Heterogeneity and patterning in the quasi-static behavior of granular materials

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Abstract Heterogeneity is classified in five categories—topologic, geometric, kinematic, static, and constitutive—and the first four categories are investigated in a numerical DEM simulation of biaxial compression. The simulation experiments show that the topology and geometric fabric become more variable during loading. The measured fluctuations in inter-particle movements are large, they increase with loading, and they extend to distances of at least eight particle diameters. Deformation and rotation heterogeneity are large and are expressed in spatial patterning. Stress heterogeneity is moderate throughout loading.

Keywords: Granular material, Heterogeneous material, Patterning, Microstructure, Discrete Element Method

1 Introduction

Perhaps the most distinguishing characteristic of granular materials is their internal heterogeneity, particularly when viewed at the micro-scale of individual particles or particle clusters. Granular materials often consist of a wide range of particle sizes and shapes, and these particles are usually arranged in an irregular manner. This geometric and topologic multiformality produce nonuniform distributions of internal force and deformation, which are often expressed in spatial and temporal patterning. In the paper, we catalog the many forms in which heterogeneity may be manifest, and we provide a classification scheme for its measurement. Examples of several forms of heterogeneity are presented, and certain expressions of their evolution and spatial patterning are described. Although the proposed classification scheme applies to both two- and three-dimensional (2D and 3D) granular materials, to particles of arbitrary shape and composition, to both sparse and dense packings, and to both dynamic and quasi-static deformations, the paper illustrates the classification within a two-dimensional framework and with a 2D example of the quasi-static deformation of a dense disk assembly.

In Section 2 we consider a classification scheme for heterogeneity and the various forms in which it can be expressed and measured. Section 3 describes the simulation methods that are used to explore several forms of heterogeneity. In the same section, we also consider a means of measuring the heterogeneity of vector and tensor objects. Section 4 presents experimental results and characterizes several types of heterogeneity and their evolution during biaxial compression.

2 Classifying heterogeneity

Table 1 gives a classification of material characteristics that can manifest heterogeneity in granular materials. The table references sample experimental studies in which these characteristics have been measured, although the short lists of references are far from exhaustive. The characteristics in the table are organized within a hierarchy of heterogeneity categories: topologic, geometric, kinematic, static, and constitutive. These categories are described in a general manner in the next paragraph. Table 2 presents a short list of informational forms that can be used for describing each characteristic. The arrangement of the forms in Table 2 reflects their complexity and the usual historical order in which measurements have been proposed and collected. The simplest form of information is some measure of central tendency: a mean, median, or modal value. Heterogeneity implies diversity and fluctuation, and this dispersion in measured values can be expressed as a variance or standard deviation, with standard graphical means such as histograms, or by fitting experimental results to an appropriate probability distribution. Of greater complexity are measurements of temporal correlation (e.g. rates of change) and spatial correlation. The most complex data analyses can also disclose the spatial and temporal patterning of heterogeneity. The paper presents data on the six characteristics that are accompanied by section numbers in Table 1 and these characteristics are explored with a range of the informational forms that are given in Table 2.

Table 1 begins with topologic characteristics, which concern the arrangement of the particles and their contacts, but without reference to their position, size, or orientation. This information can be expressed as a particle graph for both 2D and 3D assemblies, which gives the topologic connectivity of the particles in a packing, as ex-
Table 1. Heterogeneity categories and references to experimental studies

| Categorya | References |
|-----------|------------|
| Topologic (1.1) | |
| Coordination number | [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]a |
| Valence | 
| Geometric | |
| Grain size | 
| Grain shape | 
| Grain size | [13, 14, 15, 16, 17]a |
| Void ratio | [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]a |
| Void size/sha | 
| Branch vector | [18, 19, 20, 21, 22, 23, 24, 25]a |
| Branch vector length | [21, 22, 23, 24]a |
| Fabric tensor | [25, 26, 27, 28, 29, 30, 31]a |
| Loop tensor | [32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43] |
| Kinematic | |
| Particle movement | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Inter-particle motion | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Particle rotation | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Deformation | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Static | |
| Contact force | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Force potential | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Stress | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |
| Constitutive | [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]a |

a Section numbers (*,*) refer to the experimental results in this paper
b Includes statistical measures, e.g. including standard deviations or histograms
c Includes spatial correlations
d Includes spatial patternings
e Includes rates of changes or temporal patterning

Table 2. Analyses of heterogeneity

| Informational forms | Examples |
|---------------------|----------|
| Central tendency    | Mean, median, modes |
| Dispersion          | Standard deviation, variance, coefficient of variation, histograms, probability and cumulative distributions, quartile plots |
| Spatial correlation | n-point correlations, correlation lengths |
| Temporal correlation| Rates of change |
| Spatial and temporal patterning | Spatial plots, time series analyses, spatial domain transforms |

The paper presents data on the variation in local topology and its evolution during loading. A discrete metric is also proposed as a means of tracking inter-particle processes between distant particles. Geometric information includes the additional descriptors of length, shape, and angle, which relate to the positional arrangements, orientations, and sizes of particles. Together, topology and geometry describe the fabric of a granular assembly. The paper characterizes the evolution of one form of heterogeneity in this fabric. Kinematic information (Table 1) concerns the movements and rotations of particles, relative inter-particle movements, and the local deformations within small groups of particles. The paper gives examples of heterogeneous movements and deformations, the spatial correlation of inter-particle movements, and the patterning of local rotations and deformations. Static (or statistical) information (Table 1) involves the transmission of force and stress within a material, and the paper depicts the local diversity of stress and its evolution during loading. Table 1 also includes the category of constitutive heterogeneity (or, perhaps, mechanical heterogeneity), which would involve the diversity in local material stiffness. Except for simple two-particle models that rely on uniform strain assumptions, there is, as of yet, no consistent vocabulary or experimental methods for measuring and characterizing this form of heterogeneity. The reader is referred to the recent work of Gaspar and Koenders [59] and Gaspar [60], which may provide a needed framework for characterizing constitutive heterogeneity.

As a simple example of the classification scheme in Table 2, we could consider the diversity of grain size in a granular material. Methods for measuring and describing particle size, such as sieving methods, are standardized and widely applied, so that references to these methods are excluded from Table 2. These methods can readily depict a representative (central) grain size as well as the dispersion of sizes. Certain processes, such as shearing and compression, can cause particle breakage, which could be measured with temporal correlations of the size distribution. Processes that promote size segregation could be studied with methods that reveal the spatial correlation of size. Size segregation usually leads to a spatial patterning of the local size distribution, and processes that produce a periodic recurrence in such patterning would lead to both spatial and temporal patterning.

3 Methods and notation

A conventional implementation of the Discrete Element Method (DEM) was used to simulate the quasi-static behavior of a large 2D granular assembly and to illustrate different manifestations of internal heterogeneity and their evolution.

3.1 Simulation methods

The study employs a square assembly containing 10,816 circular disks of multiple diameters. The disk sizes are randomly distributed over a fairly small range of between
parameterizing events, the rates of micro-quantities will be used to compute the rates. Because time is used in quasi-stochastic boundaries, a choice that would eliminate the topological and geometric nonuniformity that might otherwise occur in the vicinity of rigid platen or assembly corners. The initial height and width of the assembly were each about 100 times the initial mean stress, \( o \), while maintaining a constant average horizontal stress, \( \bar{\sigma}_{11} = 0 \). About 200,000 time steps were required to reach the final vertical strain, \( \bar{\tau}_{22} \), of -0.01, and at this rate of loading, the average imbalance of force on a particle was less than \( 1 \times 10^{-4} \times \) times the average contact force.

During biaxial compression, a simple force mechanism was employed between contacting particles. Linear normal and tangential contact springs were assigned equal stiffnesses \( (k_n = k_t) \), and slipping between particles would occur whenever the contact friction coefficient of 0.50 was attained.

The non-uniformity of scalar, vector, and tensor quantities that can be measured within a single particle and inter-particle velocities). No contractive summation usually be expressed in a dimensionless form by dividing by an average, macro-scale rate (average strain rate, average strain rate, etc.).

### 3.2 Notation

Vectors and tensors are represented by bold Roman letters, lower and upper case respectively. Their inner products are computed as

\[
a \cdot b = a_p b_p, \quad A \cdot B = A_{pq} B_{pq},
\]

with the associated norms

\[
|a| = (a \cdot a)^{1/2}, \quad |A| = (A \cdot A)^{1/2}.
\]

A juxtaposed tensor and vector will represent the conventional product

\[
AB = A_{pq} B_{pq},
\]

and juxtaposed tensors represent the product

\[
\overline{AB} = A_{pr} \overline{B_{rq}}.
\]

Various quantities are measured at both micro and macro scales so that the variability of the micro-scale measurements can be deduced. A macro-level, assembly average is indicated with an overline \( \overline{L}, \overline{\tau}, \overline{\sigma}, \overline{\gamma}, \overline{p} \); whereas local, micro-level quantities appear with superscripts \( (L', \sigma'^k, \gamma^j, p^k) \), Table 3. The “\( k \)” superscript is used with quantities that can be measured within a single particle or its immediate vicinity; the “\( i \)” superscript is assigned to quantities that are measured within a single void cell (the dual of particles); and the “\( j \)” superscript is used for quantities associated with a pair of particles or a pair of void cells (e.g. contacts, contact forces, branch vectors, and inter-particle velocities). No contractive summation is implied with superscripts, e.g. \( a^i b^j \).

### Table 3. Superscript notation

| Index | Usage |
|-------|-------|
| \( i \) | A polygonal void cell having \( m' \) edges and vertices. An \( m \)-tuple of particles or contacts, \( i = (k_1, k_2, \ldots, k_{m'}) \) or \( i = (j_1, j_2, \ldots, j_{m'}) \) |
| \( j \) | A contacting pair of particles \( (k_1, k_2) \) |
| \( k \) | A single particle |

The initial mean stress was about 5 \( \times 10^0 \) times the initial mean stress, \( o \), and the average overlap between neighboring particles was about \( 9 \times 10^{-4} \times \) of \( D \). The assembly was surround by periodic boundaries, a choice that would eliminate the topology and geometric nonuniformity that might otherwise occur in the vicinity of rigid platen or assembly corners. The initial height and width of the assembly were each about 102 \( \times \) times the average con-

The rates of several micro-quantities (position, force, orientation, etc.) were periodically measured during the loading. These rates were calculated by first collecting the assembly’s status at two instants that were separated by 100 time steps, and the difference in these states was then used to compute the rates. Because time is used in quasi-static DEM simulations as simply a means of ordering or parameterizing events, the rates of micro-quantities will usually be expressed in a dimensionless form by dividing by an average, macro-scale rate (average strain rate, average strain rate, etc.).

### Fig. 1

Evolution of the average compressive stress within the assembly of 10,816 circular disks during biaxial compression.
assemblies

Table 4. Statistics of uniform and random vector sets

| Measure              | Vectors \(a_{\text{local}}\) |
|----------------------|-------------------------------|
|                      | Uniform, aligned | Random |
| Mean\((a_{\text{local}} || \mathbf{\mu})\) | 1 | 0 |
| Std\((a_{\text{local}} || \mathbf{\mu})\) | 0 | 1/2 |
| Mean\((a_{\text{local}} \perp \mathbf{\mu})\) | 0 | 2/\pi |
| Mean\((a_{\text{local}} \circ \mathbf{\mu})\) | 1 | 0 |

assembly-average \(\mathbf{\mu}\):

\[
a_{\text{local}} || \mathbf{\mu} = \frac{1}{|\mathbf{\mu}|} (a_{\text{local}} \cdot \mathbf{\mu})
\]

\[
a_{\text{local}} \perp \mathbf{\mu} = \frac{1}{|\mathbf{\mu}|} |a_{\text{local}}| - (a_{\text{local}} || \mathbf{\mu}) \mathbf{\mu}
\]

\[
a_{\text{local}} \circ \mathbf{\mu} = \frac{1}{|a_{\text{local}}|} (a_{\text{local}} \cdot \mathbf{\mu})
\]

The participation and non-conformity in Eqs. 5 and 6 are the dimensionless magnitudes of \(a_{\text{local}}\) in directions parallel and perpendicular to \(\mathbf{\mu}\), and relative to the length of \(\mathbf{\mu}\). The alignment \(a_{\text{local}} \cdot \mathbf{\mu}\) is the cosine of the angle separating \(a_{\text{local}}\) and \(\mathbf{\mu}\). These quantities are unambiguous when \(a\) is a vector or tensor. If \(a\) is a scalar, then \(a_{\text{local}} || \mathbf{\mu}\) is simply the quotient \(a_{\text{local}} / |\mathbf{\mu}|\); \(a_{\text{local}} \perp \mathbf{\mu}\) is zero; and \(a_{\text{local}} \circ \mathbf{\mu}\) is \(\text{sgn}(a_{\text{local}}, \mathbf{\mu})\). By reducing vector and tensor objects to the scalars in Eqs. 5-7, we can compute conventional statistical measures such as the mean, standard deviation, and coefficient of variation. These measures will be represented with the notation \(\text{Mean}(\cdot)\), \(\text{Std}(\cdot)\), and \(\text{Cov}(\cdot)\), where the coefficient of variation \(\text{Cov}(\cdot) = \text{Std}(\cdot) / \text{Mean}(\cdot)\).

As an example with vector quantities \(a\), we can consider two different sets of two-dimensional vectors \(a_{\text{local}}\), and this example can serve as a reference case for comparing the results given later in the paper. In both sets, the vectors \(a_{\text{local}}\) all have unit length. In the first set, the vectors \(a_{\text{local}}\) have a uniform direction that is aligned with the reference vector \(\mathbf{\mu}\), but in the second set, the vectors \(a_{\text{local}}\) have uniformly random directions. In the example, the reference vector \(\mathbf{\mu}\) is also assumed to have unit length. The four statistical measures \(\text{Mean}(a_{\text{local}} || \mathbf{\mu})\), \(\text{Std}(a_{\text{local}} || \mathbf{\mu})\), \(\text{Mean}(a_{\text{local}} \perp \mathbf{\mu})\), and \(\text{Mean}(a_{\text{local}} \circ \mathbf{\mu})\) are used in the paper as indicators of local non-conformity and heterogeneity, and their values for this simple example are summarized in Table 4.1.

4.1 Topologic heterogeneity

In a 2D setting, the topology of an assembly can be described by the particle graph of its particles (the graph vertices) and their contacts (the graph edges). The particle graph is associated with the Voronoi-Diirchlet tessellation of a 2D region, except that the particle graph admits only the real contacts as graph edges. The faces of the planar graph are polygonal void cells, which are enclosed by the circuits of contacting particles (an example void cell is shaded in Fig. 2). For this topologic description of a 2D granular material, the simplest local topologic measures are the local coordination number \(n_k\) and the local valence \(m_k\), defined as the number of contacts of a single particle \(k\), and the number of edges of a single void cell \(i\) (see Fig. 2 for examples of valence). Because gravity is absent in the current simulations, some particles will be unattached and, hence, excluded from the particle graph. The effective average coordination number \(\bar{n}_{\text{eff}}\) of the attached particles will be somewhat larger than the coordination number \(\bar{n}\) that includes both attached and unattached particles. \(\bar{n}_{\text{eff}}\). Dense assemblies have large coordination numbers and small valences, but during biaxial compression, the average effective coordination number is reduced, while the average valence increases.

In the simulation of 10,816 circular disks, certain local vector and tensor quantities are found to have measured values of \(\text{Std}(a_{\text{local}} || \mathbf{\mu})\) and \(\text{Mean}(a_{\text{local}} \perp \mathbf{\mu})\) that greatly exceed those of the random set, as given in the final column of Table 4. These large values are due to variations in the magnitudes of the local quantities as well as in their directions.

4 Heterogeneity measurements

The experimental results are analyzed for indications of four categories of heterogeneity: topologic, geometric (fabric), kinematic, and static.
Fig. 3. The evolution of two measures of topologic heterogeneity during biaxial compression: the coefficients of variation (Cov) of the local coordination number ($n^k$) and local valence ($m^k$).

4.2 Geometric heterogeneity

Geometric characteristics of granular materials are listed in Table I and numerous studies have shown how the assembly averages of these characteristics evolve during loading. Fewer studies indicate how the internal diversity of these characteristics changes with loading. Tsuchikura and Satake [26] have developed methods for examining the diversity of local fabric in a 2D granular material and found that void cells become more elongated during loading, but that the variation in elongation remains fairly uniform. To study this form of fabric anisotropy, they propose a method for computing the magnitude of the anisotropy of a general second order symmetric tensor $T$ by considering its deviatoric part $T'$. The self-product of $T'$ yields a scalar measure $\beta$ of anisotropy:

$$T'T' = \beta^2 I.$$  \hspace{1cm} (8)

In their experimental study, they used $\beta$ to measure the local anisotropy (elongation magnitude) of the loop tensors of individual void cells. The current study applies the same methods to analyze heterogeneity in the local fabric tensor.

Satake [34] proposed the fabric tensor as a measure of particle arrangement in a granular material, and we use a local form, $F^k$, to analyze fabric heterogeneity:

$$F^k_{pq} = \frac{1}{n^k} \sum_{j=1}^{n^k} \eta_j^p \eta_j^q,$$  \hspace{1cm} (9)

where the tensor for a particle $k$ involves its $n^k$ contacts. Superscript $j$ denotes the $j$th contact with particle $k$ (Table II). Vectors $\eta^j$ are unit vectors in the directions of the branch vectors that join the center of particle $k$ with the centers of its contacting neighbors. The assembly average $\overline{F}$ is computed from the sum of local values for all $N_{\text{eff}}$ particles that are included in (attached to) the particle graph,

$$\overline{F} = \frac{1}{2N_{\text{eff}}} \sum_{k=1}^{N_{\text{eff}}} n^k F^k.$$  \hspace{1cm} (10)

Studies have shown that $\overline{F}$ becomes increasingly anisotropic during deviatoric loading, with the major principal direction of $\overline{F}$ becoming more aligned with the direction of compressive loading [6,11].

The current study considers variability in the local anisotropy of fabric. We apply Eq. 8 to the local fabric tensor $F^k$ to compute a local measure $\alpha^k$ of fabric anisotropy: $T \rightarrow F^k$, $\beta \rightarrow \alpha^k$. Fig. 4 shows the results for the biaxial compression tests. The average fabric anisotropy of the entire assembly, $\overline{\alpha}$, increases with loading (Eqs. 8 and 10), a results that is consistent with previous experiments. As would be expected, the mean local anisotropy, $\text{Mean}(\alpha^k)$, is larger than the average assembly anisotropy $\overline{\alpha}$, and the increase in local anisotropy parallels that of the entire assembly. The results also show, however, that the standard deviation of fabric anisotropy increases with strain. The increase in $\text{Std}(\alpha^k)$ suggests that the geometric arrangement of particles becomes more varied during loading.

4.3 Inter-particle movements

The change in stress within a dry granular material is due to local changes in the inter-particle forces that result from the relative shifting of particles during assembly deformation. The simplest models of this mechanism are based upon the interactions of particle pairs that are constrained to move in accord with a homogeneous deformation field. Bathurst and Rothenburg [42] studied the inter-particle movements at small strains in the biaxial compression of a disk assembly. Their results demonstrate that, on average, the inter-particle movements at small strains are less than those that would be consistent with uniform deformation (see also [39]). The current study addresses the non-conformity of inter-particle movements relative to the average deformation, the diversity of this non-conformity, its evolution during loading, and the spatial coherence of the non-conformity. In this regard, we consider only those particles that are included in the particle graph at a particular stage of loading. The relative velocity $\hat{\nu}^j$ of two particles $k_1$ and $k_2$ is the difference in their velocities

$$\hat{\nu}^j = \nu^{k_2} - \nu^{k_1},$$  \hspace{1cm} (11)
where index \( j \) represents the contacting pair \((k_1, k_2)\). The relative movement that would be consistent with homogeneous deformation is the product \( \mathbf{L} \mathbf{v} \), where \( \mathbf{L} \) is the average velocity gradient of the assembly, and \( \mathbf{v} \) is the branch vector between the centers of particles \( k_1 \) and \( k_2 \) (Table 3).

The quantities in Eqs. (31) can be applied to describe the conformity (or non-conformity) and diversity of the local, inter-particle movements \( \mathbf{v} \) with respect to the mean-field displacement \( \mathbf{L} \mathbf{v} \). We begin by considering only pairs of particles that are in direct contact during biaxial compression (the number of these pairs ranges from 17,600 to 21,300 for the 10,816 particles), although we will consider more distant pairs in a later paragraph.

The evolution of measures (31) are shown in Fig. 5. The average inter-particle motions \( \mathbf{v} \) are consistently less than the mean-field motions, as is shown by a mean conformity \( \text{Mean}(\mathbf{v} \parallel \mathbf{L} \mathbf{v}) \) less than 1. This result is consistent with studies [39] and [42], which investigated the local behavior at small strains. Figure 5 shows that the mean conformity, \( \text{Mean}(\mathbf{v} \parallel \mathbf{L} \mathbf{v}) \), is modestly reduced during loading, from about 0.91 to about 0.82. As we will see, however, the diversity of the fluctuations can be quite large. Both the non-conformity and heterogeneity of inter-particle motions are indicated by the additional measures \( \text{Mean}(\mathbf{v} \perp \mathbf{L} \mathbf{v}) \) and \( \text{Mean}(\mathbf{v} \circ \mathbf{L} \mathbf{v}) \). If the local motions were in uniform conformance with the assembly deformation, these two measures would have values of 0 and 1 respectively. At large strains, the value of \( \text{Mean}(\mathbf{v} \perp \mathbf{L} \mathbf{v}) \) approaches 2, compared with a value of \( \text{Mean}(\mathbf{v} \parallel \mathbf{L} \mathbf{v}) \) of about 0.82. These results reveal that, on average and at large strains, the components of inter-particle movements that are orthogonal to their mean-field directions can be more than twice as large as the components that are aligned with the mean-field directions (Eqs. 3 and 4). This lack of vector alignment is also indicated by the cosine-type measure \( \text{Mean}(\mathbf{v} \circ \mathbf{L} \mathbf{v}) \), which is reduced to a value of about 0.15 (see Eq. 5). At the end of the test, fully 40\% of inter-particle motions were in the “wrong” direction, with values \( \mathbf{v} \cdot (\mathbf{L} \mathbf{v}) < 0 \). The fourth measure in Fig. 5 is \( \text{Std}((\mathbf{v} \parallel \mathbf{L} \mathbf{v})) \), which displays a rather extreme degree of nonuniformity in the components of inter-particle movements that are parallel to the mean-field movements. This nonuniformity is particularly sizable at large strains. A set of random vectors of uniform length would have a value of \( \text{Std}(\mathbf{v} \parallel \mathbf{L} \mathbf{v}) \) of only 0.5 (Table 3), a value several times smaller than those in Fig. 5. Such large values indicate a substantial heterogeneity in both the magnitudes and directions of the inter-particle movements \( \mathbf{v} \).

We can also use the biaxial compression simulation to investigate the spatial correlation of inter-particle movements and the length scale at which the inter-particle movements approximate the mean deformation field. Kruyt and Rothenburg [39] measured the spatial correlation of movements at small strains by using a 2-point correlation technique. In the current study, we do not consider all possible particle pairs, but instead use only those pairs of particles that are included in (attached to) the particle graph, as only these particles participate directly in the deformation and load-bearing mechanisms. This limitation suggests a discrete metric \( \rho \) for describing the distance between two particles \( k_1 \) and \( k_2 \). The distance \( \rho(k_1, k_2) \) is the least number of contacts (graph edges) that must be traversed to connect \( k_1 \) and \( k_2 \) (Fig. 6). The results in Fig. 5, which have already been described, were collected from the sets of all particle pairs at a discrete distance of 1, i.e. the sets \( \{(k_1, k_2): \rho(k_1, k_2) = 1\} \) at various stages of loading. The discrete metric does not provide angle or size, so all subsequent calculations with the objects \( \mathbf{v} \), \( \mathbf{L} \), and \( \rho \) were, of course, performed in Euclidean space, but only on the selected particle pairs.

Figure 6 shows the non-conformity and heterogeneity of inter-particle movements \( \mathbf{v} \) for particle pairs \( j \) at distances \( \rho \) of 1 to 10, but at the single large strain \( \overline{\varepsilon}_{22} = -0.005 \) (see Fig. 7). (The results for \( \rho = 10 \) involve over one-quarter million particle pairs.) As would be expected, the average conformity of the observed inter-particle movements with their corresponding mean-strain movements improves with an increasing discrete distance between the pairs. This improved conformity is evidenced by increases in the measures \( \text{Mean}(\mathbf{v} \parallel \mathbf{L} \mathbf{v}) \) and \( \text{Mean}(\mathbf{v} \circ \mathbf{L} \mathbf{v}) \) and in the reduction of \( \text{Mean}(\mathbf{v} \perp \mathbf{L} \mathbf{v}) \). However, at a distance of \( \rho = 10 \) and at the strain \( \overline{\varepsilon}_{22} = -0.005 \), the values of these three measures are about the same as those at distance \( \rho = 1 \) with zero strain, \( \overline{\varepsilon}_{22} \approx 0 \). That is, at the large strain of \(-0.005\), the non-conformity of motion at a dis-
and 3, at the large strain

\( \rho \) are in direct contact (i.e. with

only the

particles at small strains.

The conformity between the actual and mean-field motions is, on average, much closer conformity than the mean-field approach up the unit vector aligned with

the local deformations are, on average, far more deviant

of 1 and 3. The

standard deviation of the aligned deformations,

\( \tau_{22} = -0.005 \) (see Fig. 4). The results have been normalized by dividing by the average length \( \ell = \langle |\mathbf{V}\rangle \rangle \) for a particular separation \( \rho \) and by the strain rate \( \dot{\varepsilon}_{22} \). Figure 8 shows that, at large strains, the movements of contacting particles (\( \rho = 1 \)) are predominantly tangential, and that the mean normal motion is quite small. That is, at \( \rho = 1 \) and at large strains, the normal inter-particle movements are grossly overestimated by the mean-field motion \( \mathbf{L} \mathbf{V} \). At a distance \( \rho = 3 \), the motions are, on average, in much closer conformity with those predicted by a mean-field assumption. The apparent conformity at \( \rho = 3 \) in Fig. 8 is, however, based upon an average of movements, and the true diversity in their values is more appropriately reflected in the measures \( \text{Mean}(\mathbf{V}^\perp \mathbf{L}^i \mathbf{V}) \), \( \text{Mean}(\mathbf{V}^\parallel \mathbf{L}^i \mathbf{V}) \), and \( \text{Std}(\mathbf{V}^\parallel \mathbf{L}^i \mathbf{V}) \), which are reported in Figs. 5 and 7.

### 4.4 Deformation heterogeneity

Micro-scale deformations within a 2D granular material can be computed by considering the small polygonal void cells as being representative micro-regions among particle clusters (Fig. 2). The region of 10,816 particles can be partitioned into over 7500 of these void cells. The average velocity gradient \( \mathbf{L}^i \) within a single polygonal void cell \( i \) is computed from the motions of the particles at its vertices. These local velocity gradients can then be compared with the average assembly gradient \( \mathbf{L} \), and the measures in Eqs. 5–7 can be used to investigate the non-conformity and heterogeneity of local deformations. Figure 10 shows the evolution of these measures in the course of a biaxial compression test. At small strains, the local deformations are modestly aligned with the averaged deformation: the average cosine of alignment, \( \text{Mean}(\mathbf{L}^i \cdot \mathbf{L}) \), is 0.91, only slightly lower than 1, and the average component of the local gradient \( \mathbf{L}^i \) that is perpendicular to the assembly average \( \mathbf{L} \) is about 35% of \( \mathbf{L} \). At larger strains, the local deformations are, on average, far more deviant and exhibit a much larger dispersion of values. The standard deviation of the aligned deformations, \( \text{Mean}(\mathbf{L}^i \cdot \mathbf{L}) \), becomes more than twice its mean value of 1. Deformations that are orthogonal to \( \mathbf{L} \) become, on average, much larger than those parallel to \( \mathbf{L} \) (compare the \( \text{Mean}(\mathbf{L}^i \perp \mathbf{L}) \) in Fig. 10 with a \( \text{Mean}(\mathbf{L}^i \perp \mathbf{L}) \) of 1).

This non-conformity and heterogeneity is also illustrated in Fig. 11 which shows the distributions of aligned deformations at moderate and large compressive strains, \( \tau_{22} \) of \(-0.0005\) and \(-0.005\). In each figure, the void cells
Fig. 10. The evolution of deformation non-conformity and heterogeneity during biaxial compression. Each point represents the deformations $L_i$ in over 7500 void cells, where superscript $i$ represents an $i$th void cell.

Fig. 11. Distributions of the aligned deformation of void cells at two strains. The void cells have been grouped according to a ranking of their $L_i \parallel \bar{L}$ values (10,900 and 8300 void cells are included at the two strains).

Fig. 12. The presence of right-shear microbands at strain $\varepsilon_{22} = -0.0005$. The local void cell deformations $L_i$ have been filtered as $L_i \Phi$, where the filter $\Phi = [0.49 \ 0.41; -0.58 \ -0.49]$ captures a deformation mode that produces shearing that is downward and to the right. A complementary set of left-shear microbands would be present with the use of an alternative filter. The gray scale illustrates the magnitudes of the local filtered deformations, but some of the white regions have negative filtered values in this monochrome plot.

have been placed into 20 bins, arranged according to a ranking of the aligned deformations $L_i \parallel \bar{L}$ of each, $i$th void cell. At moderate strains, the 10% of most contributory void cells participate disproportionately in the average assembly deformation and about 6.5 times more than the lowest 10% of void cells (Fig. 11a). At the larger strain of $-0.005$, about 22% of the material makes a negative contribution to the overall assembly deformation, and, in a sense, is deforming in the “wrong” direction (Fig. 11b). As another measure of this heterogeneity at large strain, the 31% of most contributory void cells could account, by themselves, for the entire assembly deformation. This situation is akin to that of a material in which a shear band has developed, where intense shearing within the band is accompanied by unloading outside of the band. No shear bands were observed in the current simulations, although another type of localization, in the form of multiple non-persistent micro-bands, was present throughout the biaxial compression test. This type of deformation patterning, described in [9], was subtly present at the start of deformation and became more pronounced as deformation proceeded. Microband localization accounts for much of the deformation heterogeneity that is recorded in Figs. 10 and 11. An example of micro-band patterning at small strain is shown in Fig. 12 in which the local, void cell deformations $L_i$ have been filtered to highlight a right-shear deformation mode (see [9] for a discussion of the visualization technique).
Particle spins in a biaxial compression test at strain $\tau_{22} = -0.0005$. Only clockwise spinning particles are shown in the plot.

### 4.5 Particle rotation heterogeneity

Particle rotations in granular materials are known to be large, particularly in 2D assemblies of circular disks. Decker et al. [44] found that the standard deviation of the particle rotation rates could be several times larger than the average strain rate of an assembly. Calvetti et al. [30] reported that the variability of particle rotations increased consistently with increasing strain. Figure 13 shows that the average assembly stress, we instead use the (solid) disk area $\pi r^2$ and simply divide it by the assembly-average solid fraction.

**Fig. 13.** Particle spins in a biaxial compression test at strain $\tau_{22} = -0.0005$. Only clockwise spinning particles are shown in the plot.

**Fig. 14.** The evolution of stress non-conformity and heterogeneity during biaxial compression.

4.6 Stress heterogeneity

The transmission of force among particles occurs in a non-uniform manner, with certain chains of particles bearing a disproportionate share of the surface tractions. These force chains have been widely observed, and several related references are given in Table 1. The current study concerns the distribution of stress among an assembly's particles. In two previous studies, the local variation of stress within stacks of rods has been studied by withdrawing groups of rods and measuring the removal force [58]. The DEM simulations of the current study allow the direct computation of stress $\sigma^k$ within each, $k$th disk:

$$\sigma^k_{pq} = \frac{\sigma^k}{A^k} \sum_{j=1}^{n^k} \eta^k_j f^k_j,$$

where summation is over the $n^k$ contacts $j$ of the particle $k$, $r^k$ is the disk radius, $\eta^k_j$ is the unit normal vector, and $P^j$ is the contact force. Satake [64] and Kruyt and Rothenburg [39] have described a dual of the particle graph that could be used to compute a representative particle area $A^k$ that includes a portion of the void space around a particle.

**Fig. 14.** The evolution of stress non-conformity and heterogeneity during biaxial compression.

The variation in stress is greatest in its deviatoric component. Figures 15a and 15b, are histograms of the local mean stress and deviator stress, defined for particle $k$ as $p^k = (\sigma^k_{11} + \sigma^k_{22})/2$ and $q^k = (\sigma^k_{22} - \sigma^k_{11})/2$ respectively. The figure gives these components at the large strain $\tau_{22} = -0.005$. Because only compressive force can be delivered between particles, the local mean stress is uniformly positive, but the standard deviation of the local mean stress $p^k$ is about 0.60 (Fig. 15a). The standard deviation of the local deviator stress $q^k$ is 1.0 (Fig. 15b).
Large strain are compiled from the stresses in over 10,000 particles at the participation in the mean and deviator stresses. Both figures are histograms of the local participation of the local stress in the average assembly stress. Figures 15a and 15b are histograms of the local deviator stress, \( q^{k} \parallel \bar{q} \), and these particles provide a negative contribution toward bearing the average assembly deviator stress.

About 15% of particles have a negative alignment of the deviator stress, \( q^{k} \parallel \bar{q} \), and these particles provide a negative contribution toward bearing the average assembly deviator stress.

**5 Conclusion**

In the paper, we have considered several categories of heterogeneity in granular materials: topologic, geometric, kinematic, and static. In all respects, the heterogeneity can be described, at a minimum, as being moderate. Heterogeneity increases during biaxial compressive loading. In the case of inter-particle movements, the non-uniformity becomes extreme, and particle motions are only coarsely aligned with the mean-field movement. At large strains, significant fluctuations from the mean-field motion extend to distances of at least eight particle diameters. Non-uniform motion is expressed in the patterning of local movements, which includes microband patterning and rotation chain patterning. The extent and magnitude of the heterogeneity and its patterning proffer an imposing challenge to the continuum representation of granular materials at micro and macro scales, especially at large strains. Before such efforts can be productive, further statistical analyses should be undertaken to further characterize heterogeneity, to determine characteristic lengths at which heterogeneity dominates the meso-scale behavior, to quantify the heterogeneity in the local stress rates, and to establish the relationships among topologic, geometric, kinematic, and static heterogeneities.

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