51, 52], and the nonlocal granular fluidity model [53]. In this family, the length scale is typically identified as the characteristic length scale of the diffusion process of a local microstructural event, such as a shear transformation [54], due to the correlated motion of its neighbors. Recently, the hypotheses inherent to some of these formulations have been supported by micromechanics, through advanced homogenization techniques [55–59], kinematic models [31] and direct micromechanical descriptions of order parameters [60]. Yet, the micromechanical description of nonlocality within a sound theoretical framework still remains largely an open question.

In this Letter, we investigate the emergent length scale in the quasistatic flow of sand. To this end, we rely on three-dimensional Level-Set Discrete Element Method (LS-DEM) simulations of triaxial compression [61] of a sample of angular sand characterized by X-ray computed tomography [62]. We utilize complex network techniques, which have not received proper attention in 3D systems, to reveal stable and unstable mesoscale topological structures, vortex clusters and force chains, which depart from earlier observations in idealized and predominantly two-dimensional systems. Particular emphasis in placed on the cooperative evolution of these features through distinct stages of the experiment.

This Letter is organized as follows: Section 2 details the experiments and simulations furnishing the micromechanical data to be subsequently analyzed. In Sections 3–5, we present the methods used to analyze the topology, kinematics and forces in the system respectively, and discuss the outcome of each analysis. We conclude by summarizing our main findings, and discussing their implications for continuum theory in Section 6.

2. Triaxial compression experiments and simulations

The data analyzed in this work are obtained from a high-fidelity discrete element simulation of a quasi-static in-situ triaxial compression experiment reported in an earlier publication [61]. In the experiment, a cylindrical specimen of angular Hostun sand, encased in a flexible latex membrane, is subjected to a triaxial loading protocol [62]. Fig. 1 a) shows a
2-dimensional slice of the XRCT scanned specimen, which measures 11 mm in diameter and 22 mm in height, and is comprised of 53,939 angular grains. The specimen is first compressed isotropically to 100 kPa. Next, keeping the radial pressure constant, a freely rotating platen in contact with the top part of the sample enforces a vertical compression until failure.

The experiment is computationally replicated using a variant of DEM [10], termed LS-DEM [63]. Similarly to the original formulation, LS-DEM resolves the kinematics of particles interacting through frictional contacts, but also accounts for accurate particle morphology. In particular, for each physical grain in the triaxial sample, a virtual grain is generated through a level set imaging algorithm (Fig. 1a)). The resulting virtual specimen is subjected to identical boundary conditions, by modeling the membrane as well as the kinematics of the platen. The deformed virtual specimen is shown in Fig. 1a), where the formation of a shear band can be identified. For details regarding the LS-DEM simulation, the interested reader is referred to [61].

Figures 1b) and c) compare the macroscopic response of the sample in experiment and simulation, in terms of principal stress ratio and volumetric strain respectively. The sample exhibits a peak in the macroscopic stress ratio (equivalently, friction angle), only to decay later to a constant critical state value. In accordance with earlier experiments and theory [64, 65], the peak state coincides with the maximal rate of dilation of the shear band, while the volume remains constant at critical state. The peak and critical state regimes are of particular interest to this study, and are highlighted in the figures. Finally, it is worth noting that, beyond the macroscopic (stress-strain) response, LS-DEM has been shown to capture quantitatively the mesoscopic response (spatiotemporal evolution of shear band kinematics) [61], and even the particle-scale response (contact-normal and force distribution, and friction mobilization) in simple shear experiments [66].

Figure 1: a) LS-DEM simulation of a sample of Hostun sand characterized by XRCT. b) Principal stress ratio plotted against axial strain. The peak and critical state are indicated with dashed lines. c) Volumetric strain plotted against axial strain.
3. Mesoscale topological evolution

3.1. Complex networks

Our working hypothesis is that the nonlocal response of the granular assembly to externally applied loads is encoded in its evolving contact network structure. We proceed by considering the assembly as a graph, where particles serve as nodes, and contacts or contact forces serve as edges connecting the nodes (Fig. 2 a)). The use of binary contacts as edges generates the unweighted network $B$. On the other hand, the incorporation of edge weights, connecting nodes $i$ and $j$, that are given by the normalized interparticle force $W_{ij} = f_{ij}/\langle f \rangle$ generates the weighted network $W$. The weighted and unweighted contact networks have been recently used to extract interesting features [67] such as cycles [33–35] and communities [40], and to pinpoint shear band nucleation [36, 37] and force chain development [68].

In this section, we restrict our attention to the unweighted network, while the weighted network will be considered later in Section 5. In particular, we focus on identifying and characterizing the evolution of mesoscale structures during the shear-banding or unjamming transition. This is achieved through a minimal cycle analysis of the network [69]. A cycle basis is a set of simple (non-intersecting) cycles that forms a basis of the cycle space of the graph. A minimum cycle basis is a basis with minimal total length of cycles. Fig. 2 b) shows examples of minimal 3-,4-,5- and 6-cycles that pass through a given particle in the system. In a two-dimensional system, the minimal cycles would simply correspond to the faces of the contact graph.

3.2. Results

The size of our network allows us to study the statistics of cycle sizes, since even rare occasions of long minimal cycles can be accounted for. Fig. 2 c) shows the probability density function (PDF) of cycle sizes $N_c$ in the whole sample at peak and critical state. Interestingly, the density appears to decay super-exponentially with cycle size and may be well approximated by $P(N_c) \sim e^{-\alpha N_c^3}$, as shown in the same figure. In accordance with previous observations [35, 37], the density of longer cycles increases at critical state, which could be a manifestation of dilatancy.

We now turn our attention to the density of individual cycles inside the shear band, where significant topological changes occur. Fig. 2 d) shows the evolution of the density of 3-, 4-, 5- and 6-cycles (constituting $\sim80\%$ of the total number of cycles) as a function of the shear strain in the localized band. We observe that 3-,4- and 5-cycles are almost equally populous in the initially jammed configuration, hinting on their importance as stabilizing mesoscale features. This lies in contrast to previous studies on idealized two-dimensional [35] and three-dimensional [37] assemblies which showed that 3-cycles constitute the clear majority in a jammed state, due to their high rotational frustration. We conjecture that this is due to the pronounced asphericity and irregularity of the sand grains, that enhances the stability of longer cycles. Upon further deformation, 3-, 4- and 5-cycles exhibit a power-law...
Figure 2: a) Graph representation of the sample at critical state, with nodes colored by their minimal cycle coefficient. b) Example minimal 3-, 4-, 5-, and 6-cycles passing through a given center node. c) PDF of cycle size $N_c$ in the sample, and fitted distribution. d) Evolution of density of 3-, 4-, 5-, and 6-cycles inside the shear band. e) Evolution of the average minimal cycle coefficient inside the shear band. Inset: Evolution of the average coordination number.

decay to a common critical state density, also shared by 6-cycles, hinting on the existence of a common steady state in cycle birth-and-death dynamics.

Inspired by the apparent importance of several classes of cycles in our system, and in order to describe the ensuing phase transition, we introduce the average cycle membership of a particle $i$, given by $\bar{N}_c(i) = \sum_j j c_j(i) / \sum_j c_j(i)$, where $j \in [3, \infty)$ is the cycle size and $c_j(i)$ is the number of minimal cycles of size $j$ that pass through node $i$. This measure in turn gives rise to the minimal cycle coefficient $D(i) = 3/\bar{N}_c(i)$. A highly stable particle entirely surrounded by 3-cycles will have $D = 1$, while a highly unstable particle will be surrounded by long cycles such that $D \to 0$. The proposed coefficient is a generalization of the local clustering coefficient $C(i)$, which measures the density of 3-cycles surrounding a particle, and similar higher order coefficients for longer cycles [70].

We note that the minimal cycle coefficient $D$ also bears resemblance to two other mea-
sures in the complex networks literature: the loop coefficient \([71, 72]\) and the subgraph centrality \([73]\). The former is given by \(L(i) = 1/(k_i (k_i - 1)) \sum_{j,k \in \Gamma_i} 1/d_{jk/i}\), where \(\Gamma_i\) is the local subgraph of neighbors of \(i\) where node \(i\) has been excluded, and \(d_{jk/i}\) is the shortest path length between particles \(j\) and \(k\) within \(\Gamma_i\). The second relevant measure is the subgraph centrality \(SC(i) = \sum_{k=0}^{\infty} B^k_{ii}/k!\), which measures the number of closed walks starting and ending in node \(i\). The difference with \(D\) is that \(SC\) includes trivial even-sized walks, and cycles that are not simple. It has been successfully used as a proxy for fluctuating kinetic energy during failure of a granular assembly \([74]\).

Fig. 2 e) shows the evolution of the average minimal cycle coefficient \(\langle D \rangle\) within the shear band, and compares it to that of the average coordination number \(\langle Z \rangle\), the prototypical order parameter for the jamming transition \([75]\). In both cases, we observe a similar decay to a critical state value. The large Pearson’s correlation coefficient (~0.6) between the particle-scale \(D\) and \(Z\) implies that the minimal-cycle coefficient could serve as an equivalent mesoscale order parameter for this transition. In the next sections, we will address its relevance to the kinematics and kinetics of the system.

4. Nonaffine kinematics

In this section, we characterize the kinematics that accompany the topological changes within the shear band by studying the formation and evolution of vortex clusters. The majority of earlier kinematics studies have focused almost exclusively on two-dimensional vortices \([27, 30, 31]\), or have relied on simplified scalar measures of nonaffine deformation such as the nonaffine mobility \([39, 76, 77]\).

4.1. Vortex identification

We analyze the nonaffine particle displacements \(\delta u_i \equiv u_i - \epsilon \cdot \hat{x}_i\), where \(u_i\) is the displacement, and \(\hat{x}_i\) is the position of particle \(i\) with respect to a local coordinate system aligned with the shear band. The affine (approximately simple-shear) strain \(\epsilon\) dominating the band’s deformation is found in a least-squares sense \([76]\) as:

\[
\epsilon = \arg \min \sum_{i \in S} ||u_i - \epsilon \cdot \hat{x}_i||^2
\]

where the summation takes place among the set of particles \(S\) within the band.

We proceed to identify mesoscale vortex structures formed by the nonaffine displacements. As opposed to two-dimensional systems\([20, 22]\), where vorticity is parallel to the out-of-plane axis, vortices can freely rotate in 3D systems and form clusters \([78]\). To identify those clusters, we employ the methodology of \([78]\), by first computing the vorticity field:

\[
\omega(x) = \rho(x)^{-2} \sum_{i \in S} \sum_{j \in S} \phi_i(x) [\nabla \phi_j(x) \times \delta u_{ij}]
\]

where \(\phi(x) = e^{-||x-x_i||^2/\bar{d}^2}\) is the coarse-graining kernel\([79]\), \(\rho(x)\) is the coarse-grained number density field, and \(\delta u_{ij} = \delta u_i - \delta u_j\) is the relative nonaffine displacement between particles.
To identify a cluster, we choose a particle within the shear band at random and traverse its contact network using a breadth-first search algorithm. For contacting particles \( i, j \), their normalized vorticities, \( \tilde{\omega}_i, \tilde{\omega}_j \) respectively, are compared by computing the angle of their cosine similarity \( \theta_{ij} = \cos^{-1}(\tilde{\omega}_i \cdot \tilde{\omega}_j) \). The particles are included in the same cluster if \( \theta_{ij} < \theta_c = \pi/6 \), and the search continues until no more particles are included in the cluster.  

4.2. Results

The nonaffine displacement field along with the identified vortex clusters are shown in Fig. 3 a). In contrast to two-dimensional systems where there is a clear geometrically defined length scale in the form of a vortex radius [22, 31], here the complex shape of vortices requires

\[ \text{The critical angle is chosen as } \theta_c = \pi/6, \text{ following [78]. A sensitivity analysis showed that cluster sizes decrease with increasing } \theta_c, \text{ yet their distribution consistently follows a power law with exponential cutoff.} \]

Figure 3: a) Nonaffine displacement field and identified vortex clusters within the shear band. b) PDF of cluster size \( N_v \) and fitted power laws with exponential cutoff. Inset: Evolution of characteristic length \( \ell_v \) as a function of the shear strain within the band. c) PDF of the vortex strengths and fitted Maxwell-Botzmann distribution. d) PDF of the orientational order parameter \( \cos \bar{\chi} \).
an alternative definition of length scale. To this end, we compute the distribution of vortex cluster size $N_v$ throughout the stages of the experiment, and find, in accordance with [78], that it is well described by a power law with exponential cutoff, $P(N_v) \sim N_v^{-\alpha} e^{-N_v/\nu_v}$, as shown in Fig. 3 b). By analyzing the exponential tails, a characteristic vortex length scale $\ell_v \equiv \nu_v^{1/3}$ of about 4 grain diameters is obtained. Its evolution throughout the experiment is shown in the inset Fig. 3 b), where a slight increase with shear strain is identified.

Next, we characterize the vortex strength $\omega_v$, which we define as the average vorticity in each cluster. As shown in Fig. 3 c), the average vortex strength increases to a steady state value, while its density is well approximated by the Boltzmann-Maxwell distribution $P(\omega_v) \sim \omega_v^2 e^{-\omega_v^2/2}$. Finally, we characterize the directionality of these vortex clusters. This is achieved by computing the average normalized vorticity of each cluster $\tilde{\omega}_c$, and comparing it to a macroscopic 'director' $\Omega$ that is orthogonal to both the direction of shear and the normal to the shear band plane, as shown in Fig. 3 a). The distribution of their cosine similarity $\cos \tilde{\chi} = \tilde{\omega}_c \cdot \Omega$ is plotted in Fig. 3 d). We observe a slightly anisotropic distribution with some degree of preferential alignment of the vorticity with $\pm \Omega$, which would correspond to the primary (homothetic) and secondary (antithetic) vortices observed in 2D systems [27, 30, 31]. Most vortices appear to be arbitrarily oriented in space.

5. Forces

To shed light on the kinetics that accompany the kinematical (Section 4) and topological (Section 3) transition, we will now characterize the evolving force chain architecture. Driven by the lack of general agreement on what constitutes a force chain, we first reconcile the two major identification techniques in the literature: network community detection [80] and 'direct' identification [81]. We then proceed with observations on chain stability and establish direct links with topology and kinematics.

5.1. Force chain extraction via community detection

Our point of departure is the characterization of the weighted and unweighted contact networks outlined in Section 3. Following [80], we seek communities $\{s_i\}$ of grains, strongly connected via intergranular forces of similar magnitude, by maximizing the modularity function:

$$Q = \sum_{i,j} (W_{ij} - \gamma P_{ij}) \delta(s_i, s_j)$$

where $W_{ij}$ is the weighted adjacency matrix, $\gamma$ is the resolution parameter controlling the size of communities, $P_{ij}$ is the so-called null model representing the expected weight of the edge connecting nodes $i$ and $j$, and $\delta(s_i, s_j)$ is the Kronecker delta. We adopt the geographical null model [80], given by the unweighted adjacency matrix, $P_{ij} = B_{ij}$, in order to respect the spatial connectivity constraints in the granular system.
5.2. Direct force chain identification

For the ‘direct’ extraction of force chains, we employ a three-dimensional extension of the detection algorithm described in [81]. Hereby, chains are identified as quasilinear sequences of particles that reside in the strong-force network [13]. More specifically, let $\sigma_3, n_3$ denote the minor (most compressive) principal stress and its direction respectively, obtained from a spectral decomposition of the particle stress. The latter is given by $\sigma = 1/V^p \sum_c f_c \otimes x^c$, where $V^p$ is the particle volume, and $x^c$ is the location of the contact force $f_c$ with respect to the particle centroid. For a sequence of particles to constitute a force chain $S$, its members must i) exhibit a compressive stress that is higher than the sample average:

$$|\sigma_3^i| > \frac{1}{N} \sum_{j=1}^{N} |\sigma_3^j|, \ \forall i \in S$$

where $N$ is the number of particles in the sample, and ii) be sufficiently colinear:

$$\frac{\mathbf{l}_{ij} \cdot n_3^i}{||\mathbf{l}_{ij}|| \cdot ||n_3^i||} > \cos \alpha, \ \forall i, j \in S$$

where $\mathbf{l}_{ij}$ is the branch vector connecting consecutive particles $i, j$ in the chain. The angle $\alpha$ represents the maximum allowable angle between chain segments which we take as $\alpha = 45^\circ$.

5.3. Results

Fig. 4 a) shows the contact force network at critical state, along with the resulting force chains obtained via direct identification and community detection respectively. The latter is based on a resolution parameter $\gamma^* = 3.0$ (recall its definition in Section 5.1), optimized to generate chains maximally similar to those identified ‘directly’. Similarity is assessed based on the coincidence of member particles of chains determined by the two methods. We find that, for $\gamma = \gamma^*$, the chains determined by the two methods share the majority ($\sim 60\%$) of their participating members.

Fig. 4 c) shows the PDF of community sizes $N_{com}$ for varying resolution parameter $\gamma$. The sizes are found to follow a power law distribution $P(N_{com}) \sim N_{com}^{-\alpha}$, where $\alpha$ is almost linearly correlated with $\gamma$. On the other hand, in accordance with earlier studies [81], the size of chains obtained by direct identification follows an exponential distribution, as shown in Fig. 4 d). This is further evidence that for large enough $\gamma$, the two identification methods are reconciled.

Of particular importance to force transmission is the structural characterization is force chains. Fig. 4 b) shows examples of a jammed (stable) and a buckled force chain, along with several of their topological and kinematical attributes. A chain is assumed to have buckled when two criteria are met [15]: i) an increase in local chain curvature beyond a critical threshold, and ii) a reduction of the potential energy stored in the chain. On the contrary, a jammed chain is one that persists throughout loading without buckling. Fig. 4 e) shows the PDF of buckled chain segment sizes $N_b$ throughout the experiment, where we can also identify the longest segment that is prone to buckling ($N_b = 10$). It appears
that longer buckling wavelengths are not energetically favorable. Note that, in contrast to earlier studies, the stability of force chains is assessed here without recourse to numerical proxies such as rolling friction, but rather as an immediate consequence of morphology and interlocking.

Finally, we address the stability of chains in relation to the measures of topology and kinematics investigated in Sections 3 and 4. To do so, we compare these measures for buckled chains (occurring almost exclusively within the band) and persistent stable chains. Under an increase in the stored elastic energy, and a loss of lateral support due to dilatation, a chain becomes increasingly susceptible to buckling. With the help of (nonconvex) set Voronoi tesselations (Appendix A), we can identify the critical local chain packing fraction $\phi_c$ that

Figure 4: a) Force network, directly identified chains and detection of communities at critical state b) Characterization of a jammed and a buckled chain using various descriptors c) PDF of community size $N_{com}$ and fitted power law distribution. c) PDF of force chain size $N_f$ and fitted exponential distribution. c) PDF of buckled force chain size $N_b$ and fitted distribution.
induces instability in a chain, as shown in Fig. 5 a). Similarly, Fig. 5 b) compares the average minimal cycle coefficient $D_c$, in stable and buckled chains, showing that buckling is associated with a significant increase in $D_c$. Finally, Fig. 5c) shows the minimum distance (in grain diameters) of stable and buckled chains to the surface of the nearest vortex cluster. Interestingly all chains avoid forming in the interior of vortices, and most buckling events happen on the surface of vortices. This confirms that, along with topology, vortices also govern the formation of chains, in accordance with recent observations in two-dimensional systems [31].

![Figure 5](image_url)

Figure 5: PDFs of a) Packing fraction, b) Minimal cycle coefficients and c) Minimal topological distance to the surface of the nearest vortex cluster, for jammed and buckled chains.

6. Conclusion

Nonlocality is inherently linked to pattern formation such as shear banding. The objective of this study is to reveal the topological, kinematical and force signature of shear banding of a sample of angular sand. We based our investigation on high-fidelity three-dimensional simulations using the Level-Set Discrete Element Method and relied on complex networks techniques to characterize the emergent length scale.

Regarding topology, we found that longer (4-/5-) minimal cycles emerge as equally stabilizing mesoscale structures alongside the shorter well-documented 3-cycles [37]. We conjecture that this is due to particle asphericity and angularity, which enhances topological interlocking, reduces rotations, and thus increases structural stability. Our observations are in line with recent evidence of the effect of particle morphology on the continuum response [82]. We introduced the minimal cycle coefficient $D$, to collectively account for the apparent importance of several families of cycles.

With regard to kinematics, we characterized the length scale, strength and orientational order of vortex clusters within the shear band. These are essential descriptors of the nonlocal kinematics required in enhanced continuum theories. Interestingly, the vortex strength of these arbitrarily shaped clusters follows a Maxwell-Boltzmann distribution, that converges to a well-defined critical state distribution. In terms of the orientational order of this vortices,
we identified a significant departure from the primary and secondary vortices observed in earlier two-dimensional studies.

To delineate the conjugate kinetics, we relied once again on complex networks. First, we reconciled the definition of force chains as fundamental units of force transmission, by comparing the two major identification techniques. We characterized the size distribution of the critical buckling wavelength of force chains, emerging from a high-fidelity representation of morphology, and without recourse to proxies such as rolling friction. We found that the average minimal cycle coefficient in buckling is was significantly lower than in jammed chains, which verifies the relevance of this coefficient.

Several promising avenues towards a nonlocal continuum description arise from these observations. The coarsest description would rely on a mesoscale order parameter that collectively accounts for topological rearrangements, within a Landau-type framework \[49\]. The proposed minimal cycle coefficient appears to be a promising candidate. Work towards this direction would require systematically investigating its diffusive spatial coupling and its relation to the local rheology. Perhaps a more detailed description would rely on modeling, and subsequently coarse-graining, the coupled birth-and-death dynamics of force chains, cycles and vortices. We identified several constraints that these dynamics must satisfy, such as their critical state densities and rates of decay. Additional work is required in order to understand the dissipation that accompanies these birth-and-death processes. A final avenue would be to explicitly model the nonaffine kinematic field within the shear band \[31\]. Our characterization of the size, strength and orientation of vortices, can form the basis for constructing admissible nonaffine fields. Which theoretical framework can provide a consistent closure of these kinematics in terms of their conjugate kinetics remains an open question. Could this be a modified micropolar framework or, perhaps, a gradient theory of self-organization \[83\]? The road to a unified nonlocal continuum theory remains long and challenging.

Appendix A. Set Voronoi tessellation for arbitrarily shaped particles

To calculate the local packing fraction in Section 5.3, we need to compute the volume of the cell associated to each particle. To do so, we employ a generalization of the standard Voronoi tessellation \[84\] for the case of arbitrarily shaped and nonconvex particles. This involves a standard Voronoi tessellation of the particles’ discretized surface points. In other words, the points at the surface mesh of all particles are used as the input of a standard Voronoi computation \[84\], generating the example sub-cells shown in Fig. A.6. Then, all subcells belonging to the same particle are conglomerated into the nonconvex Voronoi super-cell attached to that particle. The accuracy of the scheme depends on the density of the surface discretization of each particle.

Figure A.6: Two nonconvex Voronoi cells each comprised of multiple convex subcells.
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Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: