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Homogenization methods and the mechanics of generalized continua

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1 Introduction

1.1 Scope of this work

The strong developments of the mechanics of generalized continua since the early sixties provide us with a great variety of media that involve additional degrees of freedom (higher order continua), higher order gradients of the displacement (higher grade continua) or fully non local formulations [1]. These additional features are usually supposed to account for some aspects of the underlying microstructure in a more accurate way than the classical Boltzmann continuum does. However, the links between the additional degrees of freedom for instance and the microstructure of the material generally remain unclear, except in some extreme cases (granular materials, fluid crystals...).

On the other hand, homogenization theory enables one to derive effective properties of micro-heterogeneous materials, assuming that the local behaviour of each constituent is known [2]. Accordingly, homogenization methods also provide a precise description of microstructure for random or periodic distributions of heterogenities and for both linear and non-linear local constitutive behaviours, within the framework of a Boltzmann continuum. However, the classical homogenization schemes, for which only volume fractions and spatial relative distributions of the constituents are taken into account, leave size effects and other non local effects unaccounted for.

This work aims at investigating the links between homogenization theory and the mechanics of generalized continua. It will be shown that they must be used simultaneously to describe the effective behaviour of heterogeneous materials displaying size effects.

Homogenization theory relies on the choice of a representative volume element Ω (RVE) of absolute size L which is usually taken large enough with respect to the heterogenities and much smaller than the size of the structure or component to be modelled. Furthermore, in many cases, the wavelength L_w of stress and strain variations induced in the structure can be assumed to be much bigger than L, so that the resulting homogeneous equivalent medium (HEM) can be regarded as a classical simple material. In many situations also, the Boltzmann continuum adequately accounts for the local properties of a heterogeneous material (inside the RVE). These two assumptions correspond to the first line of table 1 where different homogenization processes are listed.

mesoscopic continuum (constituents)	size of the RVE	macroscopic continuum (HEM)	reference
Boltzmann	$L \ll L_w$	Boltzmann	[2][3]
Boltzmann	$L \lesssim L_w$	generalized	section 2
generalized	$L \lesssim L_w$	generalized	section 3

Table 1 : Typology of homogenization processes

In section 2, it will be shown that, as soon as the assumption $L \ll L_w$ is dropped, the HEM must be regarded as a generalized continuum. We call *coarse grain structure* a structure made of a micro-heterogeneous material for which $L \lesssim L_w$ under the operating loading conditions. The pioneering work of Besdo [4] and coworkers [5,6,7] in that field (line 2 of table 1) has proved the necessity of resorting to generalized continua to handle coarse grain structures. They developed heuristic methods to derive the effective generalized properties of grid and composite structures. However the relation to homogenization theory had still to be established.

An elastoplastic single crystal for which a precise enough description of dislocation distribution is necessary can be regarded as an intrinsic Cosserat continuum [8]. It follows that a polycrystal is an aggregate of Cosserat media. It is then necessary to develop homogenization techniques for heterogeneous generalized continua. This is done in section 3 for heterogeneous micromorphic continua.

1.2 Kinematics and statics of three generalized continua

In this work, the analysis is restricted to three different generalized continua for which definitions and balance equations are briefly recalled whithin the framework of small perturbations.

Throughout the paper, $\underline{\boldsymbol{x}}$, $\underset{\sim}{\boldsymbol{x}}$ and $\underset{\approx}{\boldsymbol{x}}$ respectively denote a vector, a second-rank and a four-rank tensor. The third-order permutation tensor will be denoted by $\underset{\sim}{\boldsymbol{\epsilon}}$ if applied to a second-rank tensor and $\underset{\approx}{\boldsymbol{\epsilon}}$ if applied to a vector. $\underline{\boldsymbol{\nabla}}$ is the nabla operator. The divergence of $\underset{\sim}{\boldsymbol{a}}$ is denoted by $\underset{\sim}{\boldsymbol{a}}\,\underline{\boldsymbol{\nabla}}$. When the notation becomes ambiguous, indices are used.

Very similar notations for deformation and stress tensors have been adopted for the three continua so that parallels can be easily drawn. To avoid possible confusion, however, one must check in which context the tensors are used.

Second grade material

Following [9,10,11], we consider a continuum involving both first and second gradients of the displacement field $\underline{\boldsymbol{U}}(\underline{\boldsymbol{x}}, t)$. The following tensors are defined :

$$\underset{\sim}{\boldsymbol{E}} = {}^{\{}\, \underline{\boldsymbol{U}} \otimes \underline{\boldsymbol{\nabla}}\, {}^{\}} \quad (\textit{strain tensor}) \quad \text{and} \quad \underline{\underline{\underline{\boldsymbol{K}}}} = \underline{\boldsymbol{U}} \otimes \underline{\boldsymbol{\nabla}} \otimes \underline{\boldsymbol{\nabla}} \tag{1}$$

where the brackets denote the symmetric part. The previous tensors are related by

$$K_{ijk} = E_{ij,k} + E_{ki,j} - E_{jk,i}$$

The dual quantities of these two tensors respectively are the symmetric stress tensor $\underset{\sim}{\boldsymbol{\Sigma}}$ and the hyperstress tensor $\underset{\sim}{\underline{\boldsymbol{M}}}$ having the same symmetry properties as $\underset{\sim}{\underline{\boldsymbol{K}}}$. The equations of equilibrium take the form

$$\underset{\sim}{\boldsymbol{S}}\, \nabla = 0 \quad \text{where} \quad \underset{\sim}{\boldsymbol{S}} = \underset{\sim}{\boldsymbol{\Sigma}} - \underset{\sim}{\underline{\boldsymbol{M}}}\, \nabla \tag{2}$$

without volume forces nor double forces. The reader is referred to [10] for the expression of the natural traction boundary conditions. Finally, if $\varepsilon(\underset{\sim}{\boldsymbol{E}}, \underset{\sim}{\underline{\boldsymbol{K}}}, ...)$ denotes the specific energy of the system in the isothermal case, we have

$$\rho\dot{\varepsilon} = \underset{\sim}{\boldsymbol{\Sigma}} : \underset{\sim}{\dot{\boldsymbol{E}}} + \underline{\underline{\underline{\boldsymbol{M}}}} \,\vdots\, \underline{\underline{\underline{\dot{\boldsymbol{K}}}}} \tag{3}$$

additional heat production being excluded.

Cosserat material

The deformed state of a Cosserat medium $\mathcal{B}$ is described by a displacement field $\underline{\boldsymbol{U}}(\underline{\boldsymbol{x}}, t)$ and a micro-rotation field $\underset{\sim}{\boldsymbol{R}}(\underline{\boldsymbol{x}}, t)$. The latter accounts for the independent rotation of a rigid tryad attached to the microstructure of the material. In the case of small micro-rotations, the associated vector field $\underline{\boldsymbol{\Phi}}(\underline{\boldsymbol{x}}, t)$ is defined by

$$\underset{\sim}{\boldsymbol{R}} = \underset{\sim}{\boldsymbol{1}} - \underset{\approx}{\boldsymbol{\epsilon}}\, \underline{\boldsymbol{\Phi}}. \tag{4}$$

The (relative) deformation tensor $\underset{\sim}{\boldsymbol{E}}$ and the torsion-curvature tensor $\underset{\sim}{\boldsymbol{K}}$ read

$$\underset{\sim}{\boldsymbol{E}} = \underline{\boldsymbol{U}} \otimes \nabla + \underset{\approx}{\boldsymbol{\epsilon}}\, \underline{\boldsymbol{\Phi}} \quad \text{and} \quad \underset{\sim}{\boldsymbol{K}} = \underline{\boldsymbol{\Phi}} \otimes \nabla. \tag{5}$$

The dual quantities in the expression of the power of internal forces are the force-stress and couple-stress tensors $\underset{\sim}{\boldsymbol{\Sigma}}$ and $\underset{\sim}{\boldsymbol{M}}$. They must fulfill the balance equations :

$$\underset{\sim}{\boldsymbol{\Sigma}}\, \nabla = 0 \quad \text{and} \quad \underset{\sim}{\boldsymbol{M}}\, \underline{\boldsymbol{\nabla}} - \underset{\approx}{\boldsymbol{\epsilon}} \underset{\sim}{\boldsymbol{\Sigma}} = 0 \quad \forall \underline{\boldsymbol{x}} \in \mathcal{B}, \tag{6}$$

$$\underset{\sim}{\boldsymbol{\Sigma}}\, \underline{\boldsymbol{n}} = \underline{\boldsymbol{t}} \quad \text{and} \quad \underset{\sim}{\boldsymbol{M}}\, \underline{\boldsymbol{n}} = \underline{\boldsymbol{m}} \quad \forall \underline{\boldsymbol{x}} \in \partial\mathcal{B}, \tag{7}$$

where volume forces and couples have been excluded. The surface traction and moment vectors are $\underline{\boldsymbol{t}}$ and $\underline{\boldsymbol{m}}$, and $\underline{\boldsymbol{n}}$ is the normal to the surface. The previous tensors generally are not symmetric. The energy balance reads :

$$\rho\dot{\varepsilon} = \underset{\sim}{\boldsymbol{\Sigma}} : \underset{\sim}{\dot{\boldsymbol{E}}} + \underset{\sim}{\boldsymbol{M}} : \underset{\sim}{\dot{\boldsymbol{K}}}. \tag{8}$$

Micromorphic material

If the directors attached to each point of the medium are not regarded as rigid any more, a complete set of nine degrees of freedom $\underset{\sim}{\boldsymbol{X}}$ is required to account for both rotation and stretching of the tryad. This leads to the definition of three generalized deformation tensors :

$$\underset{\sim}{\boldsymbol{E}} = \underline{\boldsymbol{U}} \otimes \underline{\boldsymbol{\nabla}} - \underset{\sim}{\boldsymbol{X}}, \quad \underset{\sim}{\boldsymbol{X}}^s = ^{\{}\underset{\sim}{\boldsymbol{X}}^{\}} \quad \text{and} \quad \underset{\approx}{\boldsymbol{K}} = \underset{\sim}{\boldsymbol{X}} \otimes \underline{\boldsymbol{\nabla}}. \tag{9}$$

They are respectively called the (relative) deformation tensor, the micro - strain tensor and the micro - deformation gradient. Note that the last tensor can be decomposed into a torsion-curvature part and a micro-strain gradient part. The associated stress tensors respectively are $\underset{\sim}{\boldsymbol{S}}$, $\underset{\sim}{\boldsymbol{\Sigma}}$ (symmetric) and $\underset{\approx}{\boldsymbol{M}}$, that fulfill the following equilibrium equations :

$$\underset{\sim}{\boldsymbol{S}}\,\underline{\boldsymbol{\nabla}} = 0 \quad \text{and} \quad \underset{\approx}{\boldsymbol{M}}\,\underline{\boldsymbol{\nabla}} + \underset{\sim}{\boldsymbol{S}} - \underset{\sim}{\boldsymbol{\Sigma}} = 0 \quad \forall \underline{\boldsymbol{x}} \in \mathcal{B}, \tag{10}$$

$$\underline{\boldsymbol{t}} = \underset{\sim}{\boldsymbol{\Sigma}}\,\underline{\boldsymbol{n}} \quad \text{and} \quad \underset{\sim}{\boldsymbol{m}} = \underset{\approx}{\boldsymbol{M}}\,\underline{\boldsymbol{n}} \tag{11}$$

where surface forces and double forces $\underline{\boldsymbol{t}}$ and $\underset{\sim}{\boldsymbol{m}}$ have been introduced. The simplified form of energy balance reads

$$\rho\dot{\varepsilon} = \underset{\sim}{\boldsymbol{\Sigma}} : \dot{\underset{\sim}{\boldsymbol{X}}}^s + \underset{\sim}{\boldsymbol{S}} : \dot{\underset{\sim}{\boldsymbol{E}}} + \underline{\underline{\underline{\boldsymbol{M}}}} \,\vdots\, \dot{\underline{\underline{\underline{\boldsymbol{K}}}}} \tag{12}$$

If the micro-deformation tensor reduces to a micro-rotation, the Cosserat theory is retrieved [12] and

$$\underset{\sim}{\boldsymbol{\Sigma}}^{Cosserat} = \underset{\sim}{\boldsymbol{\Sigma}} + \underset{\sim}{\boldsymbol{S}} \quad \text{and} \quad \underset{\sim}{\boldsymbol{M}}^{Cosserat} = -\underset{\approx}{\boldsymbol{\epsilon}}\underset{\approx}{\boldsymbol{M}}. \tag{13}$$

In contrast, if $\underset{\sim}{\boldsymbol{X}}$ reduces to $\underline{\boldsymbol{U}} \otimes \underline{\boldsymbol{\nabla}}$, the micromorphic medium degenerates into a material of grade two [12]. A detailed presentation of the Cosserat and micromorphic continua can be found in [1].

2 Homogenization methods for coarse grain heterogeneous materials

In this section, heterogeneous materials for which $L \lesssim L_w$ are considered. The RVE Ω is a Boltzmann continuum but the derived HEM will be succesively a second grade, a Cosserat or a micromorphic medium. In the remaining of the paper, holes and cracks in Ω are excluded for simplicity. The origin of the coordinate system is taken as the geometric center of gravity of Ω, unless another choice is specified.

2.1 Definition of the micro-mechanical problem; Non-homogeneous boundary conditions

The constituents of Ω are classical materials with different mechanical properties. Their spatial distribution can be very intricate. We look for the displacement field

$\underline{\boldsymbol{u}}(\underline{\boldsymbol{x}}, t)$ solution of the following boundary value problem (BVP) :

$$\begin{cases} \underset{\sim}{\varepsilon} =^{\{} \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}}^{\}} \\ \textit{constitutive equations} \\ \underset{\sim}{\boldsymbol{\sigma}}\, \underline{\boldsymbol{\nabla}} = 0 \quad \forall \underline{\boldsymbol{x}} \in \Omega \\ \textit{boundary conditions} \end{cases} \tag{14}$$

where $\underset{\sim}{\varepsilon}$ and $\underset{\sim}{\boldsymbol{\sigma}}$ are the local strain and stress 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 in particular non homogeneous boundary conditions.

The main difficulty arises from the fact that there is a large variety of 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.

2.2 Homogenized medium of grade two

2.2.1 BVP with homogeneous strain gradient conditions

Let us consider the following Dirichlet boundary conditions for the problem (14)

$$\underline{\boldsymbol{u}} = \underset{\sim}{\boldsymbol{E}}\underline{\boldsymbol{x}} + \frac{1}{2}\underset{\approx}{\boldsymbol{K}}(\underline{\boldsymbol{x}} \otimes \underline{\boldsymbol{x}}), \quad \forall \underline{\boldsymbol{x}} \in \partial\Omega \tag{15}$$

where $\underset{\sim}{\boldsymbol{E}}$ and $\underset{\approx}{\boldsymbol{K}}$ are constant given second and third order tensors, $\underset{\approx}{\boldsymbol{K}}$ having the following symmetry properties $K_{ijk} = K_{ikj}$. The application of Gauss theorem leads to the following results on averaged quantities :

$$< \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}} >= \frac{1}{V}\int_\Omega \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}}\, d\Omega = \underset{\sim}{\boldsymbol{E}} \tag{16}$$

Regarding the mean work of internal forces, we get

$$< \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\varepsilon} >=< \underset{\sim}{\boldsymbol{\sigma}} >: \underset{\sim}{\boldsymbol{E}} + < \underset{\sim}{\boldsymbol{\sigma}}^{\{}\otimes^{\}}\underline{\boldsymbol{x}} > \vdots \underset{\approx}{\boldsymbol{K}} \tag{17}$$

where $\left(\underset{\sim}{\boldsymbol{\sigma}}^{\{}\otimes^{\}}\underline{\boldsymbol{x}}\right)_{ijk} = \sigma_{i(j}x_{k)}$. This expression can be interpreted as the internal work of a second grade equivalent medium, providing that $\underset{\sim}{\boldsymbol{E}}$ and $\underset{\approx}{\boldsymbol{K}}$ are the strain and second gradient tensors associated with this continuum and that the following definitions of the stress and hyperstress tensors are adopted :

$$\underset{\sim}{\boldsymbol{\Sigma}} =< \underset{\sim}{\boldsymbol{\sigma}} > \quad \text{and} \quad \underset{\approx}{\boldsymbol{M}} =< \underset{\sim}{\boldsymbol{\sigma}}^{\{}\otimes^{\}}\underline{\boldsymbol{x}} > . \tag{18}$$

It turns out that the hyperstress tensor of the HEM of grade 2 is the first moment of the local stress field. Such non-homogeneous boundary conditions have also been proposed in [13]. Contrary to the classical case, there seems to be no trivial dual boundary conditions in terms of stresses.

2.2.2 Hill-Mandel's lemma for a HEM of grade two

The previous results enable one to derive an extension of Hill-Mandel's lemma for homogeneous strain gradient conditions at the boundary. Let $\underset{\sim}{\boldsymbol{\sigma}}^\star$ be a statically admissible field (i.e. $\underset{\sim}{\boldsymbol{\sigma}}^\star \underline{\boldsymbol{\nabla}} = 0$) and $\underset{\sim}{\boldsymbol{\varepsilon}}'$ a compatible strain field. If the associated displacement field $\underline{\boldsymbol{u}}'$ satisfies Dirichlet conditions (15), then

$$\begin{aligned} < \underset{\sim}{\boldsymbol{\sigma}}^\star : \underset{\sim}{\boldsymbol{\varepsilon}}' > &= < \underset{\sim}{\boldsymbol{\sigma}}^\star >:< \underset{\sim}{\boldsymbol{\varepsilon}}' > + < \underset{\sim}{\boldsymbol{\varepsilon}}' \otimes \underline{\boldsymbol{\nabla}} > \vdots < \underset{\sim}{\boldsymbol{\sigma}}^\star \otimes \underline{\boldsymbol{x}} > \\ &= < \underset{\sim}{\boldsymbol{\sigma}}^\star >:< \underset{\sim}{\boldsymbol{\varepsilon}}' > + < \underline{\boldsymbol{u}}' \otimes \underline{\boldsymbol{\nabla}} \otimes \underline{\boldsymbol{\nabla}} > \vdots < \underset{\sim}{\boldsymbol{\sigma}}^{\star\{} \otimes {}^{\}} \underline{\boldsymbol{x}} > . \end{aligned} \tag{19}$$

Note that $\underset{\sim}{\boldsymbol{\sigma}}^\star$ and $\underset{\sim}{\boldsymbol{\varepsilon}}'$ are not necessarily related to each other by the constitutive relations. A wide use of this lemma will be made in the next section.

2.2.3 Application to heterogeneous linear elasticity

The constituents are now assumed to have a linear elastic behaviour. Let $\underset{\approx}{\boldsymbol{c}}(\underline{\boldsymbol{x}})$ be the four-rank tensor field of the local elastic properties :

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\approx}{\boldsymbol{c}}\,\underset{\sim}{\boldsymbol{\varepsilon}}. \tag{20}$$

The linearity of the BVP (14) with respect to $\underset{\sim}{\boldsymbol{E}}$ and $\underline{\underset{\sim}{\boldsymbol{K}}}$ implies the existence of two concentration tensors of fourth and fifth rank respectively such that :

$$\underset{\sim}{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}}) = \underset{\approx}{\boldsymbol{A}}^1(\underline{\boldsymbol{x}})\underset{\sim}{\boldsymbol{E}} + \underline{\underset{\approx}{\boldsymbol{A}}}^2(\underline{\boldsymbol{x}})\underline{\underset{\sim}{\boldsymbol{K}}}, \quad \forall \underline{\boldsymbol{x}} \in \Omega. \tag{21}$$

The concentration tensors fulfill the conditions :

$$< \underset{\approx}{\boldsymbol{A}}^1 >= \underset{\approx}{\boldsymbol{1}} \quad \text{and} \quad < \underline{\underset{\approx}{\boldsymbol{A}}}^2 >= 0 \tag{22}$$

where $\underset{\approx}{\boldsymbol{1}}$ is the identity tensor of fourth rank operating on symmetric second rank tensors. From (18) and (20), it follows that

$$\underset{\sim}{\boldsymbol{\Sigma}} =< \underset{\approx}{\boldsymbol{c}}\underset{\approx}{\boldsymbol{A}}^1 > \underset{\sim}{\boldsymbol{E}} + < \underset{\approx}{\boldsymbol{c}}\underline{\underset{\approx}{\boldsymbol{A}}}^2 > \underline{\underset{\sim}{\boldsymbol{K}}} \tag{23}$$

$$M_{ijk} =< c_{i(jmn} A^1_{mnpq} x_{k)} > E_{pq} + < c_{i(jmn} A^2_{mnpqr} x_{k)} > K_{pqr}. \tag{24}$$

Relations (23) and (24) represent the overall properties of the heterogeneous material. They define four tensors of effective moduli. In the following, we show that they reduce to three.

The effective properties can also be defined according to an energy-based formulation. The potential energy density of the overall medium takes the form

$$\Psi(\underset{\sim}{\boldsymbol{E}},\underline{\underline{\underline{\boldsymbol{K}}}}) = \frac{1}{2}\underset{\sim}{\boldsymbol{E}} : (\underset{\approx}{\boldsymbol{C}}^1 \underset{\sim}{\boldsymbol{E}}) + \frac{1}{2}\underline{\underline{\underline{\boldsymbol{K}}}} \vdots (\underset{\approx}{\underline{\underline{\underline{\boldsymbol{C}}}}}^2 \underset{\sim}{\underline{\boldsymbol{K}}}) + \underset{\sim}{\boldsymbol{E}} : (\underset{\approx}{\underline{\boldsymbol{C}}}^3 \underset{\sim}{\underline{\boldsymbol{K}}}) \tag{25}$$

where

$$C^1_{ijkl} =< A^1_{mnij} c_{mnpq} A^1_{pqkl} >, \quad C^2_{abc\ def} =< A^2_{mn\ abc} c_{mnpq} A^2_{pq\ def} > \tag{26}$$

$$C^3_{ij\ pqr} =< A^1_{mnij} c_{mnkl} A^2_{kl\ pqr} >=< A^2_{mn\ pqr} c_{mnkl} A^1_{klij} > . \tag{27}$$

The overall moduli have the following symmetry properties :

$$C^1_{ijkl} = C^1_{jikl} = C^1_{ijlk} = C^1_{klij}, \quad C^2_{abc\ def} = C^2_{def\ abc} \quad \text{and} \quad C^3_{ij\ pqr} = C^3_{ji\ pqr}. \tag{28}$$

The two definitions of the effective elastic moduli (23) to (27) can be shown to be equivalent by means of generalized Hill-Mandel's lemma (19).

For that purpose, we look for compatible deformation fields satisfying the Dirichlet boundary conditions (15). A set of such fields can be obtained by applying the macroscopic strains and strain gradients

$$(E^{(ij)}_{kl} = \delta_{ik}\delta_{jl}, K_{ijk} = 0) \quad \text{and} \quad (E_{kl} = 0, K^{(pqr)}_{abc} = \frac{1}{2}\delta_{ap}(\delta_{bq}\delta_{cr} + \delta_{br}\delta_{cq})) \tag{29}$$

successively, for each given fixed pair (i,j) and triplet (p,q,r). According to equations (21), we obtain the compatible strain fields

$$\varepsilon'^{(ij)}_{mn} = A^1_{mnij} \quad \text{and} \quad \varepsilon'^{(pqr)}_{mn} = A^2_{mn\ pqr}. \tag{30}$$

Similarly, self-equibrated stress fields can be worked out using the previous fields. For instance,

$$\sigma^{\star(ij)}_{mn} = c_{mnpq} A^1_{pqij} \quad \text{and} \quad \sigma^{\star(pqr)}_{mn} = c_{mnkl} A^2_{kl\ pqr} \tag{31}$$

are self-equilibrated stress fields. The application of Hill-Mandel's lemma (19) to the previous fields and the use of relations (22) lead to :

$$< A^1_{mnij} c_{mnkl} A^2_{kl\ pqr} >=< \varepsilon'^{(ij)}_{mn} >< \sigma^{\star(pqr)}_{mn} >=< c_{mnkl} A^2_{kl\ pqr} > . \tag{32}$$

Hence,

$$< \underset{\approx}{\boldsymbol{A}}^1 \underset{\approx}{\boldsymbol{c}} \underset{\approx}{\underline{\boldsymbol{A}}}^2 >=< \underset{\approx}{\boldsymbol{c}} \underset{\approx}{\underline{\boldsymbol{A}}}^2 > . \tag{33}$$

On the other hand,

$$\begin{aligned} < A^2_{klpqr} c_{klmn} A^1_{mnij} > &= < A^2_{klpqr} >< c_{klmn} A^1_{mnij} > + K^{(pqr)}_{kla} < c_{klmn} A^1_{mnij} x_a > \\ &= < c_{p(qmn} A^1_{mnij} x_{r)} > . \end{aligned} \tag{34}$$

Similarly, we get

$$< \underset{\approx}{\boldsymbol{A}}^1 \underset{\approx}{\boldsymbol{c}} \underset{\approx}{\boldsymbol{A}}^1 >=< \underset{\approx}{\boldsymbol{c}} \underset{\approx}{\boldsymbol{A}}^1 > \quad \text{and} \quad < A^2_{mnpqr} c_{mnpq} A^2_{pqabc} >=< c_{p(qmn} A^2_{mnabc} x_{r)} > . \tag{35}$$

These identities prove that the direct definition of the overall moduli and the energy-based one are equivalent. Furthermore, using (27), we establish the identity :

$$< c_{mnkl} A^2_{klpqr} >=< c_{p(qmn} A^1_{mnij} x_{r)} > . \tag{36}$$

Coupling terms between strain and strain gradient appear in the effective constitutive equations. Similar terms arise in the theory of composite beams. If the cell admits a symmetry point, the coupling terms can be shown to vanish. Otherwise, the origin of the coordinate system can be chosen such that $< c_{p(qmn} A^1_{mnij} x_{r)} >= 0$, which leads to the definition of a neutral lattice similar to the neutral fiber of a composite beam.

2.3 Cosserat HEM

An alternative choice of non-homogeneous boundary conditions can lead to the definition of a Cosserat overall medium. The complete derivation and an example in the case of heterogeneous linear elasticity can be found in [14].

2.3.1 Flexural rigidity

Consider for instance the following non-homogeneous boundary conditions

$$\underline{\boldsymbol{u}} = \underset{\sim}{\boldsymbol{E}} \underline{\boldsymbol{x}} + \underset{\sim}{\boldsymbol{F}}^{skew}(\underline{\boldsymbol{x}}) \underline{\boldsymbol{x}} \tag{37}$$

where $\underset{\sim}{\boldsymbol{F}}^{skew}$ is the following skew-symmetric tensor

$$\underset{\sim}{\boldsymbol{F}}^{skew} = (-\underset{\sim}{\underline{\boldsymbol{\epsilon}}}\, \underline{\boldsymbol{f}}(\underline{\boldsymbol{x}})) \quad \text{with} \quad \underline{\boldsymbol{f}} = \underset{\sim}{\boldsymbol{K}}\, \underline{\boldsymbol{x}}. \tag{38}$$

Vector $\underline{\boldsymbol{f}}$ is a linearly varying rotation vector so that $\underset{\sim}{\boldsymbol{K}}$ has the meaning of a prescribed curvature. Tensors $\underset{\sim}{\boldsymbol{E}}$ and $\underset{\sim}{\boldsymbol{K}}$ are given, constant and generally non-symmetric. Finally the proposed non-homogeneous boundary conditions read :

$$u_i = E_{ij} x_j + \epsilon_{ijk} K_{jl} x_l x_k, \quad \forall \underline{\boldsymbol{x}} \in \Omega. \tag{39}$$

If $\underset{\sim}{\boldsymbol{K}}$ vanishes, classical homogeneous boundary conditions are retrieved. The mean deformation in Ω reduces to $\underset{\sim}{\boldsymbol{E}}$ if the origin of the coordinate system is taken as the geometric centre of gravity. Computing now the work of internal forces and, using Gauss theorem, we get

$$< \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\boldsymbol{\varepsilon}} >= \underset{\sim}{\boldsymbol{\Sigma}} : \underset{\sim}{\boldsymbol{E}} + \underset{\sim}{\boldsymbol{M}} : \underset{\sim}{\boldsymbol{K}} \tag{40}$$

with

$$\underset{\sim}{\boldsymbol{\Sigma}} =< \underset{\sim}{\boldsymbol{\sigma}} > \quad \text{and} \quad M_{ij} =< \epsilon_{ikl} x_k \sigma_{lj} > . \tag{41}$$

As a result, if $\underset{\sim}{\boldsymbol{E}}$ and $\underset{\sim}{\boldsymbol{K}}$ are regarded as macroscopic deformation and torsion-curvature tensors, equation (40) represents a part of the work of internal forces of a Cosserat homogeneous equivalent medium (see (8)).

However, in this expression, the skew-symmetric part of $\underset{\sim}{\boldsymbol{E}}$ does not work with $\underset{\sim}{\boldsymbol{\Sigma}}$, since, according to (41), $\underset{\sim}{\boldsymbol{\Sigma}}$ is symmetric. Additional conditions are introduced in the next section to achieve the identification of the HEM with a Cosserat continuum.

Note that the previous non-homogeneous boundary conditions give a sort of flexural and torsional rigidities of the RVE. A more simple way to determine them is to perform classical flexion and torsion tests on the RVE by means of numerical simulation. Since the two methods will generally provide different effective moduli in the case of heterogeneous elastic materials, the appropriate choice of the determination method depends on the final loading conditions that the structure will undergo. Periodic conditions up to a curvature term are proposed in [14], that ultimately give a less stiff flexural rigidity than (39).

2.3.2 Cluster of RVEs

In a Cosserat theory, the translational and rotational degrees of freedom are independent. At the mesoscopic level, the translation describes 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 first neighbours (figure 1 a). Perform the test for which a rigid rotation is prescribed at the boundary of the central RVE, whereas the centre of each cell is kept fixed. It corresponds to a non-vanishing relative rotation of the microstructure with respect to the material lines. The reaction forces on each side of the RVE represent the resistance of the material to inner rotation and are used to derive the skew-symmetric part of $\underset{\sim}{\Sigma}$ (see [14]).

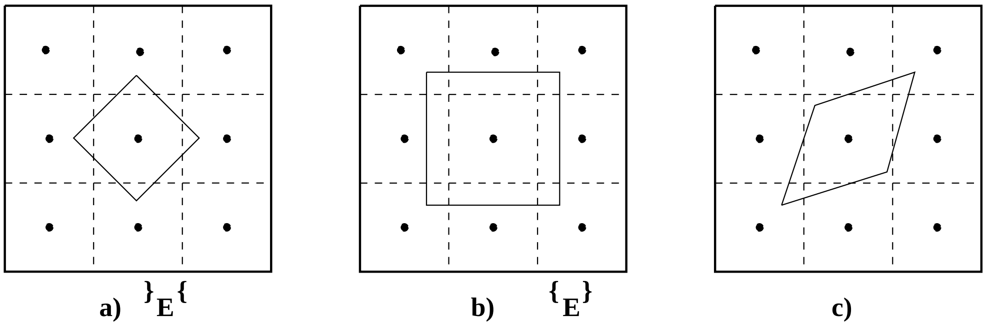

Figure 1 : Definition of a cluster of RVEs and prescribed global rotation (a) and strain (b), (c) on the central cell.

2.4 Micromorphic HEM

We want to develop non-homogeneous boundary conditions that combine the features presented for grade two and Cosserat HEMs and introduce additional ones.

The following quantities can be introduced in the case of a micromorphic medium starting from the micro-deformation tensor $\underset{\sim}{\boldsymbol{X}}$:

$$\overset{+}{K}_{ijk} = X^s_{ij,k} + X^s_{ki,j} - X^s_{jk,i} \qquad \text{and} \quad \overset{\times}{X}_i = -\frac{1}{2}\epsilon_{ijk}X_{jk}. \tag{42}$$

This prompts us to use these tensors in the definition of more general boundary conditions. In the following, the notations $X_{ij;k}$ or $\underset{\sim}{\boldsymbol{X}} \otimes \underline{\boldsymbol{\nabla}}^M$ denote partial derivation with respect to the macroscopic variables.

Let us now consider prescribed displacements on the boundary of a Boltzmann RVE of the form :

$$\underline{\boldsymbol{u}} = \underset{\sim}{\boldsymbol{X}}\,\underline{\boldsymbol{x}} + \frac{1}{2}\,\underset{\approx}{\overset{+}{\boldsymbol{K}}}(\underline{\boldsymbol{x}} \otimes \underline{\boldsymbol{x}}) + \underset{\approx}{\boldsymbol{\epsilon}}(((\underline{\overset{\times}{\boldsymbol{X}}} \otimes \underline{\boldsymbol{\nabla}}^M)\underline{\boldsymbol{x}}) \otimes \underline{\boldsymbol{x}}) \tag{43}$$

or, in index notation, $u_i = X_{ij}x_j + \frac{1}{2}K^+{}_{ijk}x_jx_k + \epsilon_{ijk}X^\times{}_{j;l}x_lx_k$.

Note that $\epsilon_{ijk}\overset{\times}{X}_{j;l} = {}^\}X^\{{}_{ik;l}$, where the inverted brackets denote the skew-symmetric part. It follows that

$$< \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}} >= \underset{\sim}{\boldsymbol{X}} \tag{44}$$

The corresponding mean internal work reads

$$< \sigma_{ij}u_{i,j} >=< \sigma_{ij} > X^s_{ij} + < \sigma_{ij}x_k > X^s_{ij;k} + < \sigma_{[ik}x_{j]} > {}^\}X^\{{}_{ij;k}. \tag{45}$$

This expression can be interpreted as a part of the work of internal forces of a micromorphic HEM provided that the overall stresses are defined as

$$\underset{\sim}{\boldsymbol{\Sigma}} =< \underset{\sim}{\boldsymbol{\sigma}} >, \quad M_{(ij)k} =< \sigma_{ij}x_k > \quad \text{and} \quad M_{[ij]k} =< \sigma_{[ik}x_{j]} > . \tag{46}$$

The contribution of the relative deformation tensor $\underset{\sim}{\boldsymbol{E}}$ does not appear in equation (45). Tensor $\underset{\sim}{\boldsymbol{E}}$ denotes the relative deformation of the RVE with respect to its immediate surroundings. To isolate this contribution to the overall energy, we consider again the cluster of RVEs introduced in the last section. Additional loading conditions are considered for which the centres of the RVEs are fixed and a relative strain is prescribed at the boundary of the central element (figure 1 b and c).

The resulting forces on the sides of the central element measure the resistance of the surrounding material to inner straining and can be used to build the components of the symmetric part of the overall stress tensor $\underset{\sim}{\boldsymbol{S}}$. The skew-symmetric part of $\underset{\sim}{\boldsymbol{S}}$ corresponds to the resistance of the material to an inner rotation that has already been investigated for the Cosserat HEM.

3 Homogenization methods for heterogeneous generalized continua

When the RVE itself is made of a heterogeneous generalized material, specific methods must be developed to define a HEM. This is the case for instance in micro-macro polycrystal modelling. As soon as the densities of statistically stored dislocations and the densities of geometrically necessary dislocations are distinguished, the single crystal must be regarded as an intrinsic generalized continuum. It is modelled as a second grade material in [15] and as a Cosserat material in [8]. Therefore, appropriate homogenization methods can lead to the derivation of a polycrystal model with non-local effects (size effects).

Homogenization techniques for heterogeneous Cosserat materials are presented in [16]. The more general case of heterogeneous micromorphic materials is treated in this work.

3.1 BVP with prescribed displacements and micro-deformation at the boundary

The RVE Ω now is a heterogeneous micromorphic continuum. The deformation, the micro-deformation, the symmetric and general stresses, and the double-force stress tensors inside Ω are respectively denoted by $\underset{\sim}{\boldsymbol{e}}, \underset{\sim}{\boldsymbol{\chi}}, \underset{\sim}{\boldsymbol{\sigma}}, \underset{\sim}{\boldsymbol{s}}$ and $\underset{\approx}{\boldsymbol{\mu}}$. The following micro-mechanical Dirichlet BVP is considered :

$$\left\{\begin{array}{l} \underset{\sim}{\boldsymbol{e}} = \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}} - \underset{\sim}{\boldsymbol{\chi}}, \quad \underset{\sim}{\boldsymbol{\chi}}^s = ^{\{} \underset{\sim}{\boldsymbol{\chi}}^{\}}, \quad \underset{\approx}{\boldsymbol{\kappa}} = \underset{\sim}{\boldsymbol{\chi}} \otimes \underline{\boldsymbol{\nabla}} \\ \textit{constitutive equations} \\ \underset{\sim}{\boldsymbol{s}}\, \underline{\boldsymbol{\nabla}} = 0, \quad \underset{\approx}{\boldsymbol{\mu}}\, \underline{\boldsymbol{\nabla}} + \underset{\sim}{\boldsymbol{s}} - \underset{\sim}{\boldsymbol{\sigma}} = 0, \quad \forall \underline{\boldsymbol{x}} \in \Omega \\ \textit{boundary conditions :} \\ \underline{\boldsymbol{u}} = \underset{\sim}{\boldsymbol{E}} \underline{\boldsymbol{x}} \quad \text{and} \quad \underset{\sim}{\boldsymbol{\chi}} = \underset{\sim}{\boldsymbol{X}}^s + \underset{\approx}{\boldsymbol{K}}\, \underline{\boldsymbol{x}}, \quad \forall \underline{\boldsymbol{x}} \in \partial\Omega \end{array}\right. \tag{47}$$

where constant tensors $\underset{\sim}{\boldsymbol{E}}, \underset{\sim}{\boldsymbol{X}}^s$(symmetric) and $\underset{\approx}{\boldsymbol{K}}$ have been introduced into the boundary conditions. It follows that

$$< \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}} >= \underset{\sim}{\boldsymbol{E}} \qquad \text{and} \qquad < \underset{\approx}{\boldsymbol{\kappa}} >= \underset{\approx}{\boldsymbol{K}}. \tag{48}$$

After noting that $(\chi_{ik} x_k)_{,j} = \kappa_{ikj} x_k + \chi_{ij}$, we get also

$$\chi^s_{ij} =< \chi_{ij} + \kappa_{ikj} x_k > . \tag{49}$$

Let us now compute the mean work of internal forces :

$$< \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\boldsymbol{\chi}}^s + \underset{\sim}{\boldsymbol{s}} : \underset{\sim}{\boldsymbol{e}} + \underline{\underline{\underline{\boldsymbol{\mu}}}} \,\vdots\, \underline{\underline{\underline{\boldsymbol{\kappa}}}} >= \underset{\sim}{\boldsymbol{E}} :< \underset{\sim}{\boldsymbol{s}} > + \underset{\sim}{\boldsymbol{X}}^s :<^{\{} \underset{\sim}{\boldsymbol{\sigma}} - \underset{\sim}{\boldsymbol{s}}^{\}} > + \underline{\underline{\underline{\boldsymbol{K}}}} \,\vdots < \underline{\underline{\underline{\boldsymbol{\mu}}}} + (\underset{\sim}{\boldsymbol{\sigma}} - \underset{\sim}{\boldsymbol{s}}) \otimes \underline{\boldsymbol{x}} > \tag{50}$$

This leads to the definitions of a micromorphic HEM for which $\underset{\sim}{\boldsymbol{E}}, \underset{\sim}{\boldsymbol{X}}$ and $\underset{\approx}{\boldsymbol{K}}$ are the macroscopic relative deformation, the (macroscopic) micro-deformation and micro-deformation gradient tensors. The associated stress tensors are :

$$\underset{\sim}{\boldsymbol{S}} =< \underset{\sim}{\boldsymbol{s}} >, \quad \underset{\sim}{\boldsymbol{\Sigma}} =<^{\{} \underset{\sim}{\boldsymbol{\sigma}} - \underset{\sim}{\boldsymbol{s}}^{\}} >, \quad \underset{\approx}{\boldsymbol{M}} =< \underset{\approx}{\boldsymbol{\mu}} + (\underset{\sim}{\boldsymbol{\sigma}} - \underset{\sim}{\boldsymbol{s}}) \otimes \underline{\boldsymbol{x}} > . \tag{51}$$

The case of a micro-heterogeneous Cosserat continuum is obtained from the previous results when $\underset{\sim}{\boldsymbol{\chi}}^s =^{\{} \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}}^{\}}$, which correponds to skew-symmetric $\underset{\sim}{\boldsymbol{e}}$ and $\underset{\sim}{\boldsymbol{s}}$. The overall medium can then be regarded as a Cosserat continuum for which

$$\underset{\sim}{\boldsymbol{\Sigma}}^{Cosserat} =< \underset{\sim}{\boldsymbol{\sigma}}^{cosserat} >=< \underset{\sim}{\boldsymbol{\sigma}} + \underset{\sim}{\boldsymbol{s}} > \tag{52}$$

$$M_{lk}^{Cosserat} = -\epsilon_{lij} M_{ijk} = < \mu_{lk}^{Cosserat} + \epsilon_{lij} \sigma_{ij}^{Cosserat} x_k > . \tag{53}$$

This was the result obtained in [16].

3.2 Hill-Mandel's lemma for heterogeneous micromorphic media

Let $(\underset{\sim}{\boldsymbol{s}}^\star, \underset{\sim}{\boldsymbol{\sigma}}^\star, \underset{\approx}{\boldsymbol{\mu}}^\star)$ be self-equilibrated force and couple stress fields on Ω, which means that

$$\underset{\sim}{\boldsymbol{s}}^\star \, \underline{\boldsymbol{\nabla}} = 0 \quad \text{and} \quad \underset{\approx}{\boldsymbol{\mu}}^\star \, \underline{\boldsymbol{\nabla}} \; + \underset{\sim}{\boldsymbol{s}}^\star - \underset{\sim}{\boldsymbol{\sigma}}^\star = 0 \tag{54}$$

Let then $(\underset{\sim}{\boldsymbol{e}}', \underset{\sim}{\boldsymbol{\chi}}^{s\prime}, \underset{\approx}{\boldsymbol{\kappa}}')$ be compatible deformation, micro-strain and micro-deformation gradient fields ($(\underline{\boldsymbol{u}}', \underset{\sim}{\boldsymbol{\chi}}')$ are the associated displacement and micro-deformation fields). Then if $(\underline{\boldsymbol{u}}', \underset{\sim}{\boldsymbol{\chi}}')$ satisfy the boundary conditions given in (14), the following relation holds :

$$\begin{aligned} < \underset{\sim}{\boldsymbol{\sigma}}^\star : \underset{\sim}{\boldsymbol{\chi}}^{s\prime} + \underset{\sim}{\boldsymbol{s}}^\star : \underset{\sim}{\boldsymbol{e}}' + \underset{\equiv}{\boldsymbol{\mu}}^\star \vdots \underset{\equiv}{\boldsymbol{\kappa}}' > \;&=\; < \underset{\sim}{\boldsymbol{s}}^\star > : < \underline{\boldsymbol{u}} \otimes \underline{\boldsymbol{\nabla}} > + <^{\{} \underset{\sim}{\boldsymbol{\sigma}}^\star - \underset{\sim}{\boldsymbol{s}}^{\star\}} > : \underset{\sim}{\boldsymbol{X}}'^s \\ &+ \; < \underset{\equiv}{\boldsymbol{\mu}}^\star + (\underset{\sim}{\boldsymbol{\sigma}}^\star - \underset{\sim}{\boldsymbol{s}}^\star) \otimes \underline{\boldsymbol{x}} > \vdots < \underset{\equiv}{\boldsymbol{\kappa}}' > \end{aligned} \tag{55}$$

where $X_{ij}'^s = < \chi_{ij}' + \kappa_{ikj} x_k >$.

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