ELSEVIER

Mechanics of Materials 22 (1996) 165–177

MECHANICS OF MATERIALS

Stress and strain in granular assemblies

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Received 7 March 1995; accepted 29 October 1995

Abstract

The aim of this paper is to clarify the meaning of the mechanical state variables stress and strain in the case of random granular assemblies. Stress and strain are expressed in terms of local, micro-level variables with the help of two complementary geometrical systems. The two expressions show a strong duality which is also analysed in the paper.

Keywords: Granular material; Microstructure; State variable; Geometry; Cell system

1. Introduction

The aim of this paper is to re-define the continuum-mechanical state variables *stress* and *strain* for a granular assembly, i.e. a material consisting of separate particles and having a characteristic discrete microstructure that changes under external loading.

We shall focus our attention on the quasi-static behavior of the material; so time effects will not be considered at all, and any part of the assembly is assumed to be in equilibrium. The results will be valid for 2D and 3D as well. The assembly consists of randomly packed separate grains having arbitrary convex shape. Contacting grains have discrete contact points transmitting concentrated contact forces. External forces act on the assembly through the contact points with its neighbourhood. For simplicity, body forces and body moments will not be considered here (however, their effect could also be included in the concepts to be discussed).

The final goal of the mechanics of granular materials is to provide relationships between the external loads acting on the material and the resulting displacements. Traditionally, the effect of external loads is expressed by the continuum-mechanical state variable *stress* (the relation between loads and the stress field is given by the equilibrium equations of continuum mechanics, for example the Cauchy equations in the simplest case); deformations are reflected by the other continuum-mechanical state variable *strain* (geometrical equations set the link between displacements and the strain field). Stress and strain are related to each other through the *constitutive equations* (which are expected to contain all the necessary information about the mechanical characteristics of the material). The geometrical and equilibrium equations are clear in continuum mechanics; but to find the proper constitutive equations for granular assemblies is not simple at all: for many years, a large number of theoretical and experimental studies have been concerned with the problem, and the results seem to be rather limited.

Recently there are two approaches that most of the researchers follow in order to solve this problem. Let us call the first one the *continuum-mechanical*, and the second one the *microstructural* approach.

The idea of the continuum-mechanical approach is to consider the assembly as a continuous domain, accept the concept of an infinitesimally small represen-

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tative volume element, and apply stress and strain as the fundamental variables that uniquely determine the state of the material in any point. Constitutive relations are searched for in such a way that they would not violate the fundamental laws of physics; and the parameters in the equations, expressing the specific properties of the material, are measured experimentally. This empirical method is the one used today for practical engineering problems.

The problem with this is the limited validity of the results. Experimentally determined relations easily become unreliable if the circumstances for which we want to apply them differ even slightly from those that existed during the experiments. (To improve the constitutive equations, either the mathematical form of the equations must be made more complicated by increasing the number of parameters; or additional state variables are introduced beside the traditional stress and strain.)

The microstructural approach is a relatively new method, and – in the long run – it may be an advantageous alternative to the previous one.

The aim of the microstructural approach is to find macro-level state variables that are based on micro-variables such as contact forces, grain displacements, and local geometrical characteristics. Since it would reflect those characteristics of the material that are most significant in determining the macro-behavior, and the relationships between its state variables would be strongly connected to the phenomena taking place in the microstructure, a microstructural theory is expected to be far more reliable and general than the existing continuum-mechanical models.

Microstructural studies are rather diverse today and the scientists working in this field do not agree even on the most fundamental questions. Different approaches to the two most important problems will shortly be summarized below.

1.1. The geometrical modelling of granular assemblies

The geometrical representation has, in many respects, always been a central problem in the microstructural approach. A summary will be given below; first on the different basic geometrical units suggested for the theoretical description; then on the best-known mathematical representations applied for modelling whole systems of grains. Finally, a short introduction will be given on two concepts that strongly inspired our efforts to work out the idea of introducing two complementary cell systems for the micromechanical analysis of granular assemblies.

So we will start with the various basic units used for the description in a geometrical representation.

Several early experiments concentrated on the analysis of micro-level geometrical characteristics and their changes under loads (see, e.g., Oda, 1972; Drescher and de Josselin de Jong, 1972, and others). The simplest unit of the description was the *contact* between two grains. It might be said that the orientation of contact normals was considered as the most important geometrical characteristic of the internal structure (the different fabric tensors, see Section 1.2, were defined to describe the orientational distribution). Branch vectors (vectors connecting the centres of neighbouring grains) also appeared in several theories (they had an important role in stress definitions for example, as seen in Section 1.2).

An other possible unit of the analysis is the individual *grain* itself. Misra (1993), for instance, suggests a theory in which a stress tensor and a strain tensor is assigned to each grain (more exactly, to a polygonal domain surrounding the grain), and an approximation of the global behavior is gained through homogenization; this approach arises in other papers too. However, our opinion is that the geometrical characteristics of a grain, even together with its contact points, cannot properly reflect the geometrical buildup of the internal structure, so this unit seems to be insufficient in itself.

A more complex unit was suggested by Chang (1983), called *micro-element.* A micro-element consists of a grain and its nearest neighbours (so this unit can be considered as the composition of the previous two). This unit is "powerful" in the sense that it is able to reflect geometrical and topological relations between grains, so it seems to be a very promising basis for building up constitutive theories.

Now turn the attention to the well-known geometric systems that are often used for modelling whole assemblies.

The widely-used *Voronoi tessalation* can be applied in several ways. In the simplest case it is defined for a set of discrete points given in the 2D or 3D Euclidean space. In the 2D problem the plane is subdivided into polygonal domains, each of them containing exactly

one point. The edges of the domains are the bisecting lines of those straight segments that connect the neighbouring points. (In 3D the system is similar: the faces of polyhedral domains are given by the bisecting planes between neighbouring points.)

Its generalized version can be applied for monosize assemblies of circular or spherical grains. For 2D assemblies of equal circles the plane can be divided into polygons whose edges are the bisecting lines of straight segments joining the centres of neighbouring grains. (The same can be done for 3D too.) A cell system ("Voronoi cells") results in such a way that there is exactly one grain in each cell. This system is especially suitable for the analysis of regular assemblies (see, e.g., Chang et al., 1989).

Dirichlet tessalation, the next system we shall introduce here, has the main advantage over the Voronoi tessalation in that the grains do not necessarily have the same size. Consider a set of non-intersecting circular grains in 2D, or non-intersecting spherical grains in 3D. A domain can be assigned to each grain, consisting of those points which have a shorter or equal tangent to that grain than to any other grain. The common faces of the domains are the power lines (power planes in 3D) of neighbouring grains. (It may be worthwhile to mention that in case of monosize assemblies the Dirichlet and Voronoi tessalations are equivalent.) A similar tessalation was suggested by Gellatly and Finney (1982), and applied by Annic et al. (1993) instead of the Voronoi cells, for the characterization of assemblies having circular grains with different sizes.

The Dirichlet tessalation, in principle, could be generalized for particles with arbitrary smooth convex shape, but as far as we know the problem was solved and construction algorithms were found only for grains and assemblies having very special regular geometry.

The *Delaunay network* can also be a useful tool in characterizing granular systems. Consider an assembly of circular or spherical grains; if the Dirichlet cells of two grains have a common side, connect the two grain centres by a straight line. These connecting lines form the Delaunay network of the assembly.

The definition can be modified to give a more physical meaning to the network if the centres of grains being in contact are connected. In this version the branches in the network correspond to the internal supports in the microstructure. However, the duality with the Dirichlet tessalation does not necessarily hold in this case.

(An interesting idea was given in Ostoja-Starzewski and Wang (1989) by the joint application of Voronoi tessalation and Delaunay network in the case when the circles degenerate into points, and the two systems show a direct duality. A structural mechanical method provided estimations on the global behavior in such a way that the branches in the Delaunay network were considered as linearly elastic two-force springs; these may correspond to contacts in a granular assembly, for example.)

In Section 2 of the present paper two new geometrical systems will be introduced as alternatives to the previous ones. They will be defined for assemblies of grains having arbitrary convex shape; and there will be a clear duality between them. Our opinion is that these advantages make the suggested cell systems more powerful for the modelling of granular assemblies than the presently applied Voronoi, Dirichlet and Delaunay systems.

Finally, two concepts will be introduced that are of a very different nature, but both based on the application of two systems dual to each other.

The first one was suggested by Tonti in 1976. He was searching for the reason of the common experience that physical theories having very different meaning show close analogies in the mathematical buildup of their basic equations. It was shown in his splendid paper (Tonti, 1976) that the differential operators used in the mathematical equations correspond to a so-called *coboundary process* executed on two complementary cell systems and this fact leads to conclusions that give the explanation for the existence of the analogies. The two systems can be introduced as follows.

To define the primal cell system, consider the analysed region Ω of the n-dimensional Euclidean space (for simplicity, this summary will be restricted to $n = 3$ only, though the considerations are valid for smaller or larger n too). Subdivide Ω into small three-dimensional cells whose faces are formed by the co-ordinate surfaces of a co-ordinate system x^1, x^2, x^3; these will be called 3-cells. Every 3-cell is composed of faces, edges and vertices that will be considered as 2-cells, 1-cells and 0-cells. To construct the dual cell system, consider the centres of the 3-cells; they become the vertices (0-cells) in the dual cell system that is built upon the dual vertices in the same way as

seen above. Obviously, for every p-cell of the primal system there corresponds a $(n-p)$-cell of the dual system, and vice versa.

The other concept was introduced by Satake (1976, 1993, 1994). In his ingenious graph-theoretical approach two complementary graphs (particle- and void-graph) are applied for the topological characterization of 2D random assemblies. The nodes in the particle graph correspond to loops in the void graph (representing the grains); branches of the two graphs correspond to each other (they represent the contacts); loops in the particle-graph correspond to nodes in the void-graph (voids). The topological structure of the graphs is expressed by two *topological matrices*. The equilibrium and compatibility equations are compiled with the help of these matrices; and it was found by Satake that the topological matrices here have the same role as the Schaefer operators in generalized continuum mechanics (Schaefer, 1967). (The correspondence between the topological matrices and Schaefer operators can be understood with the help of Tonti's results. Tonti's concept includes that the differential operators of continuum mechanics show an analogy with the coboundary processes. Indeed, the topological matrices of Satake could be considered as operators prescribing some kind of "boundary processes" in random granular assemblies.)

1.2. Macro-level state variables

The mechanical state of the assembly and its state-changing can exactly be described and predicted if the following characteristics are fully given:

- position and geometry of each grain;
- displacements (translations and rotations) of each grain;
- contact forces;
- material properties of the individual grains.

The behavior of the assembly under external loading could exactly be predicted on the level of individual grains in this case. But such a detailed description is not necessary, and too complicated from a practical point of view. Instead, the aim of the microstructural approach is to find macro-level state-variables through the proper averaging of micro-variables.

There are several different ideas in the literature on how many, and what kind of variables should be applied. It is mostly agreed upon that for practical purposes a stress–strain relationship should be given as the result of any theory; so – as a beginning – a *stress* tensor and a *strain* tensor have to be defined in terms of micro-variables. (A summary of existing suggestions will be given a few lines below.) Besides, variables expressing the geometrical state of the material are also thought to be necessary. Different *fabric tensors* were defined for this purpose to express the directions and strength of anisotropy of the microstructure (see, e.g., Satake (1983) about simple and weighted second-order fabric tensors; Konishi and Naruse (1988) on void tensors; Mehrabadi et al. (1988) on fourth-order fabric tensors). Other state variables can also be found in the literature (Cundall et al., 1983, Cambou, 1993, Koenders, 1993, and others), and not even the number of necessary variables is clarified. So the problem of finding suitable state variables is an area under active research today.

1.2.1. Stress

Several microstructural stress definitions have been given until today. The first one suggested by Drescher and de Josselin de Jong (1972) is still rather close to the continuum-mechanical approach. Consider a spherical assembly of volume V consisting of grains having arbitrary shape; the assembly is submitted to external forces $T_i^1, T_i^2, \ldots, T_i^m$ on its boundary points $x_i^1, x_i^2, \ldots, x_i^m$. The average stress of an equivalent continuum of the same V volume under the same loads is

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{k=1}^{m} x_i^k T_j^k,$$

so this expression can be applied as a definition of the stress tensor in granular assemblies.

A real microstructural definition was already given by Christoffersen et al. (1981) where the average stress of an assembly of grains with arbitrary shape is expressed with the help of the individual contact forces inside the assembly. The analysed finite-sized domain is subjected to a special load $p_i(x_j)$ having the form

$$p_i = \sigma_{ij}^{\text{load}} n_j,$$

where $\sigma_{ij}^{\text{load}}$ is a second-rank tensor and n_i is the outwards unit normal vector on the boundary of the analysed representative domain. Due to this load, contact forces $F_i^1, F_i^2, \ldots, F_i^M$ arise between the grains. The

principle of virtual work leads to a constraint for these forces:

$$\bar{\sigma}_{ij}^{\text{load}} = \frac{1}{V}\sum_{c=1}^{M} l_i^c F_j^c ,$$

where $\sigma_{ij}^{\text{load}}$ must be a symmetric tensor to ensure the moment equilibrium, and the vector l_i^c connects the centroids of the two grains forming the c-th contact. The above constraint can be applied as a definition of the $\sigma_{ij} = \sigma_{ij}^{\text{load}}$ stress tensor.

A similar definition was suggested by Rothenburg and Selvadurai (1981), from different theoretical considerations. Consider first an assembly of contacting grains of arbitrary shape; and imagine that a continuous closed shell surrounds the assembly defining its boundary this way. The shell is subjected to a special load $p_i(x_i)$ that satisfies the following condition in every point of the shell:

$$p_i = \sigma_{ij}^{\text{load}} n_i ,$$

where $\sigma_{ij}^{\text{load}}$ is a second-rank tensor and n_i is the outwards unit normal vector on the shell. The contact forces $F_i^1, F_i^2, \ldots, F_i^M$ act at the contact points between the grains. The analysis of the equilibrium equations of the grains show that $\sigma_{ij}^{\text{load}}$ can be related to the contact forces inside the assembly in the following way:

$$\bar{\sigma}_{ij}^{\text{load}} = \frac{1}{V}\sum_{c=1}^{M} l_i^c F_j^c .$$

The vector l_i^c is the branch vector belonging to contact c.

The equation is a constraint on the contact forces existing due to the specific boundary load. But this equation suggests the definition of stress in a granular assembly:

$$\bar{\sigma}_{ij} = \frac{1}{V}\sum_{c=1}^{M} l_i^c F_j^c ,$$

which is similar to the previous one. (Naturally, since the virtual work principle expresses the equilibrium condition of the system, no wonder that the two definitions are equivalent to each other.)

1.2.2. Strain

One would expect that due to the duality of stress and strain, and to the duality of contact forces and relative displacements, the microstructural definition of the strain tensor is easy to find. Unfortunately this is not the case. Though there are some interesting suggestions (a very good summary of which was given by Satake (1989)), they are rather questionable both from a theoretical and from a practical point of view (Bagi, 1991). Section 3 of the present paper tries to give a definition of the strain tensor in terms of relative displacements of neighbouring grains. Our hope is that this definition is already theoretically correct and physically well-based.

2. Geometrical representation

As a preliminary to the definition of state variables, this section introduces the suggested geometrical representation of discrete materials. First the concept of *material cell system* and *space cell system* will be explained, then the notations of geometrical microvariables used in the later sections will be defined.

2.1. The material cell system

Consider an assembly consisting of grains with convex but otherwise arbitrary shape in the 2D or 3D Euclidean space where the distance between two points is understood in the usual sense; and the $\overline{\text{PG}}$ distance between a point P and a grain G is the following:

1. If P is outside G or on its boundary, $\overline{\text{PG}}$ is the distance between P and that point of G which has the smallest distance from P. (This includes that for a Q boundary point of G the distance is zero: $\overline{\text{QG}} = 0$.)

2. By definition, if P is inside G then $\overline{\text{PG}}$ is negative and its absolute value is the smallest distance between P and the boundary points of G.

Consider now a grain G_0 and collect all those P points whose distance from is less or equal than from any other grain:

$$\overline{\text{PG}_0} \leq \overline{\text{PG}_k} \quad (k \neq 0).$$

These P points form a domain around the G_0 grain. The domain has the following important characteristics:

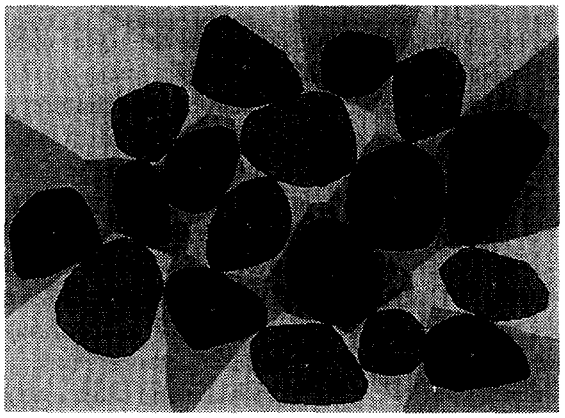

Fig. 1.

- The internal and boundary points of G_0 all belong to it.
- If $\overline{PG_0} < \overline{PG_k}$ for all $k \neq 0$, then P is an internal point of the domain; if there exists a G_i for which $\overline{PG_0} = \overline{PG_i} \leq \overline{PG_k}$ for all $k \neq 0$ and $k \neq i$, then P is a boundary point of the domains of G_0 and G_i.

Constructing these domains for all the grains the space is subdivided as illustrated in Fig. 1 for 2D. Notice the following properties:

- There is exactly one grain in each domain.
- The domains are contiguous.
- Grains on the boundary of the assembly have infinite domains while the domains are finite in the inside of the assembly.
- The common face of neighbouring domains (belonging to the grains G_1 and G_2) is the set of P points for which $\overline{PG_1} = \overline{PG_2} \leq \overline{PG_k}$ for all $k \neq 1$ and $k \neq 2$.
- If two grains have a contact point, the corresponding domains must have a common face that contains the contact point itself.

These domains will be referred to as *material cells*, and the total system given by them as the *material cell system*. The following terminology will be used in their characterisation:

(a) in 3D: The common points of neighbouring cells form *faces*; faces join each other on *edges* (note that if the face $\overline{PG_1} = \overline{PG_2} \leq \overline{PG_k}$ and the face $\overline{PG_2} = \overline{PG_3} \leq \overline{PG_k}$ have a common edge, then the face $\overline{PG_1} = \overline{PG_3} \leq \overline{PG_k}$ also joins this edge); edges intersect with each other on *nodes*.

(b) in 2D: The common points of neighbouring cells will also be referred to as *faces* (however, they are one-dimensional lines in this case); they intersect with each other on *nodes*.

Any set of grains having finite material cells will be called a *finite sub-assembly* (the cells are not required to form a contiguous domain). The boundary of the finite sub-assembly consists of finite faces, forming one or more closed surfaces (curves in 2D).

2.2. The space cell system

The construction of the space cell system is strongly based on the above definitions and characteristics. Starting from an assembly and its material cell system, the space cell system is defined by the following algorithm in 3D:

1. *Nodes* of the system are the grain centres (they correspond to the material cells).

2. If two material cells have a common face, the corresponding grain centres are connected with a straight line that will serve as an *edge* in the space cell system.

3. Consider now an edge in the material system. In the general case three faces intersect on this edge (the special geometry when there are four or more faces joining the same edge will be discussed a few lines below). The three faces define three edges in the space cell system in such a way that they form a closed triangle; this triangle will be a *face* in the space cell system.

(Returning to the special case when four or more material faces determine the same edge, notice that in this case the corresponding space-edges form a closed spatial polygon. This polygon has to be triangularized. To do this, add an imaginary small disturbance to the position of grains in order to destroy the speciality of the geometry; this way the material edge will be split into separate edges each of them belonging to three faces, while new faces will also appear. Now the problem is reduced to the general case. It should be mentioned that in general there are two or more different ways for splitting a multiple edge; any of them can arbitrarily be chosen because the solutions are equivalent from the mechanical point of view.)

4. Similarly, consider next a node in the material cell system; and consider the edges joining this node. As shown before, the edges in the material system correspond to faces in the space system; if the material edges belong to the same node, the space faces form

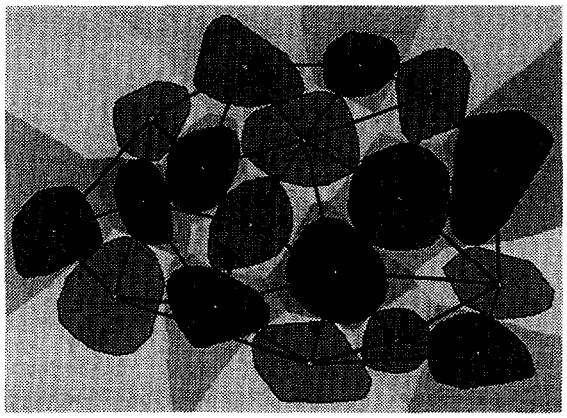

Fig. 2.

a closed *cell* in the space system corresponding to the material node.

The definition is, of course, shorter in the 2D case:

1. *Nodes* of the space cell system are the grain centres (they correspond to the material cells).

2. Where two material cells have a common face, the corresponding grain centres should be connected by a straight line, similarly to the 3D case; these lines will be the *edges* in the space cell system.

3. A node in the material system is the common point of joining faces; the corresponding edges in the space system form a closed *cell*. (Triangularization may be necessary in the case of a special geometry.)

Note that in 2D the cells are triangles, and in 3D the cells are tetrahedrons so the space cell system consists of *simplexes* in any case. Fig. 2 illustrates the space cell system of a 2D assembly.

The composition and duality of the two systems raise several beautiful geometrical problems. Since this paper concentrates on the mechanical description of the assemblies, the geometrical characterization was restricted here to only a summary of the most important features whose knowledge will be necessary for the definition of mechanical state variables. However, another paper is under preparation about the exact mathematical formulation of the two systems. It will discuss problems like triangularization, boundaries, positive and negative space cells, etc., in detail.

2.3. Geometrical micro-variables

First the micro-variables characterizing the material system will be defined.

Fig. 3.

Consider a finite sub-assembly, and a material cell in it around a grain. Some of the faces of the cell belong to "*real*" grain–grain contacts; a face like this contains the contact point itself. The rest of the faces are considered to belong to "*virtual*" contacts (there is no contact between the grain and its neighbour, but their material cells have a common face); in these cases an arbitrary internal point of the face has to be chosen as the virtual contact point. The vector showing from the centre of the grain into the grain's c-th (real or virtual) contact point will be denoted as ν_i^c.

Assume that the G_1 and G_2 grains have a (real or virtual) contact, c. The vectors ν_i^{1c} and ν_i^{2c} show from the corresponding grain centres to the contact point. The *branch vector* assigned to the contact is defined as

$$l_i^c = \nu_i^{1c} - \nu_i^{2c},$$

as illustrated in Fig. 3 for 2D. In the special case when c is on the boundary of the sub-assembly (so it is a contact between a grain and the neighbourhood of the sub-assembly), the branch vector is defined to be equal to ν_i^c (see again Fig. 3).

Now turn the attention on the characterization of the space cell system.

Consider a space cell and number its nodes as $1, 2, \ldots, (D+1)$. (The cell is a simplex so it has $(D+1)$ nodes.) Denote the faces of the cell by the number of that node which is not contained by the face (i.e. the k-th face contains all the nodes except the k-th node). Assign a vector b_i^k to each face in the following way:

- The magnitude of b_i^k is equal to the area of the face (or length in 2D).
- The direction of b_i^k is normal to the face, pointing outwards.

(It can easily be proved that $\sum_{k=1}^{D+1} b_i^k = 0$ for any cell, for both 2D and 3D.)

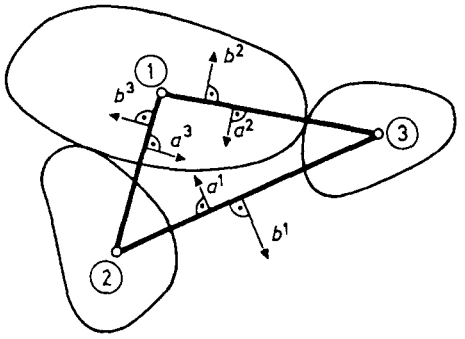

Fig. 4.

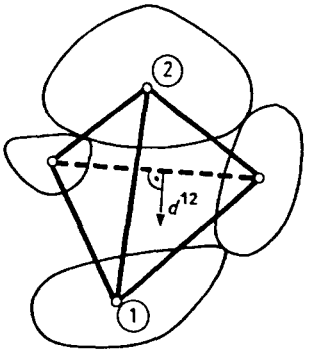

Fig. 5.

The next vector, a_i^k, is defined as

$$a_i^k = -\frac{1}{D} b_i^k .$$

These vectors are illustrated in Fig. 4 in 2D.

The a_i^k vector is the basis of the definition of the most important geometrical micro-variable of the space cell system: the so-called *complementary area vector*. To construct it, consider a pair of grains, G_1 and G_2, that have a (real or virtual) contact, so the two grain centres, 1 and 2, are connected in the space cell system. Collect now *all* those space cells that contain this edge. Assume that altogether T cells were found; denote them as cell(1), cell(2), ..., cell(t), ..., cell(T). In the next step calculate the difference $a_i^{1(t)} - a_i^{2(t)}$ separately in each cell from $t = 1$ to T; after summation over all space cells containing the 1–2 edge, the complementary area vector

$$d_i^{12} = \frac{1}{D+1} \sum_{t=1}^{T} \left(a_i^{1(t)} - a_i^{2(t)} \right)$$

is given. (Its dimension is area in 3D assemblies and length in 2D.) This vector characterizes the local geometry of the neighbourhood of the 1–2 edge.

Fig. 5 is an illustration in 2D where the 1–2 edge belongs to two cells shown by solid lines. The direction of d_i^{12} is as shown, and its magnitude is equal to the one-third of the dotted length. A similar – though more difficult to visualize – meaning can be found for d_i^{12} in 3D too.

The vectors introduced above (l_i^c, a_i^k, d_i^{mn}) will strongly be relied upon in the coming sections.

3. Strain

This section introduces the suggested definition of the strain tensor in granular assemblies. Since the definition is built up with the help of the average displacement gradient tensor of continua, first the continuum-mechanical concept will shortly be recalled; then, based on the space cell system, the definition will be given for a granular material.

3.1. Continuum

A continuous displacement field, $u_i(x_j)$ is given on a closed continuous domain (the vector $u_i(x_j)$ denotes the translation of the point having the position x_i before the displacement). As illustrated in Fig. 6, V is the volume of the domain, S is its surface, and n_i is the outwards unit normal vector on S. Let $e_{ij} = e_{ij}(x_k)$ denote the displacement gradient tensor:

$$e_{ij} = \frac{\delta u_i}{\delta x_j} .$$

According to the Gauss-Ostrogradski theorem, the volume average of $\underline{\underline{e}}$ can be expressed as a surface integral on S:

$$\bar{e}_{ij} = \frac{1}{V} \int\int\int_{(V)} e_{ij} \, \mathrm{d}V = \frac{1}{V} \int\int_{(S)} u_i n_j \, \mathrm{d}S . \qquad (1)$$

If the domain is divided into subdomains (see Fig. 7), an average displacement gradient tensor can be calculated separately for each subdomain:

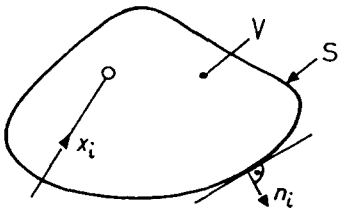

Fig. 6.

$$\bar{e}_{ij}^{L} = \frac{1}{V^L} \int\int_{(S^L)} u_i n_j \, \mathrm{d}S .$$

It is easy to see that if the domain and the displacement field is continuous, the volume-weighted average of the $\bar{e}_{ij}^{L}$ tensors will lead to the same expression as (1):

$$\bar{e}_{ij} = \frac{1}{V} \sum_{(L)} V^L \bar{e}_{ij}^{L} = \frac{1}{V} \sum_{(L)} \left(\int\int_{(S^L)} u_i n_j \, \mathrm{d}S \right)$$

$$= \frac{1}{V} \int\int_{(S)} u_i n_j \, \mathrm{d}S . \qquad (2)$$

Its skew-symmetric part is the average rigid-body rotation of the whole domain (i.e. the volume-weighted average of the rotations of individual subdomains); the symmetric part reflects the deformation of the domain and is named the *strain tensor* in the usual terminology.

3.2. Granular material

To find a state variable that can properly reflect the deformations of granular assemblies, our method is to replace the assembly by an equivalent continuum so that Eq. (2) could be applied; then after discretizing

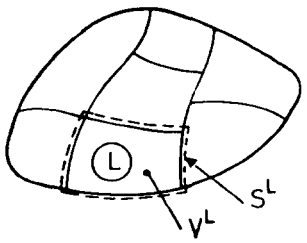

Fig. 7.

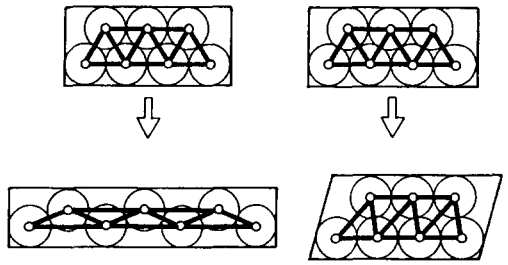

Fig. 8.

return to an expression of the displacement gradient tensor that contains the discrete micro-variables only. In this approach the application of the continuum-mechanical formalism is a tool for the averaging of the micro-variables – the resulting state variable is already of a discrete nature.

Expression (2) can be applied if the geometrical features of the equivalent continuum (division into subdomains, S, n_i) are clarified, and if a continuous displacement field (characteristic for the real displacement system of the assembly) is created on it.

Fig. 8 illustrates why the *space cell system* is the natural basis for the geometrical modelling. As shown here for simple compression and for simple shear, the global deformation of the assembly is very well represented by the deformations of the space cells since they characterise the distortions of the internal structure itself, instead of an individual grain or contact. (Note that the deformations of space cells do not loose their meaning even if there are topological changes, for example, contacts lost or created in the assembly.)

A continuous displacement field can be defined for any finite set of space cells in the following way. On the nodes of the simplexes let $u_i(x_j)$ be equal to the translation of the grain centre while inside the simplex $u_i(x_j)$ is defined as the *linear interpolation* of the node translations of that simplex. The $u_i(x_j)$ field assigned to the assembly this way is piecewise linear inside the simplexes and along the faces and edges, and continuous throughout the whole system.

So consider now the L-th space cell whose average displacement gradient tensor is

$$\bar{e}_{ij}^{L} = \frac{1}{V^L} \int\int_{(S^L)} u_i n_j \, \mathrm{d}S ,$$

which, using the fact that $u_i(x_j)$ is linear along the

boundary, can be written in the following discrete form:

$$\bar{e}_{ij}^{L} = \frac{1}{V^L} \sum_{k=1}^{D+1} u_i^k a_j^k , \tag{3}$$

where V^L and S^L are the volume and boundary of the L-th simplex, the index k runs over the nodes of this simplex, u_i^k is the translation of node k, and a_i^k was defined in Section 2. Since the sum of a_i^k vectors belonging to a simplex is zero, expression (3) can be modified by distracting the same u_i^0 vector from each nodal displacement of the cell:

$$\bar{e}_{ij}^{L} = \frac{1}{V^L} \sum_{k=1}^{D+1} \left(u_i^k - u_i^0\right) a_j^k$$

(its physical meaning is that the rigid-body translations do not change the deformation of the cell). Let u_i^0 be chosen as the average translation of the nodes:

$$u_i^0 = \frac{1}{D+1} \sum_{k=1}^{D+1} u_i^k ,$$

which gives that the average deformation gradient tensor of the L-th cell is

$$\bar{e}_{ij}^{L} = \frac{1}{D+1} \frac{1}{V^L} \sum_{m<n} \left(u_i^m - u_i^n\right) \left(a_j^m - a_j^n\right) ,$$

so after introducing the notation $\Delta u_i^{mn} = u_i^m - u_i^n$, summing over the whole system and according to the definition of d_i^{mn} in Section 2, the average displacement gradient tensor is expressed by the relative displacements of the pairs of nodes forming the edges of the cells:

$$\bar{e}_{ij} = \frac{1}{V} \sum_{m<n} \Delta u_i^{mn} d_j^{mn} \tag{4}$$

(the summation runs over all edges of the space cell system). Expression (4) contains discrete micro-variables only: relative displacements of neighbouring nodes and the corresponding complementary area vectors. The skew-symmetric part of this tensor reflects the average rigid-body rotation of the space cells. The symmetric part – similarly to the continuum-mechanical variable – expresses the deformations of the cells, and it is suggested to be the *strain tensor of granular assemblies.*

4. Stress

This section introduces the definition of the stress tensor in granular assemblies. As an introduction to that, a calculation of the average stress in a continuous domain divided into subdomains will be summarized in Section 4.1; then the stress definition for granular materials will be shown with the help of the material cell system.

4.1. Average stress in continuum

Consider a closed continuous domain with volume V loaded on its boundary S by a distributed force $p_i(x_j)$. Depending on the loads a $\sigma_{ij} = \sigma_{ij}(x_k)$ stress tensor belongs to every point of the domain satisfying the boundary conditions

$$\sigma_{ij} n_j = p_i ,$$

where n_i is the outwards unit normal vector on S. The volume average of the stress tensor can be expressed – with the help of the Gauss-Ostrogradski theorem – as a surface integral:

$$\bar{\sigma}_{ij} = \frac{1}{V} \iiint_{(V)} \sigma_{ij} \, \mathrm{d}V = \frac{1}{V} \iint_{(S)} x_i p_j \, \mathrm{d}S . \tag{5}$$

If the domain is divided into subdomains, the average stress tensor can be calculated separately for each subdomain:

$$\bar{\sigma}_{ij}^{L} = \frac{1}{V^L} \iint_{(S^L)} x_i p_j \, \mathrm{d}S ,$$

where V^L and S^L are the volume and boundary of the L-th subdomain, distributed forces $p_i(x_j)$ act on S^L from the neighbouring subdomains and the external boundary. To get a global average, volume-weighted averages of $\bar{\sigma}_{ij}^{L}$ can be calculated and it results in the same expression as (5):

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{(L)} V^L \bar{\sigma}_{ij}^{L} = \frac{1}{V} \sum_{(L)} \left(\iint_{(S^L)} x_i p_j \, \mathrm{d}S \right)$$

$$= \frac{1}{V} \iint_{(S)} x_i p_j \, \mathrm{d}S .$$

In those cases when there are concentrated forces instead of the distributed loads acting on the boundary of the domain and between the subdomains, the above expression can be written in a discrete form. Denote the forces acting from outside as $F_i^1, F_i^2, \ldots, F_i^k, \ldots$; they act at boundary points $x_i^1, x_i^2, \ldots, x_i^k, \ldots$. Expression (5) is modified as

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{(k)} x_i^k F_j^k \tag{6}$$

(the index k runs over the external loading forces). Now consider the L-th subdomain; the forces $F_i^1, F_i^2, \ldots, F_i^c, \ldots$ act on its boundary at the points $x_i^1, x_i^2, \ldots, x_i^c, \ldots$; (partly from the neighbouring subdomains and partly from outside). So the average stress here is

$$\bar{\sigma}_{ij}^L = \frac{1}{V} \sum_{(c)} x_i^c F_j^c .$$

Since the forces inside cancel out in the summation, the volume-weighted average for the whole domain – as already seen in (6) – is:

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{(L)} V^L \bar{\sigma}_{ij}^L = \frac{1}{V} \sum_{(L)} \left(\sum_{(c)} x_i^c F_j^c \right) = \frac{1}{V} \sum_{(k)} x_i^k F_j^k . \tag{7}$$

4.2. Granular material

Now turn to the definition of the stress tensor in granular assemblies. Consider any finite subassembly; expression (7) will be used for finding the proper stress tensor to describe the state of the material.

Our aim is to find a definition based on the contact forces between the grains, and on the geometrical characteristics of the assembly. Obviously the *material cell system* is the proper basis for this task: material cells divide the space into subdomains in such a way that contact forces act between them, so the above derivations and the result in (7) are directly valid. In this case V^L is the volume of the L-th material cell; $\bar{\sigma}_{ij}^L$ is its average stress; x_i^c is the co-ordinate of the contact point where the F_i^c contact force acts. (If the contact is virtual, $F_i^c = 0$ of course; and if the contact is on the boundary, F_i^c is a force acting from outside.)

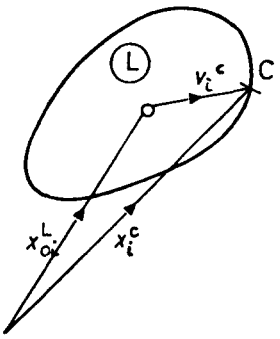

Fig. 9.

Now expression (7) will be transformed into a form containing discrete micro-variables only. First, the x_i^c vectors can be decomposed into two parts, as shown in Fig. 9,

$$x_i^c = x_{0i}^L + v_i^c ,$$

where x_{0i}^L is the co-ordinate of the centre of the L-th grain. In lack of body forces the equilibrium equation $\sum_{(c)} F_j^c = 0$ holds, so

$$\sum_{(c)} x_i^c F_j^c = \sum_{(c)} v_i^c F_j^c . \tag{8}$$

In the double sum in (7) each contact is considered twice, except from the boundary contacts. So instead of the v_i^c vectors we can apply the branch vectors defined in Section 2, hence

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{(L)} V^L \bar{\sigma}_{ij}^L = \frac{1}{V} \sum_{(c)} l_i^c F_j^c \tag{9}$$

(it is easy to show that in lack of body moments this tensor is symmetric).

Expression (9) is clearly equivalent with the previously existing results summarised in Section 1, found from different theoretical considerations. So our suggestion is to use the form (9), which is based on the material cell system, as the definition of the *stress tensor of granular assemblies.*

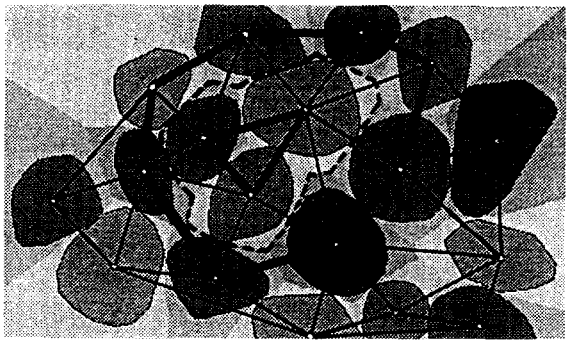

Fig. 10.

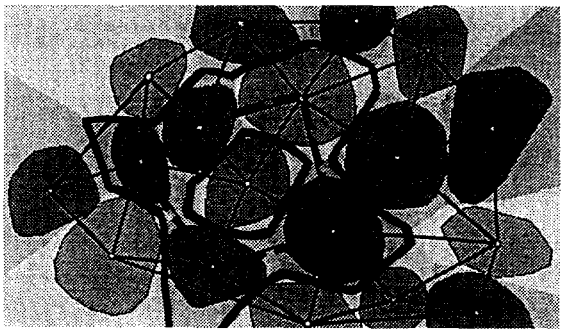

Fig. 11.

5. Duality of the state variables

A definition of the state variables in terms of discrete micro-variables was suggested in the previous sections:

$$\bar{e}_{ij} = \frac{1}{V} \sum_{(c)} \Delta u_i^c d_j^c , \tag{10}$$

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{(c)} l_i^c F_j^c . \tag{11}$$

The two forms show a strong duality. Summation with index c runs through the same contacts in both cases (except for the boundary, see below); contact forces belong to the same pairs of grains as the relative displacements; and the product of the two geometrical parameters is a volume (in 2D an area) characterizing the geometry of the local neighbourhood of the contact.

But the duality is not complete since expressions (10) and (11) cannot belong to the same domain. The strain tensor is the average of the strains in the space cells; so the boundary of a domain where strain is meaningful has to go through the centres of the particles. The solid lines in Fig. 10 illustrate the two possibilities for this type of boundary. On the other hand, the stress tensor is the average of stresses in the material cells, so any domain where stress is defined is built up of material cells (the dotted line in Fig. 10 shows that this type of boundary is always different from the previous ones).

Fig. 11 illustrates this phenomena too. The smallest unit where stress is defined is the individual material cell (solid line in the middle), but strain is not defined here: the nearest domain where the strain tensor is meaningful is shown by the dotted line. The next stress-type boundary is illustrated by a solid line again. This process can be continued, and increasing the two types of domains further and further, the difference between them, compared to the domain size, decreases. In the limit of going to infinitely large domains the difference tends to zero as the granular assembly tends to the continuum.

The fact that the two types of domains differ from each other seems to be a fundamental characteristic of granular assemblies in contrast to continua. Its physical meaning is that while the deformations of the material are carried on principally by the voids between the grains, the loads and stresses are transmitted by the grains themselves.

6. Concluding remarks

A microstructural definition of stress and strain tensors was suggested for granular assemblies in this paper. *Stress* was defined as the average of the stresses in the material cells; and *strain* was given as the average strain of the space cells. This definition is supported by the physical experience that while the forces acting on an assembly are resisted by the grains (the grains correspond to the material cells), the deformations are carried on by the internal structure and the voids (reflected by the distortions of the space cells).

As the next steps, our researches focus on two problems within the search for the relationship between stress and strain. First, statistical studies are carried on recently to predict the characteristic *distributions of micro-level variables* (contact forces, relative

displacements, geometrical micro-variables) if the macro-level state variables are prescribed. Features of these distributions are expected to be indispensable in the constitutive equations of granular assemblies. Second, theoretical efforts concentrate on the analysis of *particle rotations*, a phenomena of fundamental importance in discrete systems. Since particle rotations relate the relative displacements at the contacts to the translations of grain centres, they seem to have a peculiarly important role in establishing a link between the two complementary geometrical systems and, in the future, in finding the stress–strain relationship.

Acknowledgements

This research has been supported by the OTKA program of Hungarian Academy of Sciences, under grant number F-7641.

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