Mechanics of generalized continua: construction by homogenization

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Résumé : La mécanique des milieux continus généralisés fournit des outils pour décrire les effets d'échelle que présentent certains matériaux hétérogènes. Cependant les liens entre les nouveaux degrés de liberté que certains de ces milieux introduisent et la microstructure ne sont clairement établis que pour quelques cas extrêmes (cristaux liquides...). Dans ce travail, on essaie de construire un milieu de Cosserat homogène équivalent à un milieu classique micro-hétérogène, par des méthodes d'homogénéisation généralisées. Ces techniques permettent alors de rendre compte des champs de contraintes et de déformation dans un matériau hétérogène sollicité de telle sorte que la taille de l'élément de volume représentatif ne soit pas négligeable devant la longueur d'onde des sollicitations.

1. INTRODUCTION

Generalized continua can be used to introduce size effects in the mechanical modelling of heterogeneous materials. They involve additional degrees of freedom (higher order continua) or/and higher order gradients of the displacement fields (higher grade continua) [1,2]. In this work, we concentrate on the Cosserat continuum for which independent rotational degrees of freedom are introduced at each point of the continuum in addition to the displacement field [3]. The Cosserat rotation R can be represented by a vector Φ according to

$$R_{ij} = \delta_{ij} - \epsilon_{ijk}\Phi_k. \tag{1}$$

The (relative) deformation tensor and the torsion-curvature tensor are defined as

$$E_{ij} = U_{i,j} + \epsilon_{ijk}\Phi_k \quad \text{and} \quad K_{ij} = \Phi_{i,j}. \tag{2}$$

The dual quantities in the expression of the power of internal forces are the generally non-symmetric force-stress tensor Σ and couple-stress tensor M. The equations of balance of momentum and of balance of moment of momentum read

$$\Sigma_{ij,j} + F_i = 0 \quad \text{and} \quad M_{ij,j} - \epsilon_{ijk}\Sigma_{jk} + C_i = 0 \tag{3}$$

where volume forces F and couples C have been introduced. An illustrative way of understanding the physical meaning of couple stresses is to remark that, contrary to the classical continuum (also called Boltzmann continuum), the size of the volume element of generalized continuum mechanics is not vanishingly small. In particular, there is "enough space" on each side of the volume element to apply a linear distribution of forces (tension + flexion). The mean value of these forces divided by the small surface represents the corresponding components of the stress tensor and the slope of the distribution is related to the associated couple stress components.

There has been a long quest for the experimental determination of Cosserat elastic constants for heterogeneous materials [4]. Cosserat effects arise when the wavelength L_w of the applied stress gradients in the structure is not much larger than the size L of the representative volume element (RVE) of a heterogeneous material, which leads to very difficult experimental conditions and interpretation. Instead, we propose in this work to deduce the Cosserat elastic properties using homogenization methods starting from a classical micro-heterogeneous medium.

Classical homogenization methods are designed to derive effective properties of micro-heterogeneous materials and are valid only if $L \ll L_w$ [5]. When this hypothesis is dropped, the wanted homogeneous equivalent medium (HEM) is expected to be a generalized continuum [6]. The determination of the numerous parameters involved in constitutive equations for generalized media has been a long-standing obstacle to their use. If these constants can be determined thanks to a systematic homogenization procedure, generalized continua have a promising future in mechanics of materials.

Some pioneering work in Germany in this field [7-12] has given the incentive to the following developments. Note that, in this work, the word "homogenization" is used in a loose sense and that, in fact, the word "equivalent" refers to an estimation of the actual response of the heterogeneous material. In particular, the HEM is not expected to be unique and there exists a more adapted specific choice for each type of final structural loading conditions.

2. CONSTRUCTION OF A HOMOGENEOUS COSSERAT MEDIUM STARTING FROM A MICRO-HETEROGENEOUS BOLTZMANN CONTINUUM

2.1 Definition of the micro-mechanical problem

The constituents of the RVE Ω are classical materials with different mechanical properties. Their spatial distribution is given exactly or in a statistical sense and can be very intricate. We look for the displacement field $u(x,t)$ solution of the following boundary value problem (BVP) :

$$\left\{\begin{array}{l} \varepsilon_{ij} = u_{(i,j)} \\ \textit{constitutive equations} \\ \sigma_{ij,j} = 0 \quad \forall x \in \Omega \\ \textit{boundary conditions} \end{array}\right. \tag{4}$$

where ε and σ are the local strain and stress tensor fields. The constitutive equations are left unspecified, since the first results derived in the following do not depend on the specific local behaviour. In classical homogenization theory, one usually considers homogeneous boundary conditions or periodic ones, for which a mean strain or stress is prescribed. As soon as the hypothesis $L \ll L_w$ is dropped, more general loading conditions must be introduced and, more specifically, non homogeneous ones.

2.2 Non-homogeneous boundary conditions

The main difficulty arises from the fact that there is a large variety of possible non-homogeneous boundary conditions. A set of relevant non-homogeneous boundary conditions can be found by considering the typical loading conditions that the whole structure will eventually undergo for a specific application. Accordingly, the choice of appropriate non-homogeneous boundary conditions depends on the final structural application one aims at. Furthermore, this choice then dictates the type of generalized HEM that must be resorted to, as will be seen in the sequel.
Consider for instance the following non-homogeneous boundary conditions

$$u_i = E_{ij}x_j + F_{ij}^{skew}(x)x_j \quad \forall x \in \Omega \tag{5}$$

where F^{skew} is the following x - dependent skew-symmetric tensor

$$F_{ij}^{skew} = -\epsilon_{ijk}f_k(x) \quad \text{with} \quad f_k = K_{kl}x_l. \tag{6}$$

The third-rank permutation tensor is denoted by ϵ. Vector f is a linearly varying rotation vector so that K has the meaning of a prescribed curvature. General tensors E and K are given and constant. Finally the proposed non-homogeneous boundary conditions read :

$$u_i = E_{ij}x_j + \epsilon_{ijk}K_{jl}x_lx_k, \quad \forall x \in \partial\Omega. \tag{7}$$

If K vanishes, classical homogeneous boundary conditions are retrieved. If only K_{33} or K_{31} are non-zero, we get respectively

$$\left\{\begin{array}{l} u_1 = -K_{33}x_2x_3 \\ u_2 = K_{33}x_1x_3 \end{array}\right. \quad \text{or} \quad \left\{\begin{array}{l} u_1 = -K_{31}x_1x_2 \\ u_2 = K_{31}x_1^2 \end{array}\right. \tag{8}$$

which are torsion-like and flexion-like boundary conditions.

The mean deformation in Ω reduces to

$$< u_{i,j} >= \frac{1}{V} \int_\Omega u_{i,j}\, d\Omega = E_{ij} \tag{9}$$

if the origin of the coordinate system is taken as the geometric centre of mass. Computing now the mean work of internal forces and, using Gauss theorem,

$$< \sigma_{ij}\varepsilon_{ij} >= \frac{1}{V} \int_\Omega \sigma_{ij} u_{i,j} d\Omega = \frac{1}{V} \int_\Omega \sigma_{ij} u_i n_j dS \tag{10}$$

where n denotes the normal to the surface. The application of boundary conditions (7) leads to the expression

$$< \sigma_{ij}\varepsilon_{ij} >= \Sigma_{ij} E_{ij} + M_{ij} K_{ij} \tag{11}$$

with

$$\Sigma_{ij} =< \sigma_{ij} > \quad \text{and} \quad M_{ij} =< \epsilon_{ikl} x_k \sigma_{lj} > . \tag{12}$$

As a result, if E and K are regarded as macroscopic deformation and torsion-curvature tensors, and if relations (12) define the overall force and couple stress tensors, equation (11) represents a part of the work of internal forces of a Cosserat homogeneous equivalent medium. However, in this expression, the skew-symmetric part of E does not work with Σ, since, according to (12), Σ is symmetric. Additional conditions are introduced in the next section to achieve the identification of the HEM with a Cosserat continuum, at least in the 2D case. Note that $M_{ii} = 0$ so that K_{ii} does not work in (11). In fact, relation (11) completely defines a constrained Cosserat overall medium (couple stress theory).

3. APPLICATION TO HETEROGENEOUS LINEAR ELASTICITY

In this section, we show how the effective Cosserat elastic properties of a heterogeneous material can be worked out using the finite element method in a special case.

3.1 Unit cell and classical boundary conditions

A structural component with periodic microstructure is considered, for which the unit cell is given in figure 1. Such an element can be found for instance in a cylinder head gasket of a car engine [13] and is made of steel (E = 200000 MPa, ν = 0.3, in gray on figure 1) and of a composite latex material (E = 5500 MPa, ν = 0.45). For simplicity, we investigate the two-dimensional problem only (plane strain conditions) and periodicity is assumed in the two directions, so that there only a loose analogy to the actual head gasket. The size of the RVE is L = 5 mm. The overall symmetry of this multilayered material is orthotropic. The relevant effective elastic constants in the two-dimensional case are the following :

$$\begin{bmatrix} \Sigma \begin{cases} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \sigma_{21} \end{cases} \\ M \begin{cases} \mu_{31} \\ \mu_{32} \end{cases} \end{bmatrix} = \begin{bmatrix} Y_{1111} & Y_{1122} & 0 & 0 & 0 & 0 \\ Y_{1122} & Y_{2222} & 0 & 0 & 0 & 0 \\ 0 & 0 & Y_{1212} & Y_{1221} & 0 & 0 \\ 0 & 0 & Y_{1221} & Y_{2121} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{3131} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{3232} \end{bmatrix} \begin{bmatrix} \left. \begin{matrix} e_{11} \\ e_{22} \\ e_{12} \\ e_{21} \end{matrix} \right\} E \\ \left. \begin{matrix} \kappa_{31} \\ \kappa_{32} \end{matrix} \right\} K \end{bmatrix} \tag{13}$$

The RVE admits a centre of symmetry so that there will be no coupling between the overall Cosserat deformation and curvature tensors [6].

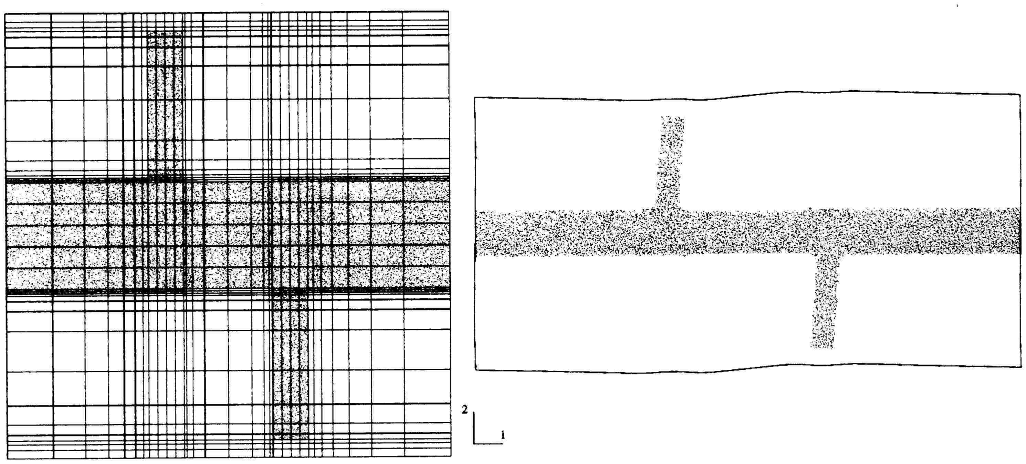
The classical orthotropic constants are deduced from two extension tests and a shear test with homogeneous (h) or periodic (p, figures 2 and 3) boundary conditions :

$$Y^h_{1111} = 79620\,\text{MPa}, Y^h_{2222} = 39470\,\text{MPa}, Y^h_{1122} = 22880\,\text{MPa and } C^h_{44} = 6890\,\text{MPa},$$

$$Y^p_{1111} = 79025\,\text{MPa}, Y^p_{2222} = 31630\,\text{MPa}, Y^p_{1122} = 21150\,\text{MPa and } C^p_{44} = 3060\,\text{MPa} \tag{14}$$

where the classical shear modulus reads

$$C_{44} = \frac{Y^2_{1221} - Y_{1212}Y_{2121}}{2Y_{1221} - Y_{1212} - Y_{2121}}. \tag{15}$$



Figures 1 and 2 : Unit cell of the coarse grain structure (left) and extension test in direction 1 (right).

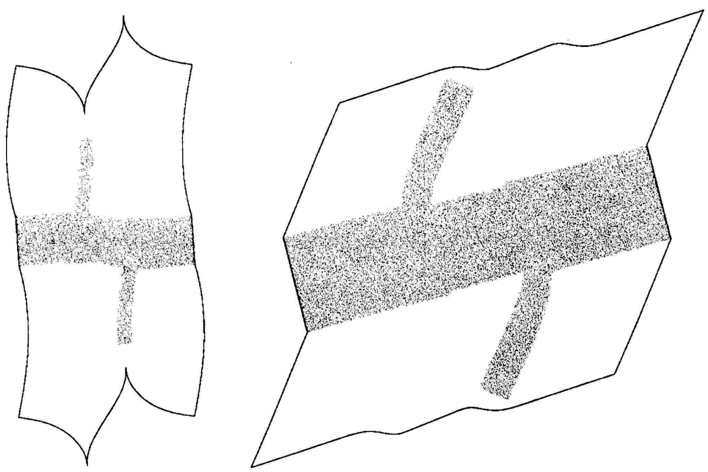


Figure 3 : Extension test in direction 2 (left) and shear test (right).

3.2 Flexural rigidity

It must be noted that a Timoshenko beam is but a one-dimensional Cosserat continuum and that there is a homogenization theory for composite beams. The homogenization procedure introduced in this work merely is a generalization to the two and three-dimensional cases. Accordingly, a flexion rigidity must be attributed to the RVE. The simplest way to determine it is to perform a flexion test with prescribed rotations of two opposite sides, the two other sides being free of forces (figure 4), from which we deduce

$$C_{3131} = 24700\,\mathrm{MPa.mm}^2 \quad \text{and} \quad C_{3232} = 24860\,\mathrm{MPa.mm}^2.$$

However, this is only an approximative way of imposing a curvature to the RVE. The explicit boundary conditions (7) lead to the deformed states of figure 5. We get

$$C_{3131} = 87500\,\mathrm{MPa.mm}^2 \quad \text{and} \quad C_{3232} = 71310\,\mathrm{MPa.mm}^2.$$

To relieve a little bit the previous conditions that provide too stiff moduli for obvious reasons (see figure 5), a certain type of periodicity conditions can be introduced :

$$u_i = E_{ij}x_j + \epsilon_{ijk}K_{jl}x_lx_k + v_i \quad \forall x \in \Omega \tag{16}$$

where v_i takes equal value on opposite sides. These conditions have been implemented in the FE code as a multipoint-constraint condition. In fact there is the additional condition that the curvature associated with v also is periodic, which is not implemented yet. The application of these periodic conditions up to a curvature term gives the deformed state of figure 6 and the effective moduli

$$C_{3131} = 25870\,\text{MPa.mm}^2 \quad \text{and} \quad C_{3232} = 42320\,\text{MPa.mm}^2.$$

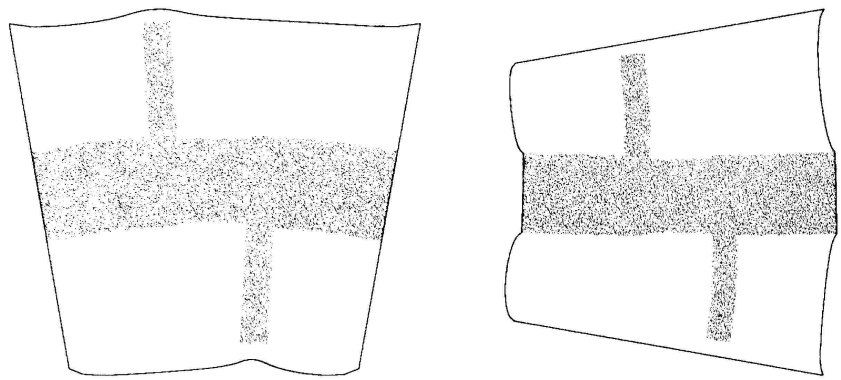


Figure 4 : Simple bending of the RVE according to directions 1 (left) and 2 (right).

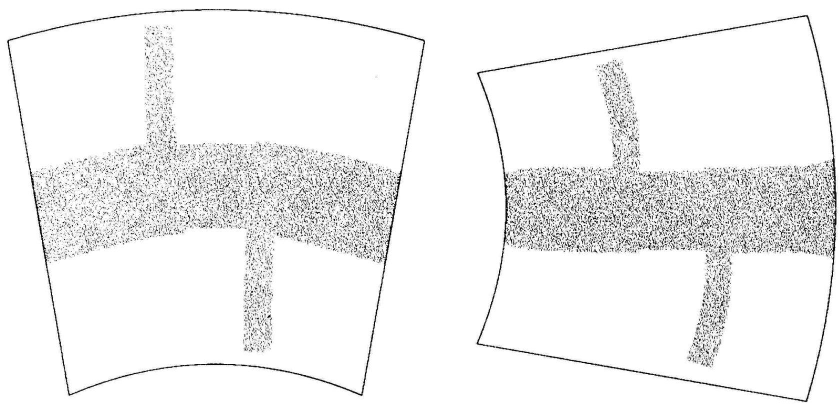


Figure 5 : Prescribed curvatures K_{31} (left) and K_{32} (right) at the boundary.

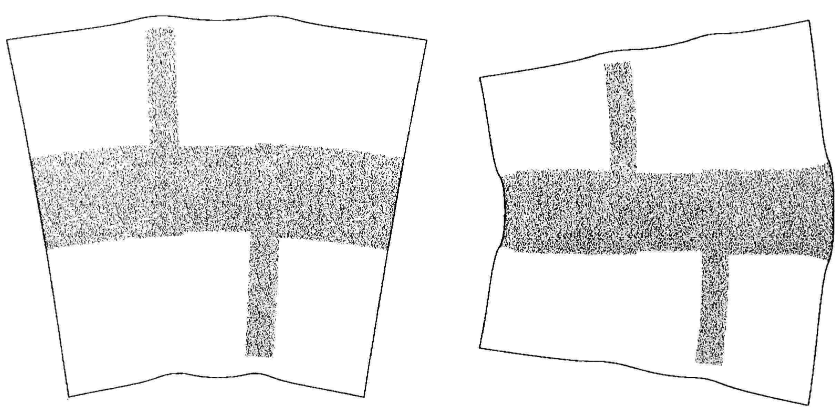


Figure 6 : Periodic conditions up to a curvature term K_{31} (left) and K_{32} (right).

3.3 Cluster of RVEs

In a Cosserat theory, the translational and rotational degrees of freedom are independent. At the mesoscopic level, the translation can describe the displacement of the centre of gravity of the RVE whereas the global rotation of each RVE is accounted for by the additional degrees of freedom. It is clear that neighbouring cells will oppose resistance to inner rotation. As a result, considering an individual RVE as in the previous sections is not sufficient to derive the overall Cosserat effective properties of the heterogeneous material. We propose to consider a *cluster of RVEs* made of one central RVE with its direct neighbours (figure 7 a).

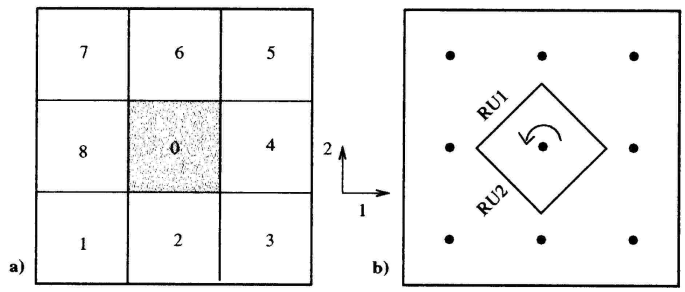


Figure 7 : (a) Definition of a cluster of RVEs and (b) prescribed global rotation of the central cell.

For the determination of the moduli Y_{1212}, Y_{1221} and Y_{2121}, the following test can be considered in addition to the shear test of figure 3. The centres of the RVE 0 to 8 are fixed and a rigid rotation is prescribed at the boundary of RVE 0 (figure 7 b). It corresponds to a non-vanishing relative rotation of the microstructure with respect to the material lines ($< e >_{\rm RVE0}$ is skew-symmetric). The FE calculation provides the reaction forces $RU1$ and $RU2$ on each side of the RVE that represent the resistance of the material to inner rotation. The wanted moduli satisfy

$$\left\{ \begin{array}{l} C_{44} = Y_{1221}^2 - Y_{1212}Y_{2121}/(2Y_{1221} - Y_{1212} - Y_{2121}) \\ Y_{1221} - Y_{1212} = 2RU1/S \\ -Y_{1221} + Y_{2121} = 2RU2/S \end{array} \right. \quad (17)$$

which gives $Y_{1212} = 4430\,\text{MPa}, Y_{2121} = 14430\,\text{MPa}, Y_{1221} = -880\,\text{MPa}$.
Figure 8 shows the deformed state of the neighbouring cells.

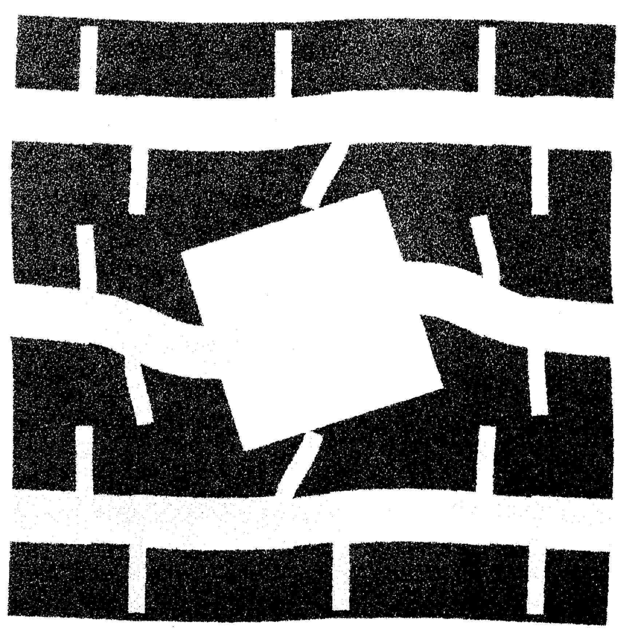


Figure 8 : Imposed inner rotation in a cluster of VERs.

4. ANALYSIS OF A "COARSE GRAIN STRUCTURE"

In general, a structure made of a heterogeneous material will be called a *coarse grain structure* if the characteristic size of the RVE L is not negligible when compared to L_ω.

Consider, for instance, a rectangular structure made of 4x5 cells (figure 9). The structure is small enough to take every heterogenity into account in a FE calculation. However such a calculation requires a mesh with 19800 quadratic elements, i.e. about 120000 d.o.f., which leads to several hours computation time on a work-station RISC6000 for the resolution of the elasticity problem. Loading conditions are prescribed that lead to strongly non-homogeneous deformations (figure 10). This will be the reference calculation.

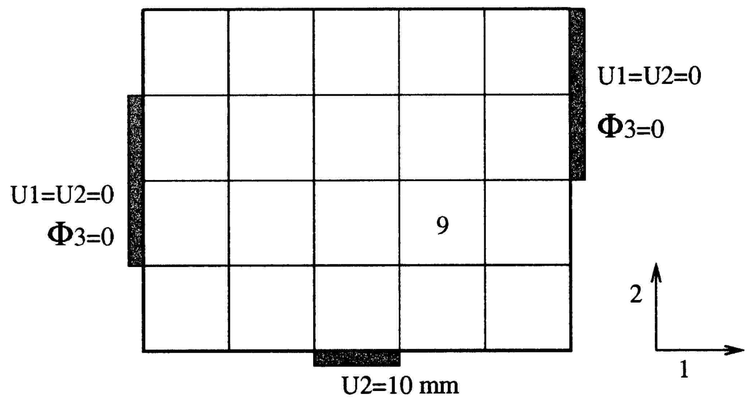


Figure 9 : Loading conditions prescribed on a coarse grain structure made of 4x5 cells.

In contrast the structure can also be modelled as a homogeneous equivalent elastic continuum. It will be successively regarded as a classical continuum using the classical effective properties (periodic assumption) and a Cosserat continuum with the effective moduli derived in section 3. Convergence is obtained with respectively 12360 and 18540 d.o.f. Note that, in the two-dimensional case, a computation with the Cosserat continuum is not really more expensive than the classical one. The calculation involving the HEM clearly is much less expensive than the reference one.

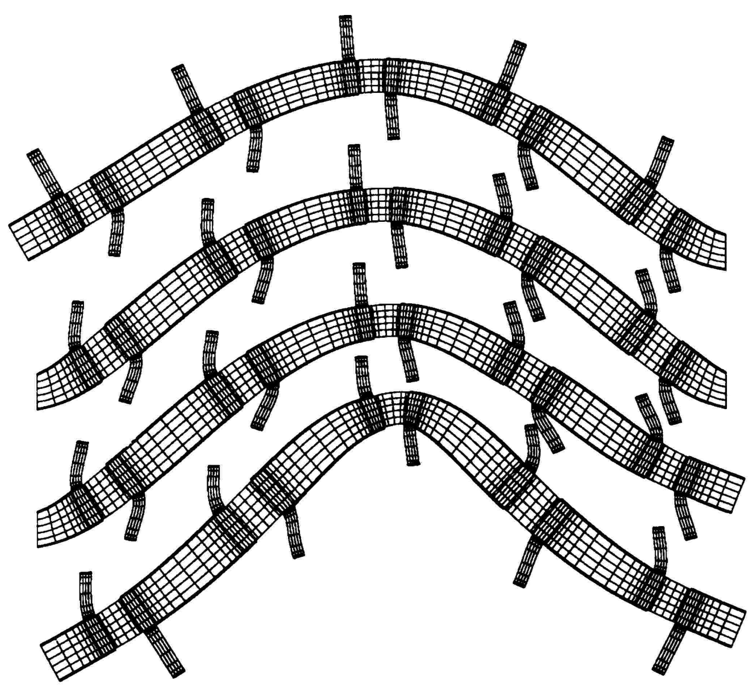
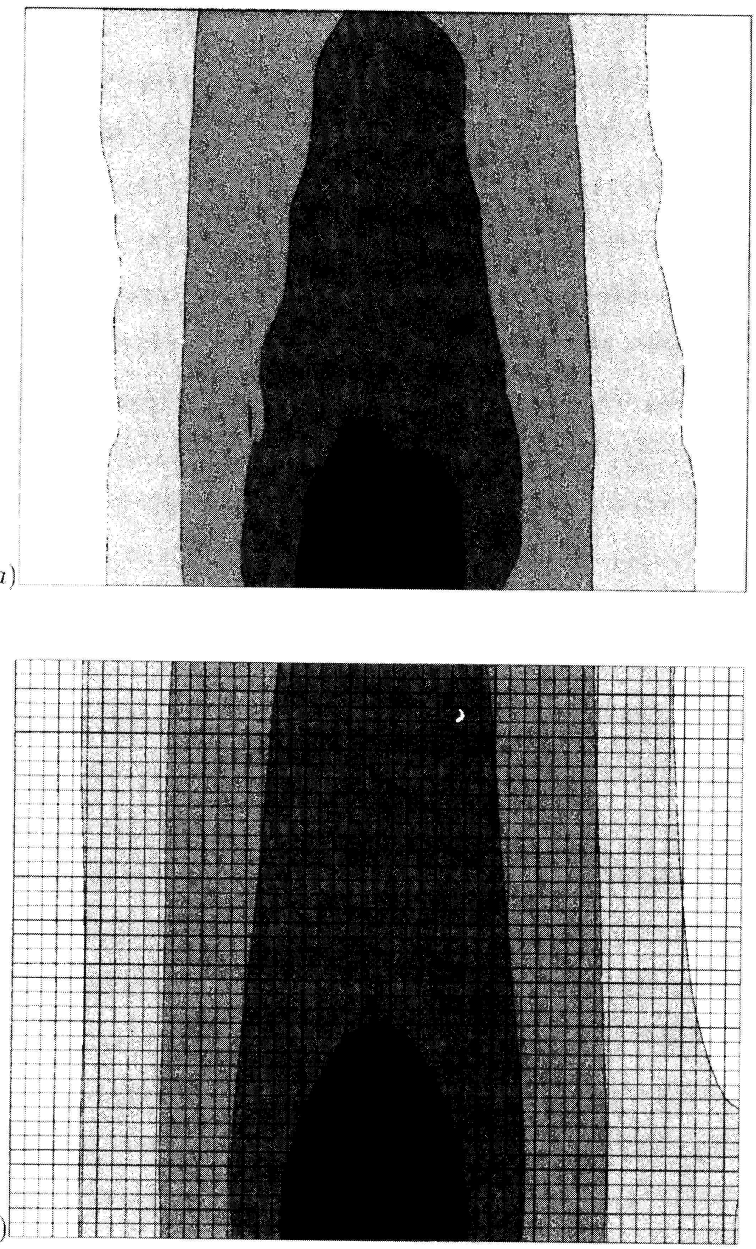


Figure 10 : Deformed state of the coarse grain structure (the soft material has not been represented).

Additional boundary conditions are needed for the Cosserat structure (figure 8). The results obtained using the HEM can be compared to the reference exact response of the material. The computation involving the Cosserat HEM is seen to provide a more realistic displacement field (figure 11). However, in some cases, the reaction forces and couples at the boundaries where displacement is prescribed are overestimated by the Cosserat prediction. Whether or not the Cosserat HME actually gives a better estimation than the classical continuum, depends on the type of non-homogeneous loading conditions in the final structure. In some situations, Jonasch [9] showed that the classical estimation can be very bad up to a factor 2. In fact, there is an appropriate generalized homogeneous equivalent medium for different types of non-homogeneous boundary conditions [6].

A decisive advantage of using a Cosserat HEM also lies in the fact that additional boundary conditions can be prescribed. The conditions $\Phi_3 = 0$ at the boundary 1 and 3 (figure 8) enable us to impose clamping conditions like in the case of a beam. This explains the better prediction of the displacement near the boundary.



a) b)

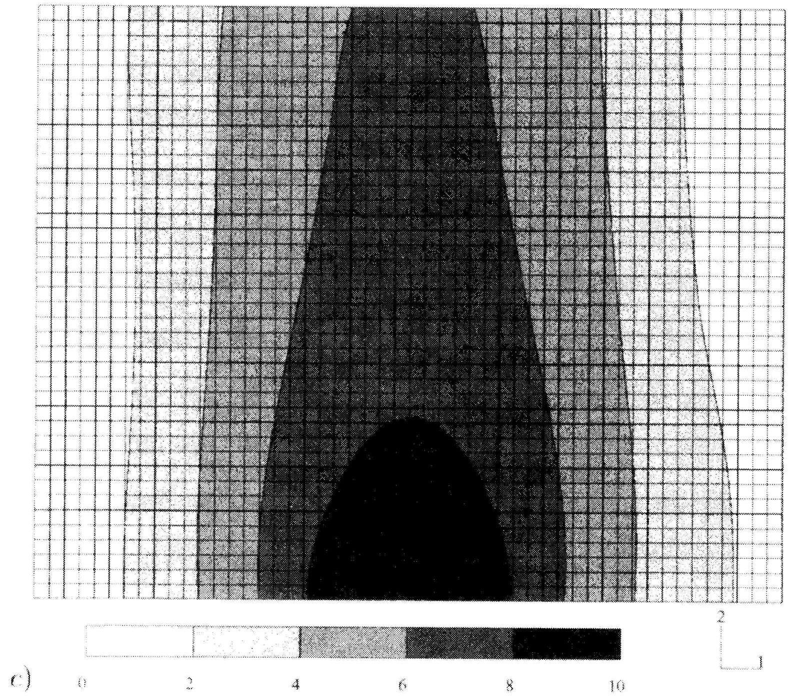


Figure 11 : Displacement field in direction 2 : reference calculation (a), classical equivalent medium (b), Cosserat equivalent medium (c).

5. CONCENTRATION PROBLEM

The concentration problem leads us back to the microstructure. The deformation and curvature at each point of the HEM are related to mean values of local quantities as explained in section 2. But if you are interested in damage initiation for instance, local values are more relevant than mean values. For that purpose, mean values of e and κ are computed on the surface occupied by each cell in the homogeneous calculation. The obtained values E and K are then prescribed to an individual RVE according to (7) or (16). The resulting deformed state of the cell 9 (for boundary conditions on the structure different from figure 8, and combining flexion and shear) is given in figure 12c and compared to the reference one (figure 12a). The same concentration problem can be solved using the classical HEM with classical periodic conditions and leads to figure 12b where flexion is not accounted for. The Cosserat HEM gives a more realistic local strain field.

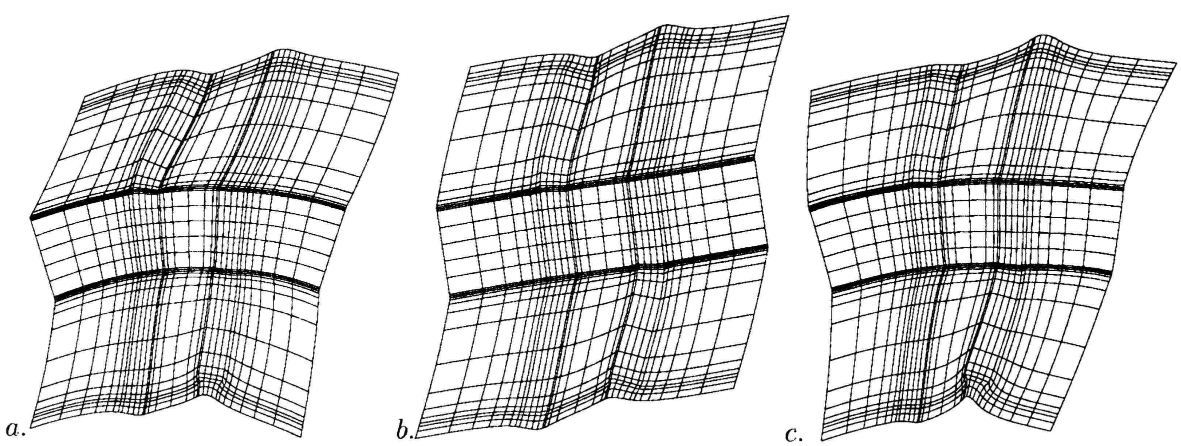


Figure 12 : Deformed state of one inidividual cell within the structure (a) and deformed states deduced from the homogeneous equivalent structure using periodic conditions (b) and curvature-periodic conditions (c).

6. CONCLUSIONS

As soon as the size of the RVE of a heterogeneous material cannot be regarded as infinitely small with respect to the wavelength of the loading conditions, which can happen in the case of localization of deformation for instance, or if the unit cell of a structural component is not small when compared to the component size, or at a crack tip, the classical homogenization schemes are not sufficient. Non-homogeneous boundary conditions must be introduced and the HEM is a generalized continuum.The type of resulting continuum depends on the choice of the applied non-homogeneous loading conditions. In [6], we have tried to give guidelines for the choice of the appropriate HEM.

In each application, very specific boundary conditions can be developed, that better represent the loading conditions under operating conditions. Instead, we have proposed general non-homogeneous boundary conditions that can be used as a basis for developing more appropriate ones. It has been necessary to resort to a *cluster of RVEs* that accounts for the interaction with neighbouring cells.

Numerical computations using the overall generalized medium can be performed to deal with such *coarse grain structures* without considering each geometrical detail of each cell. The obtained results give a precise enough description of the deformation of the aggregate. The homogenization techniques can then be used as concentration methods to work out the complex local fields in each cell. The example presented in this work is taken from structural mechanics (sandwich material). However, this approach should also be used for heterogeneous materials with microstructure (inclusions, precipitates, fibers...).

References

[1] Germain P., The method of virtual power in continuum mechanics, Part 2: Microstructure, SIAM, *J. Appl. Math.* Vol. 25, No. 3, 1973.

[2] Germain P., La méthode des puissances virtuelles en mécanique des milieux continus premiere partie : théorie du second gradient *J. de Mécanique* Vol. 12, No. 2, 1973, pp. 235-274.

[3] Borst R. de, Simulation of strain localization: A reappraisal of the Cosserat continuum, *Engineering Computations*, Vol. 8, 1991, pp. 317-332.

[4] Gauthier R.D and Jahsman W.E., A quest for micropolar elastic constants. *J. Appl. Mech.*, 1976.

[5] Sanchez-Palencia E., Zaoui A., Homogenization techniques for composite media, Lecture notes in physics, No. 272, Springer-Verlag, 1985.

[6] Forest S., Homogenization methods and the mechanics of generalized continua, International Seminar on Geometry, Continuum and Microstructure, organized by G. Maugin, Paris, 28-29 May 1997, *to be published*, Hermann, Paris.

[7] Besdo D., Inelastic behaviour of plane frictionless block-systems described as Cosserat media *Arch. Mech.* Vol. 37, 1985, pp. 603-619.

[8] Scholz S.-P., Homogenisierung einer Sandwichplatte mit rechteckigem Gitterkern, Forsch.-Ber. 2. Inst. Mech. Techn. Univ. Berlin, Nr. 8, Univ.-Bibl., 1990.

[9] Jonasch G., Zur numerischen Behandlung spezieller Scheibenstrukturen als Cosserat-Kontinuum, Fortschr.-Ber. VDI Reihe 18, Nr. 34, VDI-Verlag, 1986.

[10] Dorau H.-U., Homogene Kontinuumsmodelle für elastische orthotrope Scheibenstrukturen und Verbundmaterialien mit biegesteifen Einlagen., Diss. Univ. Hannover, 1986.

[11] Scholz S.-P., Homogenisierung einer Sandwichplatte mit rechteckigem Gitterkern, Forsch.-Ber. 2. Inst. Mech. Techn. Univ. Berlin, Nr. 8, Univ.-Bibl., 1990.

[12] Trostel R., Vektor- und Tensor- Algebra, Mathematische Grundlagen der technischen Mechanik I, Beiträge zur theoretischen Mechanik, Vieweg 1993.

[13] Dupuits M.D., Boussuge M., Forest S., Characterization and simulation of the mechanical behaviour of multilayered components composing a fibrous cylinder head gasket,EUROMECH 360, Mechanics of sandwich structures : modelling, numerical simulation, experimental identification, St. Etienne, 13-15 may, 1997.