10. INTERPRETATION OF THE RESULTS II.: STRESSES AND STRAINS

10.1 Stress tensors

10.1.1. Introductory remarks

Several stress definitions can be found in granular mechanics literature (e.g. Drescher and de Josselin de Jong, 1972, Rothenburg et al, 1981, Kanatani, 1981); they are all suitable for expressing the average stress state of a collection of separate elements. Though they may contain different restrictions regarding element shape and their definition was found by different theoretical tools (e.g. work principle, elementary consideratins etc), they are equivalent to the general definition (Bagi, 1996) which is presented below.

Now the necessary continuum-mechanical fundaments will shortly be recalled, then the microstructural stress tensor of the finite sub-assembles will be introduced, finally, two different methods will be presented for its quantitative determination.

10.1.2. Continuum mechanics overview: Average stress tensor of a finite domain

Consider an equilibrated, closed, continuous domain with volume V whose surface S is acted upon by the distributed surface loads $\mathbf{p}(\mathbf{x})$ (see Figure 1). As a result, a continuous stress field $\boldsymbol{\sigma}(\mathbf{x})$ occurs along the domain (in its interior as well as in its boundary points) for which the following boundary conditions are valid in every point of S:

$$\boldsymbol{\sigma}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x})=\mathbf{p}(\mathbf{x}) \quad .$$

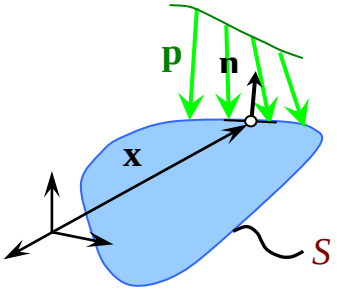

Figure 1.
Continuous domain submitted to distributed external loads

Here $\mathbf{n}(\mathbf{x})$ is the outwards unit normal of the surface.

According to the Gauss-Osztrogradszkij-theorem, the volume average of the stress in the domain can be expressed with the help of the surface loads:

$$\bar{\boldsymbol{\sigma}}=\frac{1}{V}\oint_{(V)}\boldsymbol{\sigma}(\mathbf{x})dV=\frac{1}{V}\oint_{(S)}\mathbf{x}\circ\boldsymbol{\sigma}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x})dS=\frac{1}{V}\oint_{(S)}\mathbf{x}\circ\mathbf{p}(\mathbf{x})dS \quad .$$

The surface loads may be concentrated to a few small, disjunct areas; this is the case for a smooth strictly convex element receiving contact forces from its neighbours also being strictly convex and smooth. In this case the resultants of the distributed forces are the well-known contact forces seen in the previous sections for several types of DEM models. The distributed surface forces can be replaced in the above expression by their concentrated resultants in the following way:

$$\bar{\boldsymbol{\sigma}}=\frac{1}{V}\sum_{(k)}\mathbf{x}^k\circ\mathbf{F}^k \quad ,$$

where $\mathbf{x}^k$ and $\mathbf{F}^k$ are the position and the force vector at the k-the loaded boundary point.

10.1.3. Microstructural stress tensor of a collection of discrete elements

The definition

The forthcoming derivations lead to the definition of a state variable which is able to characterise the average stress state of an equilibrated finite sub-assembly. To determine it, the contact forces and the boundary forces acting in the analysed finite sub-assembly should be known, together with the branch vectors of the contacts (i.e. the vectors connecting the reference points (centres) of contacting elements).

The material cell system subdivides the 2D or 3D space of the analysis in such a way that the contact forces are transmitted at the common faces of neighbouring material cells. A single material cell can be considered as a finite continuous domain acted upon by concentrated forces at its boundary, like the one seen in Section 10.1.2.

Consider an arbitrary finite sub-assembly of the collection of discrete elements under question. The average stress of the material cell belonging to its L-th element is:

$$\boldsymbol{\sigma}^L = \frac{1}{V^L} \sum_{(Lc \in S^L)} \mathbf{x}^{Lc} \circ \mathbf{F}^{Lc} \quad .$$

Here V^L and S^L are the volume and surface of the L-th material cell (and not of the L-th element). The summation for index Lc runs along all contacts of element L: some of them may be internal, element-to-element contacts in the sub-assembly, and some of them may be those contacts which are formed by the element and the external neighbourhood of the sub-assembly. The vector $\mathbf{x}^{Lc}$ is the position of the point-like contact Lc which may be either on an inside face, or on the boundary of the set of material cells of the sub-assembly. The vector $\mathbf{F}^{Lc}$ is the force acting on element L in its contact LC.

The same can be done for all material cells of the sub-assembly.

By definition, the ***microstructural stress tensor*** of the finite sub-assembly is the volume average of the stresses of the material cells:

$$\overline{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{(L)} V^L \boldsymbol{\sigma}^L \quad .$$

The microstructural stress tensor in terms of contact forces

In the above volume average the stresses of the elements can easily be expressed with the help of the concentrated forces acting on the elements:

$$\overline{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{(L)} V^L \boldsymbol{\sigma}^L = \frac{1}{V} \sum_{(L)} \left(\sum_{(Lc \in S^L)} \mathbf{x}^{Lc} \circ \mathbf{F}^{Lc} \right)$$

In the summation on the right those contacts which are formed by two elements of the sub-assembly are considered twice, with opposite sign; while those on the boundary are considered only once. Let us take a closer look on a contact between two elements:

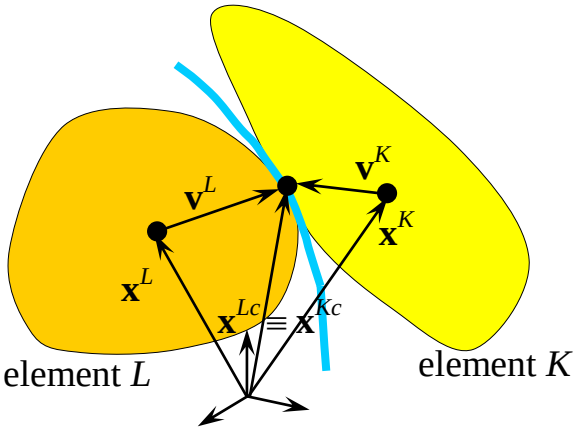

Figure 2.
Contact formed by elements L and K

Denote the positions of the reference points (practically, the centres) of elements L and K by $\mathbf{x}^{L0}$ és $\mathbf{x}^{K0}$, and the two vectors pointing from the reference points to the contact point are $\mathbf{v}^{Lc}$ and $\mathbf{v}^{Kc}$. Recognize that

$$\mathbf{x}^{Lc} = \mathbf{x}^{L0} + \mathbf{v}^{Lc} = \mathbf{x}^{Kc} = \mathbf{x}^{K0} + \mathbf{v}^{Kc} \quad .$$

In the above summation (end of Page 96) those two terms belonging to contact c are:

$$(\mathbf{x}^{L0} + \mathbf{v}^{Lc}) \circ \mathbf{F}^{Lc} + (\mathbf{x}^{K0} + \mathbf{v}^{Kc}) \circ \mathbf{F}^{Kc} \quad ,$$

where

$$\mathbf{F}^{Kc} = -\mathbf{F}^{Lc} \quad ,$$

so the two terms can further be decomposed into the following:

$$(\mathbf{x}^{L0} + \mathbf{v}^{Lc}) \circ \mathbf{F}^{Lc} + (\mathbf{x}^{K0} + \mathbf{v}^{Kc}) \circ \mathbf{F}^{Kc} = \mathbf{x}^{L0} \circ \mathbf{F}^{Lc} + \mathbf{x}^{K0} \circ \mathbf{F}^{Kc} + (\mathbf{v}^{Lc} - \mathbf{v}^{Kc}) \circ \mathbf{F}^{Lc} \quad .$$

Turn the attention now to those contacts which are formed by an element with the boundary of the sub-assembly. The term belonging to the contact c of element L is:

$$(\mathbf{x}^{L0} + \mathbf{v}^{Lc}) \circ \mathbf{F}^{Lc} \quad ,$$

which is equal to

$$\mathbf{x}^{L0} \circ \mathbf{F}^{Lc} + \mathbf{v}^{Lc} \circ \mathbf{F}^{Lc} \quad .$$

Perform now the summation. First, decompose the position vectors of the contact points into their components:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{(L)} \left(\sum_{(Lc \in S^L)} \mathbf{x}^{Lc} \circ \mathbf{F}^{Lc} \right) = \frac{1}{V} \sum_{(L)} \left(\sum_{(Lc \in S^L)} \mathbf{x}^{L0} \circ \mathbf{F}^{Lc} \right) + \left(\sum_{(Lc \in S^L)} \mathbf{v}^{Lc} \circ \mathbf{F}^{Lc} \right)$$

Since the elements are in equilibrium, hence on the right side the sum expressed by the first bracket is zero:

$$\sum_{(Lc \in S^L)} \mathbf{x}^{L0} \circ \mathbf{F}^{Lc} = 0 \quad .$$

So the summation is reduced to a simpler form:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{(L)} \left(\sum_{(Lc \in S^L)} \mathbf{v}^{Lc} \circ \mathbf{F}^{Lc} \right) \quad .$$

Introduce a few notations now. At the internal (i.e. element-to-element) contact c, arbitrarily select one of the elements to serve as “the first” and the other as “the second” element of the

contact. Let $\mathbf{l}^c$ denote the branch vector pointing from the centre of the first element to the centre of the second element. The force $\mathbf{F}^c$ acts on the first element, being expressed by the second element. For a boundary contact *c*, let $\mathbf{l}^c$ denote the vector pointing from the centre of the element to the contact point; in this case $\mathbf{F}^c$ is the external force vector acting on the boundary of the sub-assembly in *c*. Using these notations the classic form of the microstructural stress tensor is received:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\sum_{(c)} \mathbf{l}^c \circ \mathbf{F}^c \quad .$$

This expression is also valid when in addition to the contact forces, volume forces (e.g. weight) act on the elements. The proof can be found in (Bagi, 1999).

Calculation of the stresses in terms of the forces acting on the boundary

Return now to the definition of the microstructural stress tensor as the volume average of the stresses in the material cells:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\sum_{(L)} V^L \boldsymbol{\sigma}^L = \frac{1}{V}\sum_{(L)} \left(\sum_{(Lc \in S^L)} \mathbf{x}^{Lc} \circ \mathbf{F}^{Lc} \right) \quad .$$

Note that those contact forces which belong to the element-to-element contacts are considered twice, with opposite sign but with the same position vector, so they cancel out. The only remaining terms are those belonging to the boundary forces:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\sum_{(c \in S)} \mathbf{x}^c \circ \mathbf{F}^c \quad .$$

This calculation method was proposed Drescher és de Josselin de Jong (1972), and by Cundall and Strack (1983).

10.2 Strain tensors

10.2.1. Introductory remarks

Nonlinear continuum-mechanics applies several different strain versions: left or right Cauchy-Green-tensor, Piola deformation tensor, Green-Lagrange-strain, Almansi-Hamel-strain etc. All these tensors can be expressed from the ***gradient of the translation field*** of the analysed continuum: the translation gradient plays a basic role in the characterisation of the deformations.

In continuum mechanics the strains characterize the distortions of an infinitesimally small domain around the analysed point; and they are continuous functions of the position. However, when a collection of discrete elements is to be analysed, the concept of infinitesimally small domain and the application of differentiable translation field loose their applicability: each element has its own degrees of freedom, able to translate and rotate in a different way from their neighbours, and the translations and rotations show a very heterogeneous view (see Figure 3 where the result of the discrete element simulation of a biaxially loaded assembly can be seen: the arrows represent the translations of the elements for a small increment of the vertical stress component).

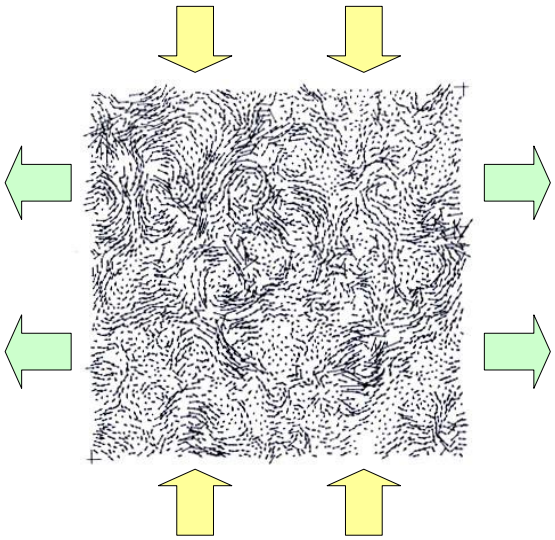

Figure 3.
Translation increments in a biaxially loaded collection of elements

Several different approaches are proposed in the literature to assign an average strain to such a collection of finite bodies. The two most important versions will be introduced below. Both of them (and all other versions for the definition of a microstructural strain tensor) are based on the initial geometry which is valid at the beginning of the incrementally small displacements of the elements, and derive an average translation gradient tensor for the assembly. The system must contain at least 4 elements whose reference points are not in the same plane (3 elements in two-dimensional analysis, with the reference points not in the same straight line). It will again be assumed for simplicity that for every element the reference point is the same as the centre of the element.

10.2.2. Continuum mechanics overview: Average strain in a finite domain

Consider a finite, closed, continuous domain with volume V and surface S whose translation field $\mathbf{u}(\mathbf{x})$ is continuously differentiable. Let $\mathbf{n}(\mathbf{x})$ denote the outwards unit vector normal to the surface S. The gradient of the translation field is:

$$\mathbf{e}(\mathbf{x}) = \left(\frac{\partial \mathbf{u}(\mathbf{x})}{\partial \mathbf{x}} \right)^T \quad .$$

According to the gradient theorem (which plays a similar role as the Gauss-Ostrogradskij theorem), the volume average of the gradient of $\mathbf{u}(\mathbf{x})$ can be expressed in the following form:

$$\bar{\mathbf{e}} = \frac{1}{V} \oint_{(V)} \mathbf{e}(\mathbf{x}) dV = \frac{1}{V} \oint_{(S)} \mathbf{n}(\mathbf{x}) \circ \mathbf{u}(\mathbf{x}) \cdot dS$$

or, in two-dimensional analysis for a domain of area A and boundary length l :

$$\bar{\mathbf{e}} = \frac{1}{A} \oint_{(A)} \mathbf{e}(\mathbf{x}) dA = \frac{1}{A} \oint_{(l)} \mathbf{n}(\mathbf{x}) \circ \mathbf{u}(\mathbf{x}) \cdot dl \quad .$$

For the validity of this expression it is not necessary that the translation field is differentiable everywhere: it is allowed that the gradient does not exist along a set of points of zero measure (i.e. surfaces in 3D or lines in 2D).

10.2.3. Strain definition based on an equivalent continuum

In the definition of the equivalent-continuum strain (Bagi, 1996) the ***space cell system*** is applied as a continuum replacing the collection of elements, to which a suitable translation gradient is assigned.

Consider a finite sub-assembly, i.e. a collection of finite-sized space cells. Define a translation field in the following way. Let the translations of the elements be the translations of the nodes of the space cell system. Since the cells are simplexes, the nodal translations uniquely define a linear translation field by interpolation. This fictitious translation field is continuously differentiable apart from the faces of the cells, and the gradient is uniform inside the cells.

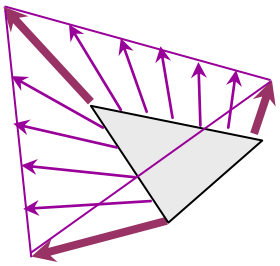

Figure 4.
Linear translation field of a space cell

For any space cell, for instance for cell L, its own translation gradient can be calculated with the help of the surface integral of the translation field:

$$d\overline{\mathbf{e}}^L = \frac{1}{V^L} \oint_{(S^L)} \mathbf{n} \circ d\mathbf{u} \, dS \ ,$$

where V^L is the volume of the L-th space cell, S^L is its surface, $d\mathbf{u}$ is the translation vector of the boundary point where the outwards unit normal vector is $\mathbf{n}$.

In two dimensions the above translation gradient is:

$$d\overline{\mathbf{e}}^L = \frac{1}{A^L} \oint_{(l^L)} \mathbf{n} \circ d\mathbf{u} \, dl \ .$$

Here A^L and l^L are the area and the boundary length of the space cell, respectively.

By taking into consideration that the translation field is the linear interpolation of the nodal translations, on the right side the integration can be expressed in terms of the nodal translations and certain geometrical data. The rather time-consuming derivations are not introduced here (the interested reader can find them in e.g. Bagi, 1996).

It is important to emphasize that the calculation is exactly the same for the negative cells, with the only difference that the volume (area in 2D) is a negative number for these cells.

Determine then the volume average of these gradients for the whole collection of space cells:

$$d\overline{\mathbf{e}} = \frac{1}{V} \sum_{(L)} V^L d\overline{\mathbf{e}}^L \ ,$$

or in 2D:

$$d\overline{\mathbf{e}} = \frac{1}{A}\sum_{(L)} A^L d\overline{\mathbf{e}}^L$$

Unlike in the stress definition, here the V volume and A area are the sum of those of the ***space cells*** and not of the material cells:

$$V = \sum_{(L)} V^L \quad , \quad \text{or in 2D:} \quad A = \sum_{(L)} A^L \quad .$$

The symmetric part of this translation gradient is, by definition, the ***microstructural strain tensor*** of the analysed finite sub-assembly.

The average translation gradient can be expressed in terms of discrete characteristics too. Without showing the details, the resulting expression is:

$$d\overline{\mathbf{e}} = \frac{1}{V}\sum_{(c)} \mathbf{d}^c \circ d\Delta\mathbf{u}^c \quad .$$

Here the summation index c runs along all edges in the considered space cell system. Similarly for the stress analysis, for every edge c select one of the elements as "the first" and the other as "the second" element of the pair. The relative translation vector $d\Delta\mathbf{u}^c$ shows the translation of the reference point of the second element with respect to the first element:

$$d\Delta\mathbf{u}^c = d\mathbf{u}^{c,second} - d\mathbf{u}^{c,first} \quad .$$

The quantity $\mathbf{d}^c$ is called the ***complementary area vector***. It is a characteristic of the local neighbourhood of edge c, and it can be considered as the dual variable of the branch vector in the sense that by summing up the $(l_i\, d_i)$ scalar product for all edges in the system, the total volume (area in 2D) can be calculated:

$$V = \sum_{(c)} \frac{1}{3}(l_i^c d_i^c) \quad \text{or} \quad A = \sum_{(c)} \frac{1}{2}(l_i^c d_i^c) \quad .$$

The tensor $d\mathbf{e}$ expressed this way is the same as the average translation gradient tensor of the considered space cells, so, again, its symmetric part gives the average strain tensor of the analysed finite sub-assembly.

10.2.4. Strain definitions based on least-square approximations

A completely different approach was proposed by P.A. Cundall and applied in TRUBAL and the commercial codes PFC 2D and 3D. He suggested to use a best-fit approximation to find a translation gradient giving the smallest deviations from the translations of the elements. Similarly to the equivalent-continuum strain, his definition is also insensitive to the shape or to the rotations of the elements; only the translations of the reference points are considered.

Let $d\mathbf{u}^p$ denote the translation increment of the centre of the p-th element during a small time step, and $\mathbf{x}^p$ the position of the centre of the p-th element at the beginning of the time step. The total number of elements is N^p. The deviation of the position of element p from the centre of the whole system is:

$$\tilde{\mathbf{x}}^p = \mathbf{x}^p - \frac{1}{N^p}\sum_{q=1}^{N^p} \mathbf{x}^q \quad ,$$

and the deviation of the translation of element p from the average translation is:

$$d\tilde{\mathbf{u}}^p = d\mathbf{u}^p - \frac{1}{N^p}\sum_{q=1}^{N^p} d\mathbf{u}^q \ .$$

In that very special case when the translations all exactly correspond to a uniform translation gradient $\boldsymbol{\alpha}$, the individual translations of the elements would be

$$d\tilde{\mathbf{u}}^p = \boldsymbol{\alpha}^T \tilde{\mathbf{x}}^p \ .$$

However, in a general case this is not valid, so for an arbitrary $\boldsymbol{\alpha}$ usually there is a deviation between the actual translation of *p* and the one which can be approximated from $\boldsymbol{\alpha}$:

$$d\tilde{\mathbf{u}}^p - \boldsymbol{\alpha}^T \tilde{\mathbf{x}}^p \neq \mathbf{0} \ .$$

Now determine that specific $\boldsymbol{\alpha}$ tensor for which the square sum of the deviations for all elements gives the smallest value:

$$\Sigma = \sum_{p=1}^{N^p} (d\tilde{\mathbf{u}}^p - \boldsymbol{\alpha}^T \tilde{\mathbf{x}}^p) \cdot (d\tilde{\mathbf{u}}^p - \boldsymbol{\alpha}^T \tilde{\mathbf{x}}^p) \rightarrow \min!$$

This particular tensor (denote it by $d\overline{\mathbf{e}}$) can easily be calculated with the help of the $\tilde{\mathbf{x}}^p$ and $d\tilde{\mathbf{u}}^p$ characteristics of the elements. (The details can be found in several papers, perhaps most easily in the manuals of the free demo versions of the PFC codes. however, these details are not necessary for the understanding of the concept of Cundall's best-fit strain tensor, so they are not introduced here.) The symmetric part of that tensor $d\overline{\mathbf{e}}$ which minimise the square sum Σ is, by definition, ***Cundall's best-fit strain tensor***.

Though the above two strain definitions are based on very different fundaments, experiments show that they give a good approximation to each other and to the overall deformation of the surrounding domain of the discrete systems.

Other authors proposed other quantities (e.g. relative translations in the contacts; relative translations of the centres of contacting or neighbouring pairs of elements etc), but these approximations turned out to be unreliable for the characterisation of the overall deformations of the assemblies (for details, see e.g. Bagi, 2005).

Questions

10.1. Define the microstructural stress tensor assigned to a finite sub-assembly! Explain how to calculate it!
10.2. Introduce the equivalent-continuum definition of the microstructural strain tensor of a finite sub-assembly!
10.3. Introduce the microstructural strain definition proposed by Cundall!