Computation of coarse grain structures using a homogeneous equivalent medium

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Abstract : This paper deals with the improvement of concentration relations when some basic hypothesis of homogenization techniques are no longer valid inducing important errors in the deduced local fields. In the first part of this work we propose a new formalism of the standard concentration rules developed in the homogenization of periodic media framework. In a second part, we insist on the fact that a homogeneous equivalent medium replacing a coarse grain material is in fact expected to be a generalized continuum. Additional stiffnesses must be attributed to the unit cell and special non-homogeneous boundary conditions and their periodic counterparts are proposed. The resulting HEM turns out to be a Cosserat continuum.

1. HOMOGENIZATION OF PERIODIC MEDIA

In order to perform a finite element analysis of a structure including a complex geometrical microstructure, like a composite material or a multiphase alloy, a homogenization technique must be developed to determine the properties of the Homogeneous Equivalent Medium (HEM). Indeed, even with high performance computational tools, it is not possible today to perform such calculations discretizing all the micro heterogeneities. It is then necessary to determine the macroscopic constitutive equations of the HEM and to perform this analysis on a macroscopic coarse mesh. In a second step, whatever the homogenization technique used in the analysis, like the homogenization of periodic media or a self consistent scheme (depending on the geometry of the microstructure), it is always possible to determine the strains and the stresses at the microscopic scale knowing the macroscopic state and using the concentration relations.
In the present analysis, the microstructure will be representative of a matrix reinforced with unidirectional long fibres perfectly aligned, propitious to make use of the homogenization of periodic media technique [1, 2], in order to determine the properties of the HEM and the 4th order concentration tensors.

1.1 General presentation and main hypothesis

Noting φ a microscopic field, the related macroscopic field is given by :

$$\Phi = <\varphi> = \frac{1}{V}\int_V \varphi \, dv$$

The macroscopic constitutive equation, in elasticity, will be the relation between the macroscopic stress tensor $\Sigma = <\sigma>$ and the macroscopic strain tensor $E = <\varepsilon>$. The homogenization of periodic media technique is based on the fundamental hypothesis of the scale separation between the micro (denoted y) and the macro (denoted x), inducing that the microscopic characteristic length, l, must be very small relative to the macroscopic length, L. This induces a local invariance by translation l and the microscopic tensors σ and ε are periodic of period l.
Denoting $\eta = \frac{l}{L}$ the ratio between both scales, the previous hypothesis leads to $\eta \ll 1$, it is then possible

to performed an asymptotic expansion of the stress and displacement fields with respect to η [3, 4]:

$$\left\{ \begin{array}{l} \sigma = \sigma_0(x,y) + \eta\, \sigma_1(x,y) + ... + \eta^i\, \sigma_i(x,y) + ... \\ u = u_0(x,y) + \eta\, u_1(x,y) + ... + \eta^i\, u_i(x,y) + ... \end{array} \right.$$

The smaller the size of the heterogeneities, the smaller the higher order terms are. Introducing these relations in the equations of a classical problem in elasticity, and equating powers of η, we get successively a set of equations solving the displacement fields $u_0, u_1, ...$. For example, the resolution of the displacement field u_0 will give the macroscopic constitutive equation and the concentration tensors. The high order displacement fields $u_1, u_2, ...$ are corrective fields allowing a better estimation of u_0 when the size of heterogeneities are not so small or when the periodicity is no longer valid (close to a free edge for example [5]). In the following, we only analyze the results obtained with the field u_0, the determination of high order displacement fields is too difficult to be easily implemented and used.
Once the field u_0 is determined solving six elementary finite element problems on the Representative Unit Cell (RUC), the concentration relation can be established as follow:

$$\varepsilon_{ij}(y) = A_{ijkh}(y)\, E_{kh}, \quad \sigma_{ij}(y) = B_{ijkh}(y)\, \Sigma_{kh} \tag{1}$$

where A and B are respectively the strain and stress concentration tensors determined as functions of the elementary displacement fields. The macroscopic constitutive equation is given by :

$$\Sigma_{ij} = L^{hom}_{ijkh}\, E_{kh}$$

with

$$L^{hom} = < L(y) : A(y) > \tag{2}$$

where L^{hom} and L are respectively the homogenized (macroscopic) and local (microscopic) stiffness matrix. Equation 2 gives the macroscopic constitutive equation introduced in the finite element analysis of the macroscopic structure and equations 1 determine the local fields. Then, with a macroscopic computation we are able to know the real state of the local stresses as if each heterogeneity had been meshed.

1.2 Limits of the homogenization technique

Very often, the main hypothesis of the scale separation is no longer valid, particularly for what we called coarse grain structures, i.e. when the applied load induces strong gradients over a small number of cells. For the concentration procedure, giving the microscopic field knowing the macroscopic one, it is no more accurate to consider a constant macroscopic field acting on the RUC because a discontinuity is observed in the local field when crossing the cells. This is not appropriate for a local post-analysis of dissipative phenomena like interfacial damage or/and plasticity.

The following example can underline the problem raised before. The structure is built up with a set of unit cells representative of a composite material which is a matrix reinforced with long fibres (see figure 1.a). In this particular case the characteristic length of the microstructure is of the same order of the macroscopic one. The structure is loaded in flexure and shear inducing very high levels of multiaxial stresses. Elastic parameters of the constitutive equation of the HEM as well as the values of the concentration tensors, were determined using the homogenization procedure presented before. Figure 2 presents the evolution of the stresses σ_{11} and σ_{12} along a vertical line crossing the four vertical cells located in the middle of the structure, and compares the results of a reference computation (where all the heterogeneities were meshed, see figure 1.b) with the results using the concentration technique (see eq. 1) without taking into account the macroscopic stress gradients inside the cells. As it was planned, there is a discontinuity in the stress field between 2 neighboring cells.

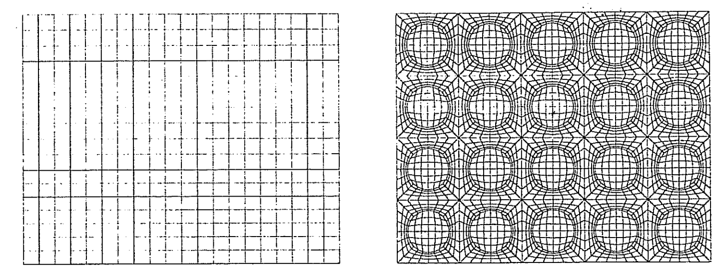

Figure 1 : Mesh used to solve the macroscopic problem with the HEM (left) and the reference mesh with all the heterogeneities (right).

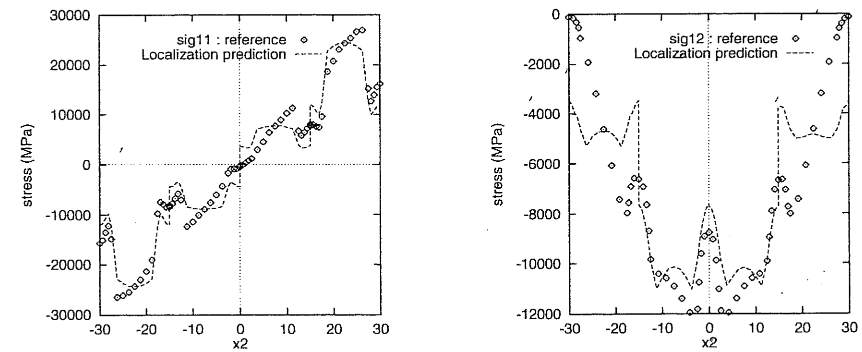

Figure 2 : σ_{11} (left) and σ_{12} (right) profiles in the composite along the middle vertical line compared with the reconstructed one.

1.3 Localization improvement

As presented before, a better way to perform the concentration process is to determine a more accurate displacement field, adding the terms $u_1, u_2, ...$ to the main one u_0. However, these resolutions involve very complex systems of equations which are difficult to manage. The new concentration technique presented here is a very simple way to take into account high macroscopic gradients in the formulation. This method modifies the relations 1 as follows:

$$\varepsilon_{ij}(y) = A_{ijkh}(y)\, E_{kh}(y), \quad \sigma_{ij}(y) = B_{ijkh}(y)\, \Sigma_{kh}(y) \tag{3}$$

The microscopic strain (stress) in a given point of the unit cell, is determined using the concentration tensor combined with the value of the macroscopic strain (stress) in this point. In this case, we don't suppose anymore that the macroscopic fields are constant over the unit cell, and their values at a given point of the cell are extrapolated from the results obtained with the macroscopic computation.
In the next figure we present the results obtained with this new formalism, concerning the evolution of the stress σ_{11} and the shear stress σ_{12}, as presented in fig. 2. As it can be shown the stresses are continuous when crossing the cells and both results are very accurate compared with the reference results.

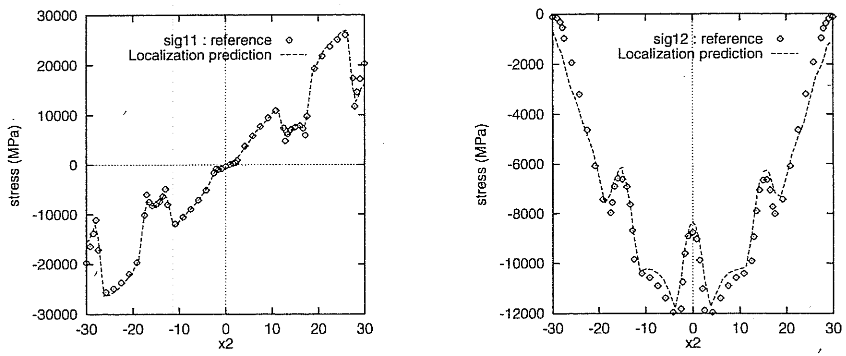

Figure 3 : σ_{11} (left) and σ_{12} (right) profiles in the composite along the middle vertical line compared with the reconstructed one.

The evolution of σ_{12} shows the influence of the free edge which is not taken into account in the present formulation. Induced by the free bound, the shear stress must be equal to 0 in the beginning and in the end of the curve, as predicted by the reference calculation. The evolution obtained with the concentration technique gives a non zero value in these points. This is directly linked to relations 3:

$$\sigma_{12} = B_{1211}\Sigma_{11} + B_{1222}\Sigma_{22} + B_{1233}\Sigma_{33} + 2B_{1212}\Sigma_{12}$$

and, in this analysis the macroscopic stresses Σ_{11} and Σ_{33} are not equal to zero on these bounds of the structure, inducing a nonzero value of σ_{12}. Another approach was developed [6], not presented here, in order to take into account the free bounds in the concentration process.

2. GENERALIZED HOMOGENEOUS EQUIVALENT MEDIUM

2.1 Homogenization techniques under non-slowly varying mean fields

Strictly speaking, the use of a homogeneous equivalent medium obtained by classical homogenization techniques may not be relevant when the size L of the representative volume element and the wavelength L_w of the variation of the applied loading conditions have the same order of magnitude. However, the previous section has shown that it can give in some cases a correct estimation of the deformed state of a coarse grain structure. A specific heuristic technique has been proposed to evaluate the local stresses in each cell with good accuracy in many cases. Nevertheless, the use of a classical HEM can lead to significant errors even in the displacement field of the structure for some microstructures and loading conditions, as shown in [7] and [8].

It is then necessary to tackle the problem of homogenization techniques under non-slowly varying mean fields. In that case, the effective medium is expected to be non local [9]. A variational approach to the problem and the derivation of bounds for the non local properties, have been proposed in [10]. An alternative method again considers a boundary value problem on the RVE with boundary conditions that take the variation of the macroscopic fields into account. This leads inevitably to non-homogeneous boundary conditions [11].

Since there is an infinite variety of possible non-homogeneous boundary conditions, one can restrict oneself to a Taylor development of the macroscopic field. Classical homogenization theory relies on a linear development of the macroscopic displacement field. The introduction of additional quadratic terms can be shown to lead to the definition of a second grade HEM [11, 12]. In the following we will consider some corrective quadratic and cubic terms that lead to the definition of a Cosserat HEM [8]. We will then focus on the concentration problem that provides the local stresses in each cell under macroscopic stress gradients like in the previous section.

2.2 Curvature of the volume element

The following quadratic boundary non-homogeneous conditions

$$u_i = E_{ij}x_j + \varepsilon_{ijk}K_{jl}x_l x_k, \quad \forall x \in \partial V \tag{4}$$

can be interpreted as combined flexion and torsion-like conditions in addition to the classical linear term [8]. This can be seen by developing explicit expressions for particular non-vanishing components of the given constant tensors $\underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{K}}$. The macroscopic deformation gradient is defined as :

$$F_{ij} =< u_{i,j} >= \frac{1}{V}\int_\Omega u_{i,j}\, d\Omega = E_{ij} + \varepsilon_{imn}K_{mj}X_n + \varepsilon_{imj}K_{mp}X_p \tag{5}$$

where $\underline{\mathbf{X}}$ is the geometric mass center of V. As a result, taking the gradient with respect to the macroscopic coordinates X_L,

$$< u_{i,j} >_{,L} = \varepsilon_{imL}K_{mj} + \varepsilon_{imj}K_{mL} \tag{6}$$

and finally

$$\varepsilon_{kij}F_{ij,L} = K_{nn}\delta_{kL} - 3K_{kL}. \tag{7}$$

In the tensorial notation, we will write

$$-2\overset{\times}{\underline{\mathbf{F}}}\otimes\underline{\nabla} = \mathrm{Tr}\,\underset{\sim}{\mathbf{K}}\,\underset{\sim}{\mathbf{1}} - 3\underset{\sim}{\mathbf{K}}. \tag{8}$$

where

$$\overset{\times}{F}_i = -\frac{1}{2}\varepsilon_{imn}F_{mn}. \tag{9}$$

It can be seen that the previous relation is equivalent to

$$\underset{\sim}{\mathbf{K}}^{deviatoric} = \frac{2}{3}\overset{\times}{\underline{\mathbf{F}}}\otimes\underline{\nabla}. \tag{10}$$

As a result, the meaning of the deviatoric part of $\underset{\sim}{\mathbf{K}}$ is that of a prescribed curvature (or torsion).

2.3 Relative rotation of the microstructure with respect to the material

Consider the following trial field on V in the two-dimensional case :

$$\tilde{u}_1 = -2\theta x_2((\frac{x_2}{L})^2 - \frac{1}{4}), \quad \tilde{u}_2 = 2\theta x_1((\frac{x_1}{L})^2 - \frac{1}{4}) \tag{11}$$

where θ is a given angle. The non-vanishing components of $\tilde{\underline{\mathbf{u}}}\otimes\underline{\nabla}$ are

$$\tilde{u}_{1,2} = -2\theta(3(\frac{x_2}{L})^2 - \frac{1}{4}), \quad \tilde{u}_{2,1} = 2\theta(3(\frac{x_1}{L})^2 - \frac{1}{4}). \tag{12}$$

so that

$$\tilde{u}_{1,2}(L/2, L/2) = -\theta, \quad \tilde{u}_{2,1}(L/2, L/2) = \theta. \tag{13}$$

This corresponds to a rotation of angle θ prescribed on the nodes of a cubic lattice of parameter L, the field being interpolated between them. This field has the following properties :

$$< \tilde{\underline{\mathbf{u}}}\otimes\underline{\nabla} >= 0, \quad < \tilde{\underline{\mathbf{u}}}\otimes\underline{\nabla}\otimes\underline{\nabla} >= 0 \tag{14}$$

provided that the origin of the coordinate system is the geometric mass center of V. The conditions (11) will be applied at the boundary ∂V. This introduces a cubic term in the expansion of the mean field.

2.4 Generalized Hill-Mandel condition

Taking the boundary conditions (4) into account, the expression of the internal work gives [8] :

$$< \underset{\sim}{\sigma} : \underset{\sim}{\varepsilon} >= \underset{\sim}{\Sigma} : \underset{\sim}{E} + \underset{\sim}{M} : \underset{\sim}{K} \tag{15}$$

where

$$\underset{\sim}{\Sigma} =< \underset{\sim}{\sigma} >, \quad M_{ij} =< \epsilon_{ikl} x_k \sigma_{lj} > . \tag{16}$$

As a result, if $\underset{\sim}{E}$ and $\underset{\sim}{K}$ are regarded as macroscopic deformation and torsion-curvature tensors, and if relations (16) define the overall force and couple stress tensors, equation (15) represents a part of the work of internal forces of a Cosserat homogeneous equivalent medium. Note that only the symmetric part $^{\{}\underset{\sim}{E}^{\}}$ of $\underset{\sim}{E}$ works with $\underset{\sim}{\Sigma}$ which is symmetric according to (16).

In the two dimensional case, the skew-symmetric part $^{\}}\underset{\sim}{E}^{\{} = \theta \underline{e}_3$ and its contribution to the internal work is introduced via the additional term $\tilde{\underline{u}}$ according to (11). Considering only this term, the energy contribution takes the form :

$$< \underset{\sim}{\sigma} : \underset{\sim}{\varepsilon} >=< \begin{bmatrix} 0 & 2\sigma_{12}(3(\frac{x_2}{L})^2 - \frac{1}{4}) & 0 \\ 2\sigma_{12}(3(\frac{x_1}{L})^2 - \frac{1}{4}) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} >: \begin{bmatrix} 0 & -\theta & 0 \\ \theta & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} . \tag{17}$$

This allows us to define the skew-symmetric part of the macroscopic force stress tensor :

$$\overset{\times}{\underset{\sim}{\Sigma}} = 3\sigma_{12}((\frac{x_2}{L})^2 - (\frac{x_1}{L})^2)\ \underline{e}_3. \tag{18}$$

The final expression of Hill-Mandel condition reads then :

$$< \underset{\sim}{\sigma} : \underset{\sim}{\varepsilon} >= ^{\{}\underset{\sim}{\Sigma}^{\}} : ^{\{}\underset{\sim}{E}^{\}} + \overset{\times}{\underline{\Sigma}} . \overset{\times}{\underline{E}} + \underset{\sim}{M} : \underset{\sim}{K}. \tag{19}$$

It must be noted that the definition of the macroscopic couple-stress tensor implies $\mathrm{Tr}\, \underset{\sim}{M} = 0$, which entails that $\mathrm{Tr}\, \underset{\sim}{K}$ does not work. This is true for a Cosserat continuum only in the two-dimensional case so that additional boundary conditions are necessary to define a complete three-dimensional overall Cosserat continuum.

Furthermore, if the curvature tensor $\underset{\sim}{K}$ actually fulfills (10) at the macroscopic level, the Cosserat medium reduces to a so-called couple-stress medium which is a second grade material involving only gradient of the rotation field [13]. But the material rotation and microstructure rotation can also be regarded as independent and the proposed homogenization procedure leads to an unconstrained Cosserat theory.

2.5 Periodic conditions and application to SiC-Ti

When the material has a periodic microstructure, the previous boundary conditions are not appropriate. Instead we look for a displacement field on V of the form :

$$u_i = E_{ij} x_j + \epsilon_{ijk} K_{jl} x_l x_k + v_i, \quad \forall x \in V, \tag{20}$$

where $\underline{v}$ takes equal values on opposite sides of the cell. It follows that the mean deformation and curvature associated with $\underline{v}$ vanish. The contribution $\tilde{u}$ has not been introduced in the periodic case yet.

In the two-dimensional case, the effective Cosserat elastic behaviour reads :

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

where the cubic symmetry of the SiCTi unit cell has been taken into account. The elastic properties of the constituents are : $E = 110000$ MPa, $\nu = 0.3$ for the matrix and $E = 410000$ MPa, $\nu = 0.25$ for the fiber. The effective constants Y_{1111}, Y_{1122} are the same as in section 1 and are determined in the same way. The relation between C_{44} and the Y_{1212}, Y_{1221} is given in [8]. The remaining constant Y_{1221} is deduced from the material response to the application of $\theta = 1.$ to the boundary of the unit cell according to (11). The flexural rigidity is determined by prescribing $K_{31} = 1$ and then computing M_{31} according to (16). The respective deformed states are shown on figure 4. Two possible representative cells have been used that give different values of the effective parameters :

$$Y_{1111} = 210\,\mathrm{GPa}, Y_{1122} = 80\,\mathrm{GPa} \text{ and } C_{44} = 59\,\mathrm{GPa},$$

$$C_{3131} = 2605600/4543419\,\mathrm{MPa.L}^2 \quad , Y_{1212} = 64580/82186\,\mathrm{MPa}, Y_{1221} = 53599/35993\,\mathrm{MPa},$$

where $L = 10\mu$m (unit used for the coordinates of the mesh).

2.6 Computation of a coarse grain structure under combined shearing and bending

The actual heterogeneous structure is submitted to combined shearing and bending. If only a small number of cells is taken into account, the calculation involving every heterogeneity remains tractable and can be compared to the response of the homogeneous equivalent medium subjected to the same loading conditions (figure 5). Additional boundary conditions are necessary in the case of the Cosserat effective medium in terms of prescribed microrotations or micro-couples. The microrotation on the side where bending is applied is taken equal to the prescribed side rotation, the remaining sides of the structure being free of force and couple stresses.

We consider now some stress components along a vertical middle line in the structure that cuts the matrix and four fibers. We try then to reproduce this distribution starting from the results obtained with the HEM. For that purpose, we first compute the mean Cosserat deformation and curvature on each cell crossed by the line. These mean values are then successively prescribed to the unit cell with periodicity conditions (concentration problem). The four deformed cells are represented on figure 6 and compared to the actual deformation. The deformation of the individual cells are of course not compatible but they give a precise enough estimation of the real state. The compared σ_{11} profiles are given on figure 7a : the Cosserat continuum provides a very accurate description of the bending response. In contrast, the Cosserat effective medium does not give a better prediction of the shear stresses σ_{12}. This is simply due to the fact that the Cosserat continuum does not account for strong gradient of shear stresses. To solve this problem, a complete second grade medium should be used to describe both bending and shear gradients.

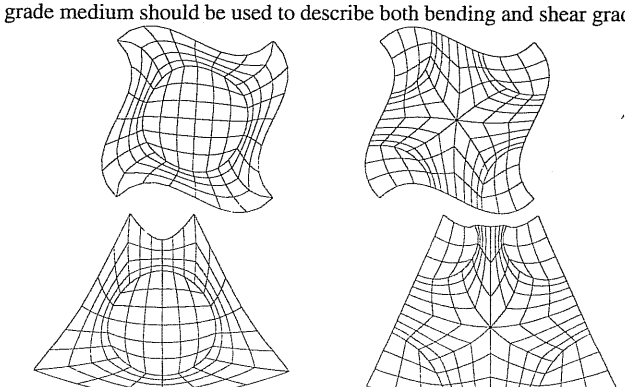

Figure 4 : Prescribed relative rotation at the boundary (above) and periodic curvature conditions (below) for two possible representative cells.

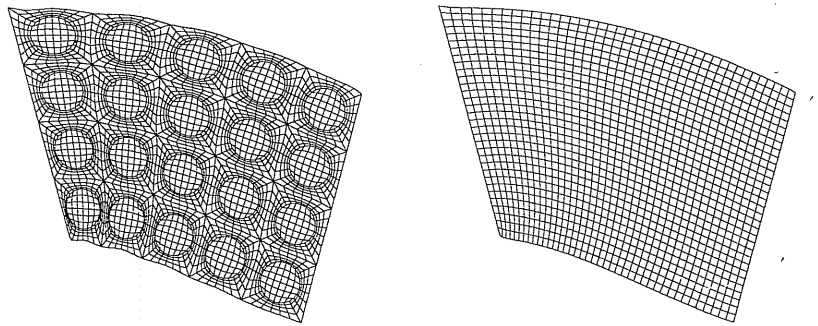

Figure 5 : Non-homogeneous deformation of the composite (left) and of the Cosserat homogeneous equivalent medium (right).

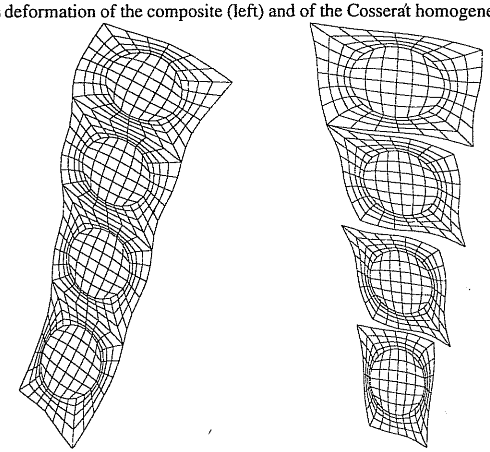

Figure 6 : Magnified deformed state of the middle row of the structure (left) and its reconstruction with unit cells (right).

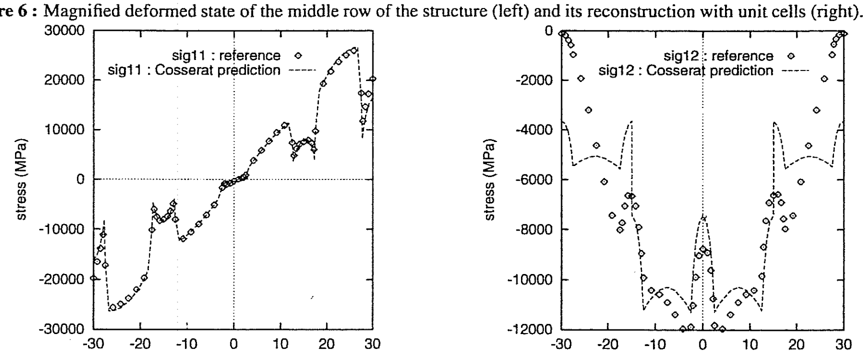

Figure 7 : σ_{11} (left) and σ_{12} (right) profiles in the composite along the middle vertical line compared with the reconstructed ones.

3. CONCLUSION

Two approaches were presented to improve the concentration techniques when the basic hypothesis of homogenization procedures are no longer verified. The first approach turns out to be a heuristic but efficient way of evaluation of local stresses, whereas the second one sets the basis of a more general framework to

build up an appropriate effective medium in the presence of strong overall stress gradients. Both approaches represent a tentative effort to cope with the computation of coarse grain structures which are common in engineering components.

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