9. INTERPRETATION OF THE RESULTS I.: GEOMETRY OF DISCRETE SYSTEMS

9.1 Introductory remarks

In the DEM models which apply perfectly rigid elements the output is rather difficult to interpret for an engineer who is used to the usual continuum-mechanical variables. These models provide a huge amount of discrete data like the displacements of each individual element, the contact forces in all contacts etc. In a system of several thousands of elements such a collection of data are practically meaningless in most cases. This is the reason why different ***microstructural state variables*** are often applied: these variables give an "averaged" impression on the geometrical, statical and kinematical state of the system.

This section will introduce the most important geometrical state variables, and gives the necessary geometrical background (i.e. the definition of the material and space cell system) for the statical and kinematical state variables to be introduced in Section 10.

9.2 Microstructural variables for the geometry

The geometrical state variables below can be calculated from data like the topological characteristics, positions of the reference points and the contacts, direction of contact normals etc. With the help of these variables phenomena like the densification of the system, the increasing degree of anisotropy etc. can be reflected.

9.2.1. Porosity

Porosity means the relation of the volume of voids in the system (V_{voids}) versus the total volume surrounded by the boundaries (V_{total}):

$$\rho = \frac{V_{voids}}{V_{total}} = \frac{V_{total} - V_{elements}}{V_{total}}$$

Porosity in the commercial softwares can usually be calculated by using a built-in routine, so that the user could follow its value throughout the whole simulation of the analysed process. Before applying such a routine, the user has to check how the overlapped domains are taken into consideration. In reality the contacting grains, stone blocks etc. change their shape, and these contacting units share a part of their boundary which separates the two material domains. For perfectly rigid DEM elements, however, the contact is formed by two elements partially occupying the same part of the space. One possibility is to calculate the void volume as shown above: i.e. gross volume minus the sum of the volume of all elements. It means that the overlapping material domains are taken into consideration twice. PFC, for instance, is a counter-example: it considers the volume of these domains only once, and calculates the void volume in the following way:

$$V_{voids} = V_{total} - \left(\sum_{p=1}^{N} V^p - \sum_{c=1}^{M} V^c \right)$$

where V^p is the volume of the p-th element, V^c is the volume of the overlapping domain at contact c, N and M are the number of elements and contacts respectively.

9.2.2. Coordination number

Coordination number is the average number of contacts per element. Let M^p denote the number of contacts of element p; the coordination number is calculated like this:

$$C = \frac{1}{N}\sum_{p=1}^{N} M^p \quad .$$

Note that in this summation the contacts formed by two elements in the analysed system are counted twice, while those between an element and the boundary (e.g. a wall supporting the system or another element outside the analysed collection of elements) is taken into consideration only once. Let M^{int} denote the number of element-to-element contacts while M^{ext} is the number of element-to-boundary contacts. Using these notations, the coordination number is:

$$C = \frac{2M^{int} + M^{ext}}{N} \quad .$$

9.2.3. Fabric tensor

A Satake-féle váztenzor

Consider a collection of M unit vectors in the 2D or 3D space. (Their position is indifferent; only their direction will have an importance.) Figure 1a. shows such a set.

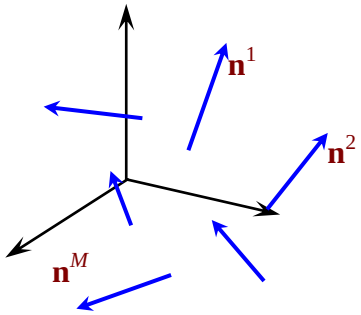

Figure 1a.
Unit normals in the space

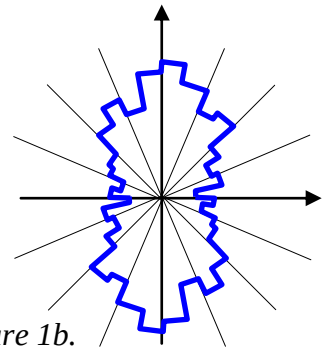

Figure 1b.
Directional distribution of the contact normal in a gravitationally equilibrated 2D granular assembly

The aim of the fabric tensor is to characterize the directional distribution of this set; in particular, to show whether there is a special direction about which a significant portion of the given vectors can be found. (If, for instance, a gravitationally deposited sand sample is analysed, there are more contact normals close to the vertical direction than to the horizontal direction; the aim of the fabric tensor is to point out this difference. Figure 1b. shows the directional distribution of the contact normals in a 2D granular assembly prepared by gravitational deposition.)

The definition of the fabric tensor is based on the dyadic product of every unit vector with itself:

$$\boldsymbol{\varphi}^c = \mathbf{v}^c \circ \mathbf{v}^c$$

and the average of these dyads has to be determined:

$$\boldsymbol{\phi} = \frac{1}{M}\sum_{c=1}^{M} \mathbf{v}^c \circ \mathbf{v}^c \quad .$$

This average is the second order fabric tensor introduced by Satake (1978). Its most important characteristics are:

→ the tensor is symmetric;
→ the tensor is positive definite, i.e. all of its eigenvalues are positive;
→ as a consequence of the symmetry, its eigenvectors are perpendicular to each other;
→ its trace is equal to 1 which means that the sum of the eigenvalues is also 1;
→ if any of the vector is turned into the opposite direction, the fabric tensor will not change.

In the special case of all of the vectors being parallel to each other, one of the eigenvalues is 1 and the others are zero; the eigenvector belonging to the unit eigenvalue has the same direction as all the vectors. If all vectors are perpendicular to a common plane, then there is an eigenvector perpendicular to the plane and the corresponding eigenvalue is zero; the other two eigenvectors are parallel to the common plane and the sum of the corresponding two eigenvalues is equal to 1.

The fabric tensor can be visualized with the help of the ***fabric ellipsoid*** (fabric ellipse in 2D). The axes of the ellipsoid are parallel to the eigenvectors, and their length is equal to the corresponding eigenvalues.

If the set of vectors is biased in a direction (e.g. vertically in the above example in Figure 1b), then the eigenvector belonging to the larges eigenvalue shows this direction. The difference between the eigenvalues reflects the strength of the anisotropy.

In discrete element analysis the fabric tensor is mostly applied for the characterisation of the distribution of contact normals. Fabric tensors can be built on any other type of unit vectors, like e.g. the long axis of non-spherical elements, or the direction of the voids in a system etc. The interested reader is advised to consult the papers Oda (1982), Satake (1982), and Konishi and Naruse (1988).

Weighted fabric tensors

The dyads belonging to the individual vectors can receive a weight which expresses some mechanical characteristic assigned to the vector. By using, for instance, the magnitude of compression force (N^c) to weight the contact normals, a fabric tensor is received which particularly emphasizes the contact directions being important in carrying the compression in the system:

$$\boldsymbol{\phi}^N = \frac{1}{M}\sum_{c=1}^{M} N^c \cdot \mathbf{v}^c \circ \mathbf{v}^c \quad .$$

The trace of this tensor is not 1, but equals to the average magnitude of contact compression, so this characteristic can also be followed during a simulation of loading processes. The l^c distance between the centres of the two contacting elements ca also be applied as a weight:

$$\boldsymbol{\phi}^l = \frac{1}{M}\sum_{c=1}^{M} l^c \cdot \mathbf{v}^c \circ \mathbf{v}^c \quad ,$$

and this way the resulting fabric tensor will emphasize the contacts of the large elements.

Higher-order fabric tensors

Already in the 1980ies, researchers like e.g. Mehrabadi et al (1988) pointed out that the second-order fabric tensors are insufficient in some cases (e.g. if there are two characteristic directions of a system, in which case the second-order fabric tensor finds the "average" of the two directions). This was why higher-order fabric tensors were suggested. The fourth-order version is, for instance, defined as

$$\boldsymbol{\phi}_4 = \frac{1}{M}\sum_{c=1}^{M} \mathbf{v}^c \circ \mathbf{v}^c \circ \mathbf{v}^c \circ \mathbf{v}^c \quad .$$

These versions can also be weighted. However, their application did not become widespread.

9.3 The material cell system and the space cell system

Now two cell systems (dual to each other) will be introduced; they will serve as the geometrical basis for the interpretation of stress and strain for discrete systems.

Consider *N* elements in the 2D or 3D space. Their shape is strictly convex, smooth, and they have point-like contacts with each other without overlaps.

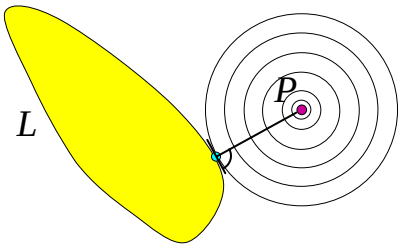

Figure 2.
Distance of point P from element L

First the distance between a point *P* and an element *L* has to be defined. Find that pint on the boundary of the element which is closest to *P*. If *P* is outside the element, then this distance is understood as the distance between *P* and *L*. If *P* is on the boundary, then this distance is zero. Finally, if *P* is inside the element, then the opposite of the distance of *P* from the closest point of the boundary is understood as the distance between *P* and *L*; in this case the distance is negative.

The two cell systems will now be defined for 2D first, and then the 3D version will be shown. More details can be found in Bagi (1995), (1996).

9.3.1. Two-dimensional analysis

The material cell system

Consider all the points of the 2D plane of the analysis. Assign every point in the plane to that element from which the point has the smallest distance. The points belonging to the same element form the ***material cell*** of that element. Those points which have equally small distance from two or more elements are assigned to all of these nearest elements.

The common face of two material cells is a line consisting of those points which have equal distance from the two elements, but do not have a smaller distance from any other element. The points of the common face belong to both cells. These faces are, in general, curved lines. The intersection point of two faces necessarily belongs to the third face going through the same point: it is a point with equal distance from the three elements. (In special cases four or even more faces can have a common intersection point, which means that the intersection point has equal distance from these four or more elements.) The intersection point belongs to all the corresponding elements. These intersection points are the nodes of the material cell system.

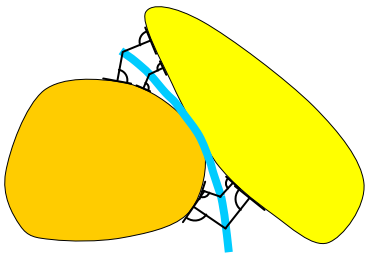

Figure 3a.
Points of the plane having equal distance from two elements: blue line

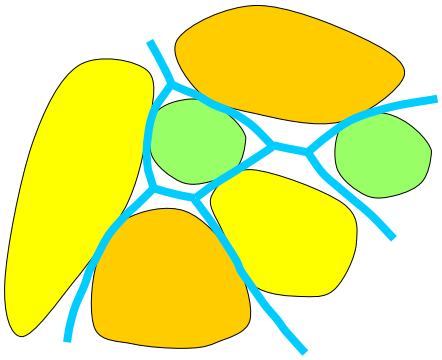

Figure 3b.
The material cell system

Add now an "***element in the infinity"*** to the system: it is, by definition, the neighbour of all those elements which have an infinite material cell (so the "element in the infinity" can be thought of as the neighbour of the boundary elements). To visualize its meaning, imagine that the plane of the analysis is the surface of a sphere with an infinitely large radius; and the "element in the infinity" is on the back side of this sphere, opposite to the analysed assembly. At an infinite distance from the analysed assembly (on the "back side" of the very large sphere), the cells of the boundary elements have a common face with the cell of the "element in the infinity", and there are common nodes defined in the usual way. Let the size of the "element in the infinity" be zero (point-like element is assumed), and its position coincides with the centre of gravity of the analysed assembly of elements.

Apart from the nodes and faces (i.e. a set with zero area), every point of the plane can uniquely be assigned to one element. So the plane is ***covered once*** by the material cell system.

In special cases a node may exist which belongs to four or more elements: four or more faces intersect in the same point. These coincidences have to be eliminated in the following way. Modify the geometry with an infinitesimally small disturbance, so that the speciality of the geometry would disappear. The multiple node splits up: new faces and nodes will appear, like those shown in Figure 4. Assign this new topology to the system.

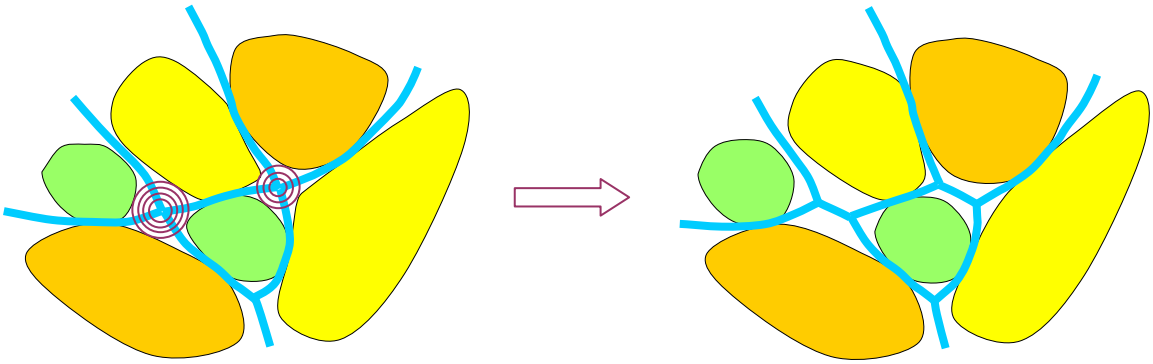

Figure 4.
Multiple nodes are split up

Depending on the applied disturbance, the multiple nodes can be split up in different ways, leading to different equally possible topologies. Any of them can arbitrarily be chosen.

The space cell system

The space cell system is dual to the system of material cells. To define it, consider now an assembly together with its material cell system (cells, faces and nodes, together with the "element in the infinity", multiple nodes already split up). The ***nodes*** of the space cell system are, by definition, the centres of the elements. (Note that there is an exact one-to-one correspondence between the material cells and the space nodes.) Where two material cells have a common face, connect the corresponding two element centres with a straight section; these will be the ***edges*** in the space cell system. (Care has to be taken on not to forget about those material faces which exist only because the multiple nodes were split up; space edges do belong to these infinitesimal material faces too.) Finally, a node in the material cell system was formed by the intersection of three faces; the corresponding three space edges determine a ***cell*** in the space cell system. The space cells are triangles, and an exact oneto-one correspondence exists between the material nodes and space cells.

A positive or negative sign is also assigned to the space cells. Consider a material node and the corresponding space cell. In clockwise direction, go around the material node, and register the elements (i.e. the material cells) in the order they were visited. Do the same with the space cell: go around through its nodes in clockwise direction, and again, register the elements (i.e. space nodes) in the order they were visited. The space cell is ***positive*** if the elements were found in the same order; and ***negative*** if they were found in the opposite order. Figure 5a. shows a system with positive space cells only, while in Figure 5b. a system containing a negative space cell can be seen.

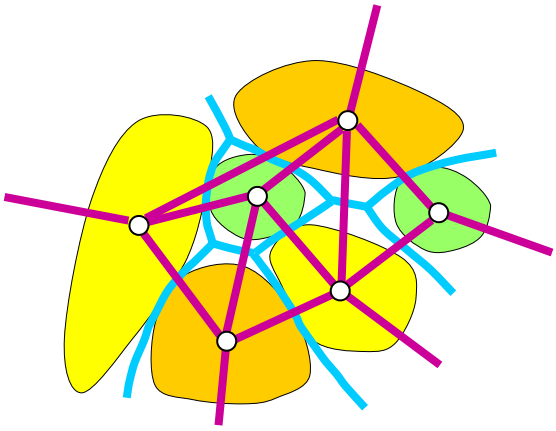

Figure 5a.
Space cell system containing positive cells only

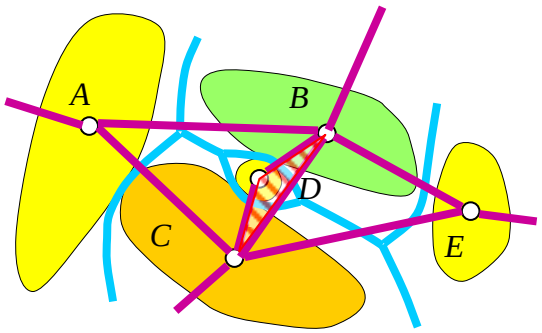

Figure 5b.
Space cell system containing a negative cell: marked area is covered by the positive cell ABC, the negative cell CBD, and the positive cell CDB.

The sign of the space cell will have two roles: the sign is assigned to the calculation of the area of the cells in 2D (negative space cell has a negative area), and to the analysis of how many time a point of the plane is covered by the space cells (a point is covered by (–1)-times by a negative cell).

With these steps a space cell system can be prepared for any collection of strictly convex, non-intersecting elements. An important characteristic of this cell system is that the space cells cover every point of the 2D plane of the analysis exactly once, apart from a zero-measure (i.e. zero area in 2D) domain.

For elements of not very different size and not very elongated shape, every edge in the space cell system usually belongs to exactly two cells, both of them being positive, which means that they are on the two different side of the edge. In this case it is trivial that the space cell system covers the space exactly once (apart from the zero-measure set given by the edges and nodes). However, there are situations e.g. if there are significant differences in the element size (e.g. at least an order of magnitude), that some of the edges can be found in the system which belong to cells more than two, or two cells being on the same side of the edge. In this case some of the cells are negative. It can be proved (Bagi, 1997) that the points of the plane are covered by one more positive than negative cells (again apart from the set of the points of the edges and nodes). In this generalized sense we may say again that the space cell system covers the plane exactly once.

9.3.2. Three-dimensional analysis

The material cell system

The above definitions can be generalized for three dimensions. To prepare the ***material cell system***, assign every point of the 3D space to the nearest element. The material cells uniquely correspond to the elements; the common face of two neighbouring cells consist of those points which have equal distance from the two elements being not larger than from any other element. The common faces are curved surfaces usually. The intersection of two faces (a curved line) consists of those points being at the same distance from three elements, so such an edge necessarily belongs to a third face also. (In special cases an edge may be formed by more than three faces; these special cases are treated by splitting up with the help of a random disturbance, similarly to the 2D case.) The nodes being formed by the intersection of four edges are at the same distance from four elements.

Add an "***element in the infinity***" to the system, similarly to the 2D case. This fictitious element has common faces, edges and nodes with those elements whose material cells are infinite, i.e. they are on the boundary.

The space cell system

The space cell system is, again, based on the material cell system. The centres of the elements are the ***nodes***, so exactly one space node belongs to every element (to every material cell). A common face of two material cells determine an ***edge*** in the space cell system: the corresponding two nodes are connected with a straight section. In the material system three faces meet on an edge; the corresponding three space edges determine a triangle, a ***face*** in the space cell system. Finally, four material edges meet in a material node; the corresponding four space faces form a ***space cell***. The space cells are tetrahedral.

A positive or negative sign can also be assigned to the 3D space cells, and it can be proved that every point of the 3D space (apart from the zero-volume set of space edges and faces) are ***covered exactly once*** in the general sense applied above. The details will not be introduced here: they can be found in e.g. Bagi, 1997.

9.3.3. The finite sub-assembly

A finite sub-assembly is a collection of elements all of them having a finite material cell (see Figure 6).

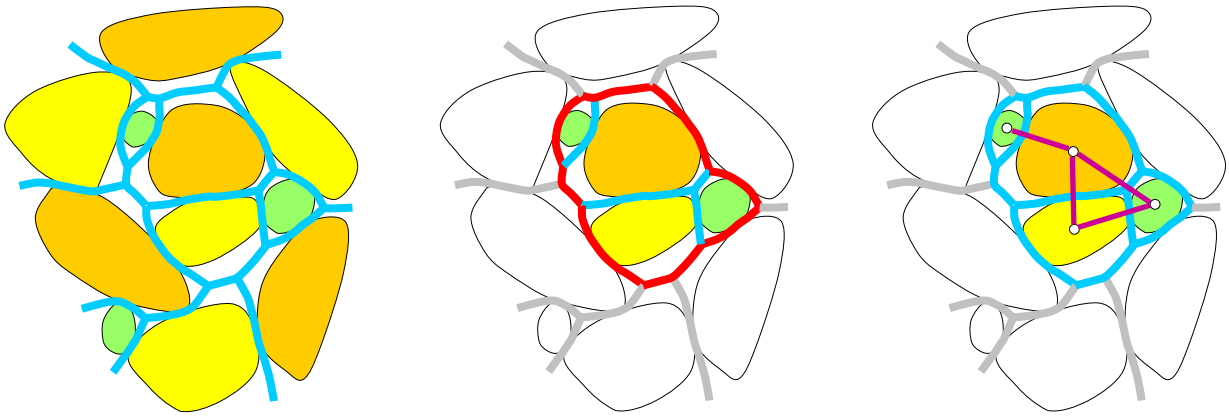

Figure 6.
The material cell system and a finite sub-assembly in it

There are several different ways to construct a finite sub-assembly from a general collection of elements. It may consist, for instance, of one single element; or or it may be formed by two groups of elements completely separated from each other etc. The material cell system of the finite sub-assembly is the collection of those (obviously finite) material cells which belong to the elements of the finite sub-assembly. Its boundary is illustrated in red in Figure 6. The space cell system of the finite sub-assembly is formed by those space cells whose nodes all belong to the elements in the finite sub-assembly. On the right in Figure 6. such a space cell system is shown; it consists of only one space cell, in spite of containing one more space edge which does not take part in forming the only cell.

Questions

9.1. Explain the meaning of porosity and coordination number!
9.2. Introduce the second-order fabric tensor of Satake, and explain its most important features!
9.3. What other fabric tensors do you know? What can they be applied for?
9.4. Define the distance between a point and an element! Introduce the material cell system!
9.5. Introduce the space cell system!
9.6. Explain the meaning of the negative space cells! What does it mean that the space cell system covers the space exactly once in generalized sense?
9.7. Explain the meaning of the finite sub-assembly, and the definition of its material and space cell system!