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Numerical Homogenization of Elastic Behavior of Fractured Rock Masses and Micro-cracked Materials by FEM

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ABSTRACT: A review of recent works on numerical homogenisation of fractured rock masses gives witness of difficulties in defining rigorously and determining numerically the *macroscopic* strain and stress that are to be used in upscaling relations. Moreover, for finite-size domains, relations between macroscopic strain and stress are dependant on boundary conditions and this constitutes an additional difficulty for upscaling. Due to these difficulties the methods used for numerical upscaling remains somehow empirical and lead to non-accurate results, for instance to *non-symmetric* elastic tensors. In this paper, some fundamental results on homogenization of finite-size heterogeneous domains established by Huet (1988) are extended to discontinuous; fractured or micro-cracked, elastic materials. Boundary conditions leading to lower and upper bounds of compliance tensors for finite-size domains are rigorously defined and, in context of Finite Elements, numerical methods for determining these tensors are given. It is shown that even for a finite-size domain the elastic tensor obtained numerically will be rigorously symmetric if correctly defined and calculated.

1 Introduction

In numerical methods used for upscaling the mechanical behaviour of heterogeneous materials, the *macroscopic behaviour* is deduced from relationships between equivalent *macroscopic* strains and stresses defined in a Representative Elementary Volume. For *continuous* heterogeneous materials, the *macroscopic strain* and *stress* are defined as the *bulk mean value* of local strain and stress in the Representative Elementary Volume (REV). But in the presence of discontinuities; fractures or cracks, which are modelled geometrically as zero thickness lines, the definition of *macroscopic* quantities relevant for determination of equivalent macroscopic behaviour must be re-examined. As a matter of fact, stress and strain are not defined on these discontinuity lines and, what is more, the contribution of quantities defined on these lines to the global volume averages would be nought since these lines have a zero volume, although they have an important effect on macroscopic behaviour. In addition, in numerical modelling the calculation domain has necessarily finite-size and it is well known that for a finite-size domain in heterogeneous materials there is not a unique compliance tensor relating bulk mean value of strain to that of stress. Indeed, different boundary conditions can create displacement fields in the domain which lead to a same value for the average strain but to different values for the average stress or *vice versa*. These difficulties are not specific to mechanical properties and are well known also for instance for permeability upscaling of porous materials (Renard and de Marsily 1997, Pouya 2005). Due to these difficulties, it can be noted in the literature that methods for determination of *macroscopic strain* and *stress* in numerical homogenization works remain somehow empirical. For instance, Pouya and Ghoreychi (2001) determined bulk mean strain and strain for a fractured domain by some boundary integrals which give only an approximate estimation of these quantities. Min and Jing (2003) determined them by taking the average values of strain and stress on a set of arbitrarily selected points in the domain. These "*empirical"* methods lead to non-accurate results for macroscopic elastic tensors and, in particular, to *non-symmetric* tensors (Min and Jing 2003). Similar problems are observed in the literature on numerical upscaling of the permeability as analysed by (Pouya and Courtois 2002).

Huet (1990, 1999) showed that for finite-size domains in heterogeneous materials, it is possible to defined two compliance tensors defining lower un upper bounds of macroscopic compliance tensors. These tensors are well symmetric and positive-definite and can be obtained by applying on the boundary of domain specific conditions. In this paper, first these results will be extended to discontinuous elastic materials. Then, in the context of Finite Elements, the numerical method for determining rigorously macroscopic strain and stress and lower and upper bounds of elastic tensors will be given. Finally, it will be shown that even in the context of numerical modelling, at least by FEM, the compliance tensor will be rigorously symmetric and positive-definite if correctly determined

from numerical strains and stresses obtained under correctly defined boundary conditions.

2 General equations

A finite-size elastic heterogeneous domain Ω containing a family of cracks Γ_κ is considered (Figure 1a). Local strain and stress fields are denoted respectively $\boldsymbol{\varepsilon}(\underline{x})$ and $\boldsymbol{\sigma}(\underline{x})$ and related by an elasticity tensor $\mathbb{C}(\underline{x})$ and displacement discontinuity and stress vector on the cracks are denoted respectively $\underline{U}(\underline{x})$ and $\underline{\sigma}(\underline{x})$ and related by the crack rigidity matrix $\mathbf{R}(\underline{x})$; $\underline{\sigma}(\underline{x})= \mathbf{R}(\underline{x}).\underline{U}(\underline{x})$. On a point $\underline{x}$ on a crack Γ_κ where the unit normal to the carck-line is $\underline{n}(\underline{x})$, we have $\underline{\sigma}(\underline{x})= \boldsymbol{\sigma}(\underline{x}).\underline{n}(\underline{x})$.

Macroscopic strain $\mathbf{E}$ and *stress* $\boldsymbol{\Sigma}$ are *defined* as follows:

$$\mathbf{E} \equiv \frac{1}{V}\int_{\partial\Omega}\frac{1}{2}(\underline{u}\otimes\underline{n}+\underline{n}\otimes\underline{u})\,ds\ , \qquad \boldsymbol{\Sigma} \equiv \frac{1}{V}\int_{\partial\Omega}\frac{1}{2}(\underline{T}\otimes\underline{x}+\underline{x}\otimes\underline{T})\,ds \tag{1}$$

where $\underline{u}$, $\underline{T}$ and $\underline{n}$ are respectively the displacement, traction and unit outward normal vector on the boundary $\partial\Omega$. The elastic strain energy potential is defined by the following expression:

$$\mathcal{W}(\underline{u}) = \frac{1}{2}\int_{\Omega}\boldsymbol{\varepsilon}:\mathbb{C}:\boldsymbol{\varepsilon}\,dv + \frac{1}{2}\sum_{\kappa}\int_{\Gamma_\kappa}\underline{U}\,.\mathbf{R}.\underline{U}\,ds \tag{2}$$

The following mathematical identity can be easily established:

$$\int_{\partial\Omega} x_i n_j\ ds\ =\ V\delta_{ij} \tag{3}$$

The fundamental Green identity for a function f in a domain Ω containing discontinuities Γ_κ reads:

$$\int_{\Omega}\partial_i f\ dv\ =\ \int_{\partial\Omega} f\ n_i\ ds\ -\sum_k\int_{\Gamma_k}[[f]]\,n_i\ ds \tag{4}$$

where in the right-side $\underline{n}$ represents the unit outward normal on $\partial\Omega$ the first integral and the unit normal vector on the crack Γ_κ in the second and $[[\,f\,]]$ represents the discontinuity or jump of f across the crack in the direction oriented by $\underline{n}$; *i.e.,* $[[\,f\,]] = f^+ - f^-$ where f^+ is the limit value of f on the upper lip Γ^+ and f^- on the lower lip Γ^- of the crack (see for instance figure 1b for f being the displacement vector $\underline{u}$).

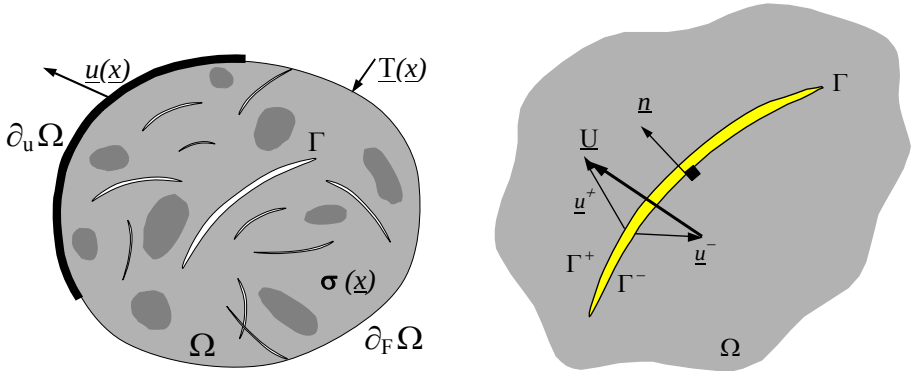


Figure 1.(a) finite-size domain in micro-cracked heterogeneous material, (b) displacement discontinuity on the crack.

By applying (4) to $(\partial_i u_j+\partial_j u_i)$ and using (3) we find:

$$\mathbf{E} = \frac{1}{V}\left[\int_{\Omega}\boldsymbol{\varepsilon}\,dv\ +\sum_k\int_{\Gamma_k}\frac{1}{2}(\underline{U}\otimes\underline{n}+\underline{n}\otimes\underline{U})\,ds\right] \tag{5}$$

From the stress balance equation $\partial_j\sigma_{ij} = 0$ we derive $\partial_j(\sigma_{ij}x_k) = \sigma_{ik}$. Then by applying (4) to $\partial_j(\sigma_{ij}x_k)$ and using $[[\boldsymbol{\sigma}]].\underline{n} = 0$ on Γ and $\boldsymbol{\sigma}.\underline{n} = \underline{T}$ on $\partial_F\Omega$ we find:

$$\boldsymbol{\Sigma} = \frac{1}{V}\int_{\Omega} \boldsymbol{\sigma}\ dv \tag{6}$$

The relations (5) and (6) mean that the *macroscopic stress* $\boldsymbol{\Sigma}$ is equal to the *volume average* of $\boldsymbol{\sigma}$ in the matrix whereas the *macroscopic strain* $\mathbf{E}$ is the sum of the *volume average* of $\boldsymbol{\varepsilon}$ in the matrix and the *crack strain* $\mathbf{E}_f$ which defined as :

$$\mathbf{E}_f = \frac{1}{V}\sum_k \int_{\Gamma_k} \frac{1}{2}(\underline{U}\otimes\underline{n} + \underline{n}\otimes\underline{U})\ ds \tag{7}$$

3 Uniform boundary conditions

As noted here-above, there is not a unique compliance tensor relating macroscopic stress to macroscopic strain obtained under general boundary conditions in a finite-size heterogeneous domain. But under some specific boundary conditions it is possible to define a unique tensor relating with together these two quantities. We define in the following two principal cases of these specific boundary conditions.

Loading cases corresponding to *linear displacement* prescribed on the boundary are defined by the condition:

$$\forall \underline{x} \in \partial\Omega;\ \ \underline{u}(\underline{x}) = \mathbf{A}.\underline{x} \tag{8}$$

where $\mathbf{A}$ is a constant symmetric second-rank tensor. In this case, the equation (3) and definition (1) imply $\mathbf{E} = \mathbf{A}$. Since all the equations are linear, the stress filed $\boldsymbol{\sigma}(\underline{x})$ and then its volume average (6) are linear functions of $\mathbf{A}$. This means that there exists a fourth-rank tensor $\mathbb{C}^u$ which allows writing $\boldsymbol{\Sigma} = \mathbb{C}^u{:}\mathbf{A}$, and since $\mathbf{E} = \mathbf{A}$:

$$\boldsymbol{\Sigma} = \mathbb{C}^u : \mathbf{E} \tag{9}$$

$\mathbb{C}^u$ represents the elastic compliance tensor under *linear displacement boundary conditions* (*ldbc*).
We define a deformation state obtained under *uniform stress boundary conditions* (*usbc)* by:

$$\forall \underline{x} \in \partial\Omega;\ \underline{T}(\underline{x}) = \mathbf{B}.\underline{n}(\underline{x}) \tag{10}$$

then substituting by (10) for $\underline{T}$ in (1) and using (3) one finds $\boldsymbol{\Sigma} = \mathbf{B}$. The linearity of all the equations imply that there exists a fourth-rank tensor $\mathbb{S}^s$ which allows writing $\mathbf{E} = \mathbb{S}^s\mathbf{:B}$, and then :

$$\mathbf{E} = \mathbb{S}^s\mathbf{:}\boldsymbol{\Sigma} \tag{11}$$

For any couple of deformation states indexed 1 and 2, by application of (4) on $\partial_i(\sigma_{ij}u_j)$ and using stress balance $\partial_i\sigma_{ij} = 0$, it can be established that :

$$\int_{\Omega} \boldsymbol{\sigma}^{(2)} : \boldsymbol{\varepsilon}^{(1)}\ dv\ + \sum_k \int_{\Gamma_k} \underline{\sigma}^{(2)}.\underline{U}^{(1)} ds = \int_{\partial\Omega} \underline{T}^{(2)}.\underline{u}^{(1)} ds \tag{12}$$

Then, if the field 1 corresponds to *ldbc*, by substituting for $\underline{u}^{(1)}$ in the right-side of (12) by $\mathbf{E}^{(1)}.\underline{x}$, and using the second equality (1), we obtain :

$$\frac{1}{V}\left(\int_{\Omega} \boldsymbol{\sigma}^{(2)} : \boldsymbol{\varepsilon}^{(1)}\ dv\ + \sum_k \int_{\Gamma_k} \underline{\sigma}^{(2)}.\underline{U}^{(1)} ds\right) = \boldsymbol{\Sigma}^{(2)}{:}\ \mathbf{E}^{(1)} \tag{13}$$

Also, if the field 2 corresponds to *usbc*, by substituting for $\underline{T}^{(2)}$ in the right-side of (12) by $\boldsymbol{\Sigma}^{(2)}.\underline{n}$ and using the first equality (1), we obtain the same relation (13). In conclusion, (12) holds for every couple of fields whereas (13) holds if the filed 1 corresponds to *ldbc* or the field 2 to *usbc*.

Now, let us replace in (13) by $\boldsymbol{\sigma}^{(2)} = \mathbb{C} : \boldsymbol{\varepsilon}^{(2)}$ and $\underline{\sigma}^{(2)} = \mathbf{R}.\underline{U}^{(2)}$ to find:

$$\frac{1}{V}\left(\int_{\Omega}\boldsymbol{\varepsilon}^{(2)}:\mathbb{C}:\boldsymbol{\varepsilon}^{(1)}\,dv+\sum_{k}\int_{\Gamma_k}\underline{U}^{(2)}.\mathbf{R}.\underline{U}^{(1)}ds\right)=\mathbf{E}^{(1)}:\mathbb{C}^{u}:\mathbf{E}^{(2)} \tag{14}$$

From the symmetry of $\mathbb{C}$ and $\mathbf{R}$ in the left-side one deduces that of $\mathbb{C}^{u}$ in the right. Besides, if the two strain fields are identical; $\boldsymbol{\varepsilon}^{(2)}=\boldsymbol{\varepsilon}^{(1)}$, $\underline{U}^{(2)}=\underline{U}^{(1)}$ and $\mathbf{E}^{(2)}=\mathbf{E}^{(1)}$, then (14) leads to :

$$\mathcal{W}(\underline{u})=\frac{1}{2V}\left(\int_{\Omega}\boldsymbol{\varepsilon}:\mathbb{C}:\boldsymbol{\varepsilon}\,dv+\sum_{k}\int_{\Gamma_k}\underline{U}.\mathbf{R}.\underline{U}ds\right)=\frac{1}{2}\mathbf{E}:\mathbb{C}^{u}:\mathbf{E} \tag{15}$$

If $\mathbf{E}:\mathbb{C}^{u}:\mathbf{E}=0$ in (15), then positive-definite property of $\mathbb{C}$ and $\mathbf{R}$ imply $\boldsymbol{\varepsilon}=0$ and $\underline{U}=0$ every where, what will imply, according to (1), that $\mathbf{E}=0$. Therefore $\mathbb{C}^{u}$ is positive-definite. We note $\mathbb{S}^{u}$ its reverse which will be also symmetric and positive-definite. With the same method it can also be shown that $\mathbb{S}^{s}$ and its reverse noted $\mathbb{C}^{s}$ are symmetric and positive-definite.

To show the bound property of $\mathbb{C}^{u}$, we consider a general state of deformation with local fields $\underline{u}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ and $\underline{U}$ obtained under general boundary conditions. Macroscopic strain and stress corresponding to this deformation state are denoted $\mathbf{E}$ and $\boldsymbol{\Sigma}$. Then, we take $\mathbf{A}^{(1)}=\mathbb{S}^{u}:\boldsymbol{\Sigma}$ and note $\boldsymbol{\varepsilon}^{(1)}$, $\boldsymbol{\sigma}^{(1)}$ and $\underline{U}^{(1)}$ the local fields obtained under *ldbc* (8) for $\mathbf{A}^{(1)}$. They can be different from respectively $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ and $\underline{U}$. But for the field indexed (1) we find, according to results shown here-above for *ldbc* fields, $\mathbf{E}^{(1)}=\mathbf{A}^{(1)}$. We note $\mathcal{W}$ and $\mathcal{W}^{(1)}$ the strain energies (2) for these two deformation states. Then we define :

$$I=\frac{1}{2V}\left(\int_{\Omega}(\boldsymbol{\sigma}-\boldsymbol{\sigma}^{(1)}):(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{(1)})\,dv+\sum_{k}\int_{\Gamma_k}(\underline{\sigma}-\underline{\sigma}^{(1)}).(\underline{U}-\underline{U}^{(1)})\mathrm{ds}\right) \tag{16}$$

Replacing in (16) by $\boldsymbol{\sigma}-\boldsymbol{\sigma}^{(1)}=\mathbb{C}:(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{(1)})$ and $\underline{\sigma}-\underline{\sigma}^{(1)}=\mathbf{R}.(\underline{U}-\underline{U}^{(1)})$ and using the positive-definiteness of $\mathbb{C}$ and $\mathbf{R}$, we find that $I\geq 0$. Then, after some manipulations, by using (13), we obtain :

$$I=\mathcal{W}+\mathcal{W}^{(1)}-\frac{1}{V}\left(\int_{\Omega}\boldsymbol{\sigma}:\boldsymbol{\varepsilon}^{(1)}\,dv+\sum_{k}\int_{\Gamma_k}\underline{\sigma}.\underline{U}^{(1)}ds\right)=\mathcal{W}+\mathcal{W}^{(1)}-\boldsymbol{\Sigma}:\mathbf{E}^{(1)} \tag{17}$$

But $\mathbf{E}^{(1)}=\mathbf{A}^{(1)}=\mathbb{S}^{u}:\boldsymbol{\Sigma}$, and according to (13), $\mathcal{W}^{(1)}=(1/2)\,\boldsymbol{\Sigma}^{(1)}:\mathbf{E}^{(1)}$, and to (9), $\boldsymbol{\Sigma}^{(1)}=\mathbb{C}^{u}:\mathbf{E}^{(1)}=\mathbb{C}^{u}:\mathbf{A}^{(1)}=\boldsymbol{\Sigma}$. Then substituting in (17), we find $I=\mathcal{W}-(1/2)\,\boldsymbol{\Sigma}:\mathbb{S}^{u}:\boldsymbol{\Sigma}$. So $I\geq 0$ implies :

$$\frac{1}{2}\boldsymbol{\Sigma}:\mathbb{S}^{u}:\boldsymbol{\Sigma}\leq\frac{1}{2V}\left(\int_{\Omega}\boldsymbol{\varepsilon}:\mathbb{C}:\boldsymbol{\varepsilon}\,dv+\sum_{k}\int_{\Gamma_k}\underline{U}.\mathbf{R}.\underline{U}\,ds\right) \tag{18}$$

Now for the same state of deformation $(\boldsymbol{\varepsilon},\underline{U})$, beginning with an auxiliary *usbc* field corresponding to (10) with $\mathbf{B}^{(2)}=\mathbb{C}^{s}:\mathbf{E}$, and by using the same methods, we obtain:

$$\frac{1}{2}\mathbf{E}:\mathbb{C}^{s}:\mathbf{E}\leq\frac{1}{2V}\left(\int_{\Omega}\boldsymbol{\varepsilon}:\mathbb{C}:\boldsymbol{\varepsilon}\,dv+\sum_{k}\int_{\Gamma_k}\underline{U}.\mathbf{R}.\underline{U}\,ds\right) \tag{19}$$

The equality in relations (18) and (19) is obtained for strain fields corresponding respectively to *ldbc* and *usbc*. These inequalities extend analogue inequalities obtained by Huet (1990) for *continue* heterogeneous materials to the case of materials containing discontinuities. Their interpretation is that $\mathbb{C}^{s}$ represents the lower bound of elasticity tensor of the domain Ω and $\mathbb{C}^{u}$ the upper bound.

In homogenization process, the difference between $\mathbb{C}^{u}$ and $\mathbb{C}^{s}$ becomes negligible when the domain's size approaches REV size. But in some applications one needs to determine a continuum equivalent model for a fractured domain which is under REV size. This occurs for instance in modelling the Excavation Damaged Zone around underground openings in fractured rocks or sometimes when studying stability of rock slopes. In theses cases un upper or lower bound of mechanical properties can be needed and the distinction between $\mathbb{C}^{u}$ and $\mathbb{C}^{s}$ can reveals to be useful.

Figure 2 presents a simple example which shows clearly why under *ldbc* the global stiffness is greater (Chalhoub 2006). As a matter of fact condition (8) imposes a continuous displacement on the boundary and so prevents opening of fractures intersecting the boundary (b) whereas this opening is free in *usbc* case (c).

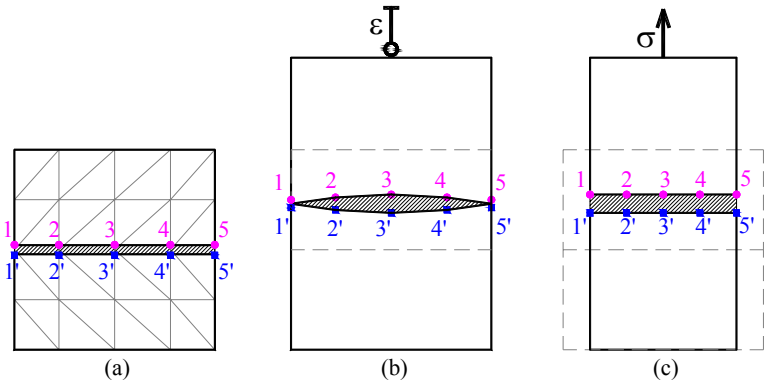


Figure 2. Loading a fractured domain (a) under linear displacement boundary conditions (b) and uniform stress boundary conditions (c). Under *ldbc* the opening at the extremity of fractures intersecting the boundary is blocked.

4 Numerical symmetry

An argument presented sometimes to explain why elastic tensors obtained numerically are not symmetric is to say that it is due to imprecision and approximate character of the numerical method and also to finite size of the domain which can be smaller than the REV size. In this section we will show that within the framework of Finite Elements Method the compliance tensors obtained numerically must be rigorously symmetric. In fact, the formulation of this method leads to expressions for $\mathbb{C}^s$ and $\mathbb{C}^u$ which are a symmetric. We will show this property for $\mathbb{C}^u$.

To show this property, we use the variational formulation of the problem. For prescribed forces $\underline{F}$ and boundary tractions $\underline{T}$ and boundary displacements, the solution of equilibrium equations minimizes the displacement potential :

$$\mathcal{A}(\underline{u}) = \mathcal{W}(\underline{u}) - \int_{\Omega} \underline{F}.\underline{u}\, dv - \int_{\partial_F\Omega} \underline{T}.\underline{u}\, ds \tag{20}$$

within the family of displacement fields satisfying the prescribed $\underline{u}$ on $\partial_u\Omega$. In *ldbc* case, volume forces and surface tractions are zero, $\mathcal{A}(\underline{u}) = \mathcal{W}(\underline{u})$ and displacement condition on the hole boundary $\partial\Omega$ is given by (8). Now consider a discretization of the domain defined by P nodes (x_p, y_p) with $1 \le p \le P$, M_1 volume elements Ω_m and M_2 joint elements Γ_k representing cracks and fractures. The elements Ω_m have J nodes with interpolation functions designated by Ψ and the joint elements Γ_k have J' nodes with interpolation function giving the *displacement discontinuity* along on the joint designated by Φ. The discrete displacement functions on Ω are defined by their nodal values $\underline{u}_p$ for $1 \le p \le P$ and the interpolation functions within elements :

$$\forall \underline{x} \in \Omega_m\ ; \qquad \underline{u}(\underline{x}) = \sum_{q=1}^{J} \Psi_m^q(\underline{x})\underline{u}_q \tag{21}$$

Along joint elements the displacement discontinuity is :

$$\forall \underline{x} \in \Gamma_k\ ; \qquad \underline{U}(\underline{x}) = \sum_{q=1}^{J'} \Phi_k^q(\underline{x})\underline{u}_q \tag{22}$$

The numerical solution minimizes $\mathcal{W}(\underline{u})$ within the family of discrete functions.

The strain and stress tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are noted by column vectors respectively $E_{3\times1}$ and $S_{3\times1}$ defined by $E^T = \{\varepsilon_{xx}, \varepsilon_{xy}, \varepsilon_{yy}\}$ and $S^T = \{\sigma_{xx}, \sigma_{xy}, \sigma_{yy}\}$. The strain in an element is given by $E = BQ$ where $B_{3\times2J}$ is the

symmetrized gradient of Ψ and $Q_{2J\times1}$ is the column of nodal displacements of the element. The elastic coefficients of the element are represented by a matrix D which allows writing S=DE. The displacement jump $\underline{U}$ on a joint element is noted by $G_{2\times1}$ where $G^T=\{U_x, U_y\}$ and related to nodal displacements $Q_{2J'\times1}$ by $G = NQ$ where the matrix $N_{2\times2J'}$ is constituted of $\Phi_k^q(\underline{x})$ functions according to (22). The elastic stiffness of the joint element is represented by $R_{2\times2}$. With these notations we have :

$$\mathcal{W}(\underline{u})= \frac{1}{2}\sum_m Q^T\left(\int_{\Omega_m} B^T D B\, dv\right)Q+\frac{1}{2}\sum_k Q^T\left(\int_{\Gamma_k} N^T R\, N\, ds\right)Q=\frac{1}{2}U^T K U \tag{23}$$

$U_{2P\times1}$ is the global column of nodal displacements and the symmetric matrix $K_{2P\times2P}$ represents the global rigidity of the system. Suppose now that P' nodes are inside the domain and P'' on the boundary, with P'+P''=P. The internal nodes are numbered from 1 to P', and those on the boundary, from P'+1 to P. The displacement vector can be separated in two parts by using bloc notation $U^T = [U_d^T, U_b^T]$, with $U_d^T=\{u_1, ..., u_{P'}\}$ and $U_b^T=\{u_{P'+1},..., u_P\}$. Correspondingly, K can be decomposed in four blocs:

$$K=\begin{bmatrix} K_d & H \\ H^T & K_b \end{bmatrix} \tag{24}$$

The symmetric blocs $K^d_{P'\times P'}$ and $K^b_{P''\times P''}$ are related respectively to the internal and boundary nodes and the bloc $H_{P'\times P''}$ to crossed terms. With this notation :

$$\mathcal{W}(\underline{u})= \frac{1}{2}UKU=\frac{1}{2}\ [\ U_d^T K_d U_d + U_d^T H U_b + U_b^T H^T U_b + U_b^T K_b U_b\ ] \tag{25}$$

Let us consider the case of *ldbc* loading of Ω with displacement on the boundary given by (8). This means that the *macroscopic strain* is equal to **A**. Let us note $A_{3\times1}$ the column vector made with the components of **A** which is symmetric, *i.e.,* $A^T = \{A_{11}, A_{12}, A_{22}\}$. The displacement for the node number p on the boundary with coordinates (x_p, y_p) is given by $u_{p,x} = A_{11}\, x_p + A_{12}\, y_p$ and $u_{p,y} = A_{12}\, x_p + A_{22}\, y_p$, what can be written as :

$$\begin{bmatrix} u_x^p \\ u_y^p \end{bmatrix}=\begin{bmatrix} x_p & y_p & 0 \\ 0 & x_p & y_p \end{bmatrix}\begin{bmatrix} A_{11} \\ A_{12} \\ A_{22} \end{bmatrix} \tag{26}$$

Using this relation, we can write $U_b = X_b A$ where $X^b_{2P''\times3}$ is constituted from rows $\{x_p, y_p, 0\}$ at the $(2p-1)_{th}$ position and $\{0, x_p, y_p\}$ at $(2p)_{th}$ position. U_d is obtained by minimisation of $\mathcal{W}(\underline{u})$ given by (25) with the fixed value of U_b. The calculus of variation of $\mathcal{W}$ for fixed values of U_b and putting $\delta\mathcal{W}=0$ lead to :

$$\delta(U\mathbf{K}U) = (\delta U_d^T)K_d U_d + U_d^T K_d \delta U_d + (\delta U_d^T) H U_b + U_d^T H^T \delta U_d = 0 \tag{27}$$

This equation has for solution :

$$U_d = -(K_d)^{-1} H U_b \tag{28}$$

Substituting in this by $U_b = X_b A$ we find :

$$U_d = -(K_d)^{-1} H\, X_b A \tag{29}$$

So finally, the global displacement solution U can be written, in bloc notation, as following:

$$U^T = [U_d^T, U_b^T]\ ; \qquad U_d = X_d A\ , \qquad U_d = -(K_d)^{-1} H\, X_b A \tag{30}$$

The *volume average stress* in the domain Ω is given by :

$$\bar{S} = \frac{1}{V} D \sum_m \left(\int_{\Omega_m} B\, dv\right) Q \tag{31}$$

and then its calculation reduces to summation upon Gauss points. According to (30) displacement U and then

every column Q in (31) are linear functions of A. Therefore $\bar{S}$; is a linear function of A, what can be written as :

$$\bar{S}; = C\,A \tag{32}$$

The objective here is to show that C is symmetric. This means that for every other $A'_{3\times1}$ we have $A'^{T}CA = A^{T}CA'$. To show this, let us consider the auxiliary displacement filed $\underline{u}'$ defined by a uniform gradient $\mathbf{A'}$ on the *hole domain* (at not only at the boundary as it was the case for $\underline{u}$), *i.e.*, $\forall \underline{x}\in\Omega$, $\underline{u}'(\underline{x}) = \mathbf{A'}.\underline{x}$. Then the corresponding displacement vector U' is given by (26) for every point, and can be written as :

$$U'^{T} = [U'_d{}^{T}, U'_b{}^{T}]\ ; \qquad U'_d = X_d A'\ , \qquad U'_d = X_d A' \tag{33}$$

Besides, for every couple of displacement fields U and U' with corresponding nodal displacements columns Q and Q', we have the identity :

$$\frac{1}{2}U'^{T}KU = \frac{1}{2}\sum_m Q'^{T}\left(\int_{\Omega_m} B^{T}DB\ dv\right)Q + \frac{1}{2}\sum_k Q'^{T}\left(\int_{\Gamma_k} N^{T}R\,N\ ds\right)Q \tag{34}$$

which is the numerical equivalent of (14). The displacement U' defined by (33) is continuous everywhere in Ω and so gives a zero jump across discontinuity lines : $N^{T}Q' = 0$ for all the joint elements in (34). Since U' defines a uniform gradient field, in the first integral in right-side of (33) we can replace $BQ'=A'$. Then, after simplifications and using (31) we can write (34) as :

$$\frac{1}{2}U'^{T}KU = \frac{1}{2V}A'^{T}\sum_m\left(\int_{\Omega_m} DB\ dv\right)Q = \frac{1}{2}A'^{T}\bar{S} = \frac{1}{2}A'^{T}CA \tag{35}$$

Now we use bloc notations (30), (33) and (24) for U, U' and K in the first side of (35) and write this relation as :

$$A'^{T}CA = U'_d{}^{T}K_dU_d + U'_d{}^{T}HU_b + U'_b{}^{T}H^{T}U_d + U'_b{}^{T}K_bU_b \tag{36}$$

Replacing in this relation by $U'_d = X_dA'$, $U'_b = X_bA'$, $U_b = X_bA$, and $U_d = -(K_d)^{-1}H\,X_bA$, and after simplification we find:

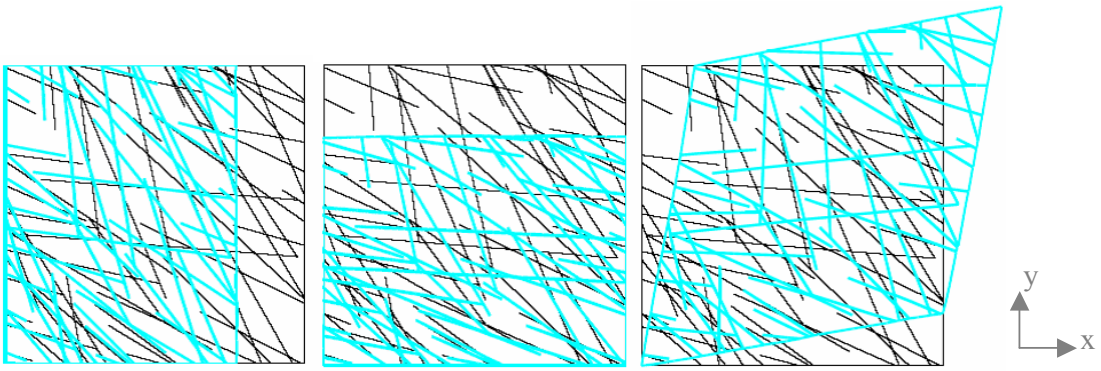
$$A'^{T}CA = -\,A'^{T}X_b{}^{T}H^{T}(K_d)^{-1}H\,X_bA + A'^{T}X_b{}^{T}K_bX_bA = A'^{T}X_b{}^{T}\left(-H^{T}(K_d)^{-1}H + K_b\right)X_b\,A \tag{37}$$

Since this relation holds for every A and A' , we deduce that :

$$C = X_b{}^{T}\left(K_b - H^{T}(K_d)^{-1}H\right)X_b \tag{38}$$

This relation gives the exact expression of C function of sub-blocs of K and the geometry (coordinates X) of the domain. Since K_b and K_d are symmetric, C is symmetric. Also, if $A^{T}CA = 0$, the equality (35) and the properties of K in the first-side imply that U must correspond to a rigid body displacement (translation and rotation). Then it is easy to show that this condition and the condition $U_b = X_bA$ for the boundary points imply $A=0$ if there are at least three non collinear point on $\partial\Omega$ *i.e.*, if Ω defines a surface and not a line). This shows that C is positive-definite. In this way C representing the value found numerically for $\mathbb{C}^{u}$ is shown to be rigorously symmetric and positive-definite.

To illustrate this result, we give in the following the example of determination of $\mathbb{C}^{u}$ for a fractured domain (Figure 3, Chalhoub 2006). The fractures have a random distribution. A FEM mesh was created for the domain with four-nodes zero-thickness joint elements (Goodman 1968) for fractures. The domain was submitted to 3 different *lbdc* cases $\underline{u} = \mathbf{A}.\underline{x}$ on $\partial\Omega$ with $\mathbf{A}$ corresponding to a contraction in *x* direction, in *y* direction and to a shear *xy*. For each loading, the macroscopic stress $\boldsymbol{\Sigma}$ was deduced from numerical results by using (31).



(a) (b) (c)

Figure 3. Three cases of linear displacements imposed on the boundary (a) : contraction in x direction, (b) in y direction and (c) : shear xy.

The three couples of values $(\mathbf{A}, \boldsymbol{\Sigma})$ obtained in this way allowed us to rigorously determine, for the fourth-rank elasticity tensor $\mathbb{C}^u$, the components C_{1111}, C_{2222}, C_{1212} and C_{1122}, C_{1112}, C_{2212} and *independently* C_{2211}, C_{1211}, C_{1222}. Since the fracture distribution was near isotropic and then the macroscopic behaviour near orthotropic, the values obtained for C_{1112}, C_{2212}, C_{1211} and C_{1222} were negligible. For matrix Young modulus 72 GPa and ν=0.25 and fracture normal stiffness K_n =4 MPa/m and tangent stiffness K_t =3 MPa/m (the size of the domain was 10 m), the values found independently for C_{1122} and C_{2211} was respectively 32.4917 GPa and 32.4918 GPa. This shows the high precision of the numerical method concerning the symmetry of $\mathbb{C}^u$ when the relative error $(C_{1122}- C_{2211})/ C_{1122}$ in the works using other methods attains sometimes about 5 %.

5 Conclusion

As shown here above, the relative errors and in particular distance to symmetry for macroscopic elastics tensors sometimes observed in the literature are not always due only to the approximate character of FEM or to finite-size of the domain. Even under these conditions, an upscaling process based on macroscopic quantities well defined and correctly determined numerically will lead to more accurate results satisfying in particular rigorously symmetry conditions for elasticity tensors.

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