Manual for open-source database of 3D printed granular materials

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This document describes the data accompanying the joural article "Open-source support toward validating and falsifying discrete mechanics models using synthetic granular materials – Part I: Experimental tests with particles manufactured by a 3D printer" published in Acta Geotechnica.

This dataset is made available to third-parties as a part of the effort to make verification and validation procedures transparent and reproducible for granular material research. This dataset includes the the microCT images of Hostun sand and the synthetic particle manufactured by 3D printer, the results of the oedometric test conducted on assembles of synthetic particles, the labelled volume and the discrete digital correlation data that provides the trajectories of individual particles in the assembles. Due to a RAID failure, the data of the original X-ray scans taken during the oedometric tests from the fifth image onward were unable to recover and hence did not include in this dataset. Nevertheless, this dataset does provide sufficient information for readers to reproduce all published results in (Gupta et al., 2018).

The name of each section heading in this document is in line with the name of the folder in the shared database for the convenience of the user/reader. Herein it is listed in processing order:

1 Grain printing

To manufacture the synthetic granular materials, the geometrical information of the grain must be stored in the format compatible to the 3D printer. In this work, we use the STL file format. The procedure that converts the x-ray tomography of a real sand grain into STL file ready to generate a morphologically equivalent 3D printed grain is listed below.

1. Obtain a high resolution ($1\,\mu\text{m/px}$) 3D image stack of a real sand grain – in this work this is obtained by a nano-tomograph.

2. Convert this image stack to a .stl extension file; an input file format for 3D printing. This is done in following sequence:

   (a) Binarise image stack

   (b) Conversion to a signed distance function

   (c) Generate a surface mesh using CDT approach

   (d) Creation of an unstructured volumetric mesh

   (e) Model repair and examination using *meshlab* (Cignoni et al., 2008) software

   (f) Conversion of mesh to STL format

3. STL file (available in shared database) upload to manufacture (SCULPTEO) website and choose parameters (like constituent material, type of finish and grain size, see paper for settings used) for printing.

4. The original grain STL file size ($470.1\,\mathrm{mm} \times 566.1\,\mathrm{mm} \times 454.2\,\mathrm{mm}$) is down-scaled to printable size ($2.5\,\mathrm{mm} \times 3.0\,\mathrm{mm} \times 2.4\,\mathrm{mm}$) satisfying the solidity check (the 'fit to print' criteria for grain).

5. Based on solidity check results, conduct an optional 'critical area thickening' procedure to eliminate the delicate details in the STL file; making it 'fit for printing' (new size – $3.1\,\mathrm{mm} \times 3.7\,\mathrm{mm} \times 3.0\,\mathrm{mm}$).

6. Use so-called 'box printing method' to print a number of grains all together instead of printing each grain separately to save significant amount of money (in our case $\approx$100 times reduced production cost.)

2   Mechanical Oedometric test

Loading system data from oedometric loading of an assembly of 1522 3D printed particles specimen (cylindrical with diameter = $45\,\mathrm{mm}$ and height = $15\,\mathrm{mm}$), compressed *in-situ* inside the x-ray micro-tomograph in Laboratoire 3SR. Oedometric (1D) compression has been performed under displacement control in a PEEK cell with a PEEK ram, ensuring low friction. A floating ring cell is not used in this case. The displacement readings are not calibrated for the stiffness of the system, meaning that the displacement readings represent certain overestimation of the compression of the material inside the cell. A strain controlled (0.1% per minute) quasi-static test is performed up to 20% of vertical strain accompanying two additional unloading steps in the course.

The analysed spreadsheet of the mechanical oedometric test is available in the shared database.

3   X-ray tomography

During the test, loading is interrupted at a total of 18 positions and x-ray CT scans are performed (at $28\,\mathrm{\mu m/px}$ resolution) were performed to capture the state of specimen at a particular stain level. These scans produced 1600 number of radiographs which are then processed into a 3D volume using filtered back-projection for each scan. Reconstructions were performed with RX-Solution's UniCT reconstruction software, allowing a software beam-hardening correction, ring filtering and source drift correction. The 3D reconstruction of each state is saved as an individual 3D TIFF file with $1700\times1700\times699$ voxels (x,y,z) each describing 16-bit greyscale values proportional (with an offset) to a frequency-lumped x-ray attenuation coefficient.

The first three reconstructed 3D image sets are available in the shared database. It is important to mention here that total 18* number of such 3D image stacks were reconstructed in the present work representing the state of specimen in the course of mechanical loading in oedometric loading. Unfortunately, 15 of them are permanently lost due to a technical incident in the image data repository. An image stack file name presents the scan number and the vertical displacement of loading platen before the beginning of that particular scan. For example, '$02 - 150um'$' means scan number '02' at '$150\,\mathrm{\mu m}$' vertical displacement.

*Note: In reality, total 19 number of X-ray CT scans were made for one sample in its complete course of mechanical loading. The very first scan was carried out at the initial state (*i.e.* 0% strain) of specimen. However, after reconstruction, it was observed that the more appropriate initial state (in terms of sample surface contact with loading platen) is presented by the second scan (at 1% axial strain). Subsequently, scan number '02' is used to produce the 'labelled volume' and to carry out 'discrete digital image correlation' (as reference image stack) described in the two following sections.

4 Labelled volume

The first step to identifying individual grains is to convert the grey scale image to a binary image. This is achieved by making threshold to appropriate grey value below which the non-grain part or the voids are present. For the present studies, the pixel value range of [46626 – 65535] is used. After thresholding, the image is converted to 8-bit binary image with '0' gray value representing voids and '255' grey value representing grain. It is important to check the contacts between grains in binary image to avoid errors and false labelling of grains in later stages. There are number of ways to deal with this issue if so ever and most commonly used in image processing are Gaussian blur filters, erosion *etc.*

Once a satisfactory binary image is obtained, the second step comes into picture called grain labelling. This is indeed the backbone of grain-based analysis including particle tracking. The grain labelling for present study has been performed using the watershed algorithm implemented in processing package **Visilog** (Bernard et al., 2011). This yields an image volume in which each grain is assigned a unique integer label such that they can subsequently be identified.

The labelled image volume obtained in this work has been shared in the open-source database.

5 Discrete digital image correlation (DDIC)

As the name signifies, this is a DIC technique suited to tracking individual particle movement between 3D images. Figure 1 below is a representation of this technique which involves correlating each discrete grain (bounded in a virtual box) in the position 'A' and 'B' for 3D translation and rotation.
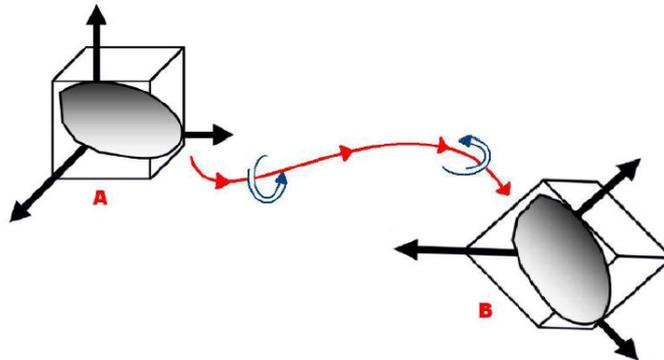

Figure 1: A general representation of Discrete DIC (Smit, 2010)

Discrete DIC uses the centre of mass of particles the measurement point. Just as in regular, local DIC approaches, the greylevel difference between the two images is minimised – in this case on a subvolume equal to the grain label in image 1 dilated twice . In this case a repeated subpixel search of 3 displacements and 3 rotations is performed using Broyden Fletcher Goldfarb Shanno (BFGS) as implemented in TomoWarp 2. A typical output result presenting from this code is shown in the figure 2 below, where node number should be interpreted as particle number:

Here, positions and displacements are in pixels, and the rotation is presented as a rotation vector in radians. 'CC' represents correlation coefficient which represents the quality of digital image correlation where the value '1' represents a perfect correlation. Moreover, the 'Error' is for the qualitative check with a particular number representing its certain specific type. In the present correlation work, Error type '32' was mostly observed for all the correlations. This is called 'search window error' which means that the size of search window was not correctly chosen for the indicated 'grain search' operation.

Starting from the labelled image, grain characteristics (label number, the centre of mass of the

NodeNumber	Zpos	Ypos	Xpos	Zdisp	Ydisp	Xdisp	Zrot	Yrot	Xrot	CC	Error
4	130.16623	166.29195	1152.67651	4.34952293	0.321917462	-1.125014111	-0.000187293	0.006727917	0.003632978	0.99889636	0
5	114.33384	205.30194	582.70026	5.357081124	0.073052073	-0.160418166	-1.30E-07	0.000283313	4.02E-05	0.999177694	0
6	131.82797	195.56383	803.35712	3.877156498	0.321744465	0.570511927	1.23E-05	-0.008611351	0.00104692	0.999027371	0
7	144.29277	129.7426	964.79541	4.704431017	-1.645846918	-0.083793391	0.006211619	-0.003152259	-0.04121811	0.999013901	0
8	114.76357	257.47028	1207.69983	6	1	2	0	0	0	0.988116264	32
9	121.79137	269.87643	785.9046	4	1	0	0	0	0	0.997450352	32
10	133.62459	254.49782	1284.08862	4.969611315	2.495030092	-0.583342984	-0.024611008	0.005898645	0.004802013	0.998696387	0
11	128.37701	228.13342	485.62991	5.423144257	-1.387230842	-0.574040138	0.000202419	0.001700162	-0.031447549	0.998925209	0

Figure 2: A typical DDIC output spreadsheet

grain as x, y, z coordinates and the coordinates of an x-y-z bounding box that contains each grain) can be computed and are saved as a TSV file. It is important to check the labelling output for unwanted labels (which may be due to two grains in contact, some small false particle due to noise in the image for example).

Notably, besides our best efforts, not all the grains are labelled representing a full grain without any split segment which is assigned a different label. This is evident from the mismatch of the total grain count in the specimen (1522 particles) and in the TSV file (1652 particles).

The TSV output spreadsheets from the DDIC operation have been added in the shared database. A typical file name includes two numbers (*e.g.* '02-09')** representing the reference image stack '02' and the image stack under treatment for DDIC. There are two sub-folders; one comprising DDIC results obtained using 'interpolation of the correlation coefficient' approach giving output for the grain translation only and the second folder comprises the results obtained using 'image interpolation' for both translation and rotations. In the second sub-folder there is another dataset which presents the additional details of computed 3D rotation in degrees using the norm of a vector approach.

Note: Figure 6(b) of the parent research article shows the X-ray CT scan number at a particular sample state. With due consideration to the outcome of note in section 3 (above), reader must add "one" to all the scan number in figure 6(b) while correlating the scan number and the corresponding spreadsheet in DDIC output file. For example, the TSV file named as '02-19' is the DDIC output file is the correlation of sample states presented by scan number '1' and '18' as per figure 6(b).

References

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