Granular vortices: identification, characterization and conditions for the localization of deformation

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Abstract

We relate the micromechanics of vortex evolution to that of force chain buckling and, on this basis, formulate the conditions for strain localization in a continuum model of dense granular media. Using the traditional bifurcation analysis of shear bands, we show that kinematic vortex fields are in fact solutions to the boundary value problem satisfying null boundary conditions. To establish an empirical basis for our study, we first develop a method to identify the location of the core and boundary of each vortex from a given displacement field in two dimensions. We then employ this method to characterize the residual deformation field (i.e., the deviation of particle motions from the continuum deformation) in a physical experiment and a discrete element simulation of dense granular samples submitted to biaxial compression. Vortices in the failure regime are essentially confined to the shear band. Primary vortices, the clear majority, rotate in the same direction as the shear band; secondary vortices, so-called wakes, rotate in the opposite direction. Primary vortices align in spatial succession along the central axis of the band; wakes form next to the band boundaries, in between and beside two adjacent primary vortices. Force chain buckling, the governing mechanism for shear bands, is responsible for vortex formation in the failure regime. Vortex dynamics are consistent with stick-slip dynamics. From quiescent conditions of jamming or stick, vortical motions arise from

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force chain buckling and associated relative particle rotations and sliding; these in turn precipitate intermittent periods of unjamming or slip, evident in the attendant drops in stress ratio and bursts in both kinetic energy and local nonaffine deformation. A kinematic vortex field inside shear bands is proposed that is consistent with the equations of continuum mechanics and the underlying instability of force chain buckling: such a field is periodic with a repeating unit cell comprising a primary vortex at the center of the band, with two trailing wakes close next to the band boundaries.

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1. Introduction

A flow pattern characteristic of failure in rate-independent materials is the localization of strain into so-called shear bands — the conditions for which was first proposed forty years ago by Rudnicki and Rice (1975). Their theory was set forth in the framework of continuum mechanics: shear band formation is treated as a bifurcation in the solution path of the boundary value problem for a continuum flow field, such that a pattern of localized deformation is permitted by the constitutive law as an additional solution to the “trivial” uniform solution. Despite its success, two key challenges remain in the mechanics and physics of shear bands in dense granular media. First, the full details of grain motions that precede and emerge in fully developed shear bands are only just beginning to come to light (Rechenmacher et al., 2011; Andò et al., 2012; Peters and Walizer, 2013; Tordesillas et al., 2014). Second, the mathematical route to bridge the dichotomy between the micromechanical description of grain-scale instabilities central to shear band formation versus the phenomenological description of continuum theory, where the practical analysis of geotechnical structures and geomaterial phenomena lie, remains unclear (Tordesillas et al., 2014). Advances in noninvasive imaging techniques (Oda and Kazama, 1998; Desrues and Viggiani, 2004; Majmudar and Behringer, 2005) and numerical discrete element methods (DEM) (Cundall and Strack, 1979; Iwashita and Oda, 1998; Oda and Iwashita, 2000) have led to extensions of the Rudnicki & Rice theory within the framework of micropolar continuum mechanics (Mühlhaus and Vardoulakis, 1987; Sulem and Vardoulakis, 1995; Tordesillas et al., 2004), yet fundamental questions remain unanswered. Foremost of these are the significance of vortex patterns in grain motions that prevalently emerge inside shear bands and the mechanisms behind the evolution of these vortices.

The connection between vortices and shear bands has attracted rife speculation (e.g. Williams and Rege, 1997; Kuhn, 1999; Alonso-Marroquín et al., 2006; Tordesillas et al., 2008a; Rechenmacher et al., 2010, 2011; Liu et al.,

2012; Peters and Walizer, 2013; Kozicki et al., 2013; Tordesillas et al., 2014). Recently, this connection was clarified from two fronts. First, Peters and Walizer (2013) observed that a slip field can be expressed as the sum of a uniform (affine) deformation field and a vortex. This is an obvious result of a simple shear field — which characterizes the deformation of the shear band — being a linear combination of a pure shear deformation and a rigid-body rotation. Though the analysis by Peters and Walizer (2013) was directed at the pre-failure and not post-localized failure regime, it holds important implications for shear band analysis. They observed vortices early in the loading history, which then implied a slip field in the area where the shear band would ultimately form. Their findings were consistent with those from analysis of high-resolution microCT data on individual grain kinematics, which demonstrated that the ultimate pattern of failure is encoded in the grains motions from the beginning of loading in a triaxial compression of Hostun sand (Tordesillas et al., 2013) and, more recently, of Ottawa and Caicos Ooid sand, as well as in a DEM simulation of simple shear (Tordesillas et al., 2015). Second, important structural building blocks of 3-cycles (i.e., three particles in mutual contact, known to provide truss-like supports to column-like force chains), exhibit similar vortex patterns early in the loading history (Tordesillas et al., 2014). A multi-scale spatio-temporal analysis of these 3-cycle structures in the pre-failure regime revealed a preferential and progressive degradation of the most stable 3-cycles (so-called persistent 3-cycles) — *where the shear band ultimately forms*. In fact, the location and strain state at which these structures became essentially depleted marked the full development of the shear band in space and time, and explained why force chains are prone to buckling *inside* the band from thereon. Use of the generalised Ripley K-function (Cressie, 1993), to quantify the existence of spatial attraction (i.e., significant statistical evidence that two distinct events frequently occur in close proximity of each other), uncovered a pattern in the dynamics of 3-cycles and force chains that is unique to the failure regime (Tordesillas et al., 2014). Once the persistent shear band is fully formed, 3-cycle “births” and “deaths” exhibit spatial attraction in the band region, as do 3-cycle deaths and buckling force chains, to within a length scale of 7-10 grain diameters, consistent with the band thickness. Energy released from these failure events then drive the vortical nonaffine motions, which are confined to the band and intensify during periods of unjamming.

These recent developments underscore the need to characterize comprehensively the relationship between vortex evolution inside shear bands and the mechanism of force chain buckling, long implicated as the root cause of shear banding (Oda and Kazama, 1998; Oda and Iwashita, 2000; Iwashita and Oda, 2000; Tordesillas et al., 2008a, 2009b; Rechenmacher et al., 2010,

2011; Liu et al., 2012; Tordesillas et al., 2014). There is compelling ground for these mechanisms to be related, after all both concentrate in shear bands in the failure regime. Moreover, micromechanical studies have implicated force chain evolution in various failure phenomena observed across the mesoscopic and macroscopic scales including: *noncoaxiality of stress and strain rate* (Collins and Muhunthan, 2003; Thornton and Zhang, 2006; Tordesillas et al., 2009a), *strain-softening under dilatation* (Oda and Kazama, 1998; Rechenmacher, 2006; Tordesillas et al., 2011b), *stick-slip dynamics* (Griffa et al., 2011), and *spatial interlacing of high and low porosity regions inside shear bands* (Oda and Kazama, 1998; Oda and Iwashita, 2000; Iwashita and Oda, 2000; Rechenmacher, 2006; Tordesillas et al., 2008a).

Here we propose that the seeds of the unstable behavior assumed in the bifurcation analysis of Rudnicki and Rice (1975) can in fact be identified from the underlying mechanism that drives the formation of vortex patterns in grain motions and, ultimately, shear bands. We choose the biaxial compression test, the principal advantage of which lies in the boundary conditions: these give rise to a known affine deformation field that serves as a backdrop on which to explore the nonaffine vortex evolution in a granular material as it transitions into failure by strain localization (Williams and Rege, 1997).

We establish the conditions for localization of deformation with respect to a kinematic vortex field inside shear bands that is consistent with the underlying particle scale instability driving vortex and shear band evolution, i.e., force chain buckling. Our analysis proceeds in three phases. In the first phase (Section 2), we develop an objective method by which to identify vortices from a given displacement field in two dimensions. Armed with this vortex detection method, we next establish the requisite empirical ground for this theoretical development in the second phase (Section 3). Here we use data on grain motions from physical experiments and discrete element (DEM) simulations of biaxial compression to characterize material behavior in the lead up to and during failure; attention is paid to the development of vortices in the *residual (nonaffine) deformation field* — the difference between the actual granular deformation and the continuum (affine) deformation. With respect to this residual field, we quantify: (i) the deformation in terms of the fundamental properties of vortices (i.e., location, direction of rotation, population and size distribution, and strength); and (ii) the relationship between vortices and key instabilities, in particular, grain rotations and force chain buckling. In the third phase (Section 4), we formulate the conditions for localization with respect to an admissible kinematic vortex field for the shear band. Additionally, we provide evidence that our proposed kinematic field is consistent not only with the governing equations of continuum mechanics but also with force chain buckling. Concluding remarks are given in Section 5.

Figure 1: (Color online) *A visual perception of vortices in a vector field.* An example vector field embodying vortices, taken from a displacement field of a sub-domain of a granular assembly to be discussed later in Section 3: the tails of the displacement vectors (blue arrows) are located at the known particle centers. Groups of vectors, circumscribed by a circle, can be discerned by a common direction of rotation of member vectors about a central point, i.e., the vortex core (green shaded area).

2. Identification of vortices

The detection of vortex patterns from a given vector field is an active research area. For a recent review of vortex detection methods from data, see Jiang et al. (2011). Here we develop a method for identifying vortices from a discrete vector field in two dimensions. For the purposes of illustration, we show an example in Figure 1. Along the forward diagonal of this vector field, individual groups of displacement vectors, each approximately circumscribed by a circle, can be seen to have member vectors rotating in the same direction around a common center — the *vortex core*. In what follows, we develop a “candidate search-and-elimination” method by which to identify objectively these circulatory or swirling patterns — the so-called *vortices*.

To aid understanding, we begin with an overview of our method before proceeding with the details. The two parts to our candidate search-and-elimination method are executed in three steps: steps 1 and 2 focus on the search part (Figure 2), while step 3 deals with the elimination part (Figure 3). In step 1, a set of *candidate vortex cores* is identified from the centroids of the triangles that partition a set of points $\mathcal{P} = \{\mathbf{p}^1, \mathbf{p}^2, \dots, \mathbf{p}^N\}$. In the context of a displacement vector field for a granular assembly of N particles, each point $\mathbf{p}^i$, $i \in \{1, 2, \dots, N\}$, represents a particle center where the

tail of the particle’s displacement vector is located. A triangle’s centroid is a candidate vortex core if the vectors at its vertices satisfy the modified direction-spanning property. This property, to be defined formally in the next section, is a geometric property of the triangle and automatically establishes the location of a candidate vortex core and the vortex direction (i.e., direction of rotation of the “first ring” member vectors around the vortex core). In step 2, *candidate vortices* that correspond to the candidate vortex cores are identified. The full extent of each vortex is established by a systematic sweep and check of the direction of neighboring vectors (in the second ring, third ring, etc.) at increasing radial distance from the vortex core, until a vector is found that rotates in the opposite direction to the corresponding vortex. The boundary of the vortex is then set by the furthest vector from the central core which rotates in the vortex direction. In step 3, the final set of vortices, so-called *resultant vortices*, is found from the candidate vortices by eliminating: (i) enclosed vortices (i.e. a vortex encapsulated within a larger vortex), and (ii) duplicate vortices (i.e., one sharing most of the same member vectors as another vortex).

2.1. Detection of vortex cores using the modified direction-spanning property

The vortex core is the center of the vortex, around which every constituent vector rotates. To find these, we search for candidates using a *modified direction-spanning property*. This property is best understood from the method originally proposed by Jiang et al. (2002) using concepts from combinatorial topology, in particular, Sperner’s lemma, used previously to identify the centers of swirling flows for a given velocity vector field (Henle, 1994). Their method begins with a triangulation of the given set of points $\mathcal{P} = \{\mathbf{p}^1, \mathbf{p}^2, \dots, \mathbf{p}^N\}$: the partitioning of the convex hull of $\mathcal{P}$ in the Euclidean plane into triangles, whose vertices are the points and which are empty of other points (De Loera et al., 2010). A popular example of such a triangulation scheme is the Delaunay triangulation which we adopt in this study.

The next step is to find the candidate vortex cores which are simply the centroids of all the triangles whose associated vectors satisfy the so-called *direction-spanning property* (Jiang et al., 2002). A set of three vectors at the vertices of a triangle satisfy the direction-spanning property if and only if each vector points to a *unique* direction range: that is, the triangle is labeled *ABC* or is said to be a “fully-labeled triangle” (Figure 4). Unfortunately, two aspects of the scheme by Jiang et al. (2002) affect the resultant label which can lead to erroneous detection (false positives): the choice of orientation or direction ranges and the choice of the value of m for the m -equally spaced Sperner direction ranges (see Appendix A for further details). To

Figure 2: (Color online) *Depiction of the search for candidate vortex cores and associated candidate vortices (steps 1, 2 of 3).* Candidate vortex cores are identified by partitioning the vector field into triangles, each analysed with respect to the modified direction-spanning property (step 1, top row). This property is satisfied if the vectors at the triangle vertices lie within a certain range of angles, as defined by the geometry of the triangle: cyan region for an anticlockwise rotation of vectors around the triangle centroid (top-left). The centroids of triangles satisfying the modified direction-spanning property are the candidate vortex cores: blue (red) dots for anticlockwise (clockwise) vortex direction (top right). Triangles that do not satisfy the modified direction-spanning property have white dots at their centroids. A candidate vortex is then identified for each candidate vortex core, with the vortex boundary set by the last member vector rotating in the vortex direction (step 2, bottom row).

Figure 3: (Color online) *Identifying vortices by candidate elimination (Step 3 of 3)*. For the example vector field in Figure 1, enclosed and duplicate candidate vortices are eliminated: (a) the vector field with blue (red) candidate vortex cores and their corresponding anti-clockwise (clockwise) vortices, with green dashed circles indicating the vortex boundaries. (b) the final resultant vortices and their cores.

overcome these limitations, we propose a vortex core detection method that does not depend on the orientation or number of direction ranges chosen for establishing candidate vortex cores, and is likewise simple and efficient to implement numerically.

In our method, we define a *modified direction-spanning property* for a set of three vectors that is based purely on the geometric properties of their associated triangle (Figure 5). Consider the triangle A with centroid O , vertices A_i and sides $A_{i,j}$ in Figure 5(a): the tails of its associated vectors $\mathbf{v}^i$ are at vertices A_i , $i \in \{1, 2, 3\}$. Each vector $\mathbf{v}^i$ assigns a label to a triangle side $A_{i,j}$ if $\mathbf{v}^i$ lies within the range of angles in $\angle OA_i E_{i,j}$: here $\angle OA_i E_{i,j}$ is bound by the median through vertex A_i on the internal side, and by the extended edge of side $A_{i,j}$, $E_{i,j}$, on the external side. As shown in Figure 5(a,b), the triangle is said to be fully-labeled if all of its sides are uniquely labeled by its constituent vectors: equivalently, we say the vectors of a fully-labeled triangle satisfy the modified direction-spanning property. By contrast, triangles in Figure 5(c,d) are not fully-labeled, as a side is left unlabeled: vectors $\mathbf{v}^1$ and $\mathbf{v}^2$ both label side $A_{1,2}$, thus leaving side $A_{2,3}$ unlabeled (Figure 5c); $\mathbf{v}^1$ does not lie in either $\angle OA_1 E_{1,2}$ or $\angle OA_1 E_{1,3}$, thus leaving side $A_{1,3}$ unlabeled (Figure 5d).

Mathematically, let $\mathbf{w}^i = \overrightarrow{A_{i-1}A_i}$ and $\mathbf{z}^i = \overrightarrow{OA_i}$, $A_0 = A_3$, $i \in \{1, 2, 3\}$

Figure 4: (Color online) *Direction-spanning property*. Displacement vectors of three particles associated with a single Delaunay triangle in a sub-domain of a granular assembly. The vectors at the vertices of the Delaunay triangle are labeled according to three equally spaced direction ranges $\{A, B, C\}$, each spanning 120° . In this case, the vectors satisfy the direction-spanning property and the triangle is fully-labeled.

(Figure 6). A modified direction-spanning property requires that, for a clockwise orientation, we have

$$w_1^i v_2^i - w_2^i v_1^i < 0, \quad z_1^i v_2^i - z_2^i v_1^i < 0, \quad i \in \{1, 2, 3\},$$

as shown in Figure 6(a); for anticlockwise orientation, we have

$$w_1^i v_2^i - w_2^i v_1^i > 0, \quad z_1^i v_2^i - z_2^i v_1^i > 0, \quad i \in \{1, 2, 3\},$$

as shown in Figure 6(b).

2.2. Algorithm for identifying vortices

The input information for our vortex algorithm is the known displacement vector field for a given equilibrium state of a deforming granular assembly comprising N particles. Based on this information, the output information of our candidate search-and-elimination scheme comprise the vortices, each defined by its vortex core and member vectors.

1. Identify candidate vortex cores (recall Figure 2):
  - (a) Perform a Delaunay triangulation of all $\mathcal{P} = \{\mathbf{p}^1, \mathbf{p}^2, \dots, \mathbf{p}^N\}$ points (i.e. known particle centers).
  - (b) For each Delaunay triangle, if vertices satisfy the modified direction-spanning property, then add the centroid to the set of candidate vortex cores $\{\mathbf{q}^1, \mathbf{q}^2, \dots, \mathbf{q}^m\}$.

Figure 5: (Color online) *Modified direction-spanning property*. (a,b) A fully-labeled triangle A with all three sides labeled $\{A_{1,2}, A_{2,3}, A_{3,1}\}$ by vectors $\mathbf{v}^i, i \in \{1, 2, 3\}$ (black lines): each vector $\mathbf{v}^i$ lies within the range of angles in $\angle OA_i E_{i,j}$ bound by the median through vertex A_i (black dashed lines) on the internal side, and by the extended edge of side $A_{i,j}$ (red dashed lines). $\angle OA_i E_{i,j}$ is shaded cyan (pink) for anticlockwise (clockwise) vortex rotation. (c) A non fully-labeled triangle, where the two vectors $\mathbf{v}^1$ and $\mathbf{v}^2$ both label side $A_{1,2}$, leaving side $A_{2,3}$ unlabeled (red line). (d) A non fully-labeled triangle, where vector $\mathbf{v}^1$ lies outside of $\angle OA_1 E_{1,2}$ and $\angle OA_1 E_{1,3}$ and thus assigns no label to any side, leaving side $A_{1,3}$ unlabeled (red line).

Figure 6: (Color online) *Vortex directions of vectors satisfying the modified direction-spanning-property.* Vectors $\mathbf{v}^i$ in $\angle OA_i E_{i,i-1}$ rotate in the same direction with respect to O and A_{i-1} : (a) clockwise (shaded pink), (b) anticlockwise (shaded cyan).

2. Identify candidate vortices from candidate vortex cores (recall Figure 2):
  - (a) Define $d_{i,j} = |\mathbf{p}^i - \mathbf{q}^j|$ as the distance between point $\mathbf{p}^i$ and vortex core $\mathbf{q}^j$.
  - (b) Given vortex core $\mathbf{q}^j$, identify the point nearest to the vortex core $\mathbf{p}^k = \arg \min_{1 \leq i \leq N} \{d_{i,j}\}$. Let S denote the set of points that rotate in the same direction with point $\mathbf{p}^k$, and $\bar{S}$ denote all other points rotating in the opposite direction.
  - (c) In S , find the furthest point $\mathbf{p}^i$ from vortex core $\mathbf{q}^j$ such that the circle centred on $\mathbf{q}^j$ with radius $r_j = d_{i,j}$ lies within the boundaries of the granular assembly under study, and $d_{l,j} > r_j$ for all $\mathbf{p}^l \in \bar{S}$.
  - (d) The radius of the candidate vortex corresponding to the candidate vortex core $\mathbf{q}^j$ is given by r_j .
3. Identify resultant vortices by elimination of candidates vortices subsumed by other candidate vortices (recall Figure 3):
  - (a) Eliminate enclosed vortices $\mathbf{q}^i$ that lie within a larger candidate vortex $\mathbf{q}^j$: that is, vortex $\mathbf{q}^i$ whose core lies inside vortex $\mathbf{q}^j$, but where the core of vortex $\mathbf{q}^j$ lies outside vortex $\mathbf{q}^i$.
  - (b) Eliminate duplicate vortices that share the same member vectors. Let $\mathcal{A} = \{\mathbf{q}^{n_1}, \dots, \mathbf{q}^{n_s}\}$ be a the set of candidate vortex cores such that for each pair $(\mathbf{q}^{n_i}, \mathbf{q}^{n_j}) \in (\mathcal{A} \times \mathcal{A})$, $|\mathbf{q}^{n_i} - \mathbf{q}^{n_j}| \leq \min\{r_{n_i}, r_{n_j}\}$. Then define a new vortex core $\frac{1}{s} \sum_{k=1}^s \mathbf{q}^{n_k}$ which replaces the vor-

tex cores in $\mathcal{A}$. The vortex corresponding to this new vortex core is found by returning to step two.

3. Characterization of vortices

We examine two systems which undergo planar deformation due to biaxial compression: System A is derived from physical experiments, while System B is from discrete element simulations. For each system, we use our method for vortex identification to characterize the evolution of vortices in the *residual displacement vector field* at distinct equilibrium states, across loading history, from the start of loading through to failure. Recall the residual displacement vector field is the difference between the actual displacement field and that dictated by the continuum (affine) deformation as determined from the motion of the boundaries. In what follows, we first describe briefly these systems and recapitulate previously established rheological features that are most relevant to this study. Next, we present the results of our analysis of vortex evolution with particular attention paid to the failure regime, during which each sample deforms in the presence of a fully developed and persistent shear band. Since the trends uncovered are common to both systems A and B, we present some of the results for one system only to avoid unnecessary repetitions.

3.1. Systems A and B: known rheological attributes

System A is from physical experiments carried out in an apparatus which has been described in some detail previously (Majmudar and Behringer, 2005; Zhang et al., 2010; Bi et al., 2011). In particular, the data set analyzed here was taken from the forward shear direction of the experiment in Zhang et al. (2010). Relevant parameters are provided in Appendix B.1. This experiment was performed on a system of bidisperse disks that were manufactured from sheets of photoelastic polymer (Vishay, Inc. PSM4). When placed between crossed (circular) polarizers, every disk shows internal patterns which encode the contact forces acting on it. We have developed nonlinear inverse algorithms (Majmudar and Behringer, 2005) which allow us to determine the contact forces acting on any given particle using the photoelastic pattern that it exhibits. The experiment was carried out by placing 1568 disks within the confining walls of a biaxial strain device. The particles rested on a smooth Plexiglas sheet, and they were confined in the horizontal direction by opposing pairs of walls whose spacing could be very precisely controlled. We then applied pure shear strain to this system of particles, through a series of very small strain steps of size $\delta x = 3.3 \times 10^{-3}$ per second. By pure shear strain, we mean compression in one direction, e.g. the x -direction, combined with

dilation in the y -direction, such that the area of the sample stayed constant. After each step, we imaged the system with polarizers in place, without polarizers in place using white light, and without polarizers in place using UV light. From the polarized images we obtained detailed inter-particle force information, as described elsewhere (Majmudar and Behringer, 2005). From the unpolarized images, we obtained the position of each particle, which we then tracked from one image/strain step to the next. Using UV light, we also tracked the rotation of each disk. To this end, we had marked each disk with a narrow diametrically placed bar of fluorescent ink. This process led to data for contact forces and branch vectors, which in turn allowed us to compute the fabric, force moment and stress tensors in the usual way.

System B is a discrete element simulation of an assembly of 5098 spherical particles under plane strain biaxial compression with constant confining pressure. Full details of this simulation have been described elsewhere (Tordesillas, 2007; Tordesillas et al., 2011a, 2014). For completeness, however, we provide a summary of the contact models used, particle size, sample preparation and loading protocol in Appendix B.2. A key aspect of this simulation is that a contact moment (or rolling resistance) is introduced to account for the effect of particle shape angularity, e.g. resistance to relative rotations due to particle interlocking (Iwashita and Oda, 1998, 2000), thus providing a closer representation of the grain kinematics encountered in real irregularly shaped grains. We have the usual discrete element output data for every one of these particles over 299 simulation time steps or strain states, spanning all regimes of the loading history through to failure.

Systems A and B exhibit stress-strain responses that are typical of densely packed granular systems (Figure 7). Both samples fail via strain localization. A single persistent shear band, inclined approximately along the main forward diagonal (from bottom left to top right corner of each sample), governs system dynamics after peak strength. In particular, stick-slip dynamics is evident from the distinct fluctuations in stress ratio after peak. Each sample undergoes cycles of unjamming (slip) and jamming (stick). During each drop in stress ratio, there is a burst in kinematical activity (i.e., large dissipative grain rearrangements) in the shear band, as characteristic of unjamming (Tordesillas, 2007; Tordesillas et al., 2014); this is then followed by a relatively quiescent period of jamming, as particles in the shear band find new stable configurations leading to a rise in stress ratio.

3.2. Vortex location, direction, population, strength and size distribution

In both systems, we observe a residual displacement field that is rich in vortices, forming intermittently across a wide range of spatial scales. We

Figure 7: (Color online) *Rheological response under quasistatic biaxial compression (Systems A and B).* (a) The stress ratio as a function of step number for System A, under constant volume. (b) The stress ratio and volumetric strain as a function of axial strain $|\varepsilon_{yy}|$ for System B, under constant confining pressure. Black dashed vertical line marks that stage in the loading history corresponding to peak stress ratio, beyond which a single persistent shear band, inclined along the forward diagonal with a global anticlockwise rotation, develops in each sample.

examined the following vortex properties: the spatial distribution and number of vortex cores, vortex direction (i.e., the common direction of rotation of constituent vectors), vortex boundary (i.e., a circle centred on the vortex core, with a radius equal to the radial distance of the member vector furthest from the vortex core), vortex size (i.e., diameter of the vortex), vortex strength (i.e., a vector property that is akin to the angular velocity of a point relative to the vortex core). Further details are given in Appendix C.

With respect to location, vortices initially emerge throughout the sample domain, including near the boundaries (Figure 8a-top), but they progressively confine themselves to the ultimate location of the persistent shear band (Figure 8a-bottom). Comparing the two distributions in Figure 8(a) shows that vortices outside the band mainly emerge prior to shear banding. In the failure regime, vortices typically align in spatial succession along the central axis of the shear band (Figure 8b).

Our studies reveal two distinct classes of vortex behavior, depending on the direction of vortex rotation (Figure 9a). We present results for System A. Class 1, comprising those vortices that rotate in the same direction as the shear band (i.e., anticlockwise), constitutes the clear majority. Class 2, comprising the so-called “wakes”, rotate in the opposite direction to the shear band (i.e., clockwise): these were first observed by Rechenmacher and co-workers (Rechenmacher, 2006; Rechenmacher et al., 2010, 2011) in their

Figure 8: (Color online) *Location of vortices (System A)*. (a) Spatial distribution of: vortex cores throughout loading (a-top), and vortex perimeters accumulated during the persistent shear banding regime (a-bottom). For clarity, only vortices with above mean diameter are shown in (a-bottom); this pattern holds true if vortices of diameter below the mean are included. (b) Residual displacement field at an unjamming step interval after peak stress ratio, with the identified vortices highlighted (green).

studies of shear band evolution in dense sand. In the failure regime, the sizes of primary vortices (Class 1) vary considerably as evident in the long-tailed distribution in Figure 9(b-top), with some vortices spanning across the shear band width ($\approx 8\langle d_{50} \rangle - 10\langle d_{50} \rangle$, where $\langle d_{50} \rangle$ is the mean grain diameter); the mean vortex diameter fluctuates about a near constant value ($\approx 3.7\langle d_{50} \rangle$). By contrast, wakes are smaller on average ($\approx 2.8\langle d_{50} \rangle$) and have a relatively narrow size distribution both before and during failure (Figure 9b-bottom). With respect to the mean absolute vortex strength, we observe no marked and persistent difference between the two classes of vortices (Figure 9c).

As shown in Figure 9(a), not only are wakes in the minority, there are also a number of states in the loading history in which there are no wakes. This is to be expected given the idealized shapes of particles in System A (i.e., circular disks) and System B (i.e., spheres). As discussed in Abedi et al. (2012), the existence of wakes is likely to be strongly dependent on particle shape. Here we find evidence to support their claim. The motions of particles in the dominant class, i.e., the primary vortices, induce the formation of wakes through drag. The primary vortices align in spatial succession along the central axis of the shear band, while granular wakes typically form next to shear band boundaries, nestled beside and in between two adjacent primary vortices (Figure 10a,b,c). In this arrangement, peripheral particles in the two

co-rotating, adjacent primary vortices drag their nearest neighbors, and drive the formation of a third vortex (the wake) that then rotates in the opposite direction. The proximity of the wake to the shear band boundary, and the opposing motions of particles at that interface, may possibly act to limit the size of the vortex (Figure 9b-bottom). Wakes can also form along the central axis of the band as shown in Figure 10(a-top), but this arrangement is rare and appears to be the result of a “misalignment” of a primary vortex away from the band axis where the majority of Class 1 vortices lie. Here again the mechanism of drag from primary vortices appears to be at play: the wake appears in the middle of three co-rotating vortices so that displacement vectors at interfacial vortex regions point in the same direction (Figure 10d). Consistent with the findings for sand (Abedi et al., 2012), we would indeed expect wake formation by drag from primary vortices to be more pronounced in systems where particles can interlock due to irregularities in shape. This, in turn, would result in more wakes forming in such systems.

3.3. Vortices and instabilities at the mesoscale and microscale

To get a better understanding of the fundamental role that vortices play in the deformation and failure of granular materials, we quantified the relationship between vortices and instabilities at both the mesoscale and the microscale (Figure 11). Force chain buckling and the microscale instabilities of interparticle rolling and sliding are not mutually exclusive. Note that we do not discuss the methods for identifying particles in individual force chains and buckling force chain segments here: these methods have been discussed in great detail in Tordesillas (2007) and Tordesillas et al. (2011a). It suffices to say that a force chain segment (i.e., a set of three consecutive contacting particles along the chain), and hence the force chain of which it is part, is considered to have buckled when its buckling angle θ (i.e., a measure of misalignment of the segment from its reference configuration) exceeds a prescribed threshold θ^* , i.e., $\theta^* < \theta$. In Figure 11(a), we show the population of such buckling segments for $\theta^* = 1^\circ$. As can be seen, buckling initiates just prior to peak stress ratio and intermittently bursts to a peak during periods of unjamming (Figure 11a). We found most of these buckling segments lie inside or close to vortices (Figure 11a-inset). As force chains serve as the principal repositories of stored energy, their failure by buckling is accompanied by sharp bursts to a peak in the mean kinetic energy (Figure 11b,c) (Appendix D.1 equations D.1-D.2), which is then dissipated through friction (Figure 11d) (Appendix D.1 equation D.3). Moreover, as previously shown in Tordesillas et al. (2008a,b), force chain buckling is a highly dissipative mode of deformation at the *local* scale, specifically, the scale of a particle and its first ring of neighbors. Here we observe that both kinetic energy of

Figure 9: (Color online) *The two classes of vortices (System A).* (a) Percentage vortex population in Class 1 (anticlockwise) and Class 2 (clockwise) versus step number. (b) Frequency distributions of vortex diameters before and after peak stress ratio for Class 1 (b-top) and Class 2 (b-bottom); grey dashed vertical line corresponds to the mean. (b-inset) Evolution with step number of the mean vortex diameter $\langle D_1 \rangle$ and $\langle D_2 \rangle$ for Class 1 and Class 2, respectively. (c) Mean absolute value of vortex strength versus step number. Note that in some stages of the loading history, no wakes form.

Figure 10: (Color online) *Granular wakes (Systems A and B)*. Alignment of primary vortices along the shear band and close-up of wake formation close to the shear band boundary: (a) System A and (b) System B. Primary vortices (blue perimeter) and wakes (red perimeter). Depiction of wake formation due to drag motion from nearby co-rotating primary vortices: (c) close to the boundary, and (d) along central shear band axis (also evident in System A in (a)-top).

Figure 11: (Color online) *Connection between vortices, buckling force chains, kinetic energy and local nonaffine deformation (System B).* (a) Number of buckling force chain (BFC) segments versus axial strain ($\theta^* = 1^\circ$). (a-inset) Percentage of BFC segments inside or in the immediate vicinity of a vortex, for threshold buckling angles $\theta^* \in [1^\circ, 10^\circ]$. Here, we count all BFC segments with at least one member particle that is “close” to a vortex, by which we mean that the distance between the perimeter of the particle and the perimeter of the nearest vortex must be no more than one mean grain diameter. Evolution with axial strain of: (b) mean translational kinetic energy of the residual field, (c) mean rotational kinetic energy, (d) dissipation rate, (e) mean local micropolar nonaffine strain, and (f) mean local micropolar nonaffine curvature (equations defined in Appendix D). Black dashed vertical lines mark the axial strain corresponding to peak stress ratio.

the residual field and local nonaffine deformation are greatest inside vortices (Figure 11e,f) (Appendix D.2 equations D.9 and D.11), where force chain buckling concentrates. Representative spatial distributions of force chain buckling, kinetic energy and local nonaffine deformation, taken during a period of unjamming, corroborate these trends (Figure 12a-d): in effect, vortices become swirling pools of energy, inside of which particles undergo motions that significantly deviate from a continuum (affine) deformation with respect to their nearest neighbors (i.e., high local nonaffine strain and curvature).

The tie between vortices and microscale instabilities of particle rotations and associated interparticle sliding and rolling can be seen in (Figures 8, 11, 13). The relationship between particle rotations and shear bands is well known (Iwashita and Oda, 1998; Oda and Kazama, 1998; Iwashita and Oda, 2000; Tordesillas, 2007; Andò et al., 2012). Particle rotations have been shown to be limited except within shear bands. Indeed, the reference homogenous deformation (or affine strain) in the biaxial configuration does not include particle rotation, hence the occurrence of rotations *must*

Figure 12: (Color online) *Representative spatial distributions of rotational kinetic energy and nonaffine deformation in and around vortices (System B).* Close-up views of spatial distribution of kinetic energy during an unjamming interval: (a) translational, and (b) rotational. Corresponding local micropolar deformation: (c) strain and (d) curvature. Residual displacement vectors (black), primary vortices (blue circles), buckling force chains (grey particles), energy and nonaffine deformation (associated Voronoi cells colored white (low) to dark red (high)).

be associated with instabilities. Our aforementioned findings that vortices concentrate inside shear bands (Figure 8) and that rotational kinetic energy is greatest inside vortices (Figure 11), suggest that particles inside vortices may themselves be rotating. Indeed we find that particle rotations are small except inside vortices and during drops in stress ratio (Figure 13a), with over half of the vortex particles rotating in the same direction as their parent vortex (Figure 13b).

3.4. Co-evolution of vortices and force chains

It was previously shown that the collapse of force chains by buckling is mainly confined to the interior or next to the boundaries of vortices (recall Figure 11a-inset). Here, we probe further force chain evolution relative to vortex evolution to establish the details of how these processes are tied to each other. We proceed by first analysing the interior of vortices, before extending our analysis to the immediate exterior of vortices in unjamming versus jamming regimes. The latter study aims to elucidate what happens at the interface between adjacent co-rotating primary vortices.

Inside primary vortices, we found that significant force chain buckling develops close to the vortex boundary (Figure 14a,b) and towards the interfacial regions with neighboring primary vortices (Figure 14a,c). We also examined the creation of new members to the force chain network by tracking the location of “newly born” force chains, which may arise from a growth or extension of an existing force chain (i.e., new member particles join a pre-existing force chain) or from the formation of an entirely new force chain (Figure 14d). In the case of extensions to a pre-existing force chain, we only account for the new members (red shaded particles in Figure 14(d)) in the analysis to accurately establish trends in the most recent nucleation sites in the force chain network. Just like buckling events, most newly born force chains lie close to the vortex perimeter (Figure 14e). The difference between buckling and creation of new force chains can be seen in the angular position histograms in Figure 14(f): new members of the force chain network typically emerge closer to the shear band boundary, whereas buckling develops close to or along the central band axis.

To understand the extent to which the instability of force chain buckling drives vortex evolution in the failure regime, we next extend our analysis to all force chains that exist both inside vortices as well as in the immediate vicinity of vortices, keeping in mind that almost all vortices after peak stress ratio lie in the shear band region. Specifically, we track the evolution of all force chain particles whose centers are at most a distance L from the nearest vortex core, where $L = r_p + r_v + \langle d_{50} \rangle$, r_p is the radius of the particle in question, r_v is the radius of nearest vortex and $\langle d_{50} \rangle$ is the mean particle diameter. To

Figure 13: (Color online) *Particle rotations inside vortices (Systems A and B)*. (a) Mean particle rotation versus: step for System A (a-left) and axial strain for System B (a-right). (b) Percentage of particles rotating in the same direction as their parent vortex versus: step for System A (b-left) and axial strain for System B (b-right). After peak stress ratio, on average, 62% (56%) of particles in Class 1 (Class 2) co-rotate with their parent vortex for System A and 64% (42%) of particles in Class 1 (Class 2) co-rotate with their parent vortex for System B. Note that no wakes form in some stages of the loading history. Black dashed vertical lines mark the stage of loading corresponding to peak stress ratio.

Figure 14: (Color online) *Force chain evolution inside vortices (System B)*. (a) Representative spatial distribution of buckling force chains (red shaded particles) relative to vortices (circular perimeter) during unjamming. (b) Position histograms of particles in buckling force chains for three threshold buckling angles $\theta^* = 1^\circ, 3^\circ$ and 5° ; (b) radial, (c) angular. (d) Spatial distribution of “newly born” force chains (red shaded particles) and pre-existing force chains (grey shaded particles). Position histograms of particles in newly born force chains: (e) radial, (f) angular. Representative spatial distributions (a,d) correspond to an unjamming interval just after peak stress ratio; the radial and angular histograms correspond to the entire loading history after peak stress ratio. Angular distributions have been rotated clockwise by the mean shear band angle of 42.5° , so that the central axis of the shear band is aligned with the x -axis.

uncover temporal as well as spatial details, we distinguish the pattern of force chain evolution in the unjamming versus jamming regimes. In Figure 15, we focus on the first unjamming-jamming cycle immediately following peak stress ratio (initial stages of the second cycle of unjamming-jamming are included for completeness). The trends shown here are representative of subsequent unjamming-jamming cycles.

During unjamming, the total area occupied by vortices reaches its peak value, though this area is small compared to the sample domain: typically below 10% as shown, for example, in Figure 15(a). The attendant buckling activity is at its most intense: note the burst to a peak in the number of buckling force chain segments during the corresponding unjamming interval in Figure 15(b). Various past studies have established that the “birth and death” evolution of structural building blocks, of which force chains are primary members, continually occurs inside shear bands: see, in particular, the quantitative spatio-temporal characterization in Tordesillas et al. (2014) which showed peaks in the births as well as deaths of 3-cycles that support force chains during unjamming. We can now add to the state of knowledge of that process from the perspective of vortex evolution. As highlighted in Figure 15(b-inset), there is a sudden growth in the number of new force chain particles that partially counteracts the loss of load-bearing capacity from the collapse of pre-existing force chains by buckling. Most of this new membership to the force chain network arises from the formation of short force chains comprising 3 particles (and, to a lesser extent, 5 particles), or the extension of existing force chains (i.e., the addition of new members), as evident in the growth in numbers of long force chains (e.g., chains of 6 particles) in Figure 15(c). These are consistent with the observed births of supporting 3-cycles during unjamming (Tordesillas et al., 2014). Overall, however, the number of particles in force chains (new and old) drops during an unjamming period, as shown in Figure 15(d).

Immediately following unjamming, we observe a quiescent period of almost negligible kinematic activity, as particles jam together and find new stable configurations. During these nascent stages of jamming, force chain buckling ceases. Without force chain buckling to drive vortex motions, vortex population drops to their lowest values, as reflected in the concomitant decline in the total area spanned by vortices during this period (Figure 15a,b); in turn, this results in the sudden drop in the population of force chains inside and in the vicinity of vortices. We emphasize that this does not imply that there are no force chains in the shear band and elsewhere in the sample: to the contrary, we observe an increase in force chains everywhere in the sample during jamming. The decline in force chain numbers seen in Figure 15(b-inset,c) is strictly confined to those inside and next to vortices of which there

are only a few or none during these stages (e.g., there are no wakes for most of this initial period of jamming as shown in Figure 15(a)). As loading advances towards the middle to late stages of a jamming period, pre-existing force chains begin to buckle; as such, vortices begin to form (Figure 15b,c) and we see a recovery in the numbers of force chains inside or near vortices. Indeed, as soon as vortices become mobilized, the number of force chains of varying lengths rise to a peak, with 3-force chains being the most dominant for most of the remaining stages of jamming (Figure 15c).

With respect to the spatial distributions of force chain particles in and around vortices, we observed a bias towards the edges and just outside vortices, with more force chains in existence during jamming than in unjamming, as expected (Figure 16a). However, as shown in Figure 16(b), regardless of regime, the force chain distribution inside vortices is roughly isotropic, albeit with a weak bias in favor of certain directions: the compressive directions opposing the shear through to the direction normal to the shear band ($40^\circ - 80^\circ$ and $220^\circ - 275^\circ$) and in the directions perpendicular to these ($140^\circ - 170^\circ$ and $320^\circ - 335^\circ$).

During unjamming, the majority of buckling force chains and birth of new force chains develop in and around vortices (Figure 17a,c), consistent with Figure 15(b). These are frequently located near the edges of vortices (Figure 17a,c): particles in buckling force chains are mostly concentrated along the central axis of the shear band, especially between $160^\circ - 215^\circ$ and $320^\circ - 0^\circ$ (Figure 17b). Although new force chains form more uniformly in all directions, biases toward 50° , 160° , 215° and 325° can be observed (Figure 17d), which are also evident in the distribution for all force chain particles (Figure 15b). Altogether, these trends suggest that, during the unjamming regimes, new force chain particles and buckling force chain particles are primarily located just inside as well as in between primary vortices.

During jamming, new force chains similarly form amidst old force chains buckling, except that both of these events are smaller in numbers than those found during unjamming. Buckling is more uniformly distributed radially during jamming (Figure 17a), although the relatively high concentration of buckling close to the central axis of the band, especially between $170^\circ - 215^\circ$ and $340^\circ - 50^\circ$, suggests that the buckling of force chains frequently takes place close to the interface with the vortex's rear neighbor. By contrast, the birth of new force chains emerge close to the band boundaries in four prominent directions: opposing the shear (60° , $210^\circ - 230^\circ$) versus with the shear ($140^\circ - 150^\circ$, $315^\circ - 340^\circ$), as shown in Figure 17(d). The latter directions are likely to be associated with force chains that form through the front and back interfacial regions with neighboring primary vortices, while the former are consistent with force chains forming inside the vortices.

Figure 15: (Color online) *Co-evolution of force chains and vortices inside the shear band.* (a) Area spanned by vortices. Temporal zoom-in of evolution across unjamming-jamming cycles of population of: (b) buckling force chain segments, and newly born force chain particles (b-inset) nearby vortices, (c) force chains classified according to length, and (d) all particles in force chains. The strain interval chosen starts at peak stress ratio, covers the complete first unjamming-jamming cycle, through to the initial stages of the next cycle of unjamming-jamming. The trends shown here are representative of subsequent unjamming-jamming cycles after peak stress ratio.

Figure 16: (Color online) *Force chains in and around vortices in unjamming versus jamming regimes.* Position histograms of *all* force chain particles located inside and in the immediate vicinity of vortex: (a) radial and (b) angular. Force chain particles analysed here are those whose center is no more than a distance L from nearest vortex core, where $L = r_v + r_p + \langle d_{50} \rangle$, r_v is the radius of nearest vortex, r_p is the radius of the particle, and $\langle d_{50} \rangle$ is the mean particle diameter. Radial distance is normalized by L . Angular distributions have been rotated clockwise by the mean shear band angle of 42.5° , so that the central axis of the shear band is aligned with the x -axis, and is normalized by the maximum count for each set in question.

4. Conditions for the localization of deformation in granular media

The multiscale characterization of the nonaffine deformation field in Section 3 suggests the formation of vortices inside shear bands is due to the mesoscale instability of force chain buckling and associated microscale instabilities of interparticle sliding and rolling. The task now is to relate this knowledge of the underlying physics to the continuum representation. Here we present the conditions for the localization of deformation, where the deformation field embodies vortex patterns consistent with the observed force chain evolution inside shear bands.

4.1. Continuum modeling of instabilities from null boundary conditions

In the absence of instabilities and inhomogeneities, the continuum deformation of a material under uniform boundary conditions would be *uniquely* described by the uniform (affine) strain. In an unstable material, however, nonunique solutions to the governing equations of deformation are possible. That is, additional deformation fields satisfying null boundary conditions can be constructed such that, when added to the uniform strain, satisfy both the governing equations of deformation and the boundary conditions. This was demonstrated by Valanis (1996, 1998) in a continuum formulation designed

Figure 17: (Color online) *Buckling and creation of new force chains in and around vortices in unjamming versus jamming regimes.* Position histograms of force chain particles located inside and close to vortices, i.e., those whose center is no more than a distance L from nearest vortex core, where $L = r_v + r_p + \langle d_{50} \rangle$, r_v is the radius of nearest vortex, r_p is the radius of the particle, and $\langle d_{50} \rangle$ is the mean particle diameter. Particles in buckling force chains and newly born force chains: (a,c) radial, (b,d) angular. Angular distributions have been rotated clockwise by the mean shear band angle of 42.5° , so that the central axis of the shear band is aligned with the x -axis; the frequency is normalized by the maximum count for each set in question.

to predict the emergence of patterned deformation or self-organization in a wide range of macroscopically uniform material domains, including in frictional materials, under uniform tractions or displacements at the boundaries. In Valanis' theory, the free energy depends not only on the observable strain and internal variables, but also the gradients of the internal variables. By introducing the gradients of the internal variables into the free energy, a separate governing equation results that satisfies an independent set of boundary conditions. In particular, Valanis introduced a deformation field $v'_i(\mathbf{x})$ that corresponds to motions that fluctuate around the mean (affine) field $\bar{v}_i(\mathbf{x})$ such that, on boundaries, the conjugate traction T'_i represents fluctuations in forces. *The deformation field $v'_i(\mathbf{x})$, viz., the residual deformation field, satisfies null boundary conditions: zero traction applies on boundaries where tractions for the mean field are specified, and zero displacement applies on boundaries where displacement for the mean field are specified.* These null boundary conditions correspond exactly to the boundary conditions leading to patterned deformation.

4.2. Vortex patterned deformation in a biaxial test

Following Valanis (1996, 1998), Peters and Walizer (2013) recently proposed a linear combination of the uniform strain field $\bar{v}_i(\mathbf{x}) = \epsilon_{ij}x_j$ and a vortex field $v'_i(\mathbf{x})$ that leads to various localized patterns of deformation in the total flow field $v_i(\mathbf{x})$ for a biaxial specimen:

$$\underbrace{v_i(\mathbf{x})}_{\text{Total field}} = \underbrace{\bar{v}_i(\mathbf{x})}_{\text{Uniform strain field}} + \underbrace{v'_i(\mathbf{x})}_{\text{Residual field}} ; \quad (1)$$

here the coordinates $\mathbf{x}$ are specified such that their origin lies at the center of the biaxial specimen. By construction, the residual field $v'_i(\mathbf{x})$ is parallel to boundaries where displacement is prescribed and imposes no forces on boundaries where tractions are prescribed. In a more general context, $v'_i(\mathbf{x})$ can be viewed as additional solutions to the governing differential equations for deformation. For the biaxial test, in the absence of instability and material inhomogeneity, the flow $v_i(\mathbf{x})$ would be uniquely described by the uniform strain: $v_i(\mathbf{x}) = \epsilon_{ij}x_j$. Thus, the residual field $v'_i(\mathbf{x})$ represents additional nonunique solutions to the deformation field that can arise under null boundary conditions.

The above construction is reminiscent of the traditional shear banding theory proposed by Rudnicki and Rice (1975), in which the shear band arises as an additional solution to the trivial uniform solution as permitted by the constitutive equations. Their approach proceeds in two steps.

First, a kinematic field for the shear band is proposed. Second, the conditions for localization are established by determining the constitutive properties that would admit the proposed kinematic field while satisfying the equations of momentum balance. The approach has been used by many researchers (e.g. Muhlhaus and Vardoulakis, 1987; Tordesillas et al., 2004), although the method is generally limited to shear bands of infinite extent making the analysis one-dimensional. The same procedure can be applied to the case of vortex patterned motions, by simply treating the uniform strain solution $\epsilon_{ij}x_j$ as the trivial solution. The problem then boils down to determining the constitutive relationship that admits the additional residual field $v'_i(\mathbf{x})$, here embodying a particular vortex pattern, while satisfying the equations of momentum balance. Below, we give a brief overview of such analysis.

Consider the following trigonometric relations for the residual deformation field in a biaxial specimen having dimensions $L_1 \times L_2$:

$$\begin{aligned} v'_1 &= \alpha_1(m, n) \sin \left[\frac{m\pi}{2} \left(\frac{x_1}{L_1} + 1 \right) \right] \cos \left[\frac{n\pi}{2} \left(\frac{x_2}{L_2} + 1 \right) \right] \\ v'_2 &= \alpha_2(m, n) \cos \left[\frac{m\pi}{2} \left(\frac{x_1}{L_1} + 1 \right) \right] \sin \left[\frac{n\pi}{2} \left(\frac{x_2}{L_2} + 1 \right) \right], \end{aligned} \quad (2)$$

where the number of vortices created in the x_1 and x_2 directions are dictated by m and n , respectively. Each one of these fields satisfy the null boundary conditions for velocities, and corresponds to a particular pattern of deformation in the total flow field $v_i(\mathbf{x})$, when superimposed on the uniform deformation field $\bar{v}_i(\mathbf{x})$, following equation (1).

For the biaxial test, momentum balance for an increment in stress is satisfied by

$$\frac{\partial \dot{\sigma}_{ij}}{\partial x_j} = 0. \quad (3)$$

Repeated subscript notation is used where the subscripts $\{i, j \in 1, 2\}$. The linearized incremental constitutive relationships are given by

$$\dot{\sigma}_{ij} = E_{ijkl} D_{kl} + \sigma_{ik} W_{kj} + \sigma_{jk} W_{ki} \quad (4)$$

with E_{ijkl} being the incremental stiffness, a quantity that depends on material state and assumed to be constant for the homogeneous specimen, σ_{ij} the prevailing stress, also assumed to be homogeneous, and D_{ij} and W_{ij} are respectively the symmetric and asymmetric parts of the deformation rate given by

$$D_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right),$$

and

$$W_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right).$$

Substitution of the constitutive equations (4) into equation (3) gives

$$\begin{aligned} E_{ijkl} \left(\frac{\partial^2 v_k}{\partial x_l \partial x_j} + \frac{\partial^2 v_l}{\partial x_k \partial x_j} \right) + \sigma_{ik} \left(\frac{\partial^2 v_k}{\partial x_j \partial x_j} - \frac{\partial^2 v_j}{\partial x_k \partial x_j} \right) + \sigma_{kj} \left(\frac{\partial^2 v_k}{\partial x_i \partial x_j} - \frac{\partial^2 v_i}{\partial x_k \partial x_j} \right) \\ = 0. \end{aligned} \quad (5)$$

In view of the second derivative terms, it is immediately verified that the trivial solution satisfies equation (5). Substitution of equation (2) yields two equations for each pair of (m, n) in terms of $\alpha_1(m, n)$ and $\alpha_2(m, n)$ and in the form $A_{ij}\alpha_j = 0$. Accordingly, the condition for the appearance of the vortex deformation field is:

$$A_{11}A_{22} - A_{21}A_{12} = 0. \quad (6)$$

The matrix A_{ij} , a function of E_{ijkl} , m and n , is similar to the acoustic matrix commonly used in traditional shear band analysis (e.g., Tordesillas et al., 2004). In addition, the condition $\dot{\sigma}_{12} = 0$ on sample boundaries where $W_{ij} = 0$ dictates that $E_{1211} = 0$ and $E_{1222} = 0$. Any constitutive state satisfying these conditions allows the appearance of vortices in the total deformation field while inherently accounting for the boundary conditions.

4.3. Vortex patterned deformation inside a shear band

Consider now the internal sub-domain of a fully formed shear band. Let the local coordinates (η, ζ) be such that η and ζ are parallel and orthogonal to the shear band, respectively. This sub-domain is subjected to the nominally uniform simple shear motion $\bar{\mathbf{v}}_{SB} = (\bar{v}_\eta, \bar{v}_\zeta)$ given by

$$\begin{aligned} \bar{v}_\eta &= \gamma \zeta, \\ \bar{v}_\zeta &= 0, \end{aligned} \quad (7)$$

where γ is the strength of the shear field. There is no reason to assume that the deformation field within the shear band is uniquely governed by the uniform simple shear field $\bar{\mathbf{v}}_{SB}$. Once the band is fully formed, it constitutes a sub-domain for which we can apply the same arguments made in Section 4.2 on the deformation of the biaxial specimen. The residual field $\mathbf{v}'_{SB}$, embodying the vortex patterns motions observed inside the shear band in Section 3, can be superimposed on the simple shear field $\bar{\mathbf{v}}_{SB}$ to give the total flow

field $\mathbf{v}_{SB}$ for the shear band — provided $\mathbf{v}'_{SB}$ meets the kinematic boundary conditions of zero velocities at the band boundaries and are permitted by the constitutive response of the material. In the subsection to follow, we propose a residual field $\mathbf{v}'_{SB}$ in accordance with the findings from the micromechanical analyses of vortex evolution in the failure regime, presented earlier in Section 3.

4.3.1. A vortex field consistent with the physics of force chain evolution

Here we combine the findings in Section 3 (Figures 8–17) and the preceding formulation to establish a refinement of the existing knowledge of continuum deformation inside shear bands. Our findings suggest a residual deformation field for the shear band that exhibits the following vortex pattern: a middle row of primary vortices aligned in spatial succession along the central axis of the shear band, with a top and bottom row of wakes forming next to the band boundaries and in between two adjacent primary vortices. We introduce a row of wakes alongside each boundary to take into account the effect of irregularities in particle shape (i.e., particle interlocking) that is inherent in naturally occurring granular media (e.g., sand). That is, consistent with the recent observations for sand in Abedi et al. (2012), we expect more wakes would form in general than those observed in the idealised systems studied here.

Mathematically, we use similar trigonometric relations as the vortex field in equation (2) to construct the pattern. For example, a variant of equation (2) that satisfies the null boundary conditions for the shear band (i.e., zero displacements at band boundaries) is given by:

$$v_\eta = \alpha_1(\beta_1 + \sin(\frac{m\pi\eta}{L_1})) \sin(\frac{2\pi\zeta}{L_2}) + \alpha_2(\beta_2 - \sin(\frac{m\pi\eta}{L_1})) \sin(\frac{4\pi\zeta}{L_2}), \quad (8)$$

$$v_\zeta = \alpha_1(\beta_3 + \cos(\frac{m\pi\eta}{L_1})) \cos(\frac{\pi\zeta}{2L_2}) + \alpha_2(\beta_4 - \cos(\frac{m\pi\eta}{L_1}))(1 - \cos(\frac{2\pi\zeta}{L_2})), \quad (9)$$

where $(\eta, \zeta) \in [-L_1, L_1] \times [-L_2, L_2]$, L_i , $i = 1, 2$, are positive constants used to specify the domain, α_i , $i = 1, 2$, and β_i , $i = 1, \dots, 4$, are given constants to specify the strength and direction of vortices, m denotes the number of vortices in the same row. In the proposed model in Figure 18, $L_1 = 40$, $L_2 = 10$, $m = 5$, $\alpha_1 = -0.9$, $\alpha_2 = 0.2$, $\beta_1 = \beta_2 = 1$ and $\beta_3 = \beta_4 = 0.1$. This one-dimensional periodic model of the residual field embodies a repeating unit cell that comprises three vortices: a primary vortex V whose core lies along the central axis of the shear band, and two smaller but equal size wakes W_1 and W_2 whose cores lie along a line normal to the shear band. The cores of the vortices form the vertices of an isosceles triangle whose vertex angle lies in V and base angles lie in W_1 and W_2 . The side lengths are given by: $\alpha_1 = \alpha_2 = r_1 + r_2$, $\alpha_3 = \sqrt{r_2(2r_1 + r_2)}$, where r_1 and r_2 denote the radii of

Figure 18: (Color online) *Proposed kinematic field inside the shear band.* The residual deformation field comprising a periodic pattern of a central primary vortex with two outer trailing wakes, as governed by equation (9).

the primary vortex and wakes, respectively. In this case, regardless of the global shear band pattern (i.e., a single band versus multiple bands that join to form different shapes), we envisage a characteristic width of d_{SB} , where $d_{SB} = 2\sqrt{r_2(2r_1 + r_2)} + 2r_2$. For both systems, the mean vortex diameter in the failure regime is: $2r_1 \approx 4\langle d_{50} \rangle$ for primary vortices and $2r_2 \approx 3\langle d_{50} \rangle$ for wakes. These correspond to $d_{SB} \approx 8\langle d_{50} \rangle - 9\langle d_{50} \rangle$, which is consistent with the shear band width observed from the particle rotation fields of both systems (Tordesillas, 2007; Zhang et al., 2010). As can be seen in the total shear band field in Figure 19, vortices which rotate in the same direction as the shear field are enhanced, whereas the wakes that rotate opposite to the shear field are somewhat subdued. Hence, ultimately, primary vortices are the main contributors to the total kinematic field inside shear bands.

The question that now arises is whether the proposed kinematic model embodying vortices in Figures 18–19 is entirely consistent with the evidence presented in Figures 15–17 on force chain evolution. Figure 20 provides a depiction of how this consistency between the evolution of vortices, as governed by equation (8), and that of force chains may be realised inside a shear band. In the initial stages of jamming, there are hardly any vortices since force chains (blue lines) that resist the shear are at their most stable configuration (Figure 20a). As shear proceeds into the middle to late stages of

Figure 19: *The total deformation field inside the shear band.* Adding the uniform simple shear field of equation (7) to the residual field of equation (9) yields the total deformation field: (a) the model and (b) System B.

jamming (Figure 20b,c), these force chains will start to overload resulting in buckling (red lines). When this occurs, secondary force chains (dashed blue lines) may also form that prop-up the buckling chain. These secondary force chains, being oriented in the direction of shear, are short-lived due to extension (i.e., particles in the chain are pulled apart by the shear). Thus, they can only provide momentary support to the buckling force chain. Consequently, buckling advances (red dashed line) leading ultimately to the collapse of force chains, in turn, resulting in the ensuing unjamming period (Figure 20d). Finally, in Figure 21, we tracked the lifetime of a representative force chain to show that the co-evolution depicted in Figure 20 is actually realised. A movie of this co-evolution is provided as a supplementary information to this paper: at various stages of the loading history, this force chain can be seen to pass through: (i) the interior of a primary vortex, or, (ii) the interface of two adjacent primary vortices. At the end of the first unjamming event, this force chain can be seen passing through the central vortex of the observed domain in Figure 14(a).

5. Summary of key findings and conclusion

Granular deformation under uniform loading conditions invariably deviates from the continuum uniform deformation. In particular, the resultant deformation field exhibits vortices that are superimposed on the deformation expected from a uniform strain. Here we relate the micromechanics of force chain evolution and vortex formation to the bifurcation analyses of equivalent continuum models. Reminiscent of traditional bifurcation analysis of

Figure 20: (Color online) *Consistency of the proposed kinematic field with force chain evolution.* A depiction of the evolution of force chains inside and at the interface of primary vortices. (a) The initial stages of jamming: stable force chains form (blue lines and blue particles). (b,c) The middle to late stages of jamming: buckling instability initiates, which manifests as vortices in the residual deformation field. (d) The collapse of force chains due to buckling during the unjamming period. A depiction of the most likely rotation field for constituent members of a buckling force chain (red particles) relative to start of jamming (d-right): central particles rotate in the same direction as the shear band (white mark), while some that are close to the band boundaries (e.g., those in wakes) may rotate opposite to the shear band (black mark).

Figure 21: (Color online) *Displacement and rotation field of a force chain in System B*. Tracking an example force chain throughout its lifetime: (a) frames from top left to bottom right are: early stage of strain-hardening regime, just before peak stress ratio, peak stress ratio, end of first unjamming, end of second jamming, collapse of force chain. This force chain is passing through the central vortex in Figure 14(a): compare fourth frame with Figure 14(a). The symbol $\perp$ in each member particle tracks its rotation relative to the first frame. Motion of constituent members of tracked force chain, from top to bottom: (b) component of displacement parallel to the shear band and rotation (positive is anticlockwise), taken from peak stress ratio to end of first unjamming. Note that the top particle, next to the band boundary, rotates clockwise, opposite to the shear band.

shear bands, we show that vortex fields are in fact solutions to the boundary value problem satisfying null boundary conditions for dense granular media.

We turned to physical experiments and discrete element simulations of biaxial compression to establish the requisite empirical ground for our study. For these systems, we characterized quantitatively the emergence of vortices in the residual deformation field (i.e., the deviation of the actual granular deformation from the continuum uniform deformation), with a focus on the failure regime. This involved, in the first instance, the development of an objective method by which to identify vortices, in particular, the central core and boundary of each vortex from a given displacement field in two dimensions. Armed with this vortex identification method, we established a set of kinematically admissible vortex fields that was consistent not only with the equations of continuum mechanics but also with the underlying particle scale instability of force chain buckling that drives both vortex and shear band evolution. The residual deformation field embodies two classes of vortices. Aligned in spatial succession along the central axis of the band are the primary vortices which rotate with the shear band. The motion of constituent particles close to the perimeter of these vortices drag nearest neighbors located next to the band boundaries, in turn mobilizing the formation of secondary vortices (the so-called wakes) that rotate in the opposite direction to the shear band.

This study has brought knowledge of the kinematic field inside shear bands into sharper focus. The affine deformation field is that of simple shear. The residual (nonaffine) deformation field embodying the vortices is periodic in form. Our findings suggest this field may comprise a repeating unit cell of three vortices: a primary vortex at the center of the band, with two trailing wakes close to the band boundary. We showed this kinematical field is consistent with the underlying instability of force chain buckling, as well as the equations of continuum mechanics. The findings here pave the way for the development of a higher level micromechanical theory of shear band evolution with an improved understanding of how the underlying micromechanics of shear bands relate to their equivalent continuum mechanics model. The extent to which these patterns hold in three-dimensions is a matter for future research. A first step in that direction would be the development of a method for identifying vortices in three-dimensional kinematic fields. This is an open problem that is continuing to attract considerable attention in dynamical systems theory (Dellnitz et al., 2009; Boltt et al., 2012) due to its immense relevance in many fields, most notably in fluid mechanics and atmospheric science.

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Appendix A. The direction-spanning property of vectors relative to various Sperner direction ranges.

There are two aspects of the scheme by Jiang et al. (2002) which can lead to erroneous detection of vortices. These aspects, which affect the resultant label, are depicted in Figure A.22: (i) choice of orientation or direction ranges (e.g., compare (a) versus (b) in Figure A.22), and (ii) the choice of m for the m -equally spaced Sperner direction ranges (e.g., compare $m = 3$ where each range spans 120° in (a,b) versus $m = 4$ where each range spans 90° in (c,d) in Figure A.22). The corresponding labels for (a-d) are shown in (e-h), respectively. With respect to the Sperner directions (a), the vectors in (e) are *not* uniquely labeled: two vectors are labeled C resulting in the triangle label ACC . Similarly, the vectors in (g) are not fully-labeled with respect to the Sperner directions (c). By contrast, the triangles in (f) and (h), labeled ABC and BCD , respectively, are fully-labeled with respect to their Sperner directions (b) and (d). Note the direction spanning-property for four equally spaced Sperner direction ranges holds for any of the following labels: ABC , ABD , BCD , or ACD . The quantization level m can also be set as high as desired, though this offers no clear benefit and becomes impractical for large m due to the exponential increase in the search space for the direction-spanning property (Jiang et al., 2002).

Appendix B. Summary of parameters for Systems A and B

Appendix B.1. System A

The data set of System A is from experiments on bidisperse photoelastic disks, described in detail in (Majmudar and Behringer, 2005; Zhang et al., 2010). In particular, the data was taken from the forward shear direction of the test in Zhang et al. (2010). A summary of all the interaction parameters governing the contacts and other quantities relevant to this study is presented in Table B.1.

Figure A.22: (Color online) The different labelling possible for a set of three vectors at the vertices of a triangle depending on the Sperner direction ranges used: three (four) equally spaced direction ranges (a) and (b) ((c) and (d)) and their corresponding direction labelling of vectors (e) and (f), respectively ((g) and (h), respectively). With respect to their Sperner direction ranges, vectors in (e) and (g) do not satisfy the direction-spanning property while those vectors in (f) and (h) satisfy the direction-spanning property.

Table B.1: System A: experimental parameters and material properties

Parameter	Value
Incremental strain along the x -axis	$\pm 3.3 \times 10^{-3}$
Timestep increment	16.67 s
Number of particles	1568
Smallest radius	3.7×10^{-3} m
Largest radius	4.3×10^{-3} m
Initial packing density	0.795 ± 0.003
Sliding friction coefficient μ^t	0.7
Rolling friction coefficient μ^r	0.1
Normal spring stiffness constant k^n	2.0×10^3 Nm $^{-1}$
Tangential spring stiffness constant k^t	0.8×10^3 Nm $^{-1}$
Rotational spring stiffness constant k^r	5.8×10^{-3} Nm rad $^{-1}$

Appendix B.2. System B

The data set of System B is from simulations of polydisperse spherical grains confined to planar motion, described in detail in Tordesillas (2007). It is governed by a classical DEM model (Cundall and Strack, 1979), modified to incorporate a moment transfer to account for rolling resistance and thus

capture the effects of non-idealised particle shapes (Iwashita and Oda, 1998, 2000). A combination of Hooke’s law, Coulomb’s friction, and hysteresis damping is used to model the interactions between contacting particles. An initially isotropic assembly of 5098 spherical particles is prepared and subject to biaxial compression with motion constrained to the plane. The ensemble is subjected to constant confining pressure, with a coefficient of rolling friction of $\mu^r = 0.02$. The initial packing fraction is 0.858. A rolling resistance and a sliding resistance act at the contacts, both of which are governed by a spring up to a limiting Coulomb value of $\mu|\mathbf{f}^n|$ and $\mu^r R_{min}|\mathbf{f}^n|$, respectively, where $\mathbf{f}^n$ is the normal contact force and R_{min} is the radius of the smaller of the two contacting particles. A summary of all the interaction parameters governing the contacts and other quantities relevant to this study is presented in Table B.2.

Table B.2: System B: DEM parameters and material properties (given per unit depth)

Parameter	Value
Applied strain rate $\dot{\epsilon}_{yy}$	-8×10^{-3} /s
Confining pressure σ_{xx} (where applicable)	7.035×10^2 N/m
Time step increment	6.81×10^{-7} s
Initial height:width ratio	1.08 : 1
Number of grains	5098
Grain density	2.65×10^3 kg/m ³
Smallest radius	0.76×10^{-3} m
Largest radius	1.52×10^{-3} m
Average radius (uniform distribution)	1.14×10^{-3} m
Initial packing density	0.858
Intergrain friction μ	0.7
Grain-wall friction (top, bottom walls) μ	0.7
Grain-wall friction (lateral walls) μ	0.0
Rolling friction μ^r	0.02
Normal spring stiffness k^n	1.05×10^5 N/m
Tangential spring stiffness k^t	5.25×10^4 N/m
Rotational spring stiffness k^r	6.835×10^{-2} N m/rad

Appendix C. Properties of vortices

Every constituent vector of the vortex rotates about the *vortex core* in the same direction. The *direction* of a vortex is the common direction of rotation of its constituent member vectors, and is either clockwise or counterclockwise.

The *boundary* of a vortex is a circle, centred on the vortex core, with a radius equal to the radial distance of the member point that is furthest from the vortex core. The *size* of a vortex is defined as its diameter.

The *strength* of a vortex is derived from a vector property that is akin to the angular velocity of a point relative to the vortex core. As shown in Figure C.23, suppose that $\mathbf{v}^P$ is the displacement vector of a particle whose center lies at point P and r denotes the distance between the particle center and the vortex core at O . We can compute, ω^P , to be the angle (measured in radians) spanned by the vector $\mathbf{v}^P$ relative to O , as follows

$$\omega^P = \frac{|\mathbf{v}^P| \sin \theta}{r}$$

where $|\cdot|$ denotes the Euclidean norm and θ denotes the angle between the vector $\mathbf{v}^P$ and the radial component $\mathbf{v}_{\parallel}^P$. As all the constituent vectors of a vortex rotate about a common center, we then define the strength of a vortex to be the average ω^P of all its constituent vectors relative to, or about the perpendicular axis through, the vortex core. Note that ω^P , as defined above, is always positive. To account for the direction of rotation of the vortex, we include a sign to the vortex strength. If the vortex rotates anticlockwise (clockwise) the vortex strength is positive (negative). Let V denote the set of particles in the same vortex and $|V|$ denote the total number of particles in the vortex. Then the strength of the vortex V is given by

$$\omega^V = \frac{\text{sgn}(V)}{|V|} \sum_{P \in V} \omega^P,$$

where $\text{sgn}(V) = 1$ if the vortex rotates anticlockwise and $\text{sgn}(V) = -1$ if the vortex rotates clockwise.

Appendix D. Properties of particles in and around vortices

Appendix D.1. Energies

The translational and rotational energy of particles is computed across intervals in both System A and System B. The intervals correspond to times and strains between data sampling of the system state. Translational and angular velocities are derived from the displacements and rotations of particles across the same intervals. The translational energy of a single particle is given by

$$E_{tr} = \frac{1}{2} m |\mathbf{v}|^2 \tag{D.1}$$

Figure C.23: (Color online) ω^P is the angle spanned by $\mathbf{v}^P$ relative to its parent vortex core O , where $\mathbf{v}^P$ is the displacement vector of a particle whose center lies at point P .

where m is the mass of the particle, and $\mathbf{v}$ is the residual (nonaffine) component of the velocity of the particle in the global reference frame. The rotational energy of a given particle is given by

$$E_{rot} = \frac{1}{2} I \omega^2 \quad (\text{D.2})$$

where I is the moment of inertia of the particle, and ω is the angular velocity of the particle in the global reference frame. For a solid sphere of radius r , this takes the form $I_{sphere} = \frac{2}{5} m r^2$, and for a solid cylinder of radius r perpendicular to the plane $I_{cylinder} = \frac{1}{2} m r^2$.

The rate of energy dissipation for System B has been discussed in some detail in Tordesillas (2007). This is computed as

$$D(\epsilon_{yy}) = \frac{(W - \Delta E_{kin} - \Delta E_{pot})}{\Delta t} \quad (\text{D.3})$$

where the global potential energy is given by

$$E_{pot} = \sum_{c=1}^{N_c} \left(\frac{|\mathbf{f}^{nc}|^2}{2k^n} + \frac{|\mathbf{f}^{tc}|^2}{2k^t} + \frac{|\mathbf{I}^c|^2}{2k^r} \right) \quad (\text{D.4})$$

where the summation is over all the contacts in the assembly N_c , $\mathbf{f}^{nc}$, $\mathbf{f}^{tc}$ and $\mathbf{I}^c$ represent respectively the normal force, tangential force and moment

of the contact c , k^n , k^t and k^r are respectively the normal, tangential and rolling spring constants, W is the work done on the system, ΔE_{kin} is the change in kinetic energy, and ΔE_{pot} is the change in potential energy over the time interval Δt (or $|\Delta \epsilon_{yy}| = 0.00038$).

Appendix D.2. Local nonaffine deformation

For any given particle, we can consider an associated small particle cluster comprising it and its first ring of neighbors. We can quantify the deviation of the motion of particles in this cluster relative to that dictated by a uniform deformation using the micromechanical Cosserat (micropolar) continuum formulation developed in Tordesillas et al. (2008b). This deviation, otherwise known as the nonaffine deformation, comprises two quantities, i.e., nonaffine strain and nonaffine curvature, as given below.

(a) Local nonaffine strain

A measure of the local strain experienced by a single particle relative to its first ring of neighbors is

$$\epsilon_{ij} = \frac{1}{2V} \sum_{c \in B} (p_i^c + p_i^{c+1}) e_{jk3} (l_k^{c+1} - l_k^c) \quad (\text{D.5})$$

where the sum is taken anticlockwise over the set of branch vectors B associated with the particle, l_i^c = branch vector between the reference particle and its neighbor “ c ”, p_i^c = vector describing the relative motion of the particle c from the frame of the reference particle, V = area of the Delaunay polygon for the particle, and e_{ijk} = is the usual Levi-Civita permutation symbol. This polygon is made up of the triangles derived from a Delaunay triangulation of the particle and its first ring of neighbors. The vector p_i^c is defined as

$$p_i^c = u_i^c - u_i + e_{ij3} l_j^c \omega \quad (\text{D.6})$$

where u_i and u_i^c denote displacement of the reference particle and its neighbor since the start of loading, respectively, and ω = rotation of the reference particle.

Although the volumetric average of strain matches the macroscopic strain, the projection of individual particle strains along branch vectors does not match the relative displacements at contacts. The difference between the relative motion of the particle c from the frame of the reference particle and the motion implied by the particle strain is given by

$$\Delta p_i^c = p_i^c - \epsilon_{ij} l_j^c \quad (\text{D.7})$$

Thus a local measure of the particle strain rate is given by

$$\dot{\epsilon}_{ij} = \frac{1}{2V} \sum_{c \in B} (\dot{p}_i^c + \dot{p}_i^{c+1}) e_{jk3} (l_k^{c+1} - l_k^c). \quad (\text{D.8})$$

Using this, a scalar measure of the nonaffine deformation experienced by each particle relative to its immediate neighbors is

$$\Delta^\epsilon = \frac{1}{2V} \sum_{c \in B} |\Delta \dot{\mathbf{p}}^c| (|\mathbf{l}^{c+1} - \mathbf{l}^c| + |\mathbf{l}^c - \mathbf{l}^{c-1}|) \quad (\text{D.9})$$

(b) *Local nonaffine curvature*

A nonaffine measure that is solely governed by rotations can be introduced by defining the local rotation gradient, the curvature κ_i , in a manner similar to the strain given in equation D.8. Thus a local measure of the particle curvature rate is given by

$$\dot{\kappa}_i = \frac{1}{2V} \sum_{c \in B} (\dot{\phi}^c + \dot{\phi}^{c+1}) e_{ij3} (l_j^{c+1} - l_j^c), \quad (\text{D.10})$$

where the rate of relative rotation is $\dot{\phi}^c = \dot{\omega}^c + \dot{\omega}^{c+1}$. Introducing $\Delta \dot{\phi}^c = \dot{\phi}^c - \dot{\kappa}_i l_i^c$, the nonaffine rotational motion is given by

$$\Delta^\kappa = \frac{1}{2V} \sum_{c \in B} |\Delta \dot{\phi}^c| (|\mathbf{l}^{c+1} - \mathbf{l}^c| + |\mathbf{l}^c - \mathbf{l}^{c-1}|). \quad (\text{D.11})$$

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