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On bounds of the effective behavior of particulate composites with imperfect interface

Sur l'encadrement du comportement effectif des composites particulaires avec interface imparfaite

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Abstract. Particulate composites are considered here as multiphase composite in which the interfaces are imperfect. When the interface mechanical properties are those of a linear elastic material, the minimum of potential and complementary energy is used in order to obtain bounds of effective elastic modulus of the composite. Test displacements or stress fields are build and characterized using Green's functions of a comparison homogeneous body, polarization fields and extension of the classical Lippmann–Schwinger equations. Then when spatial distribution of phases are known, in particular for isotropic distribution of phases or patterns, a generalization of Hashin–Shtrikman principle is obtained and lower and upper bounds are proposed.

Résumé. Les composites particulaires sont composés d'une matrice à renforts particulaires, dans cette note les interfaces entre phases sont considérées imparfaites. Lorsque les propriétés mécaniques de l'interface sont celles d'un matériau élastique linéaire, les principes de minimum de l'énergie potentielle ou complémentaire sont utilisés afin d'obtenir des bornes sur les modules effectifs d'élasticité du composite. Des champs de déplacements ou des champs de contrainte admissibles sont construits et caractérisés à l'aide des fonctions de Green d'un corps homogène de comparaison, utilisant des champs de polarisation et une extension des équations classiques de Lippmann–Schwinger à des champs discontinus. Ensuite, lorsque la distribution spatiale des phases est connue, en particulier pour une distribution isotrope des phases ou des motifs, une généralisation du principe de Hashin–Shtrikman est obtenue et des bornes inférieures et supérieures du comportement effectif sont proposées.

Keywords. Composites, Imperfect interfaces, Bounding.

Mots-clés. Composites, interfaces imparfaites, encadrement, bornes.

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1. Introduction

The determination of effective properties of non homogeneous solid requires micro-mechanical analysis.

Powerful variational methods have been developed in order to derive bounds for the overall modulus, combining an adequate statistical description of the space distribution of phases and the local mechanical properties of each phases [1–4]. For such methods, the interface between phases is assumed generally perfect. For the point of view of mechanical properties, a perfect interface is a material surface across which both the displacement and stress vector are continuous. To capture interphases properties models replace them by a zero-thickness interface models or using graded materials properties are reduced by some Taylor's expansion [5–7]. Many papers are devoted to establish averaged properties for particulate composite with imperfect interface giving estimation of the overall properties [7–10]. Bounding can be obtained using morphological patterns [11, 12] with graded interfaces, but for thin interfaces with discontinuities of displacements or stresses bounds of Voigt or Reuss type on patterns are easily obtained [8] and with isotropic spatial distribution only lower bounds are proposed [13, 14]. For thermal conductivity a lot of papers have discussed the interface behaviour and the possibility of bounding the thermal conductivity [9, 10].

It is pointed out that, apart using morphological patterns with graded interfaces with linear properties, the influence of spatial distribution of inclusion is not taking account on the overall moduli. This article proposes extension of classical bounding methods in elasticity of the effective behaviour of a multiphase media to situation of imperfect interfaces between phases described by linear constitutive behaviour on discontinuities, taking account of isotropic spatial distribution of phases. After of a short presentation of a composite with linear elastic interfaces, the displacement solution is given in terms of an integral equation with given discontinuities. Using this description and the definition of averaging process, under isotropic spatial distribution of phases, an estimation of the gobal moduli of the composite is obtained by solving problems of homogeneous inclusions and composite patterns embedded in an homogeneous comparison material. Optimal comparison materials are then determined in order to obtain bounds for the global moduli, with the definition of a generalized Hashin–Shtrikmann formulation.

2. Description of the composite

A composite is a medium with n different phases bonded across interface. To describe the arrangement of the phases indicator functions are introduced:

$$\begin{cases} x \in \Omega_r, & \phi_r(x) = 1 \\ x \notin \Omega_r & \phi_r(x) = 0 \end{cases} \tag{1}$$

The phase r is linear elastic with modulus $\mathbb{C}_r$; the local modulus inside the composite is given by

$$\mathbb{C}(x) = \sum_r \phi_r(x)\mathbb{C}(r) \tag{2}$$

In order to describe particular situations as spherical inclusions embedded in a matrix, the number of correlation functions associated to such situation is very large, direct description is more powerful, the notion of phase is then replaced by the definition of patterns $\lambda, \lambda = 1, \dots, N$. Each pattern λ is defined by a geometrical domain D_λ inside which the geometry of homogeneous constituent phases is known [11, 12]. The number of patterns λ is N^λ and the volume occupied by all patterns λ is

$$\Omega_\lambda = \sum_{i=1}^{N_\lambda} D^i_\lambda = N^\lambda D_\lambda \tag{3}$$

A point y of D^i_λ has a relative position x to the center X^i_λ with a local behaviour defined by

$$y = x + X^i_\lambda, \quad \mathbb{C}_\lambda(y) = \sum_r \phi^\lambda_r(x)\mathbb{C}_r \tag{4}$$

The whole domain is decomposed into n phases and N different patterns:

$$\Omega = \left(\bigcup_r \Omega_r\right)\left(\bigcup_{\lambda=1}^{N}\left(\bigcup_{i=1}^{N_\lambda} D_\lambda^i\right)\right) \tag{5}$$

We can introduce the proportion of phases and the proportion of pattern :

$$1-\alpha = \frac{\sum_r \Omega_r}{\Omega}, \alpha = \sum_\lambda \frac{N^\lambda D_\lambda}{\Omega} \tag{6}$$

and the volume fraction of phase r, and volume fraction of pattern λ

$$c_r = \frac{\Omega_r}{\Omega}, \quad c_\lambda = \frac{N^\lambda D_\lambda}{\Omega} \tag{7}$$

Then

$$\begin{cases} x \in \bigcup_r \Omega_r & \mathbb{C}(x) = \sum_r \phi(r)\mathbb{C}_r \\ y = x + X_\lambda^i \in \bigcup_i \bigcup_\lambda D_\lambda^i & \mathbb{C}(y) = \sum_r \sum_\lambda \phi_r^\lambda(x)\mathbb{C}_r \end{cases} \tag{8}$$

This article is decomposed in three parts, first the problem of equilibrium of a composite is investigated with the help of polarization fields, then for isotropic distributions of phases or patterns, an estimation of the global behaviour is obtained. Second, the problem of equilibrium is extended to imperfect interfaces with addition of new specific polarization fields, and an estimation of the global behaviour is obtained. Finally, using solutions of composite inclusion, with optimal polarization fields and the classical bounding of potential energy, an optimal reference medium is defined and then bounds of the modulus of composite medium. The case of anti-plan shear or of conduction is given as an example.

3. On imperfect interface

In many situations, the interface is not perfectly bonded due to the presence of local defect. Many papers are concerned with the physics and the mechanics of the interfaces. Let us consider here an interface with elastic properties, the interface is a surface across which both displacement and stress vector are discontinuous.

Along the interface S_o, displacement is discontinuous and is decomposed as a sum of a jump and an average

$$\boldsymbol{u}^+ = \bar{\boldsymbol{u}} + \frac{1}{2}|[\boldsymbol{u}]|_S,\ \boldsymbol{u}^- = \bar{\boldsymbol{u}} - \frac{1}{2}|[\boldsymbol{u}]|_S,\ |[\boldsymbol{u}]|_S = \boldsymbol{u}^+ - \boldsymbol{u}^- \tag{9}$$

Consequently, $\bar{\boldsymbol{u}} = v^\alpha \boldsymbol{A}_\alpha + w\boldsymbol{N}$ is defined only on the surface, (v^α, w) are functions of surface coordinates $(X^\alpha, \alpha = 1,2$, see Apppendix B.2) ; $\boldsymbol{A}_\alpha$ are local tangent vectors and $\boldsymbol{N}$ normal vector at a point of the surface S_o :

$$\boldsymbol{u}^\pm = \lim_{z\to 0^\pm} \boldsymbol{u}(x + z\boldsymbol{N}) \tag{10}$$

The strain $\boldsymbol{\varepsilon}_s$ along S_o is the symmetric part of displacement gradient

$$\begin{aligned} \nabla\bar{\boldsymbol{u}} &= \left(\bar{\nabla}_\beta v^\alpha - wK_\beta^\alpha\right)\boldsymbol{A}_\alpha \otimes \boldsymbol{A}^\beta + \left(\bar{\nabla}_\beta w + v^\alpha K_{\alpha\beta}\right)\boldsymbol{N}\otimes\boldsymbol{A}^\beta \\ 2\boldsymbol{\varepsilon}_s &= \nabla\bar{\boldsymbol{u}} + \nabla^T\bar{\boldsymbol{u}} \end{aligned} \tag{11}$$

For particulate composite, interface S_o for one inclusion is closed. The strain power along S_o is described by a second order symmetric tensor $\boldsymbol{\Sigma_s}$

$$\mathscr{P}_s = -\int_S \boldsymbol{\Sigma_s} : \nabla\bar{\boldsymbol{u}}^*\ \mathrm{dS} - \int_S \mathbf{T}.\left|\left[\boldsymbol{u}^*\right]\right|_S\ \mathrm{dS} \tag{12}$$

after integration by part

$$\mathscr{P}_s = \int_S \mathrm{Div}\,\boldsymbol{\Sigma_s}.\bar{\boldsymbol{u}}^*\ \mathrm{dS} - \int_S \mathbf{T}.\left|\left[\boldsymbol{u}^*\right]\right|_S\ \mathrm{dS} \tag{13}$$

and for the overall system, applying the principle of virtual work

$$\mathscr{P}_{int}+\mathscr{P}_s+\mathscr{P}_e=0,\quad \mathscr{P}_{int}=-\int_\Omega \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\left(\boldsymbol{u}^*\right)\,\mathrm{d}\Omega,\quad \mathscr{P}_\mathrm{e}=\int_{\partial\Omega}\mathbf{T}^\mathrm{d}.\boldsymbol{u}^*\,\mathrm{dS} \tag{14}$$

the conditions of static equilibrium of the whole system are obtained:

$$\begin{aligned}\mathrm{div}\,\boldsymbol{\sigma}=0,\ \text{over }\Omega,\quad \boldsymbol{\sigma}.\boldsymbol{n}=\mathbf{T}^d,\ \text{along }\partial\Omega\\ 0=|[\boldsymbol{\sigma}]|_S.\boldsymbol{N}+\mathrm{Div}\,\boldsymbol{\Sigma_s},\quad \bar{\boldsymbol{\sigma}}.\boldsymbol{N}=\mathbf{T},\ \text{along }S\end{aligned} \tag{15}$$

The components of $\boldsymbol{\Sigma_s}$ are ($\Sigma^{\alpha\beta}=\Sigma^{\beta\alpha}$, Q^α)

$$\boldsymbol{\Sigma_s}=\Sigma^{\alpha\beta}\boldsymbol{A}_\alpha\otimes\boldsymbol{A}_\beta+Q^\alpha\left(\boldsymbol{N}\otimes\boldsymbol{A}_\alpha+\boldsymbol{A}_\alpha\otimes\boldsymbol{N}\right) \tag{16}$$

and

$$\mathrm{Div}\,\boldsymbol{\Sigma_s}=\left(\bar{\nabla}_\beta\Sigma^{\alpha\beta}+Q^\beta K^\alpha_\beta\right)\boldsymbol{A}_\alpha+\left(\bar{\nabla}_\gamma Q^\gamma+K_{\alpha\beta}\Sigma^{\alpha\beta}\right)\boldsymbol{N} \tag{17}$$

Remark 1. When $Q^\alpha=0$ we recover the expression proposed by many authors [13–15].

3.1. *Strain surface energy and potential energy of the system*

The surface strain energy ϕ is assumed to be a convex function of ($|[\boldsymbol{u}]|_S,\boldsymbol{\varepsilon}_S(\bar{\boldsymbol{u}})$) as

$$\phi\left(|[\boldsymbol{u}]|_S,\boldsymbol{\varepsilon}_S(\bar{\boldsymbol{u}})\right) \tag{18}$$

and the state equations for the interface are now:

$$\mathbf{T}=\frac{\partial\phi}{\partial|[\boldsymbol{u}]|_S},\quad \boldsymbol{\Sigma_s}=\frac{\partial\phi}{\partial\boldsymbol{\varepsilon_s}} \tag{19}$$

By duality, the complementary energy associated with this potential is given by

$$\phi^*(\mathbf{T},\boldsymbol{\Sigma_s})=\min_{\boldsymbol{v},\boldsymbol{\varepsilon}_s}\left(\mathbf{T}.\boldsymbol{v}+\boldsymbol{\Sigma_s}:\boldsymbol{\varepsilon}_s-\phi(\boldsymbol{v},\boldsymbol{\varepsilon}_s)\right) \tag{20}$$

The total potential energy and the complementary energy for prescribed displacement over $\partial\Omega$ are

$$\begin{aligned}\mathscr{E}(\boldsymbol{u})&=\int_\Omega w(\boldsymbol{\varepsilon}(\boldsymbol{u}))\,\mathrm{d}\Omega+\int_\mathrm{S}\phi\left(|[\boldsymbol{u}]|_\mathrm{S},\boldsymbol{\varepsilon}_\mathrm{S}(\bar{\boldsymbol{u}})\right)\,\mathrm{dS}\\ \mathscr{E}^*(\boldsymbol{\sigma})&=\int_\Omega w^*(\boldsymbol{\sigma})\,\mathrm{d}\Omega+\int_\mathrm{S}\phi^*(\mathbf{T},\boldsymbol{\Sigma_s})\,\mathrm{dS}-\int_{\partial\Omega}\boldsymbol{n}.\boldsymbol{\sigma}.\boldsymbol{u}^\mathrm{d}\,\mathrm{dS}\end{aligned} \tag{21}$$

where $\boldsymbol{u}$ are kinematically admissible fields

$$\boldsymbol{u}\in K.A=\left\{\boldsymbol{u}|\boldsymbol{u}=\boldsymbol{u}^d\ \text{over }\partial\Omega\right\} \tag{22}$$

and $\boldsymbol{\sigma}$ statically admissible fields

$$\boldsymbol{\sigma}\in S.A=\left\{\boldsymbol{\sigma}|\,\mathrm{div}\,\boldsymbol{\sigma}=0,\ \boldsymbol{n}.\bar{\boldsymbol{\sigma}}=\mathbf{T},\ \boldsymbol{n}.|[\boldsymbol{\sigma}]|_S+\mathrm{Div}\,\boldsymbol{\Sigma_s}=0\right\} \tag{23}$$

Remark 2. $\boldsymbol{\sigma}=\mathrm{rot}^r\,\mathrm{rot}^l\,\Xi$ satisfies $\mathrm{div}\,\boldsymbol{\sigma}=0$ whatever is a symmetric second order tensor Ξ; rotational definition is given in A2. Introducing in the complementary energy, the tensor α:

$$\alpha=\frac{\partial w^*}{\partial\boldsymbol{\sigma}}=\mathbb{S}:\boldsymbol{\sigma} \tag{24}$$

by integration by part, we obtain locally

$$\mathrm{rot}^l\,\mathrm{rot}^r(\alpha)=0 \tag{25}$$

that is the compatibility conditions to define a displacement $\boldsymbol{u}$ satisfying

$$\alpha=\boldsymbol{\varepsilon}(\boldsymbol{u})=\frac{\partial w^*}{\partial\boldsymbol{\sigma}}=\mathbb{S}:\boldsymbol{\sigma}. \tag{26}$$

The minimum of complementary energy gives

$$\int_S \boldsymbol{n}.|[\boldsymbol{\sigma}.\boldsymbol{u}]|_S \, \mathrm{dS} + \int_S \frac{\partial \phi^*}{\partial \mathbf{T}^*}.|[\boldsymbol{u}]|_S + \frac{\partial \phi^*}{\partial \boldsymbol{\Sigma_s}^*} : \boldsymbol{\varepsilon}_S(\bar{\boldsymbol{u}}) \, \mathrm{dS} + \int_{\partial\Omega} \boldsymbol{n}.\boldsymbol{\sigma}.\left(\boldsymbol{u} - \boldsymbol{u}^{\mathrm{d}}\right) \mathrm{dS} = 0 \tag{27}$$

and then we recover the dual equations for the equilibrium position

$$\boldsymbol{u} = \boldsymbol{u}^d, \quad |[\boldsymbol{u}]|_S = \frac{\partial \phi^*}{\partial \mathbf{T}}, \quad \boldsymbol{\varepsilon}_s(\bar{\boldsymbol{u}}) = \frac{\partial \phi^*}{\partial \boldsymbol{\Sigma_s}} \tag{28}$$

3.2. *Integral formulation with discontinuous fields*

An homogeneous elastic medium with modulus $\mathbb{C}^o$ is introduced together with internal stresses $\boldsymbol{p}$ such that

$$\boldsymbol{\sigma} = \mathbb{C}^o : \boldsymbol{\varepsilon}(\boldsymbol{u}) + \boldsymbol{p}, \quad \boldsymbol{p} = \mathbb{C}(x) - \mathbb{C}^o \tag{29}$$

To build test fields, we assume that the fields $\boldsymbol{p}, \boldsymbol{U}, \boldsymbol{\Sigma_s}$ are known. The equilibrium state with discontinuous fields on interface S_o is to determine the displacement $\boldsymbol{u}$ which satisfies the set of local equations (PB)

- compatibility

$$2\boldsymbol{\varepsilon}(\boldsymbol{u}) = \nabla \boldsymbol{u} + \nabla^T \boldsymbol{u} \tag{30}$$

- the constitutive law,

$$\boldsymbol{\sigma} = \mathbb{C}^o : \boldsymbol{\varepsilon} + \boldsymbol{p} \tag{31}$$

- the local discontinuities along S_o

$$|[\boldsymbol{u}]|_S = \boldsymbol{U}, \quad \boldsymbol{n}.|[\boldsymbol{\sigma}]|_S + \mathrm{div}\,\boldsymbol{\Sigma_s} = 0 \tag{32}$$

- the equilibrium

$$0 = \mathrm{div}\,\boldsymbol{\sigma} \tag{33}$$

- the boundary conditions

$$\boldsymbol{u} = \boldsymbol{u}^d \text{ over } \partial\Omega \tag{34}$$

The displacement solution of (PB) is in $K.A$ and the associated stress $\boldsymbol{\sigma}$ is in $S.A$. They can be used to define bounds with applying theorem of minimum of potential energy and complementary energy.

A representation of the displacement $\boldsymbol{u}$ solution of (PB) can be given in terms of Green's function G^o :

$$\frac{\partial}{\partial y_j} \mathbb{C}^o_{pjkl} \frac{\partial}{\partial y_l} G^o_{ik}(x,y) + \delta_{ip}\delta(x-y) = 0 \quad G^o_{ij}(x,y) = 0, \forall\, y \text{ over } \partial\Omega. \tag{35}$$

Consider an homogeneous elastic body with modulus $\mathbb{C}^o$ the displacement satisfies the integral equation:

$$\boldsymbol{u} = \boldsymbol{\varepsilon}^o.x + \int_\Omega G^o.\mathrm{div}\,\boldsymbol{p}\,\mathrm{d}\Omega - \int_S \boldsymbol{n}.\Sigma.\boldsymbol{U}\,\mathrm{dS} + \int_S \mathrm{G}^o.\mathrm{div}\,\boldsymbol{\Sigma_s}\,\mathrm{dS} \tag{36}$$

where $\Sigma = \mathbb{C}^o : \nabla G^o$, and the strain becomes:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^o - \int_\Omega \Gamma^o : \boldsymbol{p}\,\mathrm{d}\Omega + \int_{S^\lambda} \boldsymbol{n}.\mathbb{C}^o : \Gamma^o.\boldsymbol{U}\,\mathrm{dS} - \int_{S^\lambda} \Gamma^o : \boldsymbol{\Sigma_s}\,\mathrm{dS} \tag{37}$$

Where we have taking account of

$$\int_\Omega G^o\,\mathrm{div}\,\boldsymbol{p}\,\mathrm{d}\Omega = \int_\Omega \mathrm{G}^o_{ip} \frac{\partial \mathrm{p_{pj}}}{\partial \mathrm{x_j}}\,\mathrm{d}\Omega = -\int_\Omega \Gamma^o_{\mathrm{ipjq}} \mathrm{p_{jq}}\,\mathrm{d}\Omega, \quad \Gamma^o_{\mathrm{ipjq}} = \frac{\partial^2 \mathrm{G}^o_{\mathrm{ip}}}{\partial \mathrm{x_j} \partial \mathrm{x_q}} \tag{38}$$

3.3. *Application to a particulate composite in an homogeneous matrix*

For spherical particulate composite, the fields $(\boldsymbol{p}, \boldsymbol{U}, \boldsymbol{\Sigma_s})$ are defined on each pattern D_λ by the same fields $P_\lambda, \boldsymbol{U}^\lambda, \boldsymbol{\Sigma_s}^\lambda$, and $\boldsymbol{p} = p_r$ in homogeneous phase r. Introducing two averaging processes, the average value for an homogeneous phase $\overline{*}^r$ and average field $f_M^\lambda(x)$ of f on pattern D_λ

$$\overline{\boldsymbol{\varepsilon}}^r = \frac{1}{\Omega_r}\int_{\Omega_r} \boldsymbol{\varepsilon}(x)\phi_r(x)\,\mathrm{d}\Omega, \quad \boldsymbol{\varepsilon}_\mathrm{M}^\lambda(\mathrm{x}) = \frac{1}{\mathrm{N}^\lambda}\sum_\mathrm{i} \boldsymbol{\varepsilon}\left(\mathrm{x}+\mathrm{X}_\lambda^\mathrm{i}\right) \tag{39}$$

Applying these averaging processes on the integral representation (37), the interaction between two homogeneous phases, two families of pattern, and between one phase and one pattern must be evaluated.

For isotropic spatial distribution of phases and patterns two by two, we have [11]:

$$\begin{aligned}
&\frac{1}{\Omega_s}\frac{1}{\Omega_r}\int_\Omega\int_\Omega \Gamma^o(x,y)\phi_r(x)\phi_s(y)\,\mathrm{d}\Omega_\mathrm{x}\,\mathrm{d}\Omega_\mathrm{y} = \delta_\mathrm{r}^\mathrm{s}\mathbb{E}\\
&\overline{\Gamma^o{}_M^\lambda}^r = \overline{\mathbb{F}_M^\lambda}^r = \sum_i \int_\Omega\int_{D_\lambda} \mathbb{F}^o\left(x, y+Y_i^\lambda\right)\mathrm{d}\Omega_\mathrm{y}\,\mathrm{d}\Omega_\mathrm{x} = \int_\Omega\int_{\mathrm{R_o}}^\infty\int_{\mathrm{S_u(R)}} \mathbb{F}(\mathrm{x},\mathrm{u})\,\mathrm{dS_u} = 0\\
&\Gamma^o{}_{MM}^{\lambda\ \mu} = N^\lambda\Gamma^o(x,y)\delta_{\lambda\mu} + \sum_i\sum_j \int_{D_\lambda}\int_{D_\mu} \mathbb{F}^o\left(x-y, X_i^\lambda - Y_j^\mu\right)\mathrm{d}\Omega_\mathrm{x}\,\mathrm{d}\Omega_\mathrm{y}\\
&\quad = N^\lambda\Gamma^o(x,y)\delta_{\lambda\mu} + \int_{R=R_o}^\infty\int_{S_u(R)}\int_{D_\lambda}\int_{D_\mu} \mathbb{F}^o(x-y,u)\,\mathrm{d}\Omega_\mathrm{x}\,\mathrm{d}\Omega_\mathrm{y}\,\mathrm{dS_u} = \mathrm{N}^\lambda\Gamma^\mathrm{o}(\mathrm{x},\mathrm{y})\delta_{\lambda\mu}
\end{aligned} \tag{40}$$

where $S_u(R)$ is the spherical surface of radius $R: S_u(R) = \{u \mid \|u\| = R\}$.

Using these properties, the average strain field on an homogeneous phase satisfies

$$\overline{\boldsymbol{\varepsilon}}^r + \mathbb{E} : p_r = \boldsymbol{\varepsilon}^o \tag{41}$$

and

$$\boldsymbol{\varepsilon}_M^\lambda(x) + \int_{D_\lambda} \Gamma^o(x-y) : P_\lambda(y)\,\mathrm{d}\Omega + \int_{\mathrm{S}^\lambda} \boldsymbol{n}.\left(\mathbb{C}_\mathrm{o} : \Gamma^\mathrm{o}\right).\boldsymbol{U}^\lambda\,\mathrm{dS} + \int_{\mathrm{S}^\lambda} \Gamma^\mathrm{o}(\mathrm{x},\mathrm{y}) : \boldsymbol{\Sigma_s}^\lambda(\mathrm{y})\,\mathrm{dS} = \boldsymbol{\varepsilon}^\mathrm{o} \tag{42}$$

$\boldsymbol{\varepsilon}_M^\lambda$ is obtained as the solution of an inhomogeneous inclusion with imperfect interface embedded in an homogeneous matrix, and submitted to internal stresses P_λ. The displacement, solution of this problem, is discontinuous as $\boldsymbol{U}^\lambda$ on S^λ, and that the stress vector is discontinuous as $\mathrm{Div}_s\,\boldsymbol{\Sigma_s}$. The local mean displacement $\bar{\boldsymbol{u}}_M^\lambda$, then $\boldsymbol{\varepsilon}_s(\bar{\boldsymbol{u}})_M^\lambda$ and also $\bar{\boldsymbol{\sigma}}_M^\lambda$ are known.

Applying the averaging process on the constitutive law for $\boldsymbol{p}, \boldsymbol{U}^\lambda, \boldsymbol{\Sigma_s}^\lambda$ we have

$$\begin{aligned}
\boldsymbol{p}_r &= (\mathbb{C}_r - \mathbb{C}_o)\overline{\boldsymbol{\varepsilon}}^r, \quad P_\lambda(x) = \left(\mathbb{C}(x) - \mathbb{C}^o\right) : \boldsymbol{\varepsilon}_M^\lambda(x)\\
|[\boldsymbol{u}]|_{SM}^{\ \lambda} &= \boldsymbol{U}^\lambda, \quad \mathbf{T}_M^\lambda = \boldsymbol{T}^\lambda = \boldsymbol{k}_s : \boldsymbol{U}^\lambda = \bar{\boldsymbol{\sigma}}_M^\lambda.\boldsymbol{n}\\
\boldsymbol{\Sigma}_s^\lambda &= \boldsymbol{K}_s : \boldsymbol{\varepsilon}_s\left(\bar{\boldsymbol{u}}_M^\lambda\right)
\end{aligned} \tag{43}$$

With the notation

$$< \boldsymbol{p} > (x) = \begin{cases} \boldsymbol{p}_r, & \text{if } \boldsymbol{x} \in \Omega_r,\\ P_\lambda(x), & \text{if } \boldsymbol{x} \in D_\lambda \end{cases} \tag{44}$$

and

$$< \boldsymbol{\varepsilon} > (x) = \begin{cases} \overline{\boldsymbol{\varepsilon}}^r & \text{if } \boldsymbol{x} \in \Omega_r\\ \boldsymbol{\varepsilon}_M^\lambda(x) & \text{if } \forall\, X_\lambda^i, \quad \boldsymbol{x} + X_\lambda^i \in D_\lambda^i \end{cases} \tag{45}$$

The dependency on x should be omitted in the following.

When the interface is perfect, the classical problem used in [11] is recovered. For imperfect interface, the constitutive laws of the interface are taken into account as

$$\begin{aligned} \boldsymbol{U}^\lambda = \boldsymbol{U}^\lambda_M \quad \boldsymbol{k}_s.\boldsymbol{U}^\lambda = \mathbf{T}^\lambda_M, \quad \mathbf{T}^\lambda_M = \boldsymbol{T}^\lambda = \frac{\partial \phi}{\partial \boldsymbol{U}} \\ 0 = \boldsymbol{n}.\left|\left[\boldsymbol{\sigma}^\lambda_M\right]\right|_s + \mathrm{Div}\,\boldsymbol{\Sigma_s}^\lambda \end{aligned} \tag{46}$$

3.4. *Estimation of the global behavior*

Now, the global mean strain and mean stress are evaluated as the usual way, taking account of possible discontinuities:

$$\boldsymbol{E} = \frac{1}{\Omega}\left(\int_\Omega \boldsymbol{\varepsilon}\,\mathrm{d}\Omega - \int_\mathrm{S} \left\{|[\boldsymbol{u}]|_\mathrm{s} \otimes \boldsymbol{n}\right\}_\mathrm{s}\,\mathrm{dS}\right), \quad \boldsymbol{\Sigma} = \frac{1}{\Omega}\left(\int_\Omega \boldsymbol{\sigma}\,\mathrm{d}\Omega - \int_{\mathrm{S}^\lambda} \left\{\boldsymbol{n}.|[\boldsymbol{\sigma}]|_\mathrm{s} \otimes \boldsymbol{x}\right\}_\mathrm{s}\,\mathrm{dS}\right) \tag{47}$$

that is

$$\begin{aligned} \boldsymbol{E} &= \sum_r c_r \overline{\boldsymbol{\varepsilon}}^r + \sum_\lambda c_\lambda \int_{D_\lambda} \boldsymbol{\varepsilon}^\lambda_M(x)\,\mathrm{d}\Omega_\mathrm{x} - \int_{\mathrm{S}^\lambda} \left\{\boldsymbol{U}^\lambda \otimes \boldsymbol{n}\right\}_\mathrm{s}\,\mathrm{dS} \\ \boldsymbol{\Sigma} &= \sum_r c_r \overline{\boldsymbol{\sigma}}^r + \sum_\lambda c_\lambda \int_{D_\lambda} \boldsymbol{\sigma}^\lambda_M(x)\,\mathrm{d}\Omega + \int_{\mathrm{S}^\lambda} \boldsymbol{\Sigma_s}\,\mathrm{dS} \end{aligned} \tag{48}$$

By elimination of $\boldsymbol{\varepsilon}^o$, an estimation of the compliance is obtained:

$$\boldsymbol{\Sigma} = \mathbb{C}^{est} : \boldsymbol{E} \tag{49}$$

3.5. *Properties of the fields solution of the integral formulation*

The discontinuity of displacement is imposed, the local value $\mathbf{T}(x + X^i_\lambda)$ defined on S^λ_i at point $x + X^i_\lambda$ fluctuates around the mean value $\mathbf{T}^\lambda_M = \boldsymbol{T}^\lambda$, by the same reasoning, the dual quantity $\boldsymbol{\varepsilon}(\bar{\boldsymbol{u}})(x + X^i_\lambda)$ associated to $\boldsymbol{\Sigma_s}(x + X^i_\lambda)$ fluctuates around the average value $\boldsymbol{\varepsilon}(\bar{\boldsymbol{u}}^\lambda_M)$.

However, it can be noticed that using the classical relation between the overall strain, and the overall stress we can estimate the homogeneous value for the particulate composite, whatever is $\mathbb{C}^o$.

For $\mathbb{C}^o$ being extremely soft or rigid, we recover the bounds of Voigt and Reuss for particular composite with imperfect interface.

Another interesting case is to consider that ϕ is decomposed into two contributions

$$\phi(\boldsymbol{U}, \boldsymbol{\Sigma_s}) = \frac{1}{2}\boldsymbol{U}.k.\boldsymbol{U} + \frac{1}{2}\boldsymbol{\Sigma_s}.K.\boldsymbol{\Sigma_s} \tag{50}$$

For k rigid, then $\boldsymbol{U} = 0$, if $K = 0$, there is no contribution of $\boldsymbol{\Sigma_s}$.

Assume $K = 0$ then the displacement is discontinuous, choosing $\boldsymbol{U}^\lambda = 0$, permits to say that an upper bound is obtained with the perfect interface. But the lower bounds is not associated to the stress field associated to this solution, because the value of ϕ^* in that case can not be determined, because no information can be given on $\mathbf{T}$.

By duality, when k is rigid, a lower bounds is obtained with perfect interface, because, we can choose $\boldsymbol{\Sigma_s}^\lambda = 0$ but the associated strain field $\boldsymbol{\varepsilon}_s$ can not be evaluate and then ϕ is not determined.

This fact is encountered for the particular interface used in [13, 14] and only one HS type bounds is obtained. To obtain the two bounds, a new scheme is proposed based on a generalized Hashin–Shtrikmann formulation.

4. On bounding of the global properties

The solution of equilibrium of the particulate composite satisfies the bounding with respect to the potential energy of the body and the complementary energy of the body:

$$\begin{aligned}\forall \boldsymbol{\sigma}^*, \forall \boldsymbol{u}^* - \int_\Omega w^*\left(\boldsymbol{\sigma}^*\right)\, \mathrm{d}\Omega - \int_S \phi^*\left(\bar{\boldsymbol{\sigma}}*.\boldsymbol{n}, \left|[\boldsymbol{\sigma}^*]\right|_S.\boldsymbol{n}\right)\, \mathrm{dS} + \int_{\partial\Omega} \boldsymbol{n}.\boldsymbol{\sigma}^*.\boldsymbol{u}^{\mathrm{d}}\, \mathrm{dS} \\ \leq -\int_\Omega w^*(\boldsymbol{\sigma})\, \mathrm{d}\Omega - \int_S \phi^*\left(\bar{\boldsymbol{\sigma}}.\boldsymbol{n}, |[\boldsymbol{\sigma}]|_S.\boldsymbol{n}\right)\, \mathrm{dS} + \int_{\partial\Omega} \boldsymbol{n}.\boldsymbol{\sigma}.\boldsymbol{u}^{\mathrm{d}}\, \mathrm{dS} \\ = \int_\Omega w(\boldsymbol{\varepsilon})\, \mathrm{d}\Omega + \int_S \phi\left(|[\boldsymbol{u}]|_S, \boldsymbol{\varepsilon}(\bar{\boldsymbol{u}})\right)\, \mathrm{dS} \\ \leq \int_\Omega w\left(\boldsymbol{\varepsilon}^*\right)\, \mathrm{d}\Omega + \int_S \phi\left(\left|[\boldsymbol{u}^*]\right|_S, \boldsymbol{\varepsilon}\left(\bar{\boldsymbol{u}^*}\right)\right)\, \mathrm{dS}\end{aligned} \tag{51}$$

Then, consider now the displacement $\boldsymbol{u}^*$ solution of the integral equation (Eq. (37)) associated to the averaging process (Eq. (43)). This field satisfies the condition to be used in (Eq. (51)) and also $\boldsymbol{\sigma}^* = \mathbb{C}^o : \boldsymbol{\varepsilon}(\boldsymbol{u}^*) + \boldsymbol{p}$ are valuable to be used too. We have

$$\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega = \int_{\partial\Omega} \boldsymbol{n}.\boldsymbol{\sigma}^* \otimes \boldsymbol{u}^*\, \mathrm{d}\Omega - \int_{\mathrm{S_o}} \boldsymbol{n}.\left|[\boldsymbol{\sigma}^*.\boldsymbol{u}^*]\right|_S\, \mathrm{dS} \tag{52}$$

The discontinuities are decomposed into two contributions

$$\boldsymbol{n}.\left|[\boldsymbol{\sigma}^*.\boldsymbol{u}^*]\right|_S = \boldsymbol{T}^*.\left|[\boldsymbol{u}^*]\right|_S + \boldsymbol{n}.\left|[\boldsymbol{\sigma}^*]\right|_S.\bar{\boldsymbol{u}}^* = \boldsymbol{T}^*.\boldsymbol{U}^\lambda - \mathrm{Div}\,\boldsymbol{\Sigma_s}.\bar{\boldsymbol{u}}^*, \quad \boldsymbol{T}^* = \boldsymbol{n}.\bar{\boldsymbol{\sigma}}^* \tag{53}$$

Then by integration and summation on the patterns, the macroscopic stress Σ^* satisfies

$$\begin{aligned}\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega = \Omega \boldsymbol{E} : \boldsymbol{\Sigma}^* + \int_{S_o} \boldsymbol{n}.\bar{\boldsymbol{\sigma}}^*.\boldsymbol{U}^\lambda\, \mathrm{dS} + \int_{\mathrm{S_o}} \mathrm{Div}\,\boldsymbol{\Sigma_s}.\bar{\boldsymbol{u}}^*\, \mathrm{dS} \\ = \Omega \boldsymbol{E} : \boldsymbol{\Sigma}^* + \int_{S_o} \boldsymbol{n}.\bar{\boldsymbol{\sigma}}^*.\boldsymbol{U}^\lambda - \boldsymbol{\Sigma_s} : \boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\, \mathrm{dS} \\ \boldsymbol{\Sigma}^* = \frac{1}{\Omega}\int_{\partial\Omega} \left(\boldsymbol{n}.\boldsymbol{\sigma}^* \otimes \boldsymbol{x}\right)_s\, \mathrm{dS}\end{aligned} \tag{54}$$

4.1. *On upper bound*

With these fields, the free energy for the field $\boldsymbol{u}^*$ takes the value

$$2w\left(\boldsymbol{\varepsilon}^*\right) = \boldsymbol{\varepsilon}^* : \mathbb{C} : \boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon}^* : \left(\mathbb{C} - \mathbb{C}^o\right) : \boldsymbol{\varepsilon}^* + \boldsymbol{\varepsilon}^* : \mathbb{C}^o : \boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon}^* : \left(\mathbb{C} - \mathbb{C}^o\right) : \boldsymbol{\varepsilon}^* + \boldsymbol{\varepsilon}^* : \left(\boldsymbol{\sigma}^* - \boldsymbol{p}\right) \tag{55}$$

and by integration

$$2\frac{1}{\Omega}\int_\Omega w\left(\boldsymbol{\varepsilon}^*\right)\, \mathrm{d}\Omega = \frac{1}{\Omega}\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega + \frac{1}{\Omega}\int_\Omega \boldsymbol{\varepsilon}^* : \left(\mathbb{C} - \mathbb{C}^{\mathrm{o}}\right) : \boldsymbol{\varepsilon}^* - \boldsymbol{p} : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega \tag{56}$$

As pointed below, the last term becomes

$$\frac{1}{\Omega}\int_\Omega \boldsymbol{p} : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega = \mathrm{c}\left\langle \boldsymbol{p} \right\rangle : \left\langle \boldsymbol{\varepsilon}^* \right\rangle = \mathrm{c}\left\langle \boldsymbol{\varepsilon}^* \right\rangle : \left(\mathbb{C} - \mathbb{C}^{\mathrm{o}}\right) : \left\langle \boldsymbol{\varepsilon}^* \right\rangle \tag{57}$$

and we obtain

$$2\frac{1}{\Omega}\int_\Omega w\left(\boldsymbol{\varepsilon}^*\right)\, \mathrm{d}\Omega = \frac{1}{\Omega}\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega + \frac{1}{\Omega}\int_\Omega \left(\boldsymbol{\varepsilon}^* - \left\langle \boldsymbol{\varepsilon}^* \right\rangle\right) : \left(\mathbb{C} - \mathbb{C}^{\mathrm{o}}\right) : \left(\boldsymbol{\varepsilon}^* - \left\langle \boldsymbol{\varepsilon}^* \right\rangle\right)\, \mathrm{d}\Omega \tag{58}$$

As

$$\frac{1}{\Omega}\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^*\, \mathrm{d}\Omega = \boldsymbol{E} : \boldsymbol{\Sigma}^* - \frac{1}{\Omega}\int_{\mathrm{S_o}} \mathbf{T} : \boldsymbol{U}^\lambda + \boldsymbol{\Sigma_s}^\lambda : \boldsymbol{\varepsilon}_{\mathrm{s}}\left(\boldsymbol{u}^*\right)\, \mathrm{dS} \tag{59}$$

and finally the total potential energy

$$\begin{aligned}2\mathscr{W}\left(\boldsymbol{u}^*\right) = \boldsymbol{E} : \boldsymbol{\Sigma}^* + \frac{1}{\Omega}\int_\Omega \left(\boldsymbol{\varepsilon}^* - \left\langle \boldsymbol{\varepsilon}^* \right\rangle\right) : \left(\mathbb{C} - \mathbb{C}^o\right) : \left(\boldsymbol{\varepsilon}^* - \left\langle \boldsymbol{\varepsilon}^* \right\rangle\right)\, \mathrm{d}\Omega\& \\ + \frac{1}{\Omega}\int_{S_o} \boldsymbol{U}^\lambda.\boldsymbol{k}_s.\boldsymbol{U}^\lambda - \boldsymbol{T}^\lambda : \boldsymbol{U}^\lambda + \boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) : \boldsymbol{K}_s : \boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) - \boldsymbol{\Sigma_s}^\lambda : \boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\, \mathrm{dS}\end{aligned} \tag{60}$$

We know that

$$\boldsymbol{T}^{\lambda} = \boldsymbol{k}_s.\boldsymbol{U}^{\lambda}, \quad \boldsymbol{\Sigma_s}^{\lambda} = \boldsymbol{K}_s : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^*\right)^{\lambda}_M = \boldsymbol{K}_s : \langle \boldsymbol{\varepsilon}_s\left(u^*\right)\rangle \tag{61}$$

then the potential energy for the trial field is reduced to

$$\begin{aligned} 2\mathscr{W}\left(\boldsymbol{u}^*\right) = \boldsymbol{E}:\boldsymbol{\Sigma}^* + \frac{1}{\Omega}\int_{\Omega}\left(\boldsymbol{\varepsilon}^* - \langle\boldsymbol{\varepsilon}^*\rangle\right):\left(\mathbb{C}-\mathbb{C}^o\right):\left(\boldsymbol{\varepsilon}^* - \langle\boldsymbol{\varepsilon}^*\rangle\right)\,\mathrm{d}\Omega \\ + \frac{1}{\Omega}\int_{S_o}\Big(\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) - \langle\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\rangle\Big):\boldsymbol{K}_s:\Big(\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) - \langle\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\rangle\Big)\,\mathrm{dS} \end{aligned} \tag{62}$$

The quantity

$$\begin{aligned} Q\left(\mathbb{C}^o\right) = \int_{\Omega}\left(\boldsymbol{\varepsilon}^* - \langle\boldsymbol{\varepsilon}^*\rangle\right):\left(\mathbb{C}-\mathbb{C}^o\right):\left(\boldsymbol{\varepsilon}^* - \langle\boldsymbol{\varepsilon}^*\rangle\right)\,\mathrm{d}\Omega \\ + \int_{S_o}\Big(\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) - \langle\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\rangle\Big):\boldsymbol{K}_s:\Big(\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right) - \langle\boldsymbol{\varepsilon}_s\left(\boldsymbol{u}^*\right)\rangle\Big)\,\mathrm{dS} \end{aligned} \tag{63}$$

can not be directly evaluated, but we can choose $\mathbb{C}^o$ in order to have $Q(\mathbb{C}^o) \leq 0$, consequently for such a $\mathbb{C}^o$ an upper bound for the potential energy is obtained. It is pointed out that an optimal value $\mathbb{C}^o$ exists, because $Q(0) > 0$ and $Q(\infty) < 0$.

By a similar reasoning, a lower bound is given considering the complementary energy.

4.2. *A lower bound*

Now, let us consider the complementary energy

$$\mathscr{W}^*\left(\boldsymbol{\sigma}^*\right) = \int_{\Omega} w^*\left(\boldsymbol{\sigma}^*\right)\,\mathrm{d}\Omega + \int_{\mathrm{S_o}}\phi^*\left(\boldsymbol{n}.\bar{\boldsymbol{\sigma}}^*, \boldsymbol{\Sigma_s}\right)\,\mathrm{dS} - \int_{\partial\Omega}\boldsymbol{n}.\boldsymbol{\sigma}^*.\boldsymbol{u}^{\mathrm{d}}\,\mathrm{dS} \tag{64}$$

$$2w^*\left(\boldsymbol{\sigma}^*\right) = \boldsymbol{\sigma}^*.\mathbb{S}\boldsymbol{\sigma}^* = \boldsymbol{\sigma}^*:\left(\mathbb{S}-\mathbb{S}^o\right):\boldsymbol{\sigma}^* + \boldsymbol{\sigma}^*:\mathbb{S}^o:\boldsymbol{\sigma}^* \tag{65}$$

and

$$\boldsymbol{\sigma}^*:\mathbb{S}^o:\boldsymbol{\sigma}^* = \boldsymbol{\sigma}^*:\left(\boldsymbol{\varepsilon}^* + \mathbb{S}^o:\boldsymbol{p}\right) \tag{66}$$

Let us consider $\mathbb{Q} = (\mathbb{S}-\mathbb{S}_o)^{-1}$

$$\begin{aligned} \left(\boldsymbol{\sigma} - \boldsymbol{p}:\mathbb{S}^o:\mathbb{Q}\right):\left(\mathbb{S}-\mathbb{S}^o\right):\left(\boldsymbol{\sigma} - \mathbb{Q}:\mathbb{S}^o:\boldsymbol{p}\right)\& \\ = \boldsymbol{\sigma}^*:\left(\mathbb{S}-\mathbb{S}^o\right):\boldsymbol{\sigma}^* + \boldsymbol{p}:\mathbb{S}^o:\boldsymbol{\sigma}^* + \boldsymbol{\sigma}^*:\mathbb{S}^o:\boldsymbol{p} - \boldsymbol{p}:\mathbb{S}^o:\mathbb{Q}:\mathbb{S}^o:\boldsymbol{p} \end{aligned} \tag{67}$$

as

$$\mathbb{S}^o:\mathbb{Q}:\mathbb{S}^o = \left(\mathbb{S}^o - \mathbb{S} + \mathbb{S}\right):\mathbb{Q}:\mathbb{S}^o = -\mathbb{S}^o + \mathbb{S}:\mathbb{Q}:\mathbb{S}^o = -\mathbb{S}^o + \left(\mathbb{C}^o - \mathbb{C}\right)^{-1} \tag{68}$$

we obtain finally

$$\begin{aligned} \left(\boldsymbol{\sigma} - \boldsymbol{p}:\mathbb{S}^o:\mathbb{Q}\right):\left(\mathbb{S}-\mathbb{S}^o\right):\left(\boldsymbol{\sigma} - \mathbb{Q}:\mathbb{S}^o:\boldsymbol{p}\right) \\ = \boldsymbol{\sigma}^*:\left(\mathbb{S}-\mathbb{S}^o\right):\boldsymbol{\sigma}^* + \boldsymbol{\sigma}^*:\mathbb{S}^o:\boldsymbol{p} + \boldsymbol{p}:\mathbb{S}^o:\left(\boldsymbol{\sigma}^* - \boldsymbol{p}\right) - \boldsymbol{p}:\left(\mathbb{C}-\mathbb{C}^o\right)^{-1}:\boldsymbol{p} \end{aligned} \tag{69}$$

the two last terms cancel due to the relation ($\boldsymbol{p} = (\mathbb{C}-\mathbb{C}^o) :< \boldsymbol{\varepsilon}^* >$). In conclusion

$$\begin{aligned} & 2\mathscr{W}^*\left(\boldsymbol{\sigma}^*\right) \\ &= \int_{\Omega}\boldsymbol{\sigma}^*:\boldsymbol{\varepsilon}^*\,\mathrm{d}\Omega - 2\int_{\partial\Omega}\boldsymbol{n}.\boldsymbol{\sigma}*.\boldsymbol{u}^{\mathrm{d}}\,\mathrm{dS} + \int_{\mathrm{S_o}}\boldsymbol{T}^*.\boldsymbol{k}_{\mathrm{s}}^{-1}.\boldsymbol{T}^* + \boldsymbol{\Sigma_s}.\boldsymbol{K}_{\mathrm{s}}^{-1}.\boldsymbol{\Sigma_s}\,\mathrm{dS} \\ &= -\Omega\boldsymbol{E}:\boldsymbol{\Sigma}^* - \int_{S_o}\boldsymbol{T}^*.\boldsymbol{U}^{\lambda} + \boldsymbol{T}^*.\boldsymbol{k}_s^{-1}.\boldsymbol{T}^*\,\mathrm{dS} + \int_{\Omega}\left(\boldsymbol{\sigma} - \boldsymbol{p}:\mathbb{S}^{\mathrm{o}}:\mathbb{Q}\right):\left(\mathbb{S}-\mathbb{S}^{\mathrm{o}}\right):\left(\boldsymbol{\sigma} - \mathbb{Q}:\mathbb{S}^{\mathrm{o}}:\boldsymbol{p}\right)\,\mathrm{d}\Omega \end{aligned} \tag{70}$$

In conclusion when

$$\begin{aligned} & Q^*\left(\mathbb{S}^o\right) \\ &= \int_{\Omega}\left(\boldsymbol{\sigma} - \boldsymbol{p}:\mathbb{S}^o:\mathbb{Q}\right):\left(\mathbb{S}-\mathbb{S}^o\right):\left(\boldsymbol{\sigma} - \mathbb{Q}:\mathbb{S}^o:\boldsymbol{p}\right)\,\mathrm{d}\Omega + \int_{\mathrm{S_o}}\left(\boldsymbol{T}^* - \boldsymbol{T}^{\lambda}\right).\boldsymbol{k}_{\mathrm{s}}^{-1}.\left(\boldsymbol{T}^* - \boldsymbol{T}^{\lambda}\right)\,\mathrm{dS} \leq 0 \end{aligned} \tag{71}$$

The value of $\mathscr{W}^*$ gives a lower bound of the potential energy of the particulate composite. The optimal value of $\mathbb{S}^o$ exists because : $Q^*(0) > 0$ and $Q^*(\infty) < 0$.

The inequalities $Q \leq 0, Q^* \leq 0$ are those obtained for classical Hashin–Shtrickman bounding, for perfect interfaces whose characteristics are $\boldsymbol{K}_s = 0, \boldsymbol{k}_s = \infty$.

4.3. *On bounding fluctuations of displacement on patterns*

To obtain bounds, it is necessary to give information on the displacement on each pattern with imperfect interface using the integral equation.

Consider the pattern D^i_λ the displacement $u(x + X^\lambda_i)$ is determined by

$$\boldsymbol{u}\left(x + X^\lambda_i\right) = \boldsymbol{u}\left(X^\lambda_i\right) + \boldsymbol{u}^\lambda(x) + \boldsymbol{u}'(x) \tag{72}$$

where $\boldsymbol{u}^\lambda$ is the displacement solution of the pattern problem, this displacement satisfies

$$\left(\boldsymbol{u}\left(x + X^\lambda_i\right) - \boldsymbol{u}\left(X^\lambda_i\right)\right)^\lambda_M = \boldsymbol{u}^\lambda(x) \tag{73}$$

It is noticed that $\boldsymbol{u}'$ is continuous on the interface, and the associated stress vector is continuous too.

Let us consider the two inequalities, let us decompose them in terms of uniform inclusions and composite inclusion with imperfect interfaces, we can impose these inequalities on all contributions separately.

Classical conclusions are obtained for uniform inclusions, we must consider a comparison material with the maximum value or the minimum value of component. For isotropic case the moduli are

$$\left(k^+_o, \mu^+_o\right) = \left(\max k_r, \max \mu_r\right), \quad \left(k^-_o, \mu^-_o\right) = \left(\min k_r, \min \mu_r\right) \tag{74}$$

But on pattern, with imperfect interface, it is necessary to determine $\mathbb{C}^o$ with respect to the inequalities. To obtain the optimal comparison material, the fluctuation $\boldsymbol{u}'(x)$ is decomposed in terms of Fourier series in 2D or spherical functions in 3D ; the associated fields, displacement and stress vector are continuous on interface S_o, the discontinuities being satisfied by the solution defined on the pattern $\boldsymbol{u}^\lambda$ with given imperfect interfaces.

With such a decomposition, the inequalities obtained with each terms of the Fourier series must be satisfied.

The process of bounding is then shown on the problem of anti-plane shear. The solution is given in two step : first, the solution of uniform circular inclusion in a uniform matrix, and solution of composite with linear elastic interface are determined ; the second step is the bounding of the fluctuations by Fourier analysis which gives the values of the optimal comparison materials for the upper and lower bounds.

5. An example

We consider the problem of anti-plane-shear for which the displacement is

$$\boldsymbol{u} = W(r,\theta)\boldsymbol{e}_z, \; \nabla W = \frac{\partial W}{\partial r}\boldsymbol{e}_r + \frac{1}{r}\frac{\partial W \, e_\theta}{\partial \theta} \tag{75}$$

and the state of stress is given by

$$\boldsymbol{\sigma} = \boldsymbol{e}_z \otimes \mathbf{q} + \mathbf{q} \otimes \boldsymbol{e}_z, \quad \mathbf{q} = K.\nabla W \tag{76}$$

finally the problem to solve is reduced to

$$\begin{aligned} &\Delta W = 0, \quad \mathbf{q} = K(x)\nabla W, \text{ in } \Omega \\ &\mathbf{q}.\boldsymbol{n} = \mathbf{Q}.\boldsymbol{n}, \text{ along } \partial\Omega \end{aligned} \tag{77}$$

The particulate composite is made of cylindrical inclusions of radius a with properties K_2 embedded in a matrix of modulus K_1. K_2, K_o are isotropic. We assumed that $\mathbf{Q} = Q\boldsymbol{e}_x$. The minimum distance between two inclusions is $2R_e$, then the composite is modelled as a family of composite cylindrical inclusions with radius R_e, in proportion c_o and a matrix with proportion c_m.

The interface has characteristics $\boldsymbol{k}_s, \boldsymbol{K}_s$ as previously. Then we must solve two problems of cylindrical inclusion embedded in the comparison material, one for the matrix, one for the pattern.

5.1. *A uniform cylindrical inclusion*

On the cylindrical inclusion of radius a, the solution satisfies

$$W(r,\theta) = A_1 r\cos\theta, r \le a, \quad W(r,\theta) = \left(A_o r + b_o \frac{a^2}{r}\right)\cos\theta,\ r \ge a \tag{78}$$

$\boldsymbol{u}$ is continuous at $r = a$ and the flux too, that is

$$K_1 \nabla \boldsymbol{u}(a).\boldsymbol{e}_r = K_o \nabla \boldsymbol{u}(a).\boldsymbol{e}_r \tag{79}$$

and the condition

$$K_o \nabla \boldsymbol{u}(\infty) = Q_o \boldsymbol{e}_x \tag{80}$$

We obtain

$$A_1 = \frac{2Q_o}{K_o + K_1}, \quad Q_o = A_o K_o, b_o = \frac{K_o - K_1}{K_o + K_1} \tag{81}$$

5.2. *On a composite cylindrical inclusion*

On the pattern, we have $W(r,\theta) = w(r)\cos\theta$, $\mathbf{q}.\boldsymbol{e}_r = q(r)\cos\theta$, $f = \frac{a^2}{R_e^2}$

$$\begin{cases} w(r) = A_2 r, & r \le a \\ w(r) = \left(A_1 r + b_1 \dfrac{a^2}{r}\right) & a \le r \le R_e \\ w(r) = \left(A_o r + b_o \dfrac{R_e^2}{r}\right), & r \ge R_e \end{cases} \tag{82}$$

On the boundary a, w and $\mathbf{q}$ are discontinuous

$$\begin{aligned} 2\bar{w} &= (A_2 + A_1 + b_1)\, a \\ 2\bar{q} &= K_2 A_2 + K_1 (A_1 - b_1) \\ 2k_s |[w]|_S &= 2k_s a (A_1 + b_1 - A_2) = K_2 A_2 + K_1 (A_1 - b_1) \\ |[q]|_S &= K_1 (A_1 - b_1) - K_2 A_2 = \frac{\boldsymbol{K}_s}{2a} (A_2 + A_1 + b_1) \end{aligned} \tag{83}$$

and the continuity of w, q at $r = R_e$

$$A_o + b_o = A_1 + b_1 f, \quad K_o (A_o - b_o) = K_1 \left(A_1 - b_1 f\right) \tag{84}$$

With the notation $\bar{K}_s = \dfrac{\boldsymbol{K}_s}{2a}, \bar{k}_s = 2a\boldsymbol{k}_s$ and $\Delta = 2K_1(\bar{K}_s - \bar{k}_s)$

$$A_1 = -\frac{A_2}{\Delta}\alpha, \quad b_1 = -\frac{A_2}{\Delta}\beta \tag{85}$$

with

$$\alpha = 2K_1K_2 + 2\bar{K}_s\bar{k}_s + \left(\bar{K}_s + \bar{k}_s\right)(K_1 + K_2) \quad \beta = 2K_1K_2 - 2\bar{K}_s\bar{k}_s + (K_1 - K_2)\left(\bar{K}_s + \bar{k}_s\right) \tag{86}$$

and finally with the condition at $r = \infty$

$$
\begin{aligned}
2K_oA_o &= \left(\alpha(K_o+K_1) + f\beta(K_o-K_1)\right)\frac{A_2}{\Delta} \\
A_1 &= \frac{2K_oA_o\alpha}{\alpha(K_o+K_1)+f\beta(K_o-K_1)} \\
b_1 &= \frac{2K_oA_o\beta}{\alpha(K_o+K_1)+f\beta(K_o-K_1)}
\end{aligned}
\tag{87}
$$

Using the relation (48), an estimation of the global modulus is obtained. Now, choosing $\mathbb{C}^o_+, \mathbb{C}^o_-$ in order to satisfy the inequalities Q, Q^* respectively, upper and lower bounds are determined.

5.3. *Determination of fluctuations*

We have now to solve the problem on fluctuations, developed in Fourier series.

$$
\begin{cases}
W(r,\theta) = A_2 r^n \cos(n\theta), & r \le a \\
W(r,\theta) = \left(A_1 r^n + b_1 \dfrac{a^{2n}}{r^n}\right)\cos(n\theta), & a \le r \le R_e
\end{cases}
\tag{88}
$$

The continuity of fields at $r = a$ determines (A_2, A_1, b_1) for a given $\mathcal{W} = \frac{W(R_e)}{R_e^n}$

$$
\mathcal{W} = A_1 + b_1 f^n, \quad A_2 = \frac{2K_1\mathcal{W}}{\delta}, \quad A_1 = \frac{K_1+K_2}{\delta}\mathcal{W}, \quad b_1 = \frac{K_1-K_2}{\delta}\mathcal{W}
\tag{89}
$$

where $\delta = K_1 + K_2 + f^n(K_1 - K_2)$. With these constants, we can evaluate $Q(K_o), Q^*(1/Ko)$

5.4. *Evaluation of $Q(K_o)$ and $Q^*(1/K_o)$*

The energy of fluctuation is

$$
q = \frac{Q(K_o)}{2n\pi R_e^{2n}} = (K_2-K_o)A_2^2 f^n + (K_1-K_o)\left(1-f^n\right)\left(A_1^2 + b_1^2 f^n\right) + \boldsymbol{K}_s a A_2^2 n f^n \le 0, \forall\, n
\tag{90}
$$

that is

$$
q\frac{\delta^2}{\mathcal{W}^2} = (K_2-K_o)4K_1^2 f^n + (K_1-K_o)\left(1-f^n\right)\left((K_1+K_2)^2 + f^n(K_1-K_2)^2\right) + \boldsymbol{K}_s a n f^n 4K_1^2 \le 0
\tag{91}
$$

Denoting $K_M = \max(K_1, K_2), K_m = \min(K_1, K_2)$, we can choose K_o such that

$$
\frac{q\delta^2}{\mathcal{W}^2} \le (K_M - K_o)\Big(4K_1^2 f^n + \left(1-f^n\right)(K_1+K_2)^2 + f^n(K_1-K_2)^2\Big) + \bar{K}_s \max\left(nf^n\right)4K_M^2 \le 0
\tag{92}
$$

As

$$
4K_m^2 \le 4K_1^2 f^n + \left(1-f^n\right)\left((K_1+K_2)^2 + f^n(K_1-K_2)^2\right) \le 4K_M^2
\tag{93}
$$

we obtain

$$
K_o \ge K_o^+ = K_M + \bar{K}_s \frac{K_M^2}{K_m^2}\max\left(nf^n\right)
\tag{94}
$$

By the same reasoning based on Q^*, we have

$$
q^* = \frac{Q^*}{2n\pi R_e^{2n}} = \frac{nf^n}{\bar{k}_s}K_2^2A_2^2 + f^n\left(\frac{1}{K_2} - \frac{1}{K_o}\right)K_2^2A_2^2 + \left(1-f^n\right)\left(\frac{1}{K_1} - \frac{1}{K_o}\right)K_1^2\left(A_1^2 + b_1^2 f^n\right) \le 0
\tag{95}
$$

then

$$
\frac{q^*\delta^2}{\mathcal{W}^2} \le \frac{nf^n}{\bar{k}_s}K_2^2 4K_1^2 + \Big(f^n 4K_2^2 + \left(1-f^n\right)\left((K_1+K_2)^2 + f^n(K_1-K_2)^2\right)\Big)\left(\frac{1}{K_m} - \frac{1}{K_o}\right)
\tag{96}
$$

then if K_o satisfies

$$
\frac{1}{K_o} \ge \frac{1}{K_o^-} = \frac{1}{K_m} + \frac{1}{\bar{k}_s}\frac{K_M^2}{K_m^2}\max nf^n
\tag{97}
$$

$q^* \leq 0$. If the interface is perfect, the classical values $K_o^+ = \max(K_1, K_2), K_o^- = \min(K_1, K_2)$ are recovered.

Remark: As $f < 1, \exists\, p,\ pf^p \geq nf^n, \forall\, n$; therefore $p \geq 1$ satisfies $\frac{p-1}{p} \leq f \leq \frac{p}{p+1}$.

The two proposed values are given as possibilities, numerically for given f more accurate value can be found.

6. Conclusion

Bounding the global behaviour of a particulate composite has been investigates when interface between phases are imperfect. When the behaviour of interface is an elastic layer, bounding methods are applied using classical theorem of minimum of potential energy or complementary energy. For isotropic distribution of phases for particulate composite, the problem is solved in order to determine estimation of global behavior using the property of a generalized Lippman–Schwinger equation taking account of discontinuities of displacement and stress-vector, based on a comparison homogeneous material and polarization fields. In this model pattern approach is useful.

Finally upper and lower bounds are obtained for an optimal choice of the reference medium. When the interface is perfect, Hashin–Shtrickman type bounds are recovered.

Fiber reinforced composite case is given as a first example of application of the method.

Appendix A. Green's functions

A.1. *Laplacian Problem*

Notations :

$$r = \|x - y\|, \quad e_j = r_{,i} = \frac{y_i - x_i}{r}, \quad r_{,ij} = \frac{1}{r}\left(\delta_{ij} - e_i e_j\right) \tag{98}$$

2D:

$$\begin{aligned} G(x,y) &= -\frac{1}{4\pi K_o}\log(r), \quad \Gamma(x,y)_{ij} = \mathbb{E}_{ij}\delta(x,y) + \mathbb{F}_{ij} \\ \mathbb{E}_{ij} &= \frac{1}{2K_o}\delta_{ij}, \mathbb{F}_{ij} = \frac{1}{4\pi K_o r}\left(\delta_{ij} - 2e_i e_j\right) \end{aligned} \tag{99}$$

3D:

$$\begin{aligned} G(x,y) &= -\frac{1}{4\pi K_o}\frac{1}{r}, \quad \Gamma(x,y)_{ij} = \mathbb{E}_{ij}\delta(x,y) + \mathbb{F}_{ij} \\ \mathbb{E}_{ij} &= \frac{1}{3K_o}\delta_{ij}, \mathbb{F}_{ij} = \frac{1}{4\pi K_o r^2}\left(\delta_{ij} - 3e_i e_j\right) \end{aligned} \tag{100}$$

A.2. *Plane strain elasticity*

$$G_i^k(x,y) = \frac{1}{8\pi\mu}\left(e_i e_k - (3-4\nu)\delta_{ik}\log r\right) \tag{101}$$

$$\Sigma_{kl}^i = -\frac{1}{4\pi\, r}\left(2e_i e_j e_k + (1-2\nu)\left(\delta_{ki}e_l + \delta_{li}e_k - \delta_{kl}e_i\right)\right) \tag{102}$$

The traction on surface with normal vector $\boldsymbol{n}$ is $T_l^i = \Sigma_{kl}^i n_k$, and the singular part is $(\kappa = \lambda + \mu)$

$$2\mu\mathbb{E}_{ijkl} = -\frac{\kappa}{\kappa+\mu}\delta_{ij}\delta_{kl} + \frac{\kappa+2\mu}{\kappa+\mu}\mathbb{I}_{ijkl} \tag{103}$$

A.3. *Tridimensional elasticity*

$$G_i^k(x,y) = \frac{1}{16\pi\mu(1-\nu)\,r}\,(e_k e_i + (3-4\nu)\delta_{ik}) \tag{104}$$

$$\Sigma_{ij}^k = -\frac{1}{8\pi(1-\nu)\,r^2}\left(3e_i e_j e_k + (1-2\nu)\left(\delta_{ki}e_j + \delta_{jk}e_i - \delta_{ij}e_k\right)\right) \tag{105}$$

Resultant value at a point x inside (outside) a sphere S of the traction

$$\int_S T_i^k \,\mathrm{dS_y} = \int_S \Sigma_{ij}^k n_j \,\mathrm{dS_y} = -\delta_{ik}\frac{\omega(S)}{4\pi} \tag{106}$$

with $\omega(S) = 0$ if $x \in S$, $\omega(S) = 4\pi$ otherwise.

$$\begin{aligned}
&\Gamma_{ikjl} = \mathbb{E}_{ikjl}\delta(x-y) + \mathbb{F}_{ikjl}, \quad 3\kappa = 3\lambda + 2\mu \\
&\mathbb{E}_{ikjl} = \frac{1}{15\mu}\left(-\frac{3\kappa+\mu}{3\kappa+4\mu}\delta_{ik}\delta_{jl} + 9\frac{\kappa+2\mu}{3\kappa+4\mu}\mathbb{I}_{ikjl}\right) \\
&\mathbb{F}_{ijkl} = -\frac{1}{8\pi\mu(3\kappa+4\mu)r^3}\Big(-6\mu\mathbb{I}_{ijkl} + (3\kappa+\mu)\,\delta_{ij}\delta_{kl} - 3\,(3\kappa+\mu)\,(e_i e_j \delta_{kl} + e_k e_l \delta_{ij}) \\
&\qquad + 15(3\kappa+\mu)e_i e_j e_k e_l - 6(3\kappa-2\mu)\,(e_i e_k \delta_{jl})_{(ij)(kl)}\Big)
\end{aligned} \tag{107}$$

Let $\mathbb{J}_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}, \mathbb{I} = \mathbb{K} + \mathbb{J}$ then

$$\mathbb{E} = \alpha\mathbb{J} + \beta\mathbb{K}, \quad \alpha = \frac{1}{3\kappa+4\mu}, \quad \beta = \frac{3}{5\mu}\frac{\kappa+2\mu}{3\kappa+4\mu} \tag{108}$$

Appendix B. Differential geometry

B.1. *Derivation along a surface*

The derivation of quantities along a surface is not directly the classical derivation, we must take into account of that the local frame is changing with its position on the surface.

Consider a surface S, any point M on the surface has local coordinates $X^\alpha, \alpha = 1,2$, and the tangent plane at point M to the surface by vectors $\boldsymbol{A}_\alpha$ with normal vector $\boldsymbol{N}$

$$\boldsymbol{A}_\alpha = \frac{\partial M}{\partial X^\alpha}, \quad \boldsymbol{N}\,\|\boldsymbol{A}_1 \wedge \boldsymbol{A}_2\| = \boldsymbol{A}_1 \wedge \boldsymbol{A}_2 \tag{109}$$

In this local frame

$$\frac{\partial \boldsymbol{A}_\alpha}{\partial X^\beta} = \Gamma^\gamma_{\alpha\beta}\boldsymbol{A}_\gamma + K_{\alpha\beta}\boldsymbol{N} \tag{110}$$

where Γ are the Christoffel symbol, and K the curvature tensor, with properties

$$\mathrm{dS} = \sqrt{\mathrm{g}}\,\mathrm{dX^1dX^2}, \quad \mathrm{g} = \|\boldsymbol{A}_1 \wedge \boldsymbol{A}_2\|, \quad \Gamma^\gamma_{\gamma\alpha} = \frac{1}{\sqrt{\mathrm{g}}}\frac{\partial\sqrt{\mathrm{g}}}{\partial \mathrm{X}^\alpha} \tag{111}$$

The covariant derivative of $\boldsymbol{A}_\alpha$ is given by

$$\bar{\nabla}\boldsymbol{A}_\alpha = \frac{\partial \boldsymbol{A}_\alpha}{\partial X^\beta} - \Gamma^\gamma_{\alpha\beta}\boldsymbol{A}_\gamma \tag{112}$$

For a vector V defines on the surface S,

$$V = V^\alpha \boldsymbol{A}_\alpha + W\boldsymbol{N} \tag{113}$$

we have

$$\nabla V = \left(\bar{\nabla}_\beta V^\alpha - WK^\alpha_\beta\right)\boldsymbol{A}_\alpha \otimes \boldsymbol{A}^\beta + \left(\bar{\nabla}_\beta W + V^\alpha K^\beta_\alpha\right)\boldsymbol{N} \otimes \boldsymbol{A}^\beta \tag{114}$$

In the same spirit, the divergence of a second order symmetric tensor Σ defined by

$$\Sigma = \Sigma^{\alpha\beta}\boldsymbol{A}_\alpha \otimes \boldsymbol{A}_\beta + T^\alpha\,(\boldsymbol{A}_\alpha \otimes \boldsymbol{N} + \boldsymbol{N} \otimes \boldsymbol{A}_\alpha) \tag{115}$$

is

$$\operatorname{Div}\boldsymbol{\Sigma} = \left(\bar{\nabla}_\beta \Sigma^{\alpha\beta} + T^\beta K^\alpha_\beta\right)\boldsymbol{A}_\alpha + \bar{\nabla}_\beta T^\beta + K_{\alpha\beta}\Sigma^{\alpha\beta} \tag{116}$$

where

$$\bar{\nabla}_\gamma \Sigma^{\alpha\beta} = \frac{\partial \Sigma^{\alpha\beta}}{\partial X^\gamma} + \Gamma^\beta_{\gamma\lambda}\Sigma^{\alpha\lambda} + \Gamma^\alpha_{\gamma\lambda}\Sigma^{\beta\lambda} \tag{117}$$

B.2. *Rotational of a second order tensor*

The rotational of a vector $\boldsymbol{v}$ is associated to the adjoin vector of $\nabla\boldsymbol{v}^T - \nabla\boldsymbol{v}$, that is in cartesian coordinates

$$\operatorname{rot}\boldsymbol{v} = R_i \boldsymbol{e}_i, \quad R_i = \boldsymbol{\varepsilon}_{ijk}\frac{\partial v^k}{\partial x^j} \tag{118}$$

where $\boldsymbol{\varepsilon}_{ijk}$ is the alternate tensor $\boldsymbol{\varepsilon}_{ijk} = 1$ or -1, following that ijk is a odd or even permutation, or in general system of coordinates

$$\operatorname{rot}\boldsymbol{v} = \nabla\wedge\boldsymbol{v}, \quad \operatorname{rot}\boldsymbol{v} = \nabla_j v^i \boldsymbol{e}_i \otimes \left(\boldsymbol{e}^j \wedge \boldsymbol{e}^k\right) \tag{119}$$

The rotational of a second order tensor must be specified right or left considering the tensor as a vector with coordinates with fixed left indices or right indices, as

$$\boldsymbol{T} = T_{ij}\boldsymbol{e}^i \otimes \boldsymbol{e}^j, \begin{cases} \operatorname{rot}^l \boldsymbol{T} & = \nabla_k T_{ij}\boldsymbol{e}^i \otimes \left(\boldsymbol{e}^j \wedge \boldsymbol{e}^k\right) \\ \operatorname{rot}^r \boldsymbol{T} & = \nabla_k T_{ij}\left(\boldsymbol{e}^i \wedge \boldsymbol{e}^k\right) \otimes \boldsymbol{e}^j \end{cases} \tag{120}$$

And consequently

$$\operatorname{rot}^r \operatorname{rot}^l T = \nabla_l \nabla_k T_{ij}\left(\boldsymbol{e}^i \wedge \boldsymbol{e}^l\right) \otimes \left(\boldsymbol{e}^j \wedge \boldsymbol{e}^k\right) \tag{121}$$

For the strain $\boldsymbol{\varepsilon}$, $\operatorname{rot}^r \operatorname{rot}^l \boldsymbol{\varepsilon} = 0$ is the condition of compatibility of the strain to ensure the existence of a field $\boldsymbol{u}$ such that $2\boldsymbol{\varepsilon} = \nabla\boldsymbol{u} + \nabla^T\boldsymbol{u}$. Then for all symmetric second order tensor Ξ and any $\boldsymbol{u}$

$$\int_\Omega \Xi : \operatorname{rot}^r \operatorname{rot}^l \boldsymbol{\varepsilon}\, \mathrm{d}\Omega = 0 = \int_\Omega \operatorname{rot}^{\mathrm{l}} \operatorname{rot}^{\mathrm{l}} \Xi : \nabla\boldsymbol{u}\, \mathrm{d}\Omega + \mathrm{B.C} \tag{122}$$

then $\boldsymbol{\sigma} = \operatorname{rot}^l \operatorname{rot}^l \Xi$ is divergence free.

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