A new variable for characterising irregular element geometries in experiments and DEM simulations

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ABSTRACT

Discrete element method (DEM) has proved to be an excellent tool for modelling bulk materials. Contrarily to the early stages of these simulations when mainly circular and spherical elements were used, extensive research is going on regarding the application of complex element shapes, e.g. polyhedra. Robust and objective geometry characterisation methods are needed to quantify the shape of virtual and real particles in order to assess the effect of particle shape on the global mechanical behaviour.

This paper proposes a weighted fabric tensor that is able to characterise the shape of individual particles in such a way that the preferred potential load-bearing direction(s) are pointed out. The three eigenvalues of this tensor express whether the stone block or grain is compact, flaky, rod-like, or is an intermediate shape in between the three basic shapes. The proposed approach has computational advantages in quantifying the results of imaging processes of stones and grains deterministically without any subjectivity. It has the advance over the traditional bounding box approaches that it is directly based on the orientations of the surface normal vectors, i.e. those directions along which an assembly of stones or grains can best transmit the internal forces.

INTRODUCTION

Particle assemblies (e.g. sand, crushed stone, gravel) and collections of stone blocks are applied as load-bearing structures in several fields of engineering. The shapes of the grains that are used in an assembly significantly affect the overall mechanical behaviour, and hence there are different shape characteristics for the classification of stone geometries that serve as a basis for the design of such structures. Masonry structures are, for example, made up of individual stone blocks whose shape, especially in case of dry joints, have a significant impact on the load-bearing capacity of the whole structure. Another typical field where the grain shape has high importance is railway ballast stone aggregates (Fischer et al., 2015). The increasing demand for understanding the role of the shape of individual components on the mechanical properties of the whole structure created the need to define quantitative parameters for describing particles shape. Thorough overviews of the different suggestions are given in (Szabó, 2013) and (Guo et al., 2019).

Discrete element method (DEM) simulations (Bagi, 2007; Cundall and Strack, 1979) are frequently applied to study the effect of particle shape. There are two ways to mimic the interlocking effect of irregular geometries in assemblies in DEM models: (i) use simple (i.e. circular or spherical) elements along with a complex contact model (e.g. rolling resistance model) (Wensrich and Katterfeld, 2012), or (ii) apply more complex element shapes. Typically, bonded spheres (i.e. *clumps* or *clusters*), ellipsoids, poly-ellipsoids or convex polyhedra are used. In the case of the second approach, again, robust and subjective shape characterising methods are needed to prove the similarity of grain shapes between reality and virtual models. The aim of the present paper is to characterise not a complete assembly, but the individual shape of each stone in the assembly.

In practice, usually, four main types of shapes are distinguished: (1) "compact" (e.g. a sphere or a cube), (2) "flaky" or "disc-like" (e.g. a disc, or a flat prism), (3) "elongated" or "rod-like" (e.g. a thin column or a needle) and (4) flat-elongated, or blade-like, as done in Zingg's fundamental publication (Zingg, 1935). The classification is performed according to the relations between the three characteristic sizes of the analysed stone (termed in different ways in the literature, e.g. length, breadth (width) and thickness in (Wadell, 1932)). There are several studies and suggestions in the literature about how these sizes should be defined, but there has been no general agreement on "the" most suitable characterisation.

However, most of these characterisations are based on the "bounding box approach" (Domokos et al., 2015) whose main idea is to include the analysed grain in "the smallest" brick-shaped enclosing domain ("smallest"

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according to, e.g. its volume or surface). There is no general agreement today in the literature on exactly how to define this enclosing domain in experiments and simulations, and this introduces ambiguities into the definition of "length", "breadth" and "thickness" of the analysed particle. In any case, the dimensions $a \geq b \geq c$ are received as the side lengths of the domain, and then based on them, several alternative characteristics can be defined in order to classify the shape of the analysed grain.
Though the bounding box approach has been applied in the literature for a wide variety of purposes, from the point of view of load-bearing capacity of assemblies, it has the disadvantage that the suggested characteristics are based on a surrounding domain, and not directly on those faces of the stone on which it can form contacts with its neighbours for force transmission. In addition, modern imaging techniques (e.g. laser scanning (Asahina and Taylor, 2011) or computer tomography (Juhasz and Fischer, 2019)) provide a set of surface triangles (nodal coordinates) as their output, and the bounding box is not entirely straightforward to determine from these data. So, the present study aims to propose a completely deterministic and computationally simple alternative to the bounding box approach in such a way that the orientations of the faces of the stone would serve as the basis of the characterisation and classification.

FABRIC TENSORS

The proposed alternative is based on defining a weighted fabric tensor. Fabric tensors (Satake, 1982, 1983) have been applied for many decades on a wide variety of fields whenever the orientational distribution of a set of unit vectors had to be described. In most applications the contact normal vectors in the assembly gave the basic vector set on which the tensor was built; as an example, a recent application for the characterisation of stress-induced anisotropy can be found in (Shi and Guo, 2018). In the three-dimensional Cartesian (x_1, x_2, x_3) coordinate system, the general definition of the second-order fabric tensor of a set of M vectors of unit length $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$, … $\mathbf{v}^{(M)}$ is the following (Here $\circ$ denotes dyadic or tensor product.):

$$\boldsymbol{\varphi} = \frac{1}{M}\sum_{k=1}^{M}\left(\mathbf{v}^{(k)} \circ \mathbf{v}^{(k)}\right) \qquad (1)$$

This is a symmetric tensor hence its eigenvalues are real numbers and its eigenvectors are perpendicular to each other; in addition, the eigenvalues are nonnegative and sum up to 1. The eigenvector belonging to the largest / smallest eigenvalue expresses the most / least preferred orientation of the $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$, … $\mathbf{v}^{(M)}$ vector set, and the strength of the bias is expressed by the magnitude of the corresponding largest / smallest eigenvalue.
The terms in the summation may receive some characteristic weight (e.g. for $\mathbf{v}^{(k)}$ being the contact normal in an assembly, the magnitude of compression in the k-th contact can be applied for weighting, which means that more significant emphasis is given to those contacts in the system which carry larger compression than others), and even on the same set of unit vectors, different weighted fabric tensors can be produced, this way carrying different physical meanings.

DEFINITION OF THE NEW VARIABLE; THE SURFACE ORIENTATION TENSOR

Consider a grain or stone represented by a polyhedron with faces 1, 2, … k, …, and denote the corresponding outwards unit normals $\mathbf{n}^{(1)}$, $\mathbf{n}^{(2)}$, … $\mathbf{n}^{(k)}$, … . They belong to the faces whose areas are $A^{(1)}$, $A^{(2)}$, … $A^{(k)}$, … respectively. The surface orientation tensor is defined as follows:

$$\mathbf{f} = \frac{1}{\sum_k A^{(k)}}\sum_{(k)}\left(A^{(k)}\mathbf{n}^{(k)} \circ \mathbf{n}^{(k)}\right) \qquad (2)$$

where the summations go along the faces of the grain with running index (k).
This tensor has the following essential properties:

1. The tensor is symmetric. Consequently, its eigenvalues are real, and the eigenvectors are perpendicular to each other.
2. Its trace is equal to 1, and its three eigenvalues are nonnegative. Hence the three eigenvalues are between 0 and 1 so that they sum up to 1.
3. Any of the vectors $\mathbf{n}^{(k)}$ can be turned to its opposite without any effect on the resulting surface orientation tensor: because of the dyadic product of $\mathbf{n}^{(k)}$ with itself in the definition, the calculated $\mathbf{f}$ will not change. Hence, in the computations, the surface normals do not have to point outwards.

Denote the three eigenvalues as $f_1 \geq f_2 \geq f_3$. The eigenvector belonging to f_1 is that orientation about which the stone mostly prefers to have contacts with its neighbourhood. For example, for a thin, flat, disc-shaped polyhedral plate, the eigenvector belonging to f_1 is the orientation of the normal vector of the two large faces (remember Property 3). For a regular polyhedron of isotropic shape (e.g. a cube), the three eigenvalues are equal. For a very long and thin column, the smallest eigenvalue, f_3, is small, close to zero (belonging to the two distant, small closing faces of the column), and the two large eigenvalues are close to each other approaching 0.5.
Based on the three eigenvalues, the following geometrical quantities can be defined and then applied for the characterisation of individual stone shapes:

$$\text{Compactness: } C := \frac{f_3}{f_1} \qquad (3)$$

$$\text{Flakiness: } F := \frac{f_1 - f_2}{f_1} \qquad (4)$$

$$\text{Rodness: } R := \frac{f_2 - f_3}{f_1} \qquad (5)$$

Note that this method of characterisation can very easily be used in post-processing the output of 3D surface imaging techniques, which produce a point cloud that represents the surface of the grain with a specific density and precision, and from this, build a triangular mesh with suitable software. The surface orientation tensor and its eigenvalues are easy to determine from this triangular mesh and then, based on the eigenvalues, the three characteristics compactness, flakiness and rodness can simply be calculated.

EXAMPLES

As an introductory example, consider a brick with its edges oriented according to the (x_1, x_2, x_3) coordinate axes, so that the sizes of this brick be $a \geq b \geq c$, respectively (Figure 2).

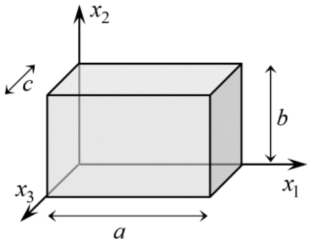

Figure 2: The Introductory Example: a Simple Brick

The areas and outward unit normals of the six faces are:

$$A_{right} = b \cdot c; \quad \mathbf{n}_{right} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad ; \tag{6}$$

$$A_{left} = b \cdot c; \quad \mathbf{n}_{left} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix} \quad ; \tag{7}$$

$$A_{top} = a \cdot c; \quad \mathbf{n}_{top} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad ; \tag{8}$$

$$A_{bottom} = b \cdot c; \quad \mathbf{n}_{bottom} = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix} \quad ; \tag{9}$$

$$A_{front} = a \cdot b; \quad \mathbf{n}_{front} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad ; \tag{10}$$

$$A_{left} = a \cdot b; \quad \mathbf{n}_{back} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix} \quad ; \tag{11}$$

From these, the surface orientation tensor is:

$$\mathbf{f} = \frac{1}{a \cdot b + a \cdot c + b \cdot c} \begin{bmatrix} b \cdot c & 0 & 0 \\ 0 & a \cdot c & 0 \\ 0 & 0 & b \cdot c \end{bmatrix} \tag{12}$$

which is a diagonal matrix so the eigenvalues can immediately be seen in the main diagonal. From them, the compactness is $C = f_3 / f_1 = c / a$; the flakiness is $F = (f_1 - f_2) / f_1 = 1 - (c / b)$; and the rodness $R = (f_2 - f_3)/f_1 = (a - b) \cdot c / a \cdot b = c / b - c / a$., A Python code was developed to analyse general geometries, which is able to process triangulated surface files in .stl format as its input and can compute the shape orientation tensor from this file. A few regular geometries were processed, which were created in a Computer-Aided Design (CAD) system to verify the code and the method. Every geometry was tested both with edges aligned parallel to the axes of the coordinate system and in a randomly chosen skew orientation. The geometries and their corresponding *C*, *F*, *R* values can be seen in Table 2. The verification was successful: even for the sphere being approximated with a finite number of triangular faces, the results provided by the code were in excellent agreement with the expectations, and the change of orientation had only a negligible effect.

Table 2: Regular Geometries in Verification Tests and their Shape Parameters

Geometry ([mm])	**Orient.**	***C***	***F***	***R***
Cube (10x10x10)	Aligned	1.000	0.000	0.000
	Random	1.000	0.000	0.000
Sphere (Ø10)	Aligned	0.9995	0.0000	0.0005
	Random	0.9995	0.0000	0.0005
Rod (50x1x1)	Aligned	0.0200	0.0000	0.9800
	Random	0.0200	0.0000	0.9800
Plate (50x50x1)	Aligned	0.0200	0.9800	0.0000
	Random	0.0200	0.9800	0.0000

For performing a more practical test of the proposed method, three representative grains were selected, one for each type of shape (Figure 3), out of 44 andesite crushed rock particles (source: KőKa andesite quarry, Komló, Hungary). DAVID structured light scanner was applied for the imaging of the surface. The triangulation and the mesh optimisation was executed with the built-in post processor belonging to the scanner.

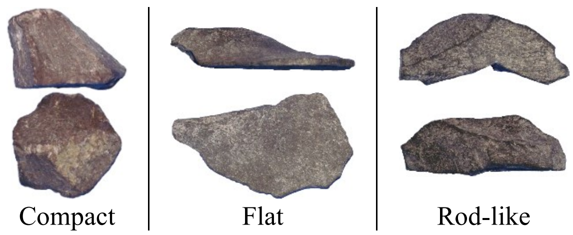

Figure 3: The Three Analysed Stones (Upper Images: Front View, Lower Images: Top View)

These grains were analysed manually as well. The three characteristic dimensions $a > b > c$ of the grains were measured with a calliper, and then their compactness, flakiness and rodness values were determined as:

$$C := \frac{c}{a} \quad ; \quad F := \frac{b - c}{a} \quad ; \quad R := \frac{a - b}{a} \tag{13}$$

These definitions are very similar to the widely used parameters of Sneed and Folk (Sneed and Folk, 1958), with the difference that they sum up to 1, similarly to those proposed parameters in Section 2 that are based on the fabric tensor. This way, these manually determined *C*, *F* and *R* parameters are directly comparable to those received from the surface orientation tensor, unlike the parameters by Sneed and Folk.
The authors note that while doing the calliper measurements, the subjective nature of measuring the necessary dimensions of the grains was experienced, and hence each dimension of each stone was measured five times, then averages were calculated for each dimension and each stone separately. The length "*a*" was understood in these measurements as the largest size that could be measured for the considered stone. Table 3 and Figure 4 present the results. The shape of a stone can be visualized as the location of a point on a triangular map, using the coordinates *C*, *F* and *E* in a similar manner as was done with other characteristics, e.g. by Sneed and Folk (Sneed and Folk, 1958).

Table 3: Characterisation of the Studied Grains with the Proposed Tensorial Method, and the Manual Method

Grain type	Method	*C*	*F*	*R*
Compact	Tensorial	0.9999	0.0000	0.0000
	Manual	0.6024	0.3383	0.0593
	Difference	0.3975	-0.3383	-0.0593
Flat	Tensorial	0.0710	0.7688	0.1602
	Manual	0.1945	0.4330	0.3725
	Difference	-0.1235	0.3358	-0.2123
Rod	Tensorial	0.2683	0.1032	0.6286
	Manual	0.3344	0.0942	0.5714
	Difference	-0.0661	0.009	0.0572

For all the three stones, the general conclusion can be drawn that the characterisation based on the surface orientation tensor was more sensitive. The results were more extreme in the sense that the three points belonging to the tensorial method were consequently closer to the corresponding vertices of the triangular map than those belonging to the manual calliper method.
This difference is particularly salient in case of the flat stone (middle one in Figure 3) which has large surfaces approximately with the same orientation, while in all other orientations the surfaces are small. The tensorial method gives a significant emphasis to the orientations of the large faces.
Regarding the compact stone (left one in Figure 3), the manual method was rather ambiguous to use: it was challenging to decide what the longest edge of the bounding box is. In addition, the significant difference between the outcome of the tensorial and the manual method can be understood if thinking of a regular cube, a perfectly compact shape according to the tensorial method. In the manual process, according to the practice, it's main diagonal serves as its longest dimension, size "*a*". Consequently, the regular cube would be characterised by the manual method as being rod-like to some extent, instead of perfectly compact. The fabric tensor approach, on the other hand, finds that none of the faces is larger than the others. Hence there is no bias in the orientational distribution of the faces, and the regular cube turns out to be perfectly compact. The left stone in Figure 3 is similar.

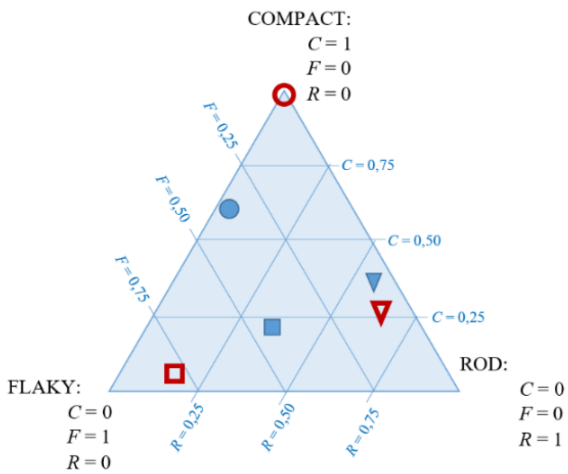

Figure 4: Shape Parameters of the Three Analysed Stones: Characterisation Based on the Surface Orientation Tensor: Hollow Circle, Square and Triangle for the Compact, Flat and Rod Grains; Characterisation Based on the Overall Grain Shape according to Sneed and Folk (1958): Solid Circle, Square and Triangle for the Compact, Flat and Rod Grains Respectively

The elongated stone (right in Figure 3) has tiny faces around the two endpoints. These faces are around perpendicular to the longest axis, while the largest part of the surface is parallel with the longest axis. No wonder that the fabric tensor pointed out the rodness shape. The manual method also found this, and as shown in the triangular map, the two results were close to each other.
An important difference between the two methods is their sensitivity to the existence of sharp, small corners. Such corners strongly influence the manual measurements because of the use of the calliper. However, these sharp corners are vulnerable from point of view of mechanics: they typically break for relatively small loads in comparison to the crushing load of the stone. Hence, these domains have low mechanical importance. An advantageous feature of the tensorial method is that since they have only a tiny contribution to the total surface, the existence of sharp corners hardly modify the surface orientation tensor, which is advantageous when the aim is to describe how the analysed grain may get into mechanical interaction with its neighbourhood.

GENERALIZATION TO SMOOTH SURFACES

The definition (Equation 2) can easily be modified to describe smooth surfaces in such a way that instead of a summation over the faces, an integration is done over the entire S surface of the stone:

$$\mathbf{f} = \frac{1}{\oint_{(S)} dS} \oint_{(S)} \mathbf{n} \circ \mathbf{n} \, dS \qquad (14)$$

After determining the eigenvalues of this tensor the same C, F and R characteristics (compactness, flakiness and rodness) can be calculated for the characterisation of the stone as for the polyhedral stones.

Equation (14) is offered basically for theoretical purposes, since recent imaging techniques result in a discretized surface description for which (2) can directly be applied.

SUMMARY OF THE RESULTS

The paper defined the surface orientation tensor as the area-weighted fabric tensor built on the outwards normal vectors of the faces of the analysed polyhedral stone. A generalized version of this tensor was given for stones with a smooth surface. Based on the three eigenvalues of the tensor, the definition of three shape characteristics (the compactness, the flakiness and the rodness) were proposed to serve as the basis of shape classification. The proposed approach has the following advantages to the bounding box methods:

1. The characterisation is completely deterministic. Human subjectivity is excluded. Randomness can be due to the finite resolution of the imaging procedure only.
2. The characterisation is based on the possible orientations of the contacts of the stone with its neighbourhood, in such a way that larger emphasis is given to the larger faces on which contacts can occur with larger probability.
3. Sharp, small corners that may strongly affect the manual calliper analysis receive only minimal weight in the quantitative results.

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