Change of scale for kinematic variables in granular materials: difficulties and limitations

Philippe Dubujet,* Cécile Nouguier-Lehon,* Bernard Cambou*

Summary

This paper is dedicated to the analysis of relations proposed in the literature for the change of scale for kinematic variables in granular materials. In a first part, numerical analyses allow the more adequate local kinematic variables to be defined. The second part is dedicated to the analysis of the local kinematic in granular material from numerical simulations. Particle rotation and loss and creation of contacts are particularly considered for different conditions of contacts.

1. Introduction

Granular materials are made up of grains in contact. These kinds of materials are then, highly discontinuous and heterogeneous with two or three phases. The macroscopic properties of these materials are obviously related to the basic structure and properties of the constituents and their interactions (grains and voids). It therefore seems of great interest to be able to derive the overall behaviour of such materials from the local properties. As is usually the case in these materials, the different phases (grains and voids) are randomly distributed: it is not possible to give a determinist description of the microstructure, so a statistical treatment is appropriate. The Representative Volume Element (RVE) will be, in this case, a statistically homogeneous specimen. Usually, only partial information on the distribution of the phases is available and so it is only possible to derive bounds or estimates for the effective behaviour of such materials. This kind of approach can be called statistical homogenization. As will be shown in the next paragraph, this approach requires the definition of some approximations. This paper deals with the analysis of the hypotheses used for the change of scale for kinematic variables.

2. General scheme of statistical homogenisation in granular materials

The goal of this approach is to use information described at the micro level to build constitutive modelling at the macro level [Cambou *et al.*, 1995]. The macro scale corresponds to a RVE for which a constitutive model written in the usual framework of continuum mechanics can be defined. The micro scale corresponds to a smaller level at which a microstructure exists and which essentially governs the material's global behaviour. In granular material, choosing this level is not easy. Two levels can be considered: one corresponds to the contact between two particles, the other to a local array including several particles. In the usual case where the local level considered corresponds to a contact between two particles, the derivation of the overall behaviour from the local properties may be described in a simplified manner by the diagram in Fig. 1.

Then the definition of the constitutive equations at the global level can be obtained using information given at the local level. This approach requires two essential elements to be developed:

- A realistic modelling at the micro scale of the local behaviour and of the microstructure,
- A technique to go between the two levels (micro and macro): the operation leading from the local level to the global one is called the "averaging process", the reverse operation (from global to local level) is called the "localization operation".

3. The usual hypotheses for the change of scale for kinematic variables

3.1. Local kinematics

Considering two rigid neighbouring particles of convex shape, the relative displacement at contact (nearest neighbouring points) and the relative rotation can be defined by (Fig. 2):

$$\begin{aligned} \delta c_i^k &= \delta u_i^m - \delta u_i^n + e_{ijl}\,(\delta\omega_j^m r_l^m - \delta\omega_j^n r_l^n), \\ \delta\omega_i^k &= \delta\omega_i^m - \delta\omega_i^n \end{aligned} \qquad (1)$$

where δc^k is the displacement of contact point C^k belonging to particle m minus the displacement of contact point C^k belonging to particle n, e_{ijl} is the

* LTDS – Ecole Centrale de Lyon, Ecully, France.

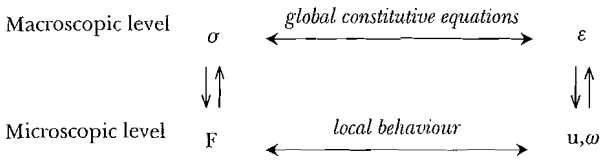

Fig. 1 – General scheme of homogenization theory.
Fig. 1 – Schema generale dei processi di omogeneizzazione.

permutation symbol, $\delta \boldsymbol{u}^m$ and $\delta \boldsymbol{u}^n$ are the displacements of the centroids G^m and $G^n$of the two particles, $\delta \boldsymbol{\omega}^m$ and $\delta \boldsymbol{\omega}^n$ are the rotations of particles m and n, $\boldsymbol{r}^m = G^mC^k$, $r^n = G^nC^k$, and $\boldsymbol{n}^k$ is oriented from particle n to particle m.

This analysis reveals that, at the local level, two very specific features of granular materials can be identified: rotations, which can occur between particles in contact, and evolution of contacts which are created or lost throughout loading. These local kinematics give rise at the global level to kinematics which are usually described by the strain tensor. The link between the kinematic variables defined at these two levels will be analysed below.

3.2. Definition of the strain tensor from the local displacement

Different approaches have been developed in the literature [KRUYT, 1996] [CHANG, 1994] [BAGI, 1996]. We will present the method proposed by [CHANG, 1994] which has been modified by [CAMBOU *et al.*, 2000]. This method is based on the hypothesis that the displacement gradient tensor defined at the macro level a_{ij} is the best estimate of the actual local displacement measured at the centre of gravity u_i^m. Then it is considered that a_{ij} is given by the minimisation of the square deviation between the two fields in volume V with N contacts between particles:

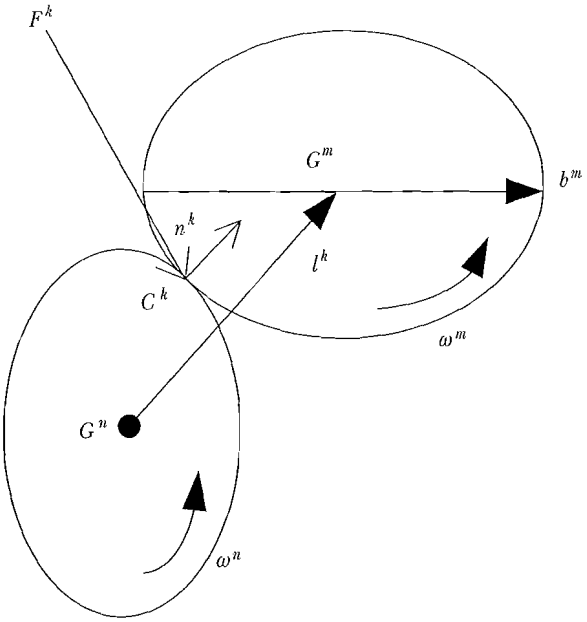

Fig. 2 – Definition of local variables at contact between two particles.
Fig. 2 – Definizione delle variabili locali relative ai contatti.

$$S=\sum_{k=1}^{N}E_i^kE_i^k=\sum_{k=1}^{N}\left[\delta a_{ij}l_j^k-(\delta u_i^m-\delta u_i^n)\right]\left[\delta a_{ip}l_p^k-(\delta u_i^m-\delta u_i^n)\right]. \quad (2)$$

To simplify the notations, $\delta l_i^k = \delta u_i^m - \delta u_i^n$ can be written, then the minimisation of S leads to the condition:

$$\frac{\partial S}{\partial a_{pq}}=\sum_{k=1}^{N}\frac{\partial(\delta a_{ij}l_j^k-\delta l_i^k)}{\partial\delta a_{pq}}(\delta a_{ir}l_r^k-\delta l_i^k)=0. \quad (3)$$

This relation can be written:

$$\sum_{k=1}^{N}(\delta a_{ir}l_r^k-\delta l_i^k)\delta_{ip}\delta_{jq}l_j^k=\sum_{k=1}^{N}(\delta a_{pr}l_r^k-\delta l_p^k)l_q^k=0, \quad (4)$$

$$\delta a_{pr}\sum_{k=1}^{N}l_r^kl_q^k=\sum_{k=1}^{N}\delta l_p^kl_q^k. \quad (5)$$

Term $\sum_{k=1}^{N}l_r^kl_q^k=NH'_{rq}$ appears in relation (5), if G'_{ij} is defined by $G'_{ij}H'_{jl} = \delta_{il}$, the following relations are obtained:

$$\begin{cases}\delta a_{ij}=\dfrac{1}{N}\left(\sum_{k=1}^{N}\delta l_i^kl_n^k\right)G'_{nj}\\ \delta\varepsilon_{ij}=\dfrac{1}{2N}\left(G'_{nj}\sum_{k=1}^{N}\delta l_i^kl_n^k+G'_{ni}\sum_{k=1}^{N}\delta l_j^kl_n^k\right)\end{cases} \quad (6)$$

In the case of isotropic materials made up of spherical or cylindrical particles, these relations can be written:

$$\delta\varepsilon_{ij}=\frac{1}{2dl_0^2N}\sum_{k=1}^{N}(\delta l_i^kl_j^k+\delta l_j^kl_i^k), \quad (7)$$

where d is the dimension of the space. These formulations can be used considering different meanings for the variable δl_i^k. Three possible expressions for δl_i^k have been analysed:

- the relative displacement of the contact point of particles in contact (the initial formulation proposed by [CHANG, 1994] is only acceptable for particles without any contact evolution or particle rotation),

- the displacement of the centres of particles in contact,
- the displacement of the centres of neighbouring particles.

The last definition of δl_i^k puts forward the notion of neighbouring particles. Two definitions can be proposed. The first one is based on the distance between two particles: two particles i and j will be considered as neighbouring particles if

$$d_{ij} \leq (R_i + R_j)(1 + a), \quad (8)$$

where d_{ij} is the distance between the two centres of particles i and j, R_i and R_j are the radii of particles i and j, and a is a parameter to be defined.

The second definition is based on the notion of local array. A Voronoï tessellation is considered: if two particles belong to the same local triangular element, they are considered as neighbouring particles.

3.3. Definition of the local displacement from the strain tensor

This definition is usually complex and only rough approximations can be proposed. The usual approximation is called the *uniform strain approximation*. In this approximation, the relative local displacement between two particles is taken to be equal to the relative displacement of two similar points in the equivalent continuum:

$$\delta l_i^k = \delta \varepsilon_{ij} l_i^k. \quad (9)$$

This relation is usually used for two particles in contact (contact k), but we will extend the use of this formulation for neighbouring particles as defined in paragraph 3.2.

3.4. Other definitions for the local kinematic variables

The local kinematic variable, which has been considered in the previous paragraphs, is the displacement between two particles. This kind of variable has been preferred because it is at this level that the static variable, the contact force, is defined. This approach seems appropriate because it should be possible to define a relation between these two kinds of variables (contact forces and displacements between two particles). Other studies [DEDECKER *et al.*, 2000] consider the local kinematic variable to be the strain tensor defined in a local array. This approach is interesting but the link between contact forces and local strain seems difficult to define and so the complete scheme of homogenization as defined in Fig. 1 seems rather difficult to perform.

4. Numerical analysis of the representative local kinematic variables

Different relations have been proposed in paragraph 3 to define the strain tensor from the local displacements (6), (7) or the inverse relation (9). The validity of these relations has been analysed from a numerical analysis using the Distinct Element Method with the *PFC2D* code. Biaxial tests are performed on 2D materials composed of cylindrical particles. Characteristics used in these numerical simulations are described in Tab. I.

These numerical analyses take into account different local kinematic variables. In particular, distributions of local strains computed in a discrete numerical simulation have been compared to the distribution given from a continuum approach in Fig. 3. In this figure, three local displacements are considered:

- the relative displacement of the contact points between particles in contact,
- the relative displacements between the centres of particles in contact,
- the relative displacement between the centres of neighbouring particles (defined by a certain distance between the centres).

All these local variables are mean values computed for a given orientation of the vector joining the centres of the considered particles. It is clear in this figure that the first two local variables are very far from the displacement field given by the continuum variable ε_{ij} if the compressive (or extensive) strain is considered. The compressive or extensive local displacement field appears to be in good agreement with the field given by the continuum, only when considering neighbouring particles with $r \leq 2.3D_m$, where r is the distance between two neighbouring particles and D_m being the mean diameter of parti-

Tab. I – Numerical parameters used in the simulations performed with the *PFC2D* code.
Tab. I – Parametri numerici (simulazioni con il programma PFC).

Variables	Numerical value
Number of particles	2500
Diameter of particles	From 1.8 to 2.2 mm
Normal and tangential stiffness $k_n=k_t$	10^8N/m
Friction ratio ball/ball	0.3
Friction ratio ball/wall	0
Confining pressure	100 kPa
Velocity of the upper wall for the compression loading	0.01m/s

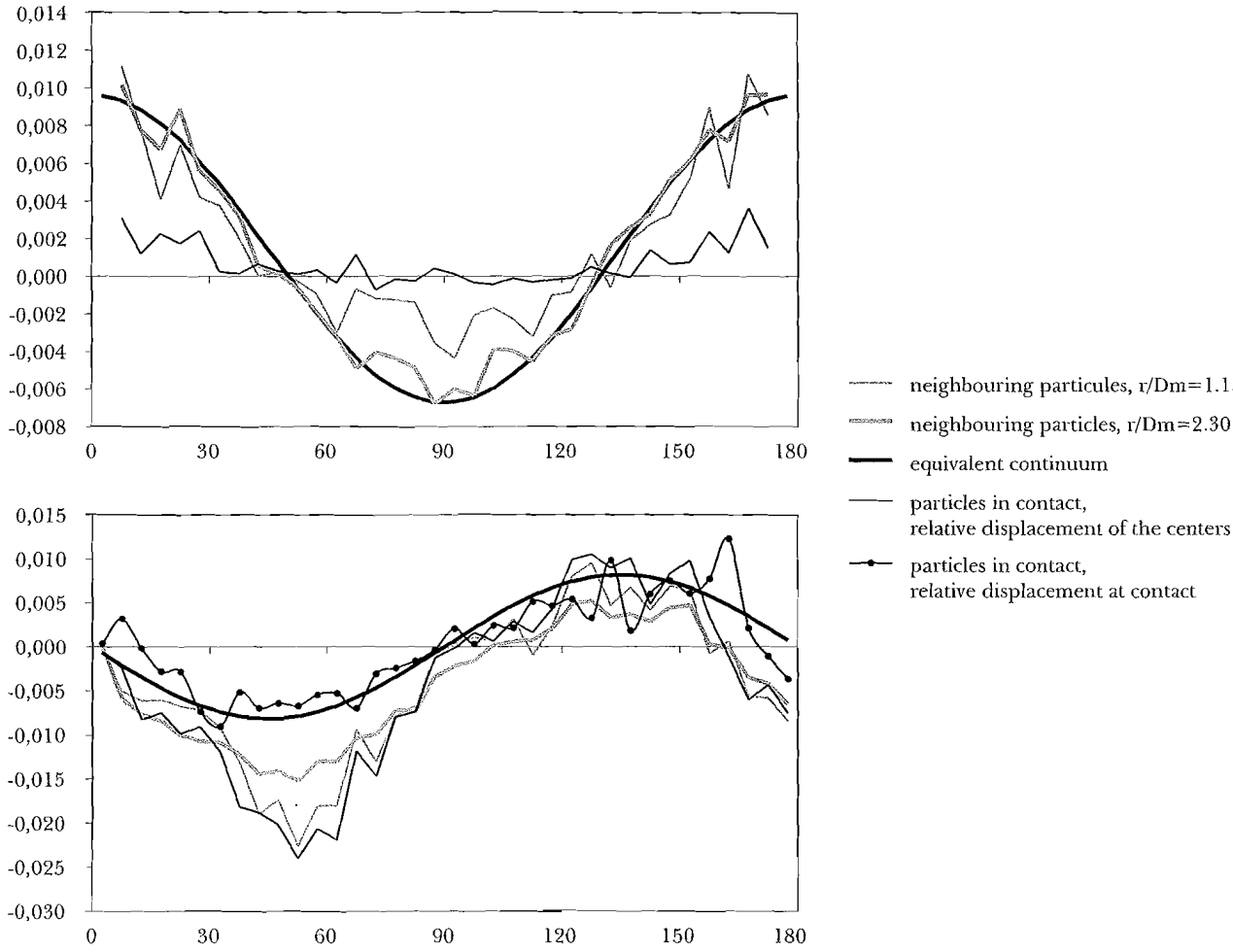

Fig. 3 – Distributions of local strain versus contact orientation (degree) computed in a discrete numerical simulation (*PFC2D*). Top: compressive (or extensive) strain, bottom: shear strain.
Fig. 3 – Distribuzione delle deformazioni locali in funzione dell'orientazione dei contatti (PFC2D). Sopra: compressione; sotto: taglio semplice.

cles. The field obtained for shearing displacements is clearly asymmetric. This is certainly due to the occurrence of shear bands. It can be pointed out that the relative displacement at the contact remains approximately symmetric, so it is clear that on the shear band the tangential field is essentially due to the preferential rotation. The same kind of conclusion has also been validated by considering the reverse link. To obtain a representative expression of the global strain tensor it is necessary to consider, in relations (6) or (7), neighbouring particles composed of particles in contact and without contact [DEDECKER *et al.*, 2000].

5. Numerical analysis of specific local phenomena occurring in granular materials

The analysis of the local kinematics in granular materials allows two specific phenomena to be pointed out: rotation of particles and loss or creation of contacts.

The rotation of particles has been analysed by considering three different materials composed of particles with different shapes. The numerical model used for these simulations has been proposed by [MOREAU, 1994]. This model has been used because it allows particles with different shapes (circular or polygonal) to be considered. This code takes into account rigid particles without any local deformation at contacts. *PFC2D* has not been used for this analsis because it can only analyse cylindrical particles (in 2D). The two codes: *PFC2D* and the Contact Dynamic Code from Moreau have been compared for quasi static loadings and give very similar results. Characteristics used in the numerical simulations obtained from the Contact Dynamic Code are described in Tab. II.

The granular distribution of the three materials is similar, the first one is composed of circular particles, the second one of convex polygonal particles without any preferential direction and the third one of convex elongated polygonal particles (with an

Tab. II – Numerical parameters used in the simulations performed with the Contact Dynamic Code.
Tab. II – Parametri numerici (simulazioni con il programma "Contact Dynamic").

Variables	Numerical value
Number of particles	2000
Diameter of particles	From 1 to 3 mm
Friction coefficient ball/ball	0.3
Friction coefficient ball/wall	0
Confining pressure	10 kPa
Local restitution coefficients	0

elongation ratio around 3). It is clear in Figs. 4 and 5 that rotations are very significantly greater for circular particles than for the polygonal ones. The mean value of the absolute value of rotation in circular particles is about 50° for a global strain of 20%, it is about 15° in polygonal particles for the same global strain level.

Other simulations have been performed to analyse the influence of rotations and loss or creation of contacts on the local displacement field, with the software *PFC2D*, developed by [CUNDALL, 1979]. For these simulations characteristics described in Tab. I are considered. Three particular conditions have been considered for an increment of load in common biaxial test:

- usual conditions of contact, free rotation of particles,
- usual conditions of contact, blocked rotation,
- unbreakable bonds at each contact, free rotation.

The global behaviour of the particular materials (contact bond and particle without rotation) is clearly stiffer than that of the usual material. It can be noted also that, for the strain increment analysed, the usual material shows dilatancy when the particular materials show contractancy. Then, it seems clear that rotation ability is linked to dilatant behaviour.

Fig. 6 shows the local displacement field given by particles with contact bonds. It is clear that the di-

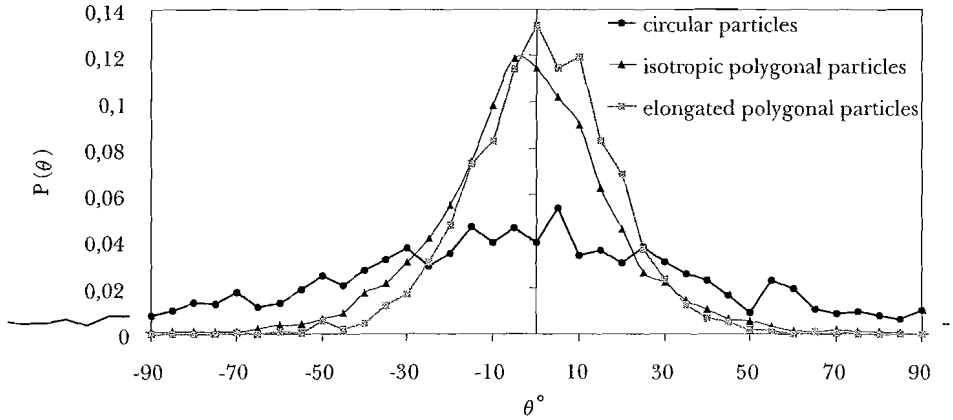

Fig. 4 – Distribution of grain rotations after 20% axial strain for the 3 samples.
Fig. 4 – Distribuzione della rotazione dei grani (deformazione 20%).

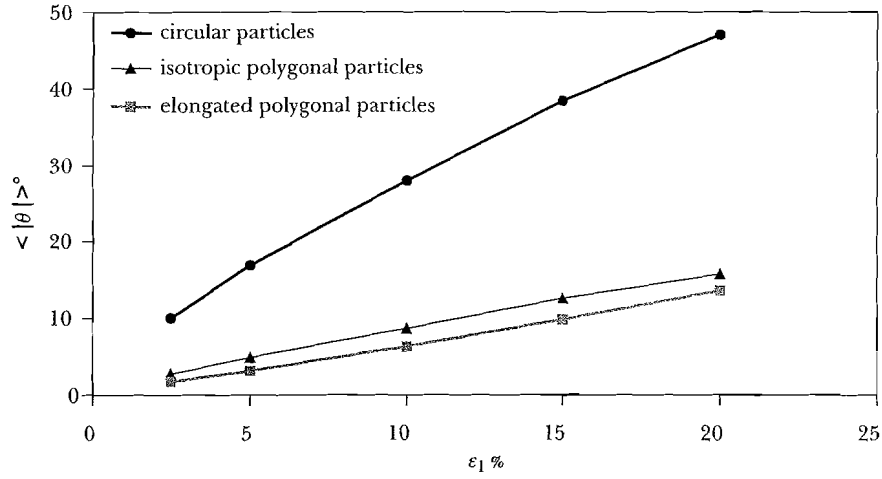

Fig. 5 – Evolution of the mean absolute value of grains rotations for the 3 samples.
Fig. 5 – Evoluzione della media delle rotazioni dei grani (valori assoluti).

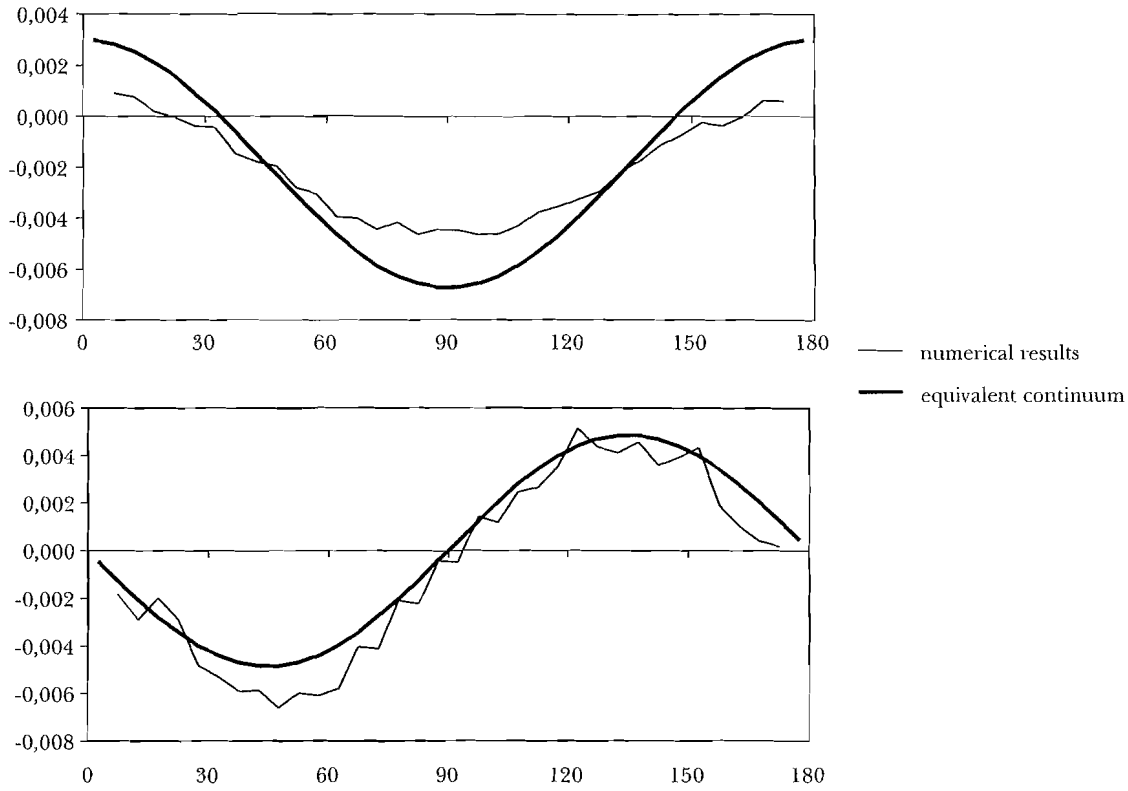

Fig. 6 – Distributions of local strain versus contact orientation (degree) computed in a discrete numerical simulation with contact bond (*PFC2D*). Top: compressive (or extensive) strain, bottom: shear strain.
Fig. 6 – Distribuzione delle deformazioni locali in funzione dell'orientazione dei contatti (PFC2D, con "bonded contacts"). Sopra: compressione; sotto: taglio semplice.

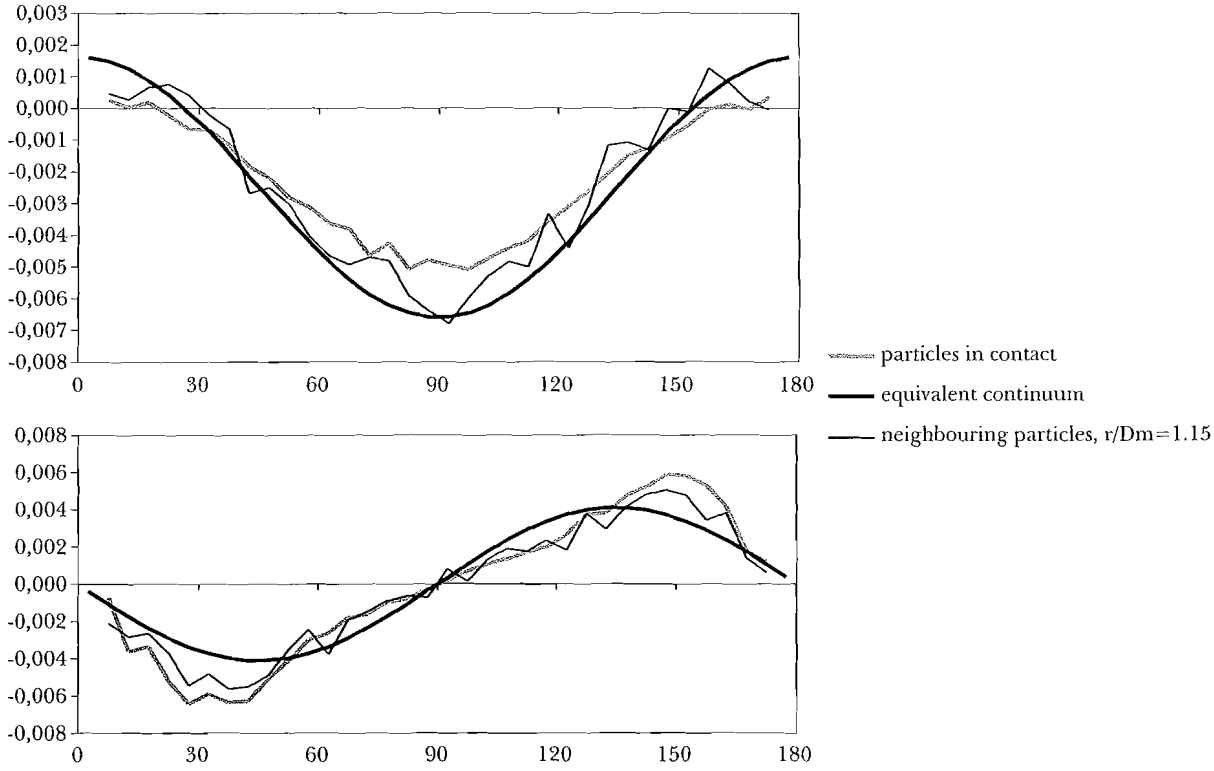

Fig. 7 – Distributions of local strain versus contact orientation (degree) computed in a discrete numerical simulation with blocked rotations (*PFC2D*). Top: compressive (or extensive) strain, bottom: shear strain.
Fig. 7 – Distribuzione delle deformazioni locali in funzione dell'orientazione dei contatti (PFC2D, rotazioni impedite). Sopra: compressione; sotto: taglio semplice.

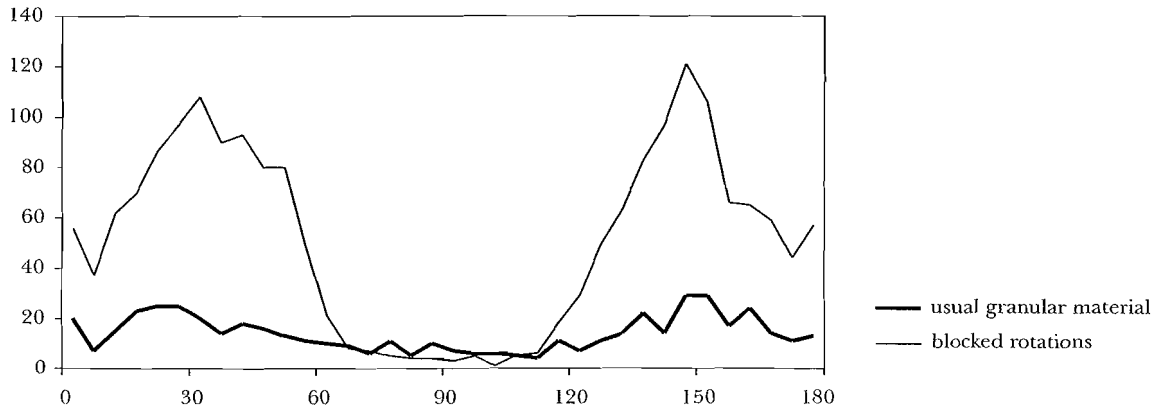

Fig. 8 – Distributions of sliding contacts versus contact orientation (degree) computed in a discrete numerical simulation (*PFC2D*).
Fig. 8 – Distribuzione angolare dei contatti al limite frizionale (PFC2D).

splacement field given by particles in contact with a contact bond is closer to the displacement field of the continuum than the displacement field given by the usual granular materials. Fig. 7 shows the local displacement field given by particles with blocked rotation. In this case also, the displacement field given by particles in contact with blocked rotation is closer to the displacement field of the continuum than the displacement field given by the usual granular materials. It can be pointed out that for orientations aroud 30° and 150°, the shearing displacement given by particles in contact is significantly greater than the continuum displacement field and corresponds to the two maxima of sliding contacts, clearly shown in Fig. 8.

Figs. 6 and 7 clearly show a very paradoxical result. Using a contact bond, which implies no loss of contact (condition on normal displacement), or blocking the rotation of a particle, leads to very similar effects on the local compressive or extensive displacement field between particles in contact.

6. Conclusion

This study allows the following conclusions to be made:

- The local displacement field between particles in contact cannot be identified with the displacement field in the equivalent continuum. This can only be done when considering neighbouring particles at a sufficiently large distance (around 2 times the mean diameter of particles).
- The local rotation of particles is much greater in circular particles than in polygonal particles.
- Rotation of particles plays an important role in the local compressive or extensive displacement field, and so in the volume change evolution.

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Relazioni micro-macro per le variabili cinematiche: difficoltà e limitazioni

Sommario

Questo articolo passa in rassegna alcune delle relazioni proposte in letteratura per descrivere il passaggio di scala micro-macro per le variabili cinematiche, alla luce dei risultati di simulazioni numeriche discrete. Le variabili cinematiche locali più rappresentative vengono individuate e studiate. In particolare l'influenza della rotazione delle particelle e della perdita di contatti è analizzata in dettaglio.