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Linking shape and rotation of grains during triaxial compression of sand

Riccardo Rorato, Dr.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering.

riccardo.rorato@upc.edu

ORCID ID: 0000-0002-4189-3058

UPC - Barcelonatech

Moduli D2 Campus Nord UPC – Office 212

C Jordi Girona 1-3

Barcelona 08034

Marcos Arroyo Alvarez de Toledo, Prof.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering

marcos.arroyo@upc.edu

ORCID ID: 0000-0001-9384-9107

Edward Carlo Giorgio Andò, Prof.

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000 Grenoble (France)

edward.ando@3sr-grenoble.fr

ORCID ID: 0000-0001-5509-5287

Antonio Gens, Prof.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering

antonio.gens@upc.edu

ORCID ID: 0000-0001-7588-7054

Gioacchino Viggiani, Prof.

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000 Grenoble (France)

cino.viggiani@3sr-grenoble.fr

ORCID ID: 0000-0002-2609-6077

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Abstract

Particle shape has a strong effect on the mechanical response of coarse soils. This has been usually observed examining specimen-scale or engineering-scale responses, which are the sum of many microscale interactions. In this work we observe the effects of particle shape directly at the microscale level. X-ray tomography (μ -CT) of two sand specimens is exploited to measure three-dimensional particle shape descriptors but also to track individual particle motions during triaxial compression. The systematic use of a discrete *Digital Volume Correlation* (DVC) algorithm allows the systematic tracking of individual grains (around 50000 for each sand specimen) during the test and measure, with good precision, their cumulated displacements and rotations. The specimens examined failed in a clearly localised shear mode. Advantage is taken of this to obtain data relevant for very different kinematical regimes: one quasi-static and the other close to critical state. A direct comparison between the shape and kinematic databases shows to what degree particle shape descriptors are related to observed kinematics. It appears that true sphericity is a good predictor of upper bound rotational restraint.

Keywords: Laboratory equipment; Microscopy; Particle-scale behaviour; Sands; Shear strength; Statistical analysis.

1 Introduction

Granular soils are made of discrete particles that interact with each other, therefore changes at the small-scale (*i.e.*, grain-scale) affect the material response at the large-scale (*i.e.*, engineering-scale) [1–3]. For granular soils, for instance, it is well-documented that

particle shape strongly affects soil properties such as extreme void ratios [4, 5], critical state friction [6] or dilatancy and peak friction [7], as well as engineering scale responses, like liquefaction resistance [8] or cone tip resistance [9].

It follows that particle shape must affect grain-scale interactions to produce those effects. This hypothesis has been repeatedly supported, from various perspectives, by the results of numerical simulation. In numerous discrete element models direct control of element shape has been shown to result in major changes in ensemble mechanical responses [10–15].

It is noteworthy, however, that similar macroscopic effects are observed when particle shape effects are represented indirectly, through appropriately modified element contact interaction laws, for instance introducing some resistance against rolling at the contact [16–19]. Both direct and indirect shape modelling strategies inevitably involve some degree of simplification, to be adjusted in applications under typically conflicting constraints of computational speed, accuracy and ease of calibration [20].

In this context, direct experimental observation of the microscale effects of particle shape appears relevant, as it may provide evidence beyond that implicit in the ensemble behaviour of the specimen. This has been a relatively unexplored avenue, because it requires relevant and accurately measured shape descriptors, as well as particle-scale resolution of internal mechanisms. There are few experimental techniques useful for that purpose [21] and the main one is relatively recent: microfocus or x-rays μ -tomography [22–25].

Despite significant difficulties, progress in 3D tomographic imaging and post-processing technologies [26–30], has made accurate grain shape determination feasible for most sands. Identification of particle-scale mechanisms is more difficult, as it requires imaging not just isolated particles, but particles in collective interaction, within specimens. Particles need to be separated from one another, within the imaged ensemble. Ideally, the existing contacts amongst particles need to be identified, as interactions between particles occur through contact forces in coarse soils. Single snapshots of microstructures (typically acquired “post-mortem”, after dismounting the test [22, 25, 31]) cannot reveal kinematics. For that purpose a sequence of images needs to be acquired during a test, and triaxial tests have been the target for most of this kind of work [32–36]. Clearly, one added difficulty here is the need to track particles confidently across different images. Progress in these tasks has been also very significant, but there are still some important obstacles, particularly in the area of contact detection and measurement. Indeed, the level of image resolution required to image particle contacts – and contact properties such as orientation – appears far more demanding than that required to image, identify and measure particles [37–39]. This has implicitly limited the scope (number of tracked particles and/or number of imaged test steps) of kinematic contact fabric imaging studies [33, 40–42].

Current technology may be exploited to obtain more statistically sound results if the focus is restricted to particle kinematics. This is the avenue explored in this work, in which we examine in detail the relations between individual grain shape and individual kinematical history of sand grains as observed during triaxial compression of two dense sand specimens that jointly provide a database of 110000 grains. For the purposes of this

study, the specimens selected for examination had the advantage of failing in sharply localised shear modes. As clearly identified in previous research [22, 24, 25] the structure and kinematics of particles within a shear band are very different from those outside, as particles in a shear band approach critical state conditions. As long as a criterion for belonging or not into the shear band could be clearly established, this experimental feature ensured that the influence of particle shape could be examined in two very different and separate kinematic settings (*i.e.*, within the band and outside it), thus making the study relevant for a larger set of conditions. In what follows, we first give some background on particle tracking and shape description terminology. We then describe the test and image analysis procedures employed and the results obtained before presenting some conclusions.

2 Background

2.1 Digital image correlation for quantifying particle kinematics

Digital Image Correlation (DIC) is the ideal tool for comparing and analysing images of deforming materials, such the ones obtained from x-ray scans. DIC is a widely used technique in experimental mechanics to deduce motion and shape features of an object by comparing its appearance in different images [43]. A first classification of DIC may be based on the dimensional support of the images employed in the comparison [44]: surface-DIC is based on bi-dimensional images, whereas volumetric DIC (or, simply, digital volume correlation, DVC), is based on three-dimensional images. Surface-DIC is widely

employed in field and laboratory experimental geotechnics [45]. DVC has seen fewer applications because of the increased difficulties associated with 3D image acquisition. In DIC a subset F of intensity values from a reference image is systematically compared with subsets G_i of the transformed image until some optimality condition is achieved [46]. This optimality condition is frequently based on a cross correlation measure, for instance searching for a maximum normalised cross correlation:

$$NCC = \frac{F * G_i}{\|F\| \|G_i\|}$$

Different algorithms are obtained depending on how the subset F is chosen, what kind of motion is assumed to relate F and G_i and how the search window (SW, the zone in which G_i is searched for) is defined.

Two broad variants of DVC have been employed in geotechnical applications: *continuum* (C-DVC) and *discrete* (D-DVC). In C-DVC, the subset F (usually referred to as correlation window, CW) is a cubical cell centred around some pre-established evaluation grid points. Although more complex transformations are sometimes used [47], the motion relating F and G is usually assumed as a simple rigid translation, and cross correlation is employed to find a displacement vector, which is assigned to the grid node. From the displacement field thus obtained, strain measures are derived using different procedures [48]. The underlying assumption is that subset F is a representative volume element RVE in a continuum; therefore, the scale of the CW should contain enough grains to make that assumption realistic.

C-DVC is not well adapted to identify particle kinematics. When the resolution of the images is such that individual grains may be identified, other alternatives are possible.

Hall et al. [24] proposed a novel discrete *grain-based* approach (D-DVC) to track individual particles. The method has as a starting point a *segmented* labelled image, in which groups of voxels are identified as grains. In D-DVC the subset F is selected considering which voxels have been previously assigned to a certain grain and is named a grain mask. The assumed motion between F and G is a rigid body motion, including translation and rotation. With D-DVC the kinematics of each identified particle is thus directly obtained. Hall et al. [24] went on to illustrate the potential of D-DVC obtaining maps of incremental displacements and rotations in a triaxial specimen of Hostun sand, showing also that the kinematic history of single grains was very different if they were involved in a shear band or not.

Andò et al. [32] proposed an alternative method to follow grain kinematics across images, called ID-track. In this method grain match between successive images is based on listed properties of grains, such as volume, surface area, etc. obtained through single-image analysis. The method requires two segmented images as input. The grain matching operation is faster than in D-DVC, as volume cross-correlation is not needed. With some modifications, ID-track has been later used by Alshibli et al. [35] and Cheng & Wang [36], amongst others. However, ID-track has some difficulties to assign precise rotation values, particularly when dealing with very spherical particles [32], and was therefore extended to include a D-DVC based technique for rotation measurement in Andò et al. [49]. For this reason, the work presented here was based on the more robust, if slower, D-DVC technique.

2.2 Particle shape description

There are different approaches to describe the shape of soil grains and, as a result, many different shape descriptors are currently in use. Table 1 summarises the 3D shape descriptors that are employed in this work whereas Table 2 lists the fundamental measures from which the shape descriptors are derived. Several shape descriptors try to measure particle similitude with a sphere (*i.e.*, sphericity), *i.e.*, the historical proposal of Wadell [50], called *true sphericity*, but also the *convexity* and *operational sphericity* descriptors. We also use some shape descriptors that are more relevant to particle *form* [51] such as *flatness index*, *elongation index* and – despite its name – *intercept sphericity*. Rorato et al. [26] present a detailed study of the relationships amongst these and other 3D and 2D shape descriptors.

Name	Symbol	Definition	Reference
<i>True Sphericity</i>	Ψ	$\frac{S_n}{S}$	[50]
<i>Flatness index</i>	FI	c/b	[52]
<i>Elongation index</i>	EI	b/a	[52]
<i>Intercept sphericity</i>	Ψ_{int}	$\sqrt[3]{\frac{bc}{a^2}} = \sqrt[3]{FI(EI)^2}$	[53]
<i>Operational Sphericity</i>	Ψ_{op}	$\sqrt[3]{\frac{V}{V_{cm}}} = \frac{D_n}{D_{cm}} \approx \frac{D_n}{a}$	[53]
<i>Convexity</i>	Co	V/V_{CH}	[30]

Table 1: Selected 3D shape descriptors [26]

Shape property	Symbol	Equivalent diameter
<i>Volume</i>	V	D_n
<i>Surface area</i>	S	

Shape property	Symbol	Equivalent diameter
<i>Surface area of the equivalent sphere (same volume)</i>	S_n	
<i>Maximum, intermediate, minimum lengths</i>	a, b, c	
<i>Convex hull volume</i>	V_{CH}	D_{CH}
<i>Volume of the maximum inscribed sphere</i>	V_{iM}	D_{iM}
<i>Volume of the minimum circumscribing sphere</i>	V_{cm}	D_{cm}

Table 2: Fundamental measures from which 3D shape descriptors are derived [26]

3 Methodology

3.1 Data acquisition

This study analyses data obtained at Laboratoire 3SR (Grenoble, France) from two sand triaxial specimens, approximately 10mm diameter and 20mm height [54]. Both specimens were prepared by dry pluviation and then subject to triaxial compression under 100kPa of confining pressure. The triaxial tests were performed “in-camera” within the x-ray scanner at Laboratoire 3SR. Results from two sand specimens that cover a wide range of particle sphericity values were selected.

The first specimen (HNEA01) was formed with Hostun HN31 sand at relative density of 83.2% (dry density value, γ_d , equal to $1.60g/cm^3$). Hostun is a quartz quarry sand whose grains appear very irregular, see Figure 1a. The grain size distribution, Figure 1c, is very narrow ($C_U = 1.41$), with a D50 equal to $338 \mu m$. The second specimen analysed (COEA04) was formed with Caicos ooids ($\gamma_d = 1.76g/cm^2$, minimum and maximum

density not recorded). This sand is a natural sand made of calcium carbonate (CaCO_3) minerals. Ooids are formed by slow chemical accretion and have a very round shape (Figure 1b). The grain size distribution (Figure 1c) is close to that of HNEA01, being also poorly graded ($C_U = 1.39$) with a D50 of $420 \mu\text{m}$.

Figure 1a-b-c: (a) Horizontal section of the scanned Hostun (a) and Caicos (b) specimens. (c) Grain Size Distribution of both sands from sieving [54]

The specimens were scanned by x-rays at several loading stages during the test (16 for test HNEA01 and 11 for COEA04). The stress-volumetric-strain curves, with indication of scanning stages are shown in Figure 2. The macroscopic responses of both specimens are typical of dense sands, with a stress peak followed by shearing at overall constant volume. Both specimens failed in a localized shear mode: Andò [32] verified that within

the shear zone constant volume was also attained (at different porosity than the overall value, see also [55]).

Figure 2: Triaxial responses of the specimens HNEA01 and COEA04 with loading stages markers. The yellow stripes indicate loading stages that are later investigated in more detail.

The pixel size selected to image the sand specimens was $15.56 \mu\text{m}/\text{px}$, to maintain a field of view of approximately $30.5 \text{ mm} \times 23.0 \text{ mm}$. For the specimens analysed, this results in about 22/26 pixels across a grain. Further details of these tests, including the scanning equipment and tomographic image acquisition procedures have been presented elsewhere [54, 56].

3.2 Single-image post-processing

The reconstruction of each x-ray scan results simply in a 3D distribution of grey-scale values which represents the frequency-lumped x-ray attenuation coefficient measured in that location. Therefore, before studying individual grains, it is necessary to *binarise*,

235 *separate* and *label* the tomographic images. The procedures applied here for these tasks
 236 are described by Andò [32]. At this point, it is possible to extract single grains from the
 237 3D labelled images. The 3D tomographic images representing Hostun (specimen
 238 HNEA01) and Caicos (specimen COEA04) sands contain respectively 48612 and 65056
 239 particles.
 240
 241 Geometrical properties (e.g. volume, surface area, inertia tensor...) of the image subset
 242 assigned to each grain are obtained through subsequent post-processing. These proper-
 243 ties may be used, in turn, to obtain different shape descriptors in 3D or 2D. The proce-
 244 dures applied for this purpose are described in detail by Rorato et al. [26]; who also pre-
 245 sented an exhaustive database of 3D shape descriptors for all the grains in this speci-
 246 mens, evaluating significant statistics. It is worth mentioning that surface area measure-
 247 ments for grains were obtained using a Marching Cubes algorithm [57], to ensure preci-
 248 sion in the evaluation of Wadell true sphericity values. Rorato [26] also verified that there
 249 were no significant shape changes during the triaxial tests.

250 **3.3 Tracking grain kinematics with D-DVC**

251 The D-DVC software that has been used in this work to obtain the grains kinematics (3D
 252 displacements and rotations) is the TomoWarp2 code [58]. In this code, grain displace-
 253 ments are expressed in pixels (the pixel-size is fixed) and 3D rotations as *rotation vectors*
 254 using a Rodrigues parametrisation [59]. In a rotation vector, the components represent
 255 the direction of the axis of rotation and the norm the magnitude of the angle of rotation

around that axis. This representation system for rigid body rotations has practical advantages over more complex alternatives, such as those based on Euler angles or quaternions [59].

To visualize the 3D unit rotation vector orientation, stereographic projection is sometimes used below. The angular coordinates used in this projection are illustrated in Figure 3. The angle θ (inclination) goes from 0° (vertical) to 90° (horizontal), while the angle φ (azimuth) goes from 0° to 360° , being the north ($\varphi=0^\circ$) the direction of the Cartesian x-axis of the specimen. Stereograms were created using the plotting tool “*orientationPlotter*” from the external open-source Python package SPAM [60].

Figure 3: Spherical coordinates system adopted for the stereoplots

Previous applications of D-DVC had focused mostly on incremental grain kinematics [24, 32]. In such approach only the incremental kinematics between two subsequent loading steps (e.g. 1-2, 2-3, 3-4, etc...) were obtained. The starting point are the two 3D greyscale images bracketing the increment (*i.e.*, initial and deformed configurations); of these two the image corresponding to the initial configuration has to be already labelled, so that grain bounding-boxes that are used as correlation windows can be extracted. This incremental or “tangent” correlation approach cannot be applied sequentially to obtain cumulative kinematics of the grains. The reason is that grain labels assigned to

the same grains by processing different scans of the same specimen will be different. To ensure consistency, a single set of grain labels, obtained from the first scan, is required. The method used here to get the history of grain displacements and rotations is based on “secant” correlation (usually referred to as “leapfrog” in C-DVC applications). In this approach, the initial labelled image is always selected for paired searches on those resulting from all the subsequent scans (*i.e.*, 1-2, 1-3, 1-4, etc...). A direct secant approach has clear limitations, being both very expensive (as the grain search window would have to increase during the process) and prone to errors. The algorithm applied here aims to overcome those difficulties using a mixed approach, in which a secant correlation scheme (1-2, 1-3, ... , 1-10) is still employed, but the search is aided by the results of the previous steps, namely the cumulative grains displacement up to the last correlation step. The initial search window is translated by a vector pointing the position of the grain in the previous correlation and can remain of a small size, saving calculation time. The inputs required in this procedure are four: two greyscale images, one labelled image and one data file with the prior grain displacements. Since initial rotations are not taken into account, for large deformations where there are large rotations, the possibility of losing grains still remains.

3.4 Validation of the D-DIC procedure

To validate the implementation of D-DVC in TomoWarp2 a simple uniform rotation check was employed [32, 61]. The rotations of all the grains contained in specimen HNEA01 were individually computed after applying a five degrees (5° *deg*) rigid rota-

tion around its vertical z-axis. The main objectives of the validation are three: (a) to evaluate the attrition rate of the algorithm (*i.e.*, the number of grains that are lost from one image to the next); (b) to evaluate the accuracy and precision with which grain rotation was measured and (c) to explore the possible relationship between the precision of the calculation and the shape of the grains (as grains masks are used as correlation windows, there is some expectation that grains closer to spherical will present a greater deviation from the imposed motion).

The check was positive from the attrition viewpoint, with more than 99.8% of the grains correctly tracked attaining a correlation coefficient between the two image subsets greater than 0.99 for each of them. Figure 4a shows the histogram of the rotations measured by D-DVC. The rotation measurements follow a normal distribution with a mean value of $4.998^{\circ}deg$ and $0.042^{\circ}deg$ standard deviation. Rotations as obtained by this code are as accurate (*i.e.*, have similar mean error), but far more precise (*i.e.*, have much smaller error standard deviation), than those obtained with the ID-track implemented by Andò [32]. Indeed, the coefficient of variation (standard deviation / mean) of measurement error is here below 1%, while it was above 400% for ID-track. Another way of conveying this information is by means of a stereogram of the computed grain rotations (Figure 4b). The radial distance from the centre of the stereoplot represents the inclination θ , whereas the angles on the external perimeter represent the azimuth φ . As expected, all the grain rotations are located at the centre of the stereoplot ($\theta = 0^{\circ}$), indicating rotations around the vertical axis, with very low deviation from the vertical. Finally, Figure 4c illustrates the relation between measured rotation and sphericity; it is clear that

the deviation from the exact solution (5° deg) increases symmetrically with the sphericity of the grains. However, the deviation remains very limited (around $\pm 0.1^\circ \text{ deg}$) and, therefore, this inbuilt bias can be safely ignored.

(a)

(b)

Figure 4a-b-c: (a) Histogram of measured rotation after rigid rotation of the specimen (b) Stereoplot showing the rotation vector of each grain (c) 2D histogram showing the correlation between grains sphericity and grains rotation.

3.5 Shear band identification

The two specimens analysed in this work showed localised deformation through shear banding [54]. In shear bands void ratio increases, coordination numbers are much reduced and the microstructural constraints on kinematics are therefore very different. Before examining the relation between grain shape and grain kinematics it was therefore necessary to first classify the grains, separating those that belonged to the shear band and those that did not. The criterion applied here to classify the grains as belonging to the shear band was based on shear strain.

To assign a nominal deviatoric strain to each grain we applied a procedure developed for DEM post-processing by Catalano et al. [62]. In this procedure, available within the code YADE [63], a Voronoi cell hosting each grain is created using a regular Delaunay triangulation having as vertices the mass centres of the labelled grains. Thus, the grain

position at the last loading increments (*i.e.*, 15-16 for HNEA01, 10-11 for COEA04) were calculated by D-DVC and then introduced in YADE. Displacements of neighbouring grains were then used to compute a nominal displacement gradient tensor for the tetrahedrons whose vertices are the grains centres of mass. A nominal averaged deviatoric strain, ε_{d_g} was projected back to each grain and a threshold value of ε_{d_g} was used to classify the grains that belonged to the shear band.

4 Results

4.1 Shear band identification

The results of the shear band identification procedure are shown in Figure 5, in which the black grains form the “shear band”: it contains 7007 grains for COEA04, and 21000 for HNEA01. The threshold value ε_{d_g} is set at 0.10; the zones identified correspond closely to those apparent in previous studies [54]. A sensitivity study to evaluate of the effect of varying this threshold value was carried out, very little changes were observed for values within the range 0.05 – 0.20.

The local reference system that will be used to define the virtual plane representing the shear band is shown in Figure 6, in which vector $\vec{n}$ is the normal to the plane and vector $\vec{a}$ indicates the steepest slope direction in the plane. According to Figure 3, showing the spherical coordinates system, both specimens present a shear band with an inclination angle (θ) of about 45°.

Figure 5: Shear band identification for specimens COEA04 (a) and HNEA01 (b). Particles are coloured black if the “micro-strain” [62] calculated on the Voronoi domain centred on the particle is greater than 0.10 (i.e., they belong to the shear band).

Figure 6: Local reference system for the shear band

Vector $\vec{b}$ is orthogonal to $\vec{n}$ and $\vec{a}$ and therefore is horizontal ($\theta = 90^\circ$). It can be used to characterise the azimuthal orientation of the shear band with respect to the global Cartesian coordinates system. The azimuth (φ) is different, being of about 135° for Hostun and 75° (from the global x -axis) for Caicos. The sections represented in Figure 5 correspond then to vertical planes orthogonal to vector $\vec{b}$.

4.2 Spatial distribution of grain shapes and shear localisation

A check was performed to verify if particle shape was spatially homogeneously distributed in the specimens. The reason was to exclude any possibility that subsequent localisation into shear bands was prompted by non-uniformity in the initial spatial distribution of grain shapes (note that a similar check was performed by Andò [54] with respect to local porosity). To do so, two vertical sections orthogonal to each other (defined respectively by vectors $\vec{n}-\vec{b}$ and $\vec{n}-\vec{a}$) are examined where the grains have been coloured by their value of degree of true sphericity, as shown in Figure 7. It is evident that grain true sphericity was initially homogeneously distributed within both specimens.

Figure 7: Sphericity spatial distribution for Hostun and Caicos sand in two vertical sections: parallel and perpendicular to the shear band.

Another check was performed on the possibility that shear banding would entrap or select particular grain shapes. To this end, histograms of the degree of true sphericity for the grains located both inside and outside the shear band were plotted; the results are shown in Figure 8. Again, it is evident that there are no significant differences of shape between the grains that were involved in the localisation process and those that remained outside the shear band.

Hostun
HNEA01

(a)

Caicos
COEA04

(b)

Figure 8: Histograms of true sphericity for Hostun (a) and Caicos (b) sands both inside and outside the shear bands.

4.3 Overall grain kinematics

Figure 9 and Figure 10 show the *cumulative* kinematic histories, in terms of vertical displacements and rotations, for Caicos ooids (specimen COEA04) and Hostun sand (specimen HNEA01) during several loading increments in the triaxial test (note that similar images, but reporting *incremental* instead of *cumulative* values were presented by Andò [32]. Results for both sands are plotted at the same scale and confirm the general observation made from incremental results by Andò [32]: within the shear band, the very rounded Caicos sand grains rotate more than the more angular grains of Hostun sand. On the other hand, it is difficult to tell the difference between the two sands outside the shear band.

Figure 9: Vertical slices of Caicos sand (specimen COEA04) showing grain vertical displacement (above) and rotation (below) *accumulated* during the test. Grains are coloured by the value of their measured z-

displacement (above) and total rotation (below). Not all the increments are shown. Stage “01” = start of deviatoric loading. Stage “11” = end of the TX test.

Figure 10: Vertical slices of Hostun sand (specimen HNEA01) showing grain vertical displacement (above) and rotation (below) **accumulated** during the test. Grains are coloured by the value of their measured z-displacement (above) and total rotation (below). Not all the increments are shown. Stage “01” = start of deviatoric loading. Stage “16” = end of the TX test.

This observation is conveyed more precisely in Figure 11, showing the histories of the cumulated mean particle rotation magnitudes, both inside and outside the shear bands. Outside the shear band, the average grain rotations of both sands are very similar and appear quite flat, with a limited increase between 1% and 5% axial strain. That increase in the average rotation outside the shear band may reflect the fact that the shear bands become somewhat narrower as deformation progresses [54], whereas the grain classification criterion is only applied in the final test stage.

409

410

411 *Figure 11: Histories of cumulated mean particle rotations inside and outside the shear bands (SB in the*
 412 *legend), measured by D-DVC throughout the triaxial tests. The green dots represent interpreted results*
 413 *from Alshibli and Alramahi (2006) for a triaxial experiment involving 400 plastic pearls.*

414 Average rotations increase much faster within the shear band. In the Caicos specimen
 415 (COEA04) average rotation magnitude raises to about 30 degrees. The trend in the
 416 Hostun specimen (HNEA01) is somewhat slower, raising to a level of about 21degrees.
 417 The distribution of cumulative rotation magnitudes in the shear bands is rather skewed
 418 (Figure 12) with the mode remaining almost constant but the high end tail progressively
 419 thickening.

Figure 12: Distribution of accumulated particle rotation magnitudes at different test stages (12-14-16) for particles within the shear band of the Hostun sand HNEA01 specimen.

The attrition rate during this sequence of image correlations is shown in Figure 13. It is clear that in this more realistic context, the D-DVC procedure has more difficulties than in the idealized uniform rotation check discussed before. The correlation problems increase as the grains rotate more, which is what happens in the shear band. Despite that, it should be noted that a) the correlation validity criterion was set at a very stringent limit ($CC = 0.98$) and b) the procedure was able to track to the end almost 80% of the grains within the shear bands and more than 95% outside them.

Figure 13: Particles with correlation maximum below 98% as a percentage of total number of particles

4.4 A comparison of secant and cumulative tangent rotations

There is a risk that the secant image correlation approach applied may lead to an underestimation of the cumulated total grains rotations, as it computes the “shortest path” of rotation (i.e., the minimum rotation angle) between the initial configuration and that of each step examined. Adding the results from tangent step-by-step correlations such as those performed by Andò [32] would avoid the underestimation problem but, as previously explained, grain re-labelling across images complicates tracking individual grains. Despite that, a meaningful statistical comparison is still possible based on the average values of rotations for all grains.

Figure 14 shows the evolution of the average magnitude of grain rotations for Hostun sand for all grains in the specimen as obtained by Andò [32] using step-by-step (i.e. tangent) correlations. This is compared with the values obtained here using the secant approach for two different scenarios. In the first one (corresponding to the results shown above) the average rotation at each step is computed only for the remaining grains (i.e.

those that are above the correlation threshold). In the second approach the average at each step is computed for all grains, assigning to those that are below the correlation threshold the last rotation value that was obtained for them.

Figure 14: History of the average magnitudes of rotations for Hostun sand measured with different approach. The error bars are magnified 10 times.

The differences between the “tangent” and “secant” correlation approaches are small. The results for the all-grain secant average are closer to those of the tangent because in the step-by-step correlations the number of grain losses was minimal, whereas in the secant approach the attrition rate is close to 20% at the end of the test. Moreover, the grains that are lost are typically those with larger rotations, which is reflected in the progressive divergence of the average restricted to the remaining grains. In any case, it is clear from the comparison that the grain rotations computed with the secant approach are not significantly underestimated.

4.5 Axes of rotation

Stereoplots (see Figure 4b) can be used to investigate the alignment of particle rotation axes during shearing. The orientations of *cumulative* rotation versors are plotted for all grains (about 110000 in total), both inside and outside the shear bands, at two different test stages in Figure 15 (at approximately 5% axial strain, corresponding to steps 01-09 in Hostun and 01-06 in Caicos) and Figure 16 (at approximately 9% axial strain, corresponding to 01-12 for Hostun and 01-09 for Caicos). The raw stereoplots are presented alongside binned frequency diagrams.

Figure 15: Stereoplots showing the rotation versor directions at 5% shortening. The green dots indicate the orientation of vector $\vec{b}$ (see Figure 6) belonging to the shear bands of Hostun and Caicos sands. The stereoplot angles markers are not shown for readability, see Figure 4b for reference.

Figure 16: Stereoplots showing the rotation vector directions at 9% shortening. The green dots indicate the orientation of vector $\vec{b}$ (see Figure 6) belonging to the shear bands of Hostun and Caicos sands. Stereoplot grid not shown for readability, see Figure 4b for reference.

Both sands exhibit similar trends (Figure 15). Outside the shear bands, the rotation axes accumulate towards the periphery of the stereoplot, with inclination angles close to 90° that indicate horizontal axes of rotation. The azimuthal angle, on the other hand, is almost homogeneously distributed around the stereoplot periphery, indicating no preferential alignment for the grain rotational axis within the horizontal plane.

The situation is different inside the shear band, which is already present at 5% strain (Figure 9; Figure 10). The rotation axes are still mainly horizontal ($\theta = 90^\circ$), but now the azimuthal angles (φ) concentrate around values of about 135° (Hostun sand) and 75° (Caicos sand). As indicated in the figures these values are, precisely, the azimuths of vector $\vec{b}$ in Figure 6 *i.e.*, those corresponding to directions orthogonal to that of steepest descent within the shear band. This alignment means that grains are rolling downslope the plane of the shear band. Another azimuthal accumulation point is observed at the diametrically opposed direction in the stereoplot, that is at 315° for Hostun and 255° for

Caicos. That position corresponds to grains rotating upslope on the plane of the shear band. These preferential orientations become sharper as localisation progresses (compare with results at 9% axial strain, shown in Figure 16) and appear generally sharper for Hostun sand than for Caicos ooids.

The results obtained contrast with those presented in Andò et al. [32] who attempted a similar analyses for the Hostun HNEA01 specimen. There the alignment of particle rotation axis and shear band normal was not evident. The difference is likely due to the superior precision of particle rotation measurement achieved by the D-DVC technique over the ID-track used in Andò et al. [32]. The presence of particle with opposite spins in shear zones, previously documented in experiments with simplified granular media (such as flat disks [64, 65] or uniform plastic beads [40]), is here confirmed for natural sands.

4.6 Relations between grain shape and magnitude of rotation

A first indication of the relationship between particle shape and rotation is already evident in Figure 11. Caicos ooids rotate – on average – far more than Hostun sand grains, but only if belonging to the shear band; for grains that remained outside the shear band there is almost no difference between the more rounded Caicos ooids and the angular Hostun sand. This insensitivity to particle shape outside the critical shearing zone is corroborated by data deduced from Alshibli and Alramahi [40], also plotted in Figure 11. Those authors reported histograms of particle rotations for 400 perforated plastic pearls, almost uniformly spherical, in a triaxial compression test that did not present a clear

shear band. The averaged rotations from that test on plastic beads plot very close to our sand data.

Although averaged values of rotation are interesting, the data collected allow a more detailed inspection of the effect of grain shape on rotation. Figure 17 presents bivariate frequency density plots exploring the effect of shape descriptors related to form on particle rotations (accumulated up to 5% axial strain). The histogram contours appear rather flat, indicating little sensitivity of particle rotations to form. The same approach is followed in Figure 18, but now using shape descriptors that measure sphericity. The histogram contours are more sensitive, particularly those at the edge, indicating larger percentiles. This is particularly evident for convexity and to true sphericity – two shape descriptors that are tightly correlated for these two sands, see [26]).

Figure 17: Normalised bivariate frequency density plots of **form** descriptors versus **cumulative** grain rotation magnitude at 5% shortening (loading stages HNEA01-09 and COEA04-06, respectively 48.612 and 65.056 grains). The contours colour bar is shown in Figure 4c.

Figure 18: Normalised bivariate frequency density plots of *sphericity* descriptors versus the *cumulative* grain rotations measured at 5% shortening (loading stages HNEA01-09 and COEA04-06, respectively 48.612 and 65.056 grains). The contours colour bar is shown in Figure 4c.

Figure 19: Normalised histograms showing the observed relation between the degrees of true sphericity and the total grains rotation measured at 5% sample shortening.

The histograms become more triangular if restricted to particles in the shear band. Figure 19 shows that the *degree of true sphericity* seems to have a significant influence on the upper limit of particle rotation, which increases as particles become more spherical. This idea is explored in more detail in Figure 20 and Figure 21, where mean and extreme values (99.5% percentiles) of rotation, measured on both Caicos sand and Hostun sand

specimens, are plotted as a function of true sphericity. The values are derived from marginal distributions, obtained at fixed true sphericity intervals (width 0.025). Because the number of particles in each interval is highly variable, error bands (plus and minus one standard error) are also represented. The error bands for the 99.5% quantile are estimated using a bootstrapping technique [66], resampling with replacement the original samples (for each interval) one thousand times. Errors band thickness increases with small sample sizes (e.g. at low values of *degree of true sphericity*) and with marginal variability (high at large values of *degree of true sphericity*, as correlating very spherical grains carries more uncertainty).

It appears that the mean values of rotation, both inside and outside the shear band are insensitive to particle sphericity, whereas the extreme upper values (the 99.5 % percentile) show a clear positive dependency between rotations and particle sphericity. There is not much difference between the mean values of Caicos and Hostun, at any given true sphericity. On the other hand, the upper limit rotations of Caicos are somewhat above those of Hostun, even at the same sphericity, and particularly for those particles inside the shear band. Andò [54] observed that porosity in the shear band was higher for Hostun than for Caicos, so it is unlikely that connectivity – which is inversely related to porosity – will explain that difference. Still, the differences between the two sands not accounted for true sphericity are less important than the common effect of sphericity on the upper bound. These trends were confirmed when other test stages were analysed, for instance at around 9% axial strain, Figure 22 and Figure 23.

Figure 20: Influence of the degree of true sphericity on the total grains rotation (at 5% shortening) outside the shear band.

Figure 21: Influence of the degree of true sphericity on the total grains rotation (at 5% shortening) inside the shear band.

Figure 22: Influence of the degree of true sphericity on the total grains rotation (at 9% shortening) outside the shear band.

Figure 23: Influence of the degree of true sphericity on the total grains rotation (at 9% shortening) inside the shear band.

5 Conclusions

This paper sets out to explore the relationship between particle shape and particle rotation at the grain scale, for all the sand grains within triaxial specimens that failed in a localised shear mode. The main findings can be summarised as follows:

- The systematic use of Discrete-Digital Volume Correlation allowed successful tracking of rotational kinematics in the large majority of grains; those measurements were far more precise than previous attempts using ID-track;
  - Kinematics within the shear bands are very different from those outside the shear band. Particle rotation magnitudes increase much faster in the bands. Rotational axes align themselves preferentially, perpendicular to the steepest descent direction of the band;
  - Sand grains in the shear plane show both positive and negative spins (upwards and downwards the plane), revealing commonalities in the shear flow mechanisms of sands with those of simpler granular materials;
  - Shape descriptors related to particle form, such as elongation or flatness indexes appear to be poorly correlated with observed particle rotation;
  - Shape descriptors related to particle sphericity have a significant effect on particle rotation. This effect is far less important on the average value than on the upper limit of rotation.
- It may be concluded that the link between particle shape and particle kinematics is only effective at the margin. This was to be expected, as it is a link necessarily mediated by particle connectivity. Despite this limitation, and until particle connectivity can be imaged with equal precision in experiments, the microscale results here presented should facilitate the calibration of advanced DEM contact models to represent shape effects, either directly [67] or indirectly [68].

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7 References

1. Jiang, M., Liu, F., Bolton, M.: Proceedings of the International Symposium on Geomechanics and Geotechnics: from Micro to Macro (IS-Shanghai 2010). CRC Press/Balkema, Shanghai (2011)
2. Soga, K., Kumar, K., Biscontin, G., Kuo, M.: Geomechanics from micro to macro : Proceedings of the TC105 ISSMGE International Symposium on Geomechanics from Micro to Macro, Cambridge, UK, 1-3 September 2014. (2014)
3. Baudet, B., Bolton, M.: Editorial Soil mechanics at the grain scale: issue 1 and 2. *Géotechnique*. 60, 313–314 (2010). doi:10.1680/geot.2010.60.5.313
4. Cho, A.G., Dodds, J., Santamarina, J.C.: Particle Shape Effects on Packing Density, Stiffness and Strength – Natural and Crushed Sands. *J. Geotech. Geoenvironmental Eng.* 132, 591–602 (2006). doi:10.1061/(ASCE)1090-0241(2006)132:5(591)
5. Santamarina, J., Cho, G.: Soil behaviour: The role of particle shape. In: *Advances in Geotechnical Engineering. Proceedings of the Skempton Conference*. pp. 1–14., London (2004)
6. Yang, J., Luo, X.D.: Exploring the relationship between critical state and particle shape for granular materials. *J. Mech. Phys. Solids*. 84, 196–213 (2015).

doi:10.1016/j.jmps.2015.08.001

7. Xiao, Y., Long, L., Matthew Evans, T., Zhou, H., Liu, H., Stuedlein, A.W.: Effect of Particle Shape on Stress-Dilatancy Responses of Medium-Dense Sands. *J. Geotech. Geoenvironmental Eng.* 145, (2019). doi:10.1061/(ASCE)GT.1943-5606.0001994

8. Vaid, Y., Chern, J., Tumi, H.: Confining pressure, Grain angularity and Liquefaction. *J. Geotech. Eng.* 111, 1229–1235 (1985)

9. Liu, Q.B., Lehane, B.M.: The influence of particle shape on the (centrifuge) cone penetration test (CPT) end resistance in uniformly graded granular soils. *Géotechnique*. 60, 111–121 (2013). doi:10.1139/t06-037

10. Rothenburg, L., Bathurst, R.J.: Micromechanical features of granular assemblies with planar elliptical particles. *Géotechnique*. 42, 79–95 (1992). doi:10.1680/geot.1992.42.1.79

11. Ng, T.-T., Lin, X.: A three-dimensional discrete element model using arrays of ellipsoids. *Géotechnique*. 47, 319–329 (1997). doi:10.1680/geot.1997.47.2.319

12. Cleary, P.W.: The effect of particle shape on simple shear flows. *Powder Technol.* 179, 144–163 (2008). doi:10.1016/j.powtec.2007.06.018

13. Ferrellec, J.-F., McDowell, G.R.: A method to model realistic particle shape and inertia in DEM. *Granul. Matter.* 12, 459–467 (2010). doi:10.1007/s10035-010-0205-8

14. Jiang, M.J., Liu, J.D., Arroyo, M.: Numerical evaluation of three non-coaxial kinematic models using the distinct element method for elliptical granular materials. *Int. J. Numer. Anal. Methods Geomech.* 40, 2468–2488 (2016). doi:10.1002/nag.2540

15. Matsushima, T., Chang, C.S.: Quantitative evaluation of the effect of irregularly shaped particles in sheared granular assemblies. *Granul. Matters.* 13, 269–276

(2011). doi:10.1007/s10035-011-0263-6

16. Iwashita, K., Oda, M.: Rolling resistance at contacts in simulation of shear band development by DEM. *J. Eng. Mech.* 124, 285–292 (1998). doi:10.1061/(ASCE)0733-9399(1998)124:3(285)
17. Jiang, M.J.J., Yu, H.-S., Harris, D.: A novel discrete model for granular material incorporating rolling resistance. *Comput. Geotech.* 32, 340–357 (2005). doi:10.1016/j.compgeo.2005.05.001
18. Belheine, N., Plassiard, J.P., Donzé, F. V., Darve, F., Seridi, A.: Numerical simulation of drained triaxial test using 3D discrete element modeling. *Comput. Geotech.* 36, 320–331 (2009). doi:10.1016/j.compgeo.2008.02.003
19. Huang, X., Hanley, K.J., O’Sullivan, C., Kwok, C.Y.: Implementation of rotational resistance models: A critical appraisal. *Particuology.* 34, 14–23 (2017). doi:10.1016/j.partic.2016.08.007
20. Coetzee, C.J.: Calibration of the discrete element method and the effect of particle shape. *Powder Technol.* 297, 50–70 (2016). doi:10.1016/j.powtec.2016.04.003
21. Guillard, F., Marks, B., Einav, I.: Dynamic X-ray radiography reveals particle size and shape orientation fields during granular flow. *Sci. Rep.* 7, 1–11 (2017). doi:10.1038/s41598-017-08573-y
22. Oda, M., Takemura, T., Takahashi, M.: Microstructure in shear band observed by microfocus X-ray computed tomography. *Géotechnique.* 54, 539–542 (2004)
23. Matsushima, T., Uesugi, K., Nakano, T., Tsuchiyama, A.: Visualization of Grain Motion inside a Triaxial Specimen by Micro X-ray CT at SPring-8. In: Desrues, J., Besuelle, P., and Viggiani, G. (eds.) *Advances in X-ray Tomography for Geomaterials.* pp. 35–52. , London (2006)

- 662 24. Hall, S.A., Bornert, M., Desrues, J., Pannier, Y., Lenoir, N., Viggiani, G., Bésuelle,
663 P.: Discrete and continuum analysis of localised deformation in sand using X-ray
664 μ CT and volumetric digital image correlation. *Géotechnique*. 60, 315–322 (2010).
665 doi:10.1680/geot.2010.60.5.315
- 666 25. Hasan, A., Alshibli, K.A.: Experimental assessment of 3D particle-to-particle
667 interaction within sheared sand using synchrotron microtomography.
668 *Géotechnique*. 60, 369–379 (2010). doi:10.1680/geot.2010.60.5.369
- 669 26. Rorato, R., Arroyo, M., Andò, E., Gens, A.: Sphericity measures of sand grains.
670 *Eng. Geol.* 254, 43–53 (2019). doi:10.1016/j.enggeo.2019.04.006
- 671 27. Alshibli, K.A., Druckrey, A.M., Al-Raoush, R.I., Weiskittel, T., Lavrik, N. V.:
672 Quantifying Morphology of Sands Using 3D Imaging. *J. Mater. Civ. Eng.* 27,
673 (2015). doi:10.1061/(ASCE)MT.1943-5533.0001246
- 674 28. Zhao, B., Wang, J.: 3D quantitative shape analysis on form, roundness, and
675 compactness with micro-CT. *Powder Technol.* 291, 262–275 (2016).
676 doi:10.1016/j.powtec.2015.12.029
- 677 29. Kong, D., Fonseca, J.: Quantification of the morphology of shelly carbonate sands
678 using 3D images. *Géotechnique*. 68, 249–261 (2018). doi:10.1680/jgeot.16.P.278
- 679 30. Fonseca, J., O’Sullivan, C., Coop, M.R., Lee, P.D.: Non-invasive characterization
680 of particle morphology of natural sands. *Soils Found.* 52, 712–722 (2012).
681 doi:10.1016/j.sandf.2012.07.011
- 682 31. Fonseca, J., O’Sullivan, C., Coop, M.R., Lee, P.D.: Quantifying the evolution of soil
683 fabric during shearing using directional parameters. *Géotechnique*. 63, 818–829
684 (2013). doi:10.1680/geot.11.P.150
- 685 32. Andò, E., Hall, S.A., Viggiani, G., Desrues, J., Bésuelle, P.: Grain-scale

- experimental investigation of localised deformation in sand: A discrete particle tracking approach. *Acta Geotech.* 7, 1–13 (2012). doi:10.1007/s11440-011-0151-6
33. Hasan, A., Alshibli, K.: Three dimensional fabric evolution of sheared sand. *Granul. Matter.* 14, 469–482 (2012). doi:10.1007/s10035-012-0353-0
34. Higo, Y., Oka, F., Sato, T., Matsushima, Y., Kimoto, S.: Investigation of localized deformation in partially saturated sand under triaxial compression using microfocus X-ray CT with digital image correlation. *Soils Found.* 53, 181–198 (2013). doi:10.1016/j.sandf.2013.02.001
35. Alshibli, K.A., Jarrar, M.F., Druckrey, A.M., Al-Raoush, R.I.: Influence of Particle Morphology on 3D Kinematic Behavior and Strain Localization of Sheared Sand. *J. Geotech. Geoenvironmental Eng.* 143, 04016097 (2017). doi:10.1061/(ASCE)GT.1943-5606.0001601
36. Cheng, Z., Wang, J.: A particle-tracking method for experimental investigation of kinematics of sand particles under triaxial compression. *Powder Technol.* 328, 436–451 (2018). doi:10.1016/j.powtec.2017.12.071
37. Wiebicke, M., Andò, E., Herle, I., Viggiani, G.: On the metrology of interparticle contacts in sand from x-ray tomography images. *Meas. Sci. Technol.* 28, 124007 (2018)
38. Wiebicke, M., Andò, E., Salvatore, E., Viggiani, G., Herle, I.: Experimental measurement of granular fabric and its evolution under shearing. In: Radjai, F., Nezamabadi, S., Luding, S., and Delenne, J.Y. (eds.) *European Physical Journal Web of Conferences.* p. 02020. EDP Sciences (2017)
39. Wiebicke, M., Andò, E., Šmilauer, V., Herle, I., Viggiani, G.: A benchmark strategy for the experimental measurement of contact fabric. *Granul. Matter.* 21:54, 1–13

- 710 (2019). doi:10.1007/s10035-019-0902-x
- 711 40. Alshibli, K.A., Alramahi, B.A.: Microscopic Evaluation of Strain Distribution in
712 Granular Materials during Shear. *J. Geotech. Geoenvironmental Eng.* 132, 80–91
713 (2006). doi:10.1061/(asce)1090-0241(2006)132:1(80)
- 714 41. Vlahinić, I., Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E.: From computed
715 tomography to mechanics of granular materials via level set bridge. *Acta Geotech.*
716 12, 85–95 (2017). doi:10.1007/s11440-016-0491-3
- 717 42. Cheng, Z., Wang, J.: Experimental investigation of inter-particle contact evolution
718 of sheared granular materials using X-ray micro-tomography. *Soils Found.* 58,
719 1492–1510 (2018). doi:10.1016/j.sandf.2018.08.008
- 720 43. Sutton, M.A., Schreier, H.W., Orteu, J.-J.: Image correlation for shape, motion and
721 deformation measurements: basic concepts, theory and applications. Springer
722 (2009)
- 723 44. Hall, S.A.: Digital Image Correlation in Experimental Geomechanics. In:
724 Gioacchino Viggiani, Stephen A. Hall, and Enrique Romero (eds.) *ALERT*
725 *Doctoral School 2012 Advanced experimental techniques in geomechanics.* pp.
726 69–102. , Aussois (France) (2012)
- 727 45. Take, W.A.: Thirty-Sixth Canadian Geotechnical Colloquium: Advances in
728 visualization of geotechnical processes through digital image correlation. *Can.*
729 *Geotech. J.* 52, 1199–1220 (2015). doi:10.1139/cgj-2014-0080
- 730 46. Pan, B., Qian, K., Xie, H., Asundi, A.: Two-dimensional digital image correlation
731 for in-plane displacement and strain measurement: a review. *Meas. Sci. Technol.*
732 20, (2009). doi:10.1088/0957-0233/20/6/062001
- 733 47. Stanier, S.A., Blaber, J., Take, W.A., White, D.J.: Improved image-based

- 734 deformation measurement for geotechnical applications. *Can. Geotech. J.* 53, 727–
735 739 (2016). doi:10.1139/cgj-2015-0253
- 736 48. Pinyol, N.M., Alvarado, M.: Novel analysis for large strains based on particle
737 image velocimetry. *Can. Geotech. J.* 54, 933–944 (2017)
- 738 49. Andò, E., Hall, S.A., Viggiani, G., Desrues, J., Bésuelle, P.: Experimental
739 micromechanics: grain-scale observation of sand deformation. *Géotechnique Lett.*
740 2, 107–112 (2012). doi:10.1680/geolett.12.00027
- 741 50. Wadell, H.: Volume, Shape, and Roundness of Rock Particles. *J. Geol.* 40, 443–451
742 (1932)
- 743 51. Barret, P.J.: The shape of rock particle, a critical review. *Sedimentology.* 27, 291–
744 303 (1980). doi:10.1111/j.1365-3091.1980.tb01179.x
- 745 52. Zingg, T.: Beitrag zur Schotteranalyse, [http://e-](http://e-collection.library.ethz.ch/view/eth:21472)
746 [collection.library.ethz.ch/view/eth:21472](http://e-collection.library.ethz.ch/view/eth:21472), (1935)
- 747 53. Krumbein, W.C.: Measurement and Geological Significance of Shape and
748 Roundness of Sedimentary Particles. *J. Sediment. Res.* 11, 64–72 (1941)
- 749 54. Andò, E.: Experimental investigation of microstructural changes in deforming
750 granular media using x-ray tomography, (2013)
- 751 55. Salvatore, E., Modoni, G., Andò, E., Albano, M., Viggiani, G.: Determination of
752 the critical state of granular materials with triaxial tests. *Soils Found.* 57, 733–744
753 (2017). doi:10.1016/j.sandf.2017.08.005
- 754 56. Viggiani, G., Andò, E., Takano, D., Santamarina, J.C.: Laboratory X-ray
755 Tomography: A Valuable Experimental Tool for Revealing Processes in Soils.
756 *Geotech. Test. J.* 38, 61–71 (2015). doi:10.1520/GTJ20140060
- 757 57. Lorensen, W.E., Cline, H.E.: Marching cubes: A high resolution 3D surface

- 758 construction algorithm. ACM siggraph Comput. Graph. 21, 163–169 (1987).
- 759 doi:10.1145/37402.37422
- 760 58. Tudisco, E., Andò, E., Cailletaud, R., Hall, S.A.: TomoWarp2: A local digital
- 761 volume correlation code. SoftwareX. 6, 267–270 (2017).
- 762 doi:10.1016/J.SOFTX.2017.10.002
- 763 59. Campello, E.M.B.: A description of rotations for DEM models of particle systems.
- 764 Comp. Part. Mech. 2, 109–125 (2015). doi:10.1007/s40571-015-0041-z
- 765 60. Andò, E., Cailletaud, R., Roubin, E., Stamati, O., the spam contributors: SPAM:
- 766 The Software for the Practical Analysis of Materials, (2017)
- 767 61. Pannier, Y., Lenoir, N., Bornert, M.: Discrete volumetric digital image correlation
- 768 for the investigation of granular type media at microscale: accuracy assessment.
- 769 EPJ Web Conf. 6, (2010). doi:10.1051/epjconf/20100635003
- 770 62. Catalano, E., Chareyre, B., Barthélémy, E.: Pore-scale modeling of fluid-particles
- 771 interaction and emerging poromechanical effects. Int. J. Numer. Anal. Methods
- 772 Geomech. 38, 51–71 (2014). doi:10.1002/nag.2198
- 773 63. Šmilauer, V. et al.: Yade Documentation 2nd ed. The Yade Project. (2015)
- 774 64. Veje, C.T., Howell, D.W., Behringer, R.P.: Kinematics of a two-dimensional
- 775 granular Couette experiment at the transition to shearing. Phys. Rev. E - Stat.
- 776 Physics, Plasmas, Fluids, Relat. Interdiscip. Top. 59, 739–745 (1999).
- 777 doi:10.1103/PhysRevE.59.739
- 778 65. Pasternak, E., Dyskin, A. V., Esin, M., Hassan, G.M., MacNish, C.: Rotations and
- 779 pattern formation in granular materials under loading. Philos. Mag. 95, 3122–3145
- 780 (2015). doi:10.1080/14786435.2015.1059517
- 781 66. Efron, B., Tibshirani, R.: An introduction to the bootstrap. Chapman & Hall (1994)

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2
3
4
5
6
7
8
9
10
11
12
13
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46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
65

782 67. Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E.: All you need is shape:
783 Predicting shear banding in sand with LS-DEM. J. Mech. Phys. Solids. 111, 375–
784 392 (2018). doi:10.1016/j.jmps.2017.10.003
785 68. Rorato, R., Arroyo, M., Gens, A., Andò, E., Viggiani, G.: Particle Shape
786 Distribution Effects on the Triaxial Response of Sands: A DEM Study. In: Giovine,
787 P. and et al. (eds.) micro to MACRO Mathematical Modelling in Soil Mechanics,
788 Trends in Mathematics. pp. 277–286. , Reggio Calabria (Italy) (2018)
789

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Linking shape and rotation of grains during triaxial compression of sand

Riccardo Rorato, Dr.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering.

riccardo.rorato@upc.edu

ORCID ID: 0000-0002-4189-3058

UPC - Barcelonatech

Moduli D2 Campus Nord UPC – Office 212

C Jordi Girona 1-3

Barcelona 08034

Marcos Arroyo Alvarez de Toledo, Prof.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering

marcos.arroyo@upc.edu

ORCID ID: 0000-0001-9384-9107

Edward Carlo Giorgio Andò, Prof.

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000 Grenoble (France)

edward.ando@3sr-grenoble.fr

ORCID ID: 0000-0001-5509-5287

Antonio Gens, Prof.

Universitat Politècnica de Catalunya (UPC), Barcelona (Spain) - Department of Civil and Environmental Engineering

antonio.gens@upc.edu

ORCID ID: 0000-0001-7588-7054

Gioacchino Viggiani, Prof.

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000 Grenoble (France)

cino.viggiani@3sr-grenoble.fr

ORCID ID: 0000-0002-2609-6077

35 **Declaration**

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43 *Availability of data and material (data transparency):* Available on request.

45 *Code availability (software application or custom code):* Open-source Python programming
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47 **Compliance with ethical standards**

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Abstract

Particle shape has a strong effect on the mechanical response of coarse soils. This has been usually observed examining specimen-scale or engineering-scale responses, which are the sum of many microscale interactions. In this work we observe the effects of particle shape directly at the microscale level. X-ray tomography (μ -CT) of two sand specimens is exploited to measure three-dimensional particle shape descriptors but also to track individual particle motions during triaxial compression. A discrete *Digital Volume Correlation* (DVC) algorithm is employed to track the motion of individual grains (around 50000 for each sand specimen) during the test and measure, with good precision, their cumulated displacements and rotations. The specimens examined failed in a clearly localised shear mode. Advantage is taken of this to obtain data relevant for very different kinematical regimes: one uniform and more constrained and the other close to critical state. A direct comparison between the shape and kinematic databases shows to what degree particle shape descriptors are related to observed kinematics. It appears that true sphericity is a good predictor of upper bound rotational restraint.

Keywords: Laboratory equipment; Microscopy; Particle-scale behaviour; Sands; Shear strength; Statistical analysis.

1 Introduction

Granular soils are made of discrete particles that interact with each other, therefore changes at the small-scale (*i.e.*, grain-scale) affect the material response at the large-scale (*i.e.*, engineering-scale) [1–3]. For granular soils, for instance, it is well-documented that

particle shape strongly affects soil properties such as extreme void ratios [4, 5], critical state friction [6] or dilatancy and peak friction [7], as well as engineering scale responses, like liquefaction resistance [8] or cone tip resistance [9].

It follows that particle shape must affect grain-scale interactions to produce those effects. This hypothesis has been repeatedly supported, from various perspectives, by the results of numerical simulation. In numerous discrete element models direct control of element shape has been shown to result in major changes in ensemble mechanical responses [10–15].

It is noteworthy, however, that similar macroscopic effects are observed when particle shape effects are represented indirectly, through appropriately modified element contact interaction laws, for instance introducing some resistance against rolling at the contact [16–19]. Both direct and indirect shape modelling strategies inevitably involve some degree of simplification, to be adjusted in applications under typically conflicting constraints of computational speed, accuracy and ease of calibration [20].

In this context, direct experimental observation of the microscale effects of particle shape appears relevant, as it may provide evidence beyond that implicit in the ensemble behaviour of the specimen. This has been a relatively unexplored avenue, because it requires relevant and accurately measured shape descriptors, as well as particle-scale resolution of internal mechanisms. There are few experimental techniques useful for that purpose [21] and the main one is relatively recent: microfocus or x-rays μ -tomography [22–25].

Despite significant difficulties, progress in 3D tomographic imaging and post-processing technologies [26–30], has made accurate grain shape determination feasible for most sands. Identification of particle-scale mechanisms is more difficult, as it requires imaging not just isolated particles, but particles in collective interaction, within specimens. Particles need to be separated from one another, within the imaged ensemble. Ideally, the existing contacts amongst particles need to be identified, as interactions between particles occur through contact forces in coarse soils. Single snapshots of microstructures (typically acquired “post-mortem”, after dismounting the test [22, 25, 31]) cannot reveal kinematics. For that purpose a sequence of images needs to be acquired during a test, and triaxial tests have been the target for most of this kind of work [32–36]. Clearly, one added difficulty here is the need to track particles confidently across different images. Progress in these tasks has been also very significant, but there are still some important obstacles, particularly in the area of contact detection and measurement. Indeed, the level of image resolution required to image particle contacts – and contact properties such as orientation – appears far more demanding than that required to image, identify and measure particles [37–39]. This has implicitly limited the scope (number of tracked particles and/or number of imaged test steps) of kinematic contact fabric imaging studies [33, 40–42].

Current technology may be exploited to obtain more statistically sound results if the focus is restricted to particle kinematics. This is the avenue explored in this work, in which we examine in detail the relations between individual grain shape and individual kinematical history of sand grains as observed during triaxial compression of two dense sand specimens that jointly provide a database of 110000 grains. For the purposes of this

study, the specimens selected for examination had the advantage of failing in sharply localised shear modes. As clearly identified in previous research [22, 24, 25] the structure and kinematics of particles within a shear band are very different from those outside, as particles in a shear band approach critical state conditions. As long as a criterion for belonging or not into the shear band could be clearly established, this experimental feature ensured that the influence of particle shape could be examined in two very different and separate kinematic settings (*i.e.*, within the band and outside it), thus making the study relevant for a larger set of conditions. In what follows, we first give some background on particle tracking and shape description terminology. We then describe the test and image analysis procedures employed and the results obtained before presenting some conclusions.

2 Background

2.1 *Digital image correlation for quantifying particle kinematics*

Digital Image Correlation (DIC) is the ideal tool for comparing and analysing images of deforming materials, such the ones obtained from x-ray scans. DIC is a widely used technique in experimental mechanics to deduce motion and shape features of an object by comparing its appearance in different images [43]. A first classification of DIC may be based on the dimensional support of the images employed in the comparison [44]: surface-DIC is based on bi-dimensional images, whereas volumetric DIC (or, simply, digital volume correlation, DVC), is based on three-dimensional images. Surface-DIC is widely

employed in field and laboratory experimental geotechnics [45]. DVC has seen fewer applications because of the increased difficulties associated with 3D image acquisition. In DIC a subset F of intensity values from a reference image is systematically compared with subsets G_i of the transformed image until some optimality condition is achieved [46]. This optimality condition is frequently based on a cross correlation measure, for instance searching for a maximum normalised cross correlation:

$$NCC = \frac{F * G_i}{\|F\| \|G_i\|}$$

Different algorithms are obtained depending on how the subset F is chosen, what kind of motion is assumed to relate F and G_i and how the search window (SW, the zone in which G_i is searched for) is defined.

Two broad variants of DVC have been employed in geotechnical applications: *continuum* (C-DVC) and *discrete* (D-DVC). In C-DVC, the subset F (usually referred to as correlation window, CW) is a cubical cell centred around some pre-established evaluation grid points. Although more complex transformations are sometimes used [47], the motion relating F and G is usually assumed as a simple rigid translation, and cross correlation is employed to find a displacement vector, which is assigned to the grid node. From the displacement field thus obtained, strain measures are derived using different procedures [48]. The underlying assumption is that subset F is a representative volume element RVE in a continuum; therefore, the scale of the CW should contain enough grains to make that assumption realistic.

C-DVC is not well adapted to identify particle kinematics. When the resolution of the images is such that individual grains may be identified, other alternatives are possible.

Hall et al. [24] proposed a novel discrete *grain-based* approach (D-DVC) to track individual particles. The method has as a starting point a *segmented* labelled image, in which groups of voxels are identified as grains. In D-DVC the subset F is selected considering which voxels have been previously assigned to a certain grain and is named a grain mask. The assumed motion between F and G is a rigid body motion, including translation and rotation. With D-DVC the kinematics of each identified particle is thus directly obtained. Hall et al. [24] went on to illustrate the potential of D-DVC obtaining maps of incremental displacements and rotations in a triaxial specimen of Hostun sand, showing also that the kinematic history of single grains was very different if they were involved in a shear band or not.

Andò et al. [32] proposed an alternative method to follow grain kinematics across images, called ID-track. In this method grain match between successive images is based on listed properties of grains, such as volume, surface area, etc. obtained through single-image analysis. The method requires two segmented images as input. The grain matching operation is faster than in D-DVC, as volume cross-correlation is not needed. With some modifications, ID-track has been later used by Alshibli et al. [35] and Cheng & Wang [36], amongst others. However, ID-track has some difficulties to assign precise rotation values, particularly when dealing with very spherical particles [32], and was therefore extended to include a D-DVC based technique for rotation measurement in Andò et al. [49]. For this reason, the work presented here was based on the more robust, if slower, D-DVC technique.

2.2 Particle shape description

There are different approaches to describe the shape of soil grains and, as a result, many different shape descriptors are currently in use. Table 1 summarises the 3D shape descriptors that are employed in this work whereas Table 2 lists the fundamental measures from which the shape descriptors are derived. Several shape descriptors try to measure particle similitude with a sphere (*i.e.*, sphericity), *i.e.*, the historical proposal of Wadell [50], called *true sphericity*, but also the *convexity* and *operational sphericity* descriptors. We also use some shape descriptors that are more relevant to particle *form* [51] such as *flatness index*, *elongation index* and – despite its name – *intercept sphericity*. Rorato et al. [26] present a detailed study of the relationships amongst these and other 3D and 2D shape descriptors.

Name	Symbol	Definition	Reference
<i>True Sphericity</i>	Ψ	$\frac{S_n}{S}$	[50]
<i>Flatness index</i>	FI	c/b	[52]
<i>Elongation index</i>	EI	b/a	[52]
<i>Intercept sphericity</i>	Ψ_{int}	$\sqrt[3]{\frac{bc}{a^2}} = \sqrt[3]{FI(EI)^2}$	[53]
<i>Operational Sphericity</i>	Ψ_{op}	$\sqrt[3]{\frac{V}{V_{cm}}} = \frac{D_n}{D_{cm}} \approx \frac{D_n}{a}$	[53]
<i>Convexity</i>	Co	V/V_{CH}	[30]

Table 1: Selected 3D shape descriptors [26]

Shape property	Symbol	Equivalent diameter
<i>Volume</i>	V	D_n
<i>Surface area</i>	S	

Shape property	Symbol	Equivalent diameter
<i>Surface area of the equivalent sphere (same volume)</i>	S_n	
<i>Maximum, intermediate, minimum lengths</i>	a, b, c	
<i>Convex hull volume</i>	V_{CH}	D_{CH}
<i>Volume of the maximum inscribed sphere</i>	V_{iM}	D_{iM}
<i>Volume of the minimum circumscribing sphere</i>	V_{cm}	D_{cm}

Table 2: Fundamental measures from which 3D shape descriptors are derived [26]

3 Methodology

3.1 Data acquisition

This study analyses data obtained at Laboratoire 3SR (Grenoble, France) from two sand triaxial specimens, approximately 10mm diameter and 20mm height [54]. Both specimens were prepared by dry pluviation and then subject to triaxial compression under 100kPa of confining pressure. The triaxial tests were performed “in-camera” within the x-ray scanner at Laboratoire 3SR. Results from two sand specimens that cover a wide range of particle sphericity values were selected.

The first specimen (HNEA01) was formed with Hostun HN31 sand at relative density of 83.2% (initial void ratio, $e = 0.658$; dry density, $\gamma_d = 1.60g/cm^3$). Hostun is a quartz quarry sand whose grains appear very irregular, see Figure 1a. The grain size distribution, Figure 1c, is very narrow ($C_U = 1.41$), with a D50 equal to $338 \mu m$. The second specimen analysed (COEA04) was formed with Caicos ooids ($e = 0.468$; $\gamma_d = 1.76g/cm^2$).

Due to lack of material, minimum and maximum void ratios were not measured for this sand, but comparison with relevant database results [6] suggest that the specimen void ratio was close to its likely minimum. This sand is a natural sand made of calcium carbonate (CaCO_3) minerals. Ooids are formed by slow chemical accretion and have a very round shape (Figure 1b). The grain size distribution (Figure 1c) is close to that of HNEA01, being also poorly graded ($C_U = 1.39$) with a D_{50} of $420 \mu\text{m}$.

Figure 1a-b-c: (a) Horizontal section of the scanned Hostun (a) and Caicos (b) specimens. (c) Grain Size Distribution of both sands from sieving [54]

The specimens were scanned by x-rays at several loading stages during the test (16 for test HNEA01 and 11 for COEA04). The stress-volumetric-strain curves, with indication of scanning stages are shown in Figure 2. The macroscopic responses of both specimens are typical of dense sands, with a stress peak followed by shearing at overall constant

volume. Both specimens failed in a localized shear mode: Andò [32] verified that within the shear zone constant volume was also attained (at different porosity than the overall value, see also [55]). No breakage was visible in any of the tomographic images. Rorato et al (2019) compared the initial and final images to show that the statistics of all shape parameters remained practically invariant during the tests.

Figure 2: Triaxial responses of the specimens HNEA01 and COEA04 with loading stages markers. The yellow stripes indicate loading stages that are later investigated in more detail.

The pixel size selected to image the sand specimens was $15.56 \mu\text{m}/\text{px}$, to maintain a field of view of approximately $30.5 \text{ mm} \times 23.0 \text{ mm}$. For the specimens analysed, this results in about 22/26 pixels across a grain. Further details of these tests, including the scanning equipment and tomographic image acquisition procedures have been presented elsewhere [54, 56].

3.2 Single-image post-processing

The reconstruction of each x-ray scan results simply in a 3D distribution of grey-scale values which represents the frequency-lumped x-ray attenuation coefficient measured in that location. Therefore, before studying individual grains, it is necessary to *binarise*, *separate* and *label* the tomographic images. The procedures applied here for these tasks are described by Andò [32]. At this point, it is possible to extract single grains from the 3D labelled images. The 3D tomographic images representing Hostun (specimen HNEA01) and Caicos (specimen COEA04) sands contain respectively 48612 and 65056 particles.

Geometrical properties (e.g. volume, surface area, inertia tensor...) of the image subset assigned to each grain are obtained through subsequent post-processing. These properties may be used, in turn, to obtain different shape descriptors in 3D or 2D. The procedures applied for this purpose are described in detail by Rorato et al. [26]; who also presented an exhaustive database of 3D shape descriptors for all the grains in this specimens, evaluating significant statistics. It is worth mentioning that surface area measurements for grains were obtained using a Marching Cubes algorithm [57], to ensure precision in the evaluation of Wadell true sphericity values. Rorato [26] also verified that there were no significant shape changes during the triaxial tests.

3.3 Tracking grain kinematics with D-DVC

The D-DVC software that has been used in this work to obtain the grains kinematics (3D displacements and rotations) is the TomoWarp2 code [58]. In this code, grain displacements are expressed in pixels (the pixel-size is fixed) and 3D rotations as *rotation vectors* using a Rodrigues parametrisation [59]. In a rotation vector, the components represent the direction of the axis of rotation and the norm the magnitude of the angle of rotation around that axis. This representation system for rigid body rotations has practical advantages over more complex alternatives, such as those based on Euler angles or quaternions [59].

To visualize the 3D unit rotation vector orientation, stereographic projection is sometimes used below. The angular coordinates used in this projection are illustrated in Figure 3. The angle θ (inclination) goes from 0° (vertical) to 90° (horizontal), while the angle φ (azimuth) goes from 0° to 360° , being the north ($\varphi=0^\circ$) the direction of the Cartesian x -axis of the specimen. Stereograms were created using the plotting tool “*orientationPlotter*” from the external open-source Python package SPAM [60].

Figure 3: Spherical coordinates system adopted for the stereoplots

Previous applications of D-DVC had focused mostly on incremental grain kinematics [24, 32]. In such approach only the incremental kinematics between two subsequent

loading steps (e.g. 1-2, 2-3, 3-4, etc...) were obtained. The starting point are the two 3D greyscale images bracketing the increment (*i.e.*, initial and deformed configurations); of these two the image corresponding to the initial configuration has to be already labelled, so that grain bounding-boxes that are used as correlation windows can be extracted. This incremental or “tangent” correlation approach cannot be applied sequentially to obtain cumulative kinematics of the grains. The reason is that grain labels assigned to the same grains by processing different scans of the same specimen will be different. To ensure consistency, a single set of grain labels, obtained from the first scan, is required. The method used here to get the history of grain displacements and rotations is based on “secant” correlation (usually referred to as “leapfrog” in C-DVC applications). In this approach, the initial labelled image is always selected for paired searches on those resulting from all the subsequent scans (*i.e.*, 1-2, 1-3, 1-4, etc...). A direct secant approach has clear limitations, being both very expensive (as the grain search window would have to increase during the process) and prone to errors. The algorithm applied here aims to overcome those difficulties using a mixed approach, in which a secant correlation scheme (1-2, 1-3, ... , 1-10) is still employed, but the search is aided by the results of the previous steps, namely the cumulative grains displacement up to the last correlation step. The initial search window is translated by a vector pointing the position of the grain in the previous correlation and can remain of a small size, saving calculation time. The inputs required in this procedure are four: two greyscale images, one labelled image and one data file with the prior grain displacements. Since the rotations that precede the analysed step are not taken into account for the correlation, it is still possible to lose grains when large rotations are present..

3.4 Validation of the D-DIC procedure

To validate the implementation of D-DVC in TomoWarp2 a simple uniform rotation check was employed [32, 61]. The rotations of all the grains contained in specimen HNEA01 were individually computed after applying a five degrees (5° deg) rigid rotation around its vertical z-axis. The main objectives of the validation are three: (a) to evaluate the attrition rate of the algorithm (*i.e.*, the number of grains that are lost from one image to the next); (b) to evaluate the accuracy and precision with which grain rotation was measured and (c) to explore the possible relationship between the precision of the calculation and the shape of the grains (as grains masks are used as correlation windows, it is expected that grains closer to a spherical shape will be tracked with less precision). The check was positive from the attrition viewpoint, with more than 99.8% of the grains correctly tracked attaining a correlation coefficient between the two image subsets greater than 0.99 for each of them. Figure 4a shows the histogram of the rotations measured by D-DVC. The rotation measurements follow a normal distribution with a mean value of 4.998° deg and 0.042° deg standard deviation. Rotations as obtained by this code are as accurate (*i.e.*, have similar mean error), but far more precise (*i.e.*, have much smaller error standard deviation), than those obtained with the ID-track implemented by Andò [32]. Indeed, the coefficient of variation (standard deviation / mean) of measurement error is here below 1%, while it was above 400% for ID-track. Another way of conveying this information is by means of a stereogram of the computed grain rotations (Figure 4b). The radial distance from the centre of the stereoplot represents the inclination θ , whereas the angles on the external perimeter represent the azimuth φ . As ex-

pected, all the grain rotations are located at the centre of the stereoplot ($\theta = 0^\circ$), indicating rotations around the vertical axis, with very low deviation from the vertical. Finally, Figure 4c illustrates the relation between measured rotation and sphericity; it is clear that the deviation from the exact solution (5° deg) increases symmetrically with the sphericity of the grains. However, the deviation remains very limited (around $\pm 0.1^\circ \text{ deg}$) and, therefore, this inbuilt bias can be safely ignored.

(a)

(b)

Figure 4a-b-c: (a) Histogram of measured rotation after rigid rotation of the specimen (b) Stereoplot showing the rotation vector of each grain (c) 2D histogram showing the correlation between grains sphericity and grains rotation.

3.5 Shear band identification

The two specimens analysed in this work showed localised deformation through shear banding [54]. In shear bands void ratio increases, coordination numbers are much reduced and the microstructural constraints on kinematics are therefore very different. Before examining the relation between grain shape and grain kinematics it was therefore necessary to first classify the grains, separating those that belonged to the shear band and those that did not. The criterion applied here to classify the grains as belonging to the shear band was based on shear strain.

To assign a nominal deviatoric strain to each grain we applied a procedure developed for DEM post-processing by Catalano et al. [62]. In this procedure, available within the code YADE [63], a Voronoi cell hosting each grain is created using a regular Delaunay triangulation having as vertices the mass centres of the labelled grains. Thus, the grain

position at the last loading increments (*i.e.*, 15-16 for HNEA01, 10-11 for COEA04) were calculated by D-DVC and then introduced in YADE. Displacements of neighbouring grains were then used to compute a nominal displacement gradient tensor for the tetrahedrons whose vertices are the grains centres of mass. A nominal averaged deviatoric strain, ε_{d_g} was projected back to each grain and a threshold value of ε_{d_g} was used to classify the grains that belonged to the shear band.

4 Results

4.1 Shear band identification

The results of the shear band identification procedure are shown in Figure 5, in which the black grains form the “shear band”: it contains 7007 grains for COEA04, and 21000 for HNEA01. The threshold value ε_{d_g} is set at 0.10; the zones identified correspond closely to those apparent in previous studies [54]. A sensitivity study to evaluate of the effect of varying this threshold value was carried out, very little changes were observed for values within the range 0.05 – 0.20.

The local reference system that will be used to define the virtual plane representing the shear band is shown in Figure 6, in which vector $\vec{n}$ is the normal to the plane and vector $\vec{a}$ indicates the steepest slope direction in the plane. According to Figure 3, showing the spherical coordinates system, both specimens present a shear band with an inclination angle (θ) of about 45°.

Figure 5: Shear band identification for specimens COEA04 (a) and HNEA01 (b). Particles are coloured black if the “micro-strain” [62] calculated on the Voronoi domain centred on the particle is greater than 0.10 (i.e., they belong to the shear band).

Figure 6: Local reference system for the shear band

Vector $\vec{b}$ is orthogonal to $\vec{n}$ and $\vec{a}$ and therefore is horizontal ($\theta = 90^\circ$). It can be used to characterise the azimuthal orientation of the shear band with respect to the global Cartesian coordinates system. The azimuth (φ) is different, being of about 135° for Hostun and 75° (from the global x -axis) for Caicos. The sections represented in Figure 5 correspond then to vertical planes orthogonal to vector $\vec{b}$.

4.2 Spatial distribution of grain shapes and shear localisation

A check was performed to verify if particle shape was spatially homogeneously distributed in the specimens. The reason was to exclude any possibility that subsequent localisation into shear bands was prompted by non-uniformity in the initial spatial distribution of grain shapes (note that a similar check was performed by Andò [54] with respect to local porosity). To do so, two vertical sections orthogonal to each other (defined respectively by vectors $\vec{n}-\vec{b}$ and $\vec{n}-\vec{a}$) are examined where the grains have been coloured by their value of degree of true sphericity, as shown in Figure 7. It is evident that grain true sphericity was initially homogeneously distributed within both specimens.

Figure 7: Sphericity spatial distribution for Hostun and Caicos sand in two vertical sections: parallel and perpendicular to the shear band.

Another check was performed on the possibility that shear banding would entrap or select particular grain shapes. To this end, histograms of the degree of true sphericity for the grains located both inside and outside the shear band were plotted; the results are shown in Figure 8. Again, it is evident that there are no significant differences of shape between the grains that were involved in the localisation process and those that remained outside the shear band.

Hostun
HNEA01

(a)

Caicos
COEA04

(b)

Figure 8: Histograms of true sphericity for Hostun (a) and Caicos (b) sands both inside and outside the shear bands.

4.3 Overall grain kinematics

Figure 9 and Figure 10 show the *cumulative* kinematic histories, in terms of vertical displacements and rotations, for Caicos ooids (specimen COEA04) and Hostun sand (specimen HNEA01) during several loading increments in the triaxial test (note that similar images, but reporting *incremental* instead of *cumulative* values were presented by Andò [32]. Results for both sands are plotted at the same scale and confirm the general observation made from incremental results by Andò [32]: within the shear band, the very rounded Caicos sand grains rotate more than the more angular grains of Hostun sand. On the other hand, it is difficult to tell the difference between the two sands outside the shear band.

Figure 9: Vertical slices of Caicos sand (specimen COEA04) showing grain vertical displacement (above) and rotation (below) *accumulated* during the test. Grains are coloured by the value of their measured z-

displacement (above) and total rotation (below). Not all the increments are shown. Stage “01” = start of deviatoric loading. Stage “11” = end of the TX test.

Figure 10: Vertical slices of Hostun sand (specimen HNEA01) showing grain vertical displacement (above) and rotation (below) **accumulated** during the test. Grains are coloured by the value of their measured z-displacement (above) and total rotation (below). Not all the increments are shown. Stage “01” = start of deviatoric loading. Stage “16” = end of the TX test.

This observation is conveyed more precisely in Figure 11, showing the histories of the cumulated mean particle rotation magnitudes, both inside and outside the shear bands. Outside the shear band, the average grain rotations of both sands are very similar and appear quite flat, with a limited increase between 1% and 5% axial strain. That increase in the average rotation outside the shear band may reflect the fact that the shear bands become somewhat narrower as deformation progresses [54], whereas the grain classification criterion is only applied in the final test stage.

Figure 11: Histories of cumulated mean particle rotations inside and outside the shear bands (SB in the legend), measured by D-DVC throughout the triaxial tests. The green dots represent interpreted results from Alshibli and Alramahi (2006) for a triaxial experiment involving 400 plastic pearls.

Average rotations increase much faster within the shear band. In the Caicos specimen (COEA04) average rotation magnitude raises to about 30 degrees. The trend in the Hostun specimen (HNEA01) is somewhat slower, raising to a level of about 21 degrees. The distribution of cumulative rotation magnitudes in the shear bands is rather skewed (Figure 12) with the mode remaining almost constant but the high end tail progressively thickening.

Figure 12: Distribution of accumulated particle rotation magnitudes at different test stages (12-14-16) for particles within the shear band of the Hostun sand HNEA01 specimen.

The attrition rate during this sequence of image correlations is shown in Figure 13. It is clear that in this more realistic context, the D-DVC procedure has more difficulties than in the idealized uniform rotation check discussed before. The correlation problems increase as the grains rotate more, which is what happens in the shear band. Despite that, it should be noted that a) the correlation validity criterion was set at a very stringent limit ($CC = 0.98$) and b) the procedure was able to track to the end almost 80% of the grains within the shear bands and more than 95% outside them.

Figure 13: Particles with correlation maximum below 98% as a percentage of total number of particles

4.4 A comparison of secant and cumulative tangent rotations

There is a risk that the secant image correlation approach applied may lead to an under-estimation of the cumulated total grains rotations, as it computes the “shortest path” of rotation (i.e., the minimum rotation angle) between the initial configuration and that of each step examined. Adding the results from tangent step-by-step correlations such as those performed by Andò [32] would avoid the underestimation problem but, as previously explained, grain re-labelling across images complicates tracking individual grains. Despite that, a meaningful statistical comparison is still possible based on the average values of rotations for all grains.

Figure 14 shows the evolution of the average magnitude of grain rotations for Hostun sand for all grains in the specimen as obtained by Andò [32] using step-by-step (i.e. tangent) correlations. This is compared with the values obtained here using the secant approach for two different scenarios. In the first one (corresponding to the results shown above) the average rotation at each step is computed only for the remaining grains (i.e.

those that are above the correlation threshold). In the second approach the average at each step is computed for all grains, assigning to those that are below the correlation threshold the last rotation value that was obtained for them.

Figure 14: History of the average magnitudes of rotations for Hostun sand measured with different approach. The error bars are magnified 10 times.

The differences between the “tangent” and “secant” correlation approaches are small. The results for the all-grain secant average are closer to those of the tangent because in the step-by-step correlations the number of grain losses was minimal, whereas in the secant approach the attrition rate is close to 20% at the end of the test. Moreover, the grains that are lost are typically those with larger rotations, which is reflected in the progressive divergence of the average restricted to the remaining grains. In any case, it is clear from the comparison that the grain rotations computed with the secant approach are not significantly underestimated.

4.5 Axes of rotation

Stereoplots (see Figure 4b) can be used to investigate the alignment of particle rotation axes during shearing. The orientations of *cumulative* rotation versors are plotted for all grains (about 110000 in total), both inside and outside the shear bands, at two different test stages in Figure 15 (at approximately 5% axial strain, corresponding to steps 01-09 in Hostun and 01-06 in Caicos) and Figure 16 (at approximately 9% axial strain, corresponding to 01-12 for Hostun and 01-09 for Caicos). The raw stereoplots are presented alongside binned frequency diagrams.

Figure 15: Stereoplots showing the rotation versor directions at 5% shortening. The green dots indicate the orientation of vector $\vec{b}$ (see Figure 6) belonging to the shear bands of Hostun and Caicos sands. The stereoplot angles markers are not shown for readability, see Figure 4b for reference.

Figure 16: Stereoplots showing the rotation vector directions at 9% shortening. The green dots indicate the orientation of vector $\vec{b}$ (see Figure 6) belonging to the shear bands of Hostun and Caicos sands. Stereoplot grid not shown for readability, see Figure 4b for reference.

Both sands exhibit similar trends (Figure 15). Outside the shear bands, the rotation axes accumulate towards the periphery of the stereoplot, with inclination angles close to 90° that indicate horizontal axes of rotation. The azimuthal angle, on the other hand, is almost homogeneously distributed around the stereoplot periphery, indicating no preferential alignment for the grain rotational axis within the horizontal plane.

The situation is different inside the shear band, which is already present at 5% strain (Figure 9; Figure 10). The rotation axes are still mainly horizontal ($\theta = 90^\circ$), but now the azimuthal angles (φ) concentrate around values of about 135° (Hostun sand) and 75° (Caicos sand). As indicated in the figures these values are, precisely, the azimuths of vector $\vec{b}$ in Figure 6 *i.e.*, those corresponding to directions orthogonal to that of steepest descent within the shear band. This alignment means that grains are rolling downslope the plane of the shear band. Another azimuthal accumulation point is observed at the diametrically opposed direction in the stereoplot, that is at 315° for Hostun and 255° for

Caicos. That position corresponds to grains rotating upslope on the plane of the shear band. These preferential orientations become sharper as localisation progresses (compare with results at 9% axial strain, shown in Figure 16) and appear generally sharper for Hostun sand than for Caicos ooids.

The results obtained contrast with those presented in Andò et al. [32] who attempted a similar analyses for the Hostun HNEA01 specimen. There the alignment of particle rotation axis and shear band normal was not evident. The difference is likely due to the superior precision of particle rotation measurement achieved by the D-DVC technique over the ID-track used in Andò et al. [32]. The presence of particle with opposite spins in shear zones, previously documented in experiments with simplified granular media (such as flat disks [64, 65] or uniform plastic beads [40]), is here confirmed for natural sands.

4.6 Relations between grain shape and magnitude of rotation

A first indication of the relationship between particle shape and rotation is already evident in Figure 11. Caicos ooids rotate – on average – far more than Hostun sand grains, but only if belonging to the shear band; for grains that remained outside the shear band there is almost no difference between the more rounded Caicos ooids and the angular Hostun sand. This insensitivity to particle shape outside the critical shearing zone is corroborated by data deduced from Alshibli and Alramahi [40], also plotted in Figure 11. Those authors reported histograms of particle rotations for 400 perforated plastic pearls, almost uniformly spherical, in a triaxial compression test that did not present a clear

shear band. The averaged rotations from that test on plastic beads plot very close to our sand data.

Although averaged values of rotation are interesting, the data collected allow a more detailed inspection of the effect of grain shape on rotation. Figure 17 presents bivariate frequency density plots exploring the effect of shape descriptors related to form on particle rotations (accumulated up to 5% axial strain). The histogram contours appear rather flat, indicating little sensitivity of particle rotations to form. The same approach is followed in Figure 18, but now using shape descriptors that measure sphericity. The histogram contours are more sensitive, particularly those at the edge, indicating larger percentiles. This is particularly evident for convexity and to true sphericity – two shape descriptors that are tightly correlated for these two sands, see [26]).

Figure 17: Normalised bivariate frequency density plots of **form** descriptors versus **cumulative** grain rotation magnitude at 5% shortening (loading stages HNEA01-09 and COEA04-06, respectively 48.612 and 65.056 grains). The contours colour bar is shown in Figure 4c.

Figure 18: Normalised bivariate frequency density plots of *sphericity* descriptors versus the *cumulative* grain rotations measured at 5% shortening (loading stages HNEA01-09 and COEA04-06, respectively 48.612 and 65.056 grains). The contours colour bar is shown in Figure 4c.

Figure 19: Normalised histograms showing the observed relation between the degrees of true sphericity and the total grains rotation measured at 5% sample shortening.

The histograms become more triangular if restricted to particles in the shear band. Figure 19 shows that the *degree of true sphericity* seems to have a significant influence on the upper limit of particle rotation, which increases as particles become more spherical. This idea is explored in more detail in Figure 20 and Figure 21, where mean and extreme values (99.5% percentiles) of rotation, measured on both Caicos sand and Hostun sand

specimens, are plotted as a function of true sphericity. The values are derived from marginal distributions, obtained at fixed true sphericity intervals (width 0.025). Because the number of particles in each interval is highly variable, error bands (plus and minus one standard error) are also represented. The error bands for the 99.5% quantile are estimated using a bootstrapping technique [66], resampling with replacement the original samples (for each interval) one thousand times. Errors band thickness increases with small sample sizes (e.g. at low values of *degree of true sphericity*) and with marginal variability (high at large values of *degree of true sphericity*, as correlating very spherical grains carries more uncertainty).

It appears that the mean values of rotation, both inside and outside the shear band are insensitive to particle sphericity, whereas the extreme upper values (the 99.5 % percentile) show a clear positive dependency between rotations and particle sphericity. There is not much difference between the mean values of Caicos and Hostun, at any given true sphericity. On the other hand, the upper limit rotations of Caicos are somewhat above those of Hostun, even at the same sphericity, and particularly for those particles inside the shear band. Andò [54] observed that porosity in the shear band was higher for Hostun than for Caicos, so it is unlikely that connectivity – which is inversely related to porosity – will explain that difference. Still, the differences between the two sands not accounted for true sphericity are less important than the common effect of sphericity on the upper bound. These trends were confirmed when other test stages were analysed, for instance at around 9% axial strain, Figure 22 and Figure 23.

Figure 20: Influence of the degree of true sphericity on the total grains rotation (at 5% shortening) outside the shear band.

Figure 21: Influence of the degree of true sphericity on the total grains rotation (at 5% shortening) inside the shear band.

Figure 22: Influence of the degree of true sphericity on the total grains rotation (at 9% shortening) outside the shear band.

Figure 23: Influence of the degree of true sphericity on the total grains rotation (at 9% shortening) inside the shear band.

5 Discussion

From the previous result it may be concluded that the link between particle shape and particle kinematics is only effective at the margin. This was to be expected, as it is a link necessarily mediated by particle connectivity. Particle shape cannot control particle rotation on its own, as rotational equilibrium is a result of contact force magnitudes and

positions and, as such, a result of particle shape and particle connectivity. In a shear band, particle connectivity is low and therefore the role of particle shape in controlling rotation is increased. The same reasoning suggests that particle shape effects should be more intense in loose than in dense sand. This may explain the different effect of particle shape dependency of extreme void ratios, which is even stronger for the minimum than for the maximum void ratio [4].

The interplay of connectivity and particle shape can also be related to the stress-strain response of the sand specimens illustrated in Figure 2. It is apparent that both specimens reach a similar value of peak strength, despite the Caicos specimen being initially denser than Hostun ($e = 0.468$ vs $e = 0.658$). The inter-granular contact friction angle of Caicos is likely similar to that of Hostun [67; 68]. This leaves the more spherical shape of Caicos as the likely cause of a peak appearing at lower densities than in the more angular Hostun. Other mesoscopic effects of shape are apparent in the lower residual strength of Caicos, which may be related to the larger rotations observed for this material in the shear band.

The previous observations cannot be proved by image analysis only, at least until particle connectivity can be imaged in experiments with equal precision as shape. The alternative, obviously, is to use DEM. The particle scale results presented here may be used to calibrate and/or verify DEM models in which shape effects are represented. If a direct representation of shape is used [69] it may be expected that the differential trends in particle kinematics noted here would also emerge from the simulations. A different approach is proposed in [70, 71] where the observed particle kinematics are used to calibrate a general link between moment-rotation contact law parameters and particle sphericity.

6 Conclusions

This paper set out to explore the relationship between particle shape and particle rotation at the grain scale, for all the sand grains within triaxial specimens that failed in a localised shear mode. The main findings can be summarised as follows:

- The systematic use of Discrete-Digital Volume Correlation allowed successful tracking of rotational kinematics in the large majority of grains; those measurements were far more precise than previous attempts using ID-track;
- Kinematics within the shear bands are very different from those outside the shear band. Particle rotation magnitudes increase much faster in the bands. Rotational axes align themselves preferentially, perpendicular to the steepest descent direction of the band;
- Sand grains in the shear plane show both positive and negative spins (upwards and downwards the plane), revealing commonalities in the shear flow mechanisms of sands with those of simpler granular materials;
- Shape descriptors related to particle form, such as elongation or flatness indexes appear to be poorly correlated with observed particle rotation;
- Shape descriptors related to particle sphericity have a significant effect on particle rotation. This effect is far less important on the average value than on the upper limit of rotation.

These findings are applicable to particles of relatively rotund shapes, such as the sand grains examined here, and may not necessarily apply to flatter or more elongated particles.

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8 References

1. Jiang, M., Liu, F., Bolton, M.: Proceedings of the International Symposium on Geomechanics and Geotechnics: from Micro to Macro (IS-Shanghai 2010). CRC Press/Balkema, Shanghai (2011)
2. Soga, K., Kumar, K., Biscontin, G., Kuo, M.: Geomechanics from micro to macro : Proceedings of the TC105 ISSMGE International Symposium on Geomechanics from Micro to Macro, Cambridge, UK, 1-3 September 2014. (2014)
3. Baudet, B., Bolton, M.: Editorial Soil mechanics at the grain scale: issue 1 and 2. *Géotechnique*. 60, 313–314 (2010). doi:10.1680/geot.2010.60.5.313
4. Cho, A.G., Dodds, J., Santamarina, J.C.: Particle Shape Effects on Packing Density, Stiffness and Strength – Natural and Crushed Sands. *J. Geotech. Geoenvironmental Eng.* 132, 591–602 (2006). doi:10.1061/(ASCE)1090-0241(2006)132:5(591)
5. Santamarina, J., Cho, G.: Soil behaviour: The role of particle shape. In: *Advances in Geotechnical Engineering. Proceedings of the Skempton Conference*. pp. 1–14., London (2004)
6. Yang, J., Luo, X.D.: Exploring the relationship between critical state and particle shape for granular materials. *J. Mech. Phys. Solids*. 84, 196–213 (2015).

doi:10.1016/j.jmps.2015.08.001

7. Xiao, Y., Long, L., Matthew Evans, T., Zhou, H., Liu, H., Stuedlein, A.W.: Effect of Particle Shape on Stress-Dilatancy Responses of Medium-Dense Sands. *J. Geotech. Geoenvironmental Eng.* 145, (2019). doi:10.1061/(ASCE)GT.1943-5606.0001994
8. Vaid, Y., Chern, J., Tumi, H.: Confining pressure, Grain angularity and Liquefaction. *J. Geotech. Eng.* 111, 1229–1235 (1985)
9. Liu, Q.B., Lehane, B.M.: The influence of particle shape on the (centrifuge) cone penetration test (CPT) end resistance in uniformly graded granular soils. *Géotechnique*. 60, 111–121 (2013). doi:10.1139/t06-037
10. Rothenburg, L., Bathurst, R.J.: Micromechanical features of granular assemblies with planar elliptical particles. *Géotechnique*. 42, 79–95 (1992). doi:10.1680/geot.1992.42.1.79
11. Ng, T.-T., Lin, X.: A three-dimensional discrete element model using arrays of ellipsoids. *Géotechnique*. 47, 319–329 (1997). doi:10.1680/geot.1997.47.2.319
12. Cleary, P.W.: The effect of particle shape on simple shear flows. *Powder Technol.* 179, 144–163 (2008). doi:10.1016/j.powtec.2007.06.018
13. Ferrellec, J.-F., McDowell, G.R.: A method to model realistic particle shape and inertia in DEM. *Granul. Matter.* 12, 459–467 (2010). doi:10.1007/s10035-010-0205-8
14. Jiang, M.J., Liu, J.D., Arroyo, M.: Numerical evaluation of three non-coaxial kinematic models using the distinct element method for elliptical granular materials. *Int. J. Numer. Anal. Methods Geomech.* 40, 2468–2488 (2016). doi:10.1002/nag.2540
15. Matsushima, T., Chang, C.S.: Quantitative evaluation of the effect of irregularly shaped particles in sheared granular assemblies. *Granul. Matters.* 13, 269–276

(2011). doi:10.1007/s10035-011-0263-6

16. Iwashita, K., Oda, M.: Rolling resistance at contacts in simulation of shear band development by DEM. *J. Eng. Mech.* 124, 285–292 (1998). doi:10.1061/(ASCE)0733-9399(1998)124:3(285)
17. Jiang, M.J.J., Yu, H.-S., Harris, D.: A novel discrete model for granular material incorporating rolling resistance. *Comput. Geotech.* 32, 340–357 (2005). doi:10.1016/j.compgeo.2005.05.001
18. Belheine, N., Plassiard, J.P., Donzé, F. V., Darve, F., Seridi, A.: Numerical simulation of drained triaxial test using 3D discrete element modeling. *Comput. Geotech.* 36, 320–331 (2009). doi:10.1016/j.compgeo.2008.02.003
19. Huang, X., Hanley, K.J., O’Sullivan, C., Kwok, C.Y.: Implementation of rotational resistance models: A critical appraisal. *Particuology.* 34, 14–23 (2017). doi:10.1016/j.partic.2016.08.007
20. Coetzee, C.J.: Calibration of the discrete element method and the effect of particle shape. *Powder Technol.* 297, 50–70 (2016). doi:10.1016/j.powtec.2016.04.003
21. Guillard, F., Marks, B., Einav, I.: Dynamic X-ray radiography reveals particle size and shape orientation fields during granular flow. *Sci. Rep.* 7, 1–11 (2017). doi:10.1038/s41598-017-08573-y
22. Oda, M., Takemura, T., Takahashi, M.: Microstructure in shear band observed by microfocus X-ray computed tomography. *Géotechnique.* 54, 539–542 (2004)
23. Matsushima, T., Uesugi, K., Nakano, T., Tsuchiyama, A.: Visualization of Grain Motion inside a Triaxial Specimen by Micro X-ray CT at SPring-8. In: Desrues, J., Besuelle, P., and Viggiani, G. (eds.) *Advances in X-ray Tomography for Geomaterials.* pp. 35–52. , London (2006)

- 691 24. Hall, S.A., Bornert, M., Desrues, J., Pannier, Y., Lenoir, N., Viggiani, G., Bésuelle,
692 P.: Discrete and continuum analysis of localised deformation in sand using X-ray
693 μ CT and volumetric digital image correlation. *Géotechnique*. 60, 315–322 (2010).
694 doi:10.1680/geot.2010.60.5.315
- 695 25. Hasan, A., Alshibli, K.A.: Experimental assessment of 3D particle-to-particle
696 interaction within sheared sand using synchrotron microtomography.
697 *Géotechnique*. 60, 369–379 (2010). doi:10.1680/geot.2010.60.5.369
- 698 26. Rorato, R., Arroyo, M., Andò, E., Gens, A.: Sphericity measures of sand grains.
699 *Eng. Geol.* 254, 43–53 (2019). doi:10.1016/j.enggeo.2019.04.006
- 700 27. Alshibli, K.A., Druckrey, A.M., Al-Raoush, R.I., Weiskittel, T., Lavrik, N. V.:
701 Quantifying Morphology of Sands Using 3D Imaging. *J. Mater. Civ. Eng.* 27,
702 (2015). doi:10.1061/(ASCE)MT.1943-5533.0001246
- 703 28. Zhao, B., Wang, J.: 3D quantitative shape analysis on form, roundness, and
704 compactness with micro-CT. *Powder Technol.* 291, 262–275 (2016).
705 doi:10.1016/j.powtec.2015.12.029
- 706 29. Kong, D., Fonseca, J.: Quantification of the morphology of shelly carbonate sands
707 using 3D images. *Géotechnique*. 68, 249–261 (2018). doi:10.1680/jgeot.16.P.278
- 708 30. Fonseca, J., O’Sullivan, C., Coop, M.R., Lee, P.D.: Non-invasive characterization
709 of particle morphology of natural sands. *Soils Found.* 52, 712–722 (2012).
710 doi:10.1016/j.sandf.2012.07.011
- 711 31. Fonseca, J., O’Sullivan, C., Coop, M.R., Lee, P.D.: Quantifying the evolution of soil
712 fabric during shearing using directional parameters. *Géotechnique*. 63, 818–829
713 (2013). doi:10.1680/geot.11.P.150
- 714 32. Andò, E., Hall, S.A., Viggiani, G., Desrues, J., Bésuelle, P.: Grain-scale

- 715 experimental investigation of localised deformation in sand: A discrete particle
716 tracking approach. *Acta Geotech.* 7, 1–13 (2012). doi:10.1007/s11440-011-0151-6
- 717 33. Hasan, A., Alshibli, K.: Three dimensional fabric evolution of sheared sand.
718 *Granul. Matter.* 14, 469–482 (2012). doi:10.1007/s10035-012-0353-0
- 719 34. Higo, Y., Oka, F., Sato, T., Matsushima, Y., Kimoto, S.: Investigation of localized
720 deformation in partially saturated sand under triaxial compression using
721 microfocus X-ray CT with digital image correlation. *Soils Found.* 53, 181–198
722 (2013). doi:10.1016/j.sandf.2013.02.001
- 723 35. Alshibli, K.A., Jarrar, M.F., Druckrey, A.M., Al-Raoush, R.I.: Influence of Particle
724 Morphology on 3D Kinematic Behavior and Strain Localization of Sheared Sand.
725 *J. Geotech. Geoenvironmental Eng.* 143, 04016097 (2017).
726 doi:10.1061/(ASCE)GT.1943-5606.0001601
- 727 36. Cheng, Z., Wang, J.: A particle-tracking method for experimental investigation of
728 kinematics of sand particles under triaxial compression. *Powder Technol.* 328,
729 436–451 (2018). doi:10.1016/j.powtec.2017.12.071
- 730 37. Wiebicke, M., Andò, E., Herle, I., Viggiani, G.: On the metrology of interparticle
731 contacts in sand from x-ray tomography images. *Meas. Sci. Technol.* 28, 124007
732 (2018)
- 733 38. Wiebicke, M., Andò, E., Salvatore, E., Viggiani, G., Herle, I.: Experimental
734 measurement of granular fabric and its evolution under shearing. In: Radjai, F.,
735 Nezamabadi, S., Luding, S., and Delenne, J.Y. (eds.) *European Physical Journal*
736 *Web of Conferences.* p. 02020. EDP Sciences (2017)
- 737 39. Wiebicke, M., Andò, E., Šmilauer, V., Herle, I., Viggiani, G.: A benchmark strategy
738 for the experimental measurement of contact fabric. *Granul. Matter.* 21:54, 1–13

- 739 (2019). doi:10.1007/s10035-019-0902-x
- 740 40. Alshibli, K.A., Alramahi, B.A.: Microscopic Evaluation of Strain Distribution in
741 Granular Materials during Shear. *J. Geotech. Geoenvironmental Eng.* 132, 80–91
742 (2006). doi:10.1061/(asce)1090-0241(2006)132:1(80)
- 743 41. Vlahinić, I., Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E.: From computed
744 tomography to mechanics of granular materials via level set bridge. *Acta Geotech.*
745 12, 85–95 (2017). doi:10.1007/s11440-016-0491-3
- 746 42. Cheng, Z., Wang, J.: Experimental investigation of inter-particle contact evolution
747 of sheared granular materials using X-ray micro-tomography. *Soils Found.* 58,
748 1492–1510 (2018). doi:10.1016/j.sandf.2018.08.008
- 749 43. Sutton, M.A., Schreier, H.W., Orteu, J.-J.: Image correlation for shape, motion and
750 deformation measurements: basic concepts, theory and applications. Springer
751 (2009)
- 752 44. Hall, S.A.: Digital Image Correlation in Experimental Geomechanics. In:
753 Gioacchino Viggiani, Stephen A. Hall, and Enrique Romero (eds.) *ALERT*
754 *Doctoral School 2012 Advanced experimental techniques in geomechanics.* pp.
755 69–102. , Aussois (France) (2012)
- 756 45. Take, W.A.: Thirty-Sixth Canadian Geotechnical Colloquium: Advances in
757 visualization of geotechnical processes through digital image correlation. *Can.*
758 *Geotech. J.* 52, 1199–1220 (2015). doi:10.1139/cgj-2014-0080
- 759 46. Pan, B., Qian, K., Xie, H., Asundi, A.: Two-dimensional digital image correlation
760 for in-plane displacement and strain measurement: a review. *Meas. Sci. Technol.*
761 20, (2009). doi:10.1088/0957-0233/20/6/062001
- 762 47. Stanier, S.A., Blaber, J., Take, W.A., White, D.J.: Improved image-based

- 763 deformation measurement for geotechnical applications. *Can. Geotech. J.* 53, 727–
764 739 (2016). doi:10.1139/cgj-2015-0253
- 765 48. Pinyol, N.M., Alvarado, M.: Novel analysis for large strains based on particle
766 image velocimetry. *Can. Geotech. J.* 54, 933–944 (2017)
- 767 49. Andò, E., Hall, S.A., Viggiani, G., Desrues, J., Bésuelle, P.: Experimental
768 micromechanics: grain-scale observation of sand deformation. *Géotechnique Lett.*
769 2, 107–112 (2012). doi:10.1680/geolett.12.00027
- 770 50. Wadell, H.: Volume, Shape, and Roundness of Rock Particles. *J. Geol.* 40, 443–451
771 (1932)
- 772 51. Barret, P.J.: The shape of rock particle, a critical review. *Sedimentology.* 27, 291–
773 303 (1980). doi:10.1111/j.1365-3091.1980.tb01179.x
- 774 52. Zingg, T.: Beitrag zur Schotteranalyse, [http://e-](http://e-collection.library.ethz.ch/view/eth:21472)
775 [collection.library.ethz.ch/view/eth:21472](http://e-collection.library.ethz.ch/view/eth:21472), (1935)
- 776 53. Krumbein, W.C.: Measurement and Geological Significance of Shape and
777 Roundness of Sedimentary Particles. *J. Sediment. Res.* 11, 64–72 (1941)
- 778 54. Andò, E.: Experimental investigation of microstructural changes in deforming
779 granular media using x-ray tomography, (2013)
- 780 55. Salvatore, E., Modoni, G., Andò, E., Albano, M., Viggiani, G.: Determination of
781 the critical state of granular materials with triaxial tests. *Soils Found.* 57, 733–744
782 (2017). doi:10.1016/j.sandf.2017.08.005
- 783 56. Viggiani, G., Andò, E., Takano, D., Santamarina, J.C.: Laboratory X-ray
784 Tomography: A Valuable Experimental Tool for Revealing Processes in Soils.
785 *Geotech. Test. J.* 38, 61–71 (2015). doi:10.1520/GTJ20140060
- 786 57. Lorensen, W.E., Cline, H.E.: Marching cubes: A high resolution 3D surface

- 787 construction algorithm. ACM siggraph Comput. Graph. 21, 163–169 (1987).
- 788 doi:10.1145/37402.37422
- 789 58. Tudisco, E., Andò, E., Cailletaud, R., Hall, S.A.: TomoWarp2: A local digital
790 volume correlation code. SoftwareX. 6, 267–270 (2017).
791 doi:10.1016/J.SOFTX.2017.10.002
- 792 59. Campello, E.M.B.: A description of rotations for DEM models of particle systems.
793 Comp. Part. Mech. 2, 109–125 (2015). doi:10.1007/s40571-015-0041-z
- 794 60. Andò, E., Cailletaud, R., Roubin, E., Stamati, O., the spam contributors: SPAM:
795 The Software for the Practical Analysis of Materials, (2017)
- 796 61. Pannier, Y., Lenoir, N., Bornert, M.: Discrete volumetric digital image correlation
797 for the investigation of granular type media at microscale: accuracy assessment.
798 EPJ Web Conf. 6, (2010). doi:10.1051/epjconf/20100635003
- 799 62. Catalano, E., Chareyre, B., Barthélémy, E.: Pore-scale modeling of fluid-particles
800 interaction and emerging poromechanical effects. Int. J. Numer. Anal. Methods
801 Geomech. 38, 51–71 (2014). doi:10.1002/nag.2198
- 802 63. Šmilauer, V. et al.: Yade Documentation 2nd ed. The Yade Project. (2015)
- 803 64. Veje, C.T., Howell, D.W., Behringer, R.P.: Kinematics of a two-dimensional
804 granular Couette experiment at the transition to shearing. Phys. Rev. E - Stat.
805 Physics, Plasmas, Fluids, Relat. Interdiscip. Top. 59, 739–745 (1999).
806 doi:10.1103/PhysRevE.59.739
- 807 65. Pasternak, E., Dyskin, A. V., Esin, M., Hassan, G.M., MacNish, C.: Rotations and
808 pattern formation in granular materials under loading. Philos. Mag. 95, 3122–3145
809 (2015). doi:10.1080/14786435.2015.1059517
- 810 66. Efron, B., Tibshirani, R.: An introduction to the bootstrap. Chapman & Hall (1994)

- 811 67. Cole, D. M. (2015). Laboratory observations of frictional sliding of individual
812 contacts in geologic materials. *Granular Matter*, 17(1), 95-110.
- 813 68. Nardelli, V., & Coop, M. R. (2019). The experimental contact behaviour of natural
814 sands: normal and tangential loading. *Géotechnique*, 69(8), 672-686.
- 815 69. Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E.: All you need is shape:
816 Predicting shear banding in sand with LS-DEM. *J. Mech. Phys. Solids*. 111, 375–
817 392 (2018). doi:10.1016/j.jmps.2017.10.003
- 818 70. Rorato, R., Arroyo, M., Gens, A., Andò, E., Viggiani, G.: Particle Shape
819 Distribution Effects on the Triaxial Response of Sands: A DEM Study. In: Giovine,
820 P. and et al. (eds.) *micro to MACRO Mathematical Modelling in Soil Mechanics*,
821 *Trends in Mathematics*. pp. 277–286. , Reggio Calabria (Italy) (2018)
- 822 71. Rorato, R., Arroyo, M., Gens, A., Andó, E. & Viggiani, G. (2020) Image-based
823 calibration of rolling resistance in discrete element models of sand, under review
824 *Computers & Geotechnics*