TOPOLOGICAL SENSITIVITY ANALYSIS APPLIED IN THE CONTEXT OF MULTI-SCALE CONSTITUTIVE MODELS

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Abstract. *The main purpose of the present work is to carry out a topological sensitivity analysis in constitutive multi-scale models. The derivation of the proposed sensitivity relies on the concept of topological derivative, applied within a variational multi-scale constitutive framework where the macroscopic variables at each point of the macroscopic continuum are defined as volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material associated with that point. As a fundamental result of the topological sensitivity analyses carried out, tensorial fields were identified that represent the topological derivative of the macroscopic constitutive tensor when a singular perturbation is introduced at the micro-scale. The components of such tensorial fields depend on the solution of the canonical variational problems associated to the original unperturbed domain. In particular, in this work, several classical computational modeling problems are addressed within the proposed framework, such as, stationary heat conduction problem, linear elasticity and fracture solid mechanics. The final format of the proposed analytical formulas are strikingly simple and can be potentially used in applications such as the synthesis and optimal design of microstructures to meet a specified macroscopic behavior.*

Keywords: *: Topological derivative, topological sensitivity analysis, multi-scale modeling, synthesis of microstructures.*

1. Introduction

Composite materials have become one of the most important classes of engineering materials. In a broad sense, one can argue that much of material science is about improving macroscopic material properties by means of topological and shape changes at a microstructural level. In this context, the ability to accurately predict the macroscopic mechanical behavior from the corresponding microscopic properties as well as its sensitivity to changes in microstructure becomes essential in the analysis and potential purpose-design and optimisation of heterogeneous media. Such concepts have been successfully used, for instance, in Sigmund (1994); Silva et al. (1997) and Kikuchi et al. (1998) by means of a relaxation-based technique in the design of periodic microstructural topologies. This paper proposes a general *exact* analytical expression for the topological sensitivity of the two-dimensional macroscopic elasticity tensor to topological changes of the microstructure of the underlying material. The macroscopic linear elastic response is estimated by means of a well-established homogenisation-based multi-scale constitutive theory for elasticity problems, see the works by Germain et al. (1983) and Michel et al. (1999), where the macroscopic strain and stress tensors at each point of the macroscopic continuum are defined as the volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material associated with that point. The proposed sensitivity is a symmetric fourth order tensor field over the RVE that measures how the macroscopic elasticity parameters estimated within the multi-scale framework changes when a small circular inclusion is introduced at the micro-scale. Its analytical formula is derived by making use of the concepts of *topological asymptotic expansion* and *topological derivative*, Sokołowski and Żochowski (1999) and Céa et al. (2000), within a variational formulation of the adopted multi-scale theory. The final format of the proposed analytical formula is strikingly simple and can be potentially used in applications such as the synthesis and optimal design of microstructures to meet a specified macroscopic behavior.

The paper is organised as follows. The multi-scale constitutive framework adopted in the estimation of the macroscopic elasticity tensor is briefly described in Section 2. The main contribution of the paper is presented in Section 3. Here, an overview of the topological derivative concept is given. Finally, some concluding remarks are made in Section 4.

2. Multi-scale modelling

In this section we briefly describe the multi-scale constitutive model for classical elasticity problems which allows estimating the macroscopic elasticity tensor using a homogenisation-based variational framework with the complete description of a local Representative Volume Element (RVE) of material. This constitutive modelling approach follows closely the strategy presented, among others, by Germain et al. (1983), Miehe et al. (1999) and Michel et al. (1999) – and whose variational structure is described in detail in de Souza Neto and Feijóo (2006). In this context, the main concept is the assumption that any point x of the macroscopic continuum (refer to Fig. 1) is associated to a local RVE whose

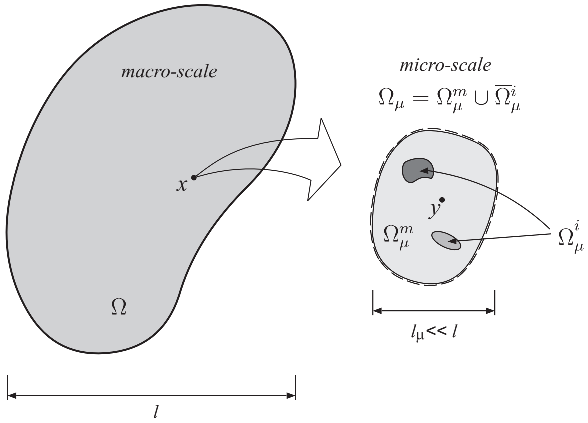

Figure 1. Macroscopic continuum with a locally attached microstructure.

domain Ω_μ, with smooth boundary $\partial\Omega_\mu$, has characteristic length l_μ, much smaller than the characteristic length l of the macro-continuum domain, Ω. For simplicity, we consider that the RVE domain consist of a matrix, Ω_μ^m, containing inclusions of different materials occupying a domain Ω_μ^i (see Fig.1), but the formulation is completely analogous to the one presented here if the RVE contains voids instead.

Using the concept of *homogenization* we define the macroscopic strain tensor $\mathbf{E}$ at a point $\boldsymbol{x}$ of the macroscopic continuum as the volume average of its microscopic counterpart $\mathbf{E}_\mu$ over the domain of the RVE:

$$\mathbf{E} := \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{E}_\mu, \tag{1}$$

where V_μ is a total volume of the RVE and

$$\mathbf{E}_\mu := \nabla^s \mathbf{u}_\mu, \tag{2}$$

with $\mathbf{u}_\mu$ denoting the microscopic displacement field of the RVE. Tacking into account the Green's Theorem in definitions (2) and (1) we obtain the following equivalent expression for the homogenized (macroscopic) strain tensor $\mathbf{E}$

$$\mathbf{E} = \frac{1}{V_\mu} \int_{\partial\Omega_\mu} \mathbf{u}_\mu \otimes_s \mathbf{n}, \tag{3}$$

where $\mathbf{n}$ is the outward unit normal to the boundary $\partial\Omega_\mu$ and $\otimes_s$ denotes the symmetric tensor product of vectors.

Now, without loss of generality, it is possible split $\mathbf{u}_\mu$ into a sum

$$\mathbf{u}_\mu(\boldsymbol{y}) = \mathbf{u} + \bar{\mathbf{u}}(\boldsymbol{y}) + \tilde{\mathbf{u}}_\mu(\boldsymbol{y}), \tag{4}$$

of a constant (rigid) RVE displacement coinciding with the macro displacement $\mathbf{u}$, a field $\bar{\mathbf{u}}(\boldsymbol{y}) := \mathbf{E}\,\boldsymbol{y}$, and a fluctuation displacement field $\tilde{\mathbf{u}}_\mu(\boldsymbol{y})$. With the above split, the microscopic strain field (2) can be written as a sum

$$\mathbf{E}_\mu = \mathbf{E} + \tilde{\mathbf{E}}_\mu, \tag{5}$$

of a homogeneous strain (uniform over the RVE) coinciding with the macroscopic strain $\mathbf{E}$ and a field $\tilde{\mathbf{E}}_\mu$ corresponding to a fluctuation of the microscopic strain about the homogenised (average) value.

2.1 Admissible and virtual microscopic displacement fields

Naturally, assumptions (1) and (2) places a constraint on the admissible displacement fields of the RVE. These conditions can be expressed by requiring the set $\mathcal{K}_\mu$ of kinematically admissible displacements of the RVE to satisfy

$$\mathcal{K}_\mu \subset \mathcal{K}_\mu^* := \left\{ \boldsymbol{v} \in \left[H^1(\Omega_\mu)\right]^2 : \int_{\Omega_\mu} \boldsymbol{v} = V_\mu \mathbf{u}\,, \int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \mathbf{n} = V_\mu\,\mathbf{E},\ [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\Omega_\mu^i \right\}, \tag{6}$$

where $\mathcal{K}_\mu^*$ is the *minimally constrained set of kinematically admissible RVE displacement fields* and $[\![\boldsymbol{v}]\!]$ denotes the *jump* of function $\boldsymbol{v}$ across the matrix/inclusion interface $\partial\Omega_\mu^i$, defined as

$$[\![(\cdot)]\!] := (\cdot)|_m - (\cdot)|_i\,, \tag{7}$$

with subscripts m and i associated, respectively, with quantity values on the matrix and inclusion.

The split presented in (4), allows to express constraint (6), without loss of generality, by requiring that the space $\tilde{\mathcal{K}}_\mu$ of admissible displacement fluctuations of the RVE be a subspace of the *minimally constrained space of displacement fluctuations*, $\tilde{\mathcal{K}}_\mu^*$:

$$\tilde{\mathcal{K}}_\mu \subset \tilde{\mathcal{K}}_\mu^* := \left\{ \boldsymbol{v} \in \left[H^1(\Omega_\mu)\right]^2 : \int_{\Omega_\mu} \boldsymbol{v} = \mathbf{0}, \int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \mathbf{n} = \mathbf{0},\ [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\Omega_\mu^i \right\}. \tag{8}$$

Then, we have that the space of virtual displacement of the RVE can be defined as

$$\mathcal{V}_\mu := \left\{ \boldsymbol{\eta} \in \left[H^1(\Omega_\mu)\right]^2 : \boldsymbol{\eta} = \boldsymbol{v}_1 - \boldsymbol{v}_2;\ \forall \boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathcal{K}_\mu \right\}, \tag{9}$$

coinciding with the space of microscopic displacement fluctuations, i.e., $\mathcal{V}_\mu = \tilde{\mathcal{K}}_\mu$.

2.2 Macroscopic stress and the Hill-Mandel Principle

In the same way that the macroscopic strain tensor (1), the macroscopic stress tensor $\mathbf{T}$, is defined as the volume average of the microscopic stress field $\mathbf{T}_\mu$ over the RVE, i.e.,

$$\mathbf{T} := \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{T}_\mu. \tag{10}$$

In order to introduce the Hill-Mandel Principle of Macro-Homogeneity (Hill (1965) and Mandel (1971)) let us consider a generic RVE with body force field $\mathbf{b}_\mu = \mathbf{b}_\mu(\boldsymbol{y})$ in Ω_μ and an external traction field $\mathbf{q}_\mu = \mathbf{q}_\mu(\boldsymbol{y})$ on $\partial\Omega_\mu$. That principle establishes that the power of the macroscopic stress tensor at an arbitrary point of the macro-continuum must be equal to the volume average of the power of the microscopic stress over the RVE associated with that point for any kinematically admissible motion of the RVE. In view of the Hill-Mandel principle, we have that the body force and external traction fields of the RVE belong to the functional space orthogonal to the chosen $\mathcal{V}_\mu$ – they are reactions to the constraints imposed upon the possible displacement fields of the RVE. That is, the body force $\mathbf{b}_\mu$ and the external traction $\mathbf{q}_\mu$ must satisfy the variational equations, see de Souza Neto and Feijóo (2006),

$$\int_{\Omega_\mu} \mathbf{b}_\mu \cdot \boldsymbol{\eta} = 0 \quad \text{and} \quad \int_{\partial\Omega_\mu} \mathbf{q}_\mu \cdot \boldsymbol{\eta} = 0 \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{11}$$

2.3 The RVE mechanical equilibrium problem

For this work, materials that satisfy the classical linear elastic constitutive law will be used to describe the behaviour of the RVE matrix and inclusions. That is, the microscopic stress tensor field $\mathbf{T}_\mu$ satisfies

$$\mathbf{T}_\mu = \mathbb{C}_\mu \mathbf{E}_\mu, \tag{12}$$

where $\mathbb{C}_\mu$ is the fourth order elasticity tensor, for isotropic and homogeneous materials, defined as:

$$\mathbb{C}_\mu = \frac{E}{1-\nu^2} \left[(1-\nu)\, \mathbb{I} + \nu\, (\mathbf{I} \otimes \mathbf{I}) \right], \tag{13}$$

with E and ν denoting, respectively, the Young's moduli and the Poisson's ratio of the domain Ω_μ. These parameters are given by

$$E := \begin{cases} E_m & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^m \\ E_i & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^i \end{cases} \quad \text{and} \quad \nu := \begin{cases} \nu_m & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^m \\ \nu_i & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^i \end{cases}. \tag{14}$$

If the RVE has more than one inclusion, the parameters E_i and ν_i are piecewise constant. In addition, in eq.(13), we use $\mathbf{I}$ and $\mathbb{I}$ to denote the second and fourth order identity tensors, respectively.

The linearity of (12) together with the additive decomposition (5), allows the microscopic stress field to be split as

$$\mathbf{T}_\mu = \bar{\mathbf{T}}_\mu + \tilde{\mathbf{T}}_\mu, \tag{15}$$

where $\bar{\mathbf{T}}_\mu$ is the microscopic stress field associated with the uniform strain induced by $\bar{\mathbf{u}}\,(\boldsymbol{y})$, i.e., $\bar{\mathbf{T}}_\mu = \mathbb{C}_\mu \mathbf{E}$, and $\tilde{\mathbf{T}}_\mu$ is the microscopic stress fluctuation field associated with $\tilde{\mathbf{u}}_\mu\,(\boldsymbol{y})$, i.e., $\tilde{\mathbf{T}}_\mu = \mathbb{C}_\mu \tilde{\mathbf{E}}_\mu$.

In view of expressions (11), (12) and (15), we have that the *RVE mechanical equilibrium problem* consists of finding, for a given macroscopic strain $\mathbf{E}$, an admissible microscopic displacement fluctuation field $\tilde{\mathbf{u}}_\mu \in \mathcal{V}_\mu$, such that

$$\int_{\Omega_\mu} \tilde{\mathbf{T}}_\mu \cdot \nabla^s \boldsymbol{\eta} = -\int_{\Omega_\mu} \bar{\mathbf{T}}_\mu \cdot \nabla^s \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu, \quad \text{with} \quad \tilde{\mathbf{T}}_\mu = \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_\mu. \tag{16}$$

2.4 Classes of multi-scale constitutive models

The characterisation of a multi-scale model of the present type is completed with the choice of a suitable space of kinematically admissible displacement fluctuations $\mathcal{V}_\mu \subset \tilde{\mathcal{K}}^*_\mu$. We list below three classical possible choices:

- *Linear boundary displacement model*. For this class of models the choice is

$$\mathcal{V}_\mu = \mathcal{V}^{\mathcal{L}}_\mu := \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}^*_\mu : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}) = \mathbf{0} \; \forall \boldsymbol{y} \in \partial\Omega_\mu \right\}. \tag{17}$$

  The only possible reactive body force over Ω_μ orthogonal to $\mathcal{V}^{\mathcal{L}}_\mu$ is $\mathbf{b}_\mu = \mathbf{0}$. On $\partial\Omega_\mu$, the resulting reactive external traction, $\mathbf{q}_\mu \in \left(\mathcal{V}^{\mathcal{L}}_\mu\right)^\perp$, may be any function.

- *Periodic boundary fluctuations model*. The space of displacement fluctuations is defined as

$$\mathcal{V}_\mu = \mathcal{V}^{\mathcal{P}}_\mu := \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}^*_\mu : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^+) = \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^-) \; \forall \text{pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu \right\}. \tag{18}$$

  Again, only the zero body force field is orthogonal to the chosen space of fluctuations. In order to satisfy $(11)_2$ the external traction fields must be *anti-periodic*, i.e.,

$$\mathbf{q}_\mu(\boldsymbol{y}^+) = -\mathbf{q}_\mu(\boldsymbol{y}^-) \quad \forall \text{pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu. \tag{19}$$

- *Minimally constrained* or *Uniform RVE boundary traction model*. In this case, we chose,

$$\mathcal{V}_\mu = \mathcal{V}^{\mathcal{U}}_\mu := \tilde{\mathcal{K}}^*_\mu. \tag{20}$$

  Again only the zero body force field is orthogonal to the chosen space. The boundary traction orthogonal to the space of fluctuations satisfy the *uniform boundary traction condition*, de Souza Neto and Feijóo (2006):

$$\mathbf{q}_\mu(\boldsymbol{y}) = \mathbf{T}\mathbf{n}(\boldsymbol{y}) \quad \forall \boldsymbol{y} \in \partial\Omega_\mu, \tag{21}$$

  where $\mathbf{T}$ is the macroscopic stress tensor defined in (10).

2.5 The homogenised elasticity tensor

In the constitutive multi-scale model introduced in the previous sections, was presented how use the macroscopic information (strain tensor $\mathbf{E}$) to obtain the microscopic displacement field $\mathbf{u}_\mu$. However, using the same concepts it is possible to obtain a closed form of the macroscopic constitutive response, in our case, the homogenized elasticity tensor $\mathbb{C}$. This methodology was suggested by Michel et al. (1999) and is based on re-write the problem (16) as a superposition of linear problems associated with the individual Cartesian components of the macroscopic strain tensor. Then, the macroscopic (homogenized) tensor $\mathbb{C}$ can be written as a sum

$$\mathbb{C} = \bar{\mathbb{C}} + \tilde{\mathbb{C}}, \tag{22}$$

of an homogenized (volume average) macroscopic elasticity tensor $\bar{\mathbb{C}}$, given by

$$\bar{\mathbb{C}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu, \tag{23}$$

and a contribution $\tilde{\mathbb{C}}$ associated to the choice of space $\mathcal{V}_\mu$, defined as:

$$\tilde{\mathbb{C}} := \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\tilde{\mathbf{T}}_{\mu_{kl}})_{ij} \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l), \tag{24}$$

where $\tilde{\mathbf{T}}_{\mu_{ij}} = \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}}$ is the fluctuation stress field associated with the fluctuation displacement field $\tilde{\mathbf{u}}_{\mu_{ij}}$, being the vector fields $\tilde{\mathbf{u}}_{\mu_{ij}} \in \mathcal{V}_\mu$ the solutions of the linear variational equations

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} \cdot \nabla^s \boldsymbol{\eta} = -\int_{\Omega_\mu} \mathbb{C}_\mu (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \nabla^s \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu, \tag{25}$$

for $i, j = 1, 2$ (in the two-dimensional case). In the above expressions the elements $\{\mathbf{e}_i\}$ are the orthonormal basis of the two-dimensional Euclidean space. For a more detailed description on the derivation of expressions (22 – 25) we refer the reader to Michel et al. (1999); de Souza Neto and Feijóo (2006) and Giusti et al. (2009).

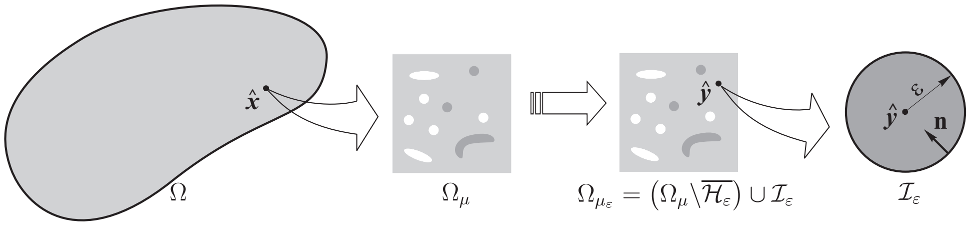

Figure 2. Microstructure perturbed with a inclusion $\mathcal{I}_\varepsilon$.

3. The topological sensitivity of the homogenised elasticity tensor

The main result of this paper – a closed formula for the sensitivity of the homogenised elasticity tensor (22) to the introduction of a circular inclusion centered at an arbitrary point of the RVE domain is presented in this section. To this end, let ψ be a functional that depends on a given domain and let it have sufficient regularity so that the following expansion is possible

$$\psi\left(\varepsilon\right) = \psi\left(0\right) + f\left(\varepsilon\right) D_T\psi + o\left(f\left(\varepsilon\right)\right), \tag{26}$$

where $\psi(0)$ is the functional evaluated in the original domain and $\psi(\varepsilon)$ denotes the functional for a topologically perturbed domain. The parameter ε defines the size of the topological perturbation, so that the original domain is retrieved when $\varepsilon = 0$. In addition, $f(\varepsilon)$ is a *regularising function* defined such that $f(\varepsilon) \to 0$ with $\varepsilon \to 0^+$ and $o\left(f\left(\varepsilon\right)\right)$ contains all terms of higher order in $f(\varepsilon)$. The term $D_T\psi$ of (26) is defined as the *topological derivative* of ψ at the unperturbed (original) RVE domain. The concept of topological derivative was rigorously introduced by Sokołowski and Żochowski (1999). Since then, the notion of topological derivative has proved extremely useful in the treatment of a wide range of problems in mechanics, optimisation, inverse analysis and image processing and has become a subject of intensive research.

3.1 Application to the multi-scale elasticity model

To begin the topological sensitivity analysis, it is appropriate to define the following functional

$$\psi(\varepsilon) := V_\mu \mathbf{T}^\varepsilon \cdot \mathbf{E}, \quad \Rightarrow \quad \psi(0) = V_\mu \mathbf{T} \cdot \mathbf{E}, \tag{27}$$

where $\mathbf{T}^\varepsilon$ denotes the macroscopic stress tensor associated with a RVE topologically perturbed by a small inclusion of radius ε defined by $\mathcal{I}_\varepsilon$ and $\mathbf{T}$ is the macroscopic stress tensor associated to the unperturbed domain Ω_μ. More precisely, the perturbed domain is obtained when a circular hole $\mathcal{H}_\varepsilon$ of radius ε is introduced at an arbitrary point $\hat{\boldsymbol{y}} \in \Omega_\mu$. Next, this region is replaced with the circular inclusion $\mathcal{I}_\varepsilon$ with different material. Then, the perturbed domain is defined as $\Omega_{\mu_\varepsilon} = (\Omega_\mu \backslash \mathcal{H}_\varepsilon) \cup \mathcal{I}_\varepsilon$ (refer to Fig. 2). Thus, the asymptotic topological expansion of the functional $(27)_1$ reads

$$\mathbf{T}^\varepsilon \cdot \mathbf{E} = \mathbf{T} \cdot \mathbf{E} + \frac{1}{V_\mu} f\left(\varepsilon\right) D_T\psi + o\left(f\left(\varepsilon\right)\right). \tag{28}$$

Our purpose here is to derive the closed formula for the topological sensitivity of the macroscopic elasticity tensor (22). Then, we start deriving a closed formula for the associated topological derivative $D_T\psi$, which characterizes the asymptotic expansion (28). To this end, we write the shape functional $\psi(\varepsilon)$ in terms of the microscopic strain and stress tensors as:

$$\psi(\varepsilon) := \mathcal{J}_{\Omega_{\mu_\varepsilon}}\left(\mathbf{u}_{\mu_\varepsilon}\right) = \int_{\Omega_{\mu_\varepsilon}} \mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \mathbf{u}_{\mu_\varepsilon}, \tag{29}$$

where $\mathbf{T}_{\mu_\varepsilon}$ is the microscopic stress field associated to perturbed domain Ω_{μ_ε}. Analogously to the presented in the previous section, the stress tensor field $\mathbf{T}_{\mu_\varepsilon}$ is defined as

$$\mathbf{T}_{\mu_\varepsilon} = \mathbb{C}^*_\mu \mathbf{E}_{\mu_\varepsilon}, \tag{30}$$

with $\mathbf{E}_{\mu_\varepsilon} = \nabla^s \mathbf{u}_{\mu_\varepsilon}$ denoting the microscopic strain field in Ω_{μ_ε} and the constitutive fourth order tensor $\mathbb{C}^*_\mu$, for $\gamma \in \mathbb{R}^+$, is given by

$$\mathbb{C}^*_\mu = \begin{cases} \mathbb{C}_\mu & \forall \boldsymbol{y} \in \Omega_\mu \backslash \overline{\mathcal{H}_\varepsilon} \\ \gamma \mathbb{C}_\mu & \forall \boldsymbol{y} \in \mathcal{I}_\varepsilon \end{cases}. \tag{31}$$

Particularly, the microscopic displacement field $\mathbf{u}_{\mu_\varepsilon} \in \mathcal{K}_{\mu_\varepsilon} := \{\boldsymbol{v} \in \mathcal{K}_\mu : [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\mathcal{I}_\varepsilon\}$, associated to the perturbed RVE, is decomposed as

$$\mathbf{u}_{\mu_\varepsilon} = \mathbf{u} + \mathbf{E}\boldsymbol{y} + \tilde{\mathbf{u}}_{\mu_\varepsilon}, \tag{32}$$

where the fluctuation displacement field $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ is the solution of the variational problem for the perturbed domain Ω_{μ_ε}: find $\tilde{\mathbf{u}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon} := \{\boldsymbol{\xi} \in \mathcal{V}_\mu : [\![\boldsymbol{\xi}]\!] = \mathbf{0} \text{ on } \partial\mathcal{I}_\varepsilon\}$ such that:

$$\int_{\Omega_{\mu_\varepsilon}} \tilde{\mathbf{T}}_{\mu_\varepsilon} \cdot \nabla^s \boldsymbol{\eta}_\varepsilon = -\int_{\Omega_{\mu_\varepsilon}} \bar{\mathbf{T}}^*_\mu \cdot \nabla^s \boldsymbol{\eta}_\varepsilon \quad \forall \boldsymbol{\eta}_\varepsilon \in \mathcal{V}_{\mu_\varepsilon}, \quad \text{with} \quad \tilde{\mathbf{T}}_{\mu_\varepsilon} = \mathbb{C}^*_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_\varepsilon}, \tag{33}$$

where $\mathcal{V}_{\mu_\varepsilon}$ is the space of kinematically admissible displacement fluctuations of the perturbed RVE and $\bar{\mathbf{T}}^*_\mu$ is the microscopic stress field, associated to Ω_{μ_ε}, induced by the macroscopic strain $\mathbf{E}$, i.e., $\bar{\mathbf{T}}^*_\mu = \mathbb{C}^*_\mu \mathbf{E}$.

For the calculation of the topological derivative, we shall adopt the approach presented by Novotny et al. (2003), whereby the topological derivative is obtained as

$$D_T\psi = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}). \tag{34}$$

The derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ with respect to the perturbation parameter ε can be seen as the sensitivity of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$, in the classical sense, to the change in shape produced by a uniform expansion of the inclusion $\mathcal{I}_\varepsilon$. Then, the shape derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ results exclusively in terms of a integral over the boundary $\partial\mathcal{I}_\varepsilon$ of the inclusion (Giusti et al. (2008); de Faria et al. (2009)):

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = -\int_{\partial\mathcal{I}_\varepsilon} [\![\boldsymbol{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n}. \tag{35}$$

In order to derive an explicit expression for the integrand on the right hand side of (35), we consider a curvilinear coordinate system along $\partial\mathcal{I}_\varepsilon$, characterised by the orthonormal vectors $\mathbf{n}$ and $\mathbf{t}$. Then, we can decompose the stress tensor $\mathbf{T}_{\mu_\varepsilon}$ and the strain tensor $\mathbf{E}_{\mu_\varepsilon}$ on the boundary $\partial\mathcal{I}_\varepsilon$ as follows

$$\begin{aligned} \mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} &= \mathrm{T}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n}) + \mathrm{T}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t}) + \mathrm{T}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n}) + \mathrm{T}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}), \\ \mathbf{E}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} &= \mathrm{E}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n}) + \mathrm{E}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t}) + \mathrm{E}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n}) + \mathrm{E}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}). \end{aligned} \tag{36}$$

Using decomposition $(36)_1$, note that the Neumann boundary condition along $\partial\mathcal{I}_\varepsilon$ gives

$$[\![\tilde{\mathbf{T}}_{\mu_\varepsilon}]\!]\mathbf{n}|_{\partial\mathcal{I}_\varepsilon} = -[\![\bar{\mathbf{T}}^*_\mu]\!]\mathbf{n} \quad \Rightarrow \quad [\![\mathbf{T}_{\mu_\varepsilon}]\!]\mathbf{n}|_{\partial\mathcal{I}_\varepsilon} = \mathbf{0}, \tag{37}$$

$$\Rightarrow \qquad \mathrm{T}^{nn}_{\mu_\varepsilon}|_m = \mathrm{T}^{nn}_{\mu_\varepsilon}|_i \quad \text{and} \quad \mathrm{T}^{tn}_{\mu_\varepsilon}|_m = \mathrm{T}^{nn}_{\mu_\varepsilon}|_i \quad \text{on} \quad \partial\mathcal{I}_\varepsilon. \tag{38}$$

Similarly to eq. (36), the fluctuation displacement field $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ can be decomposed on $\partial\mathcal{I}_\varepsilon$ as

$$\tilde{\mathbf{u}}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} = \tilde{\mathrm{u}}^n_{\mu_\varepsilon}\mathbf{n} + \tilde{\mathrm{u}}^t_{\mu_\varepsilon}\mathbf{t}. \tag{39}$$

Therefore, the continuity condition of $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ along $\partial\mathcal{I}_\varepsilon$ implies

$$[\![\tilde{\mathbf{u}}_{\mu_\varepsilon}]\!]|_{\partial\mathcal{I}_\varepsilon} = \mathbf{0} \quad \Rightarrow \quad \left.\frac{\partial\tilde{\mathbf{u}}_{\mu_\varepsilon}}{\partial t}\right|_m = \left.\frac{\partial\tilde{\mathbf{u}}_{\mu_\varepsilon}}{\partial t}\right|_i \text{ on } \partial\mathcal{I}_\varepsilon. \tag{40}$$

Alternatively, the above condition can be written in terms of the components, in the base *n–t*, of the fluctuation strain tensor $\tilde{\mathbf{E}}_{\mu_\varepsilon}$ as follows

$$\tilde{\mathrm{E}}^{tt}_{\mu_\varepsilon}|_m = \tilde{\mathrm{E}}^{tt}_{\mu_\varepsilon}|_i, \quad \Rightarrow \quad \mathrm{E}^{tt}_{\mu_\varepsilon}|_m = \mathrm{E}^{tt}_{\mu_\varepsilon}|_i. \tag{41}$$

Tacking into account the decompositions (36) and (39), and the continuity condition (38), (40) and (41), the jump of the Eshelby tensor flux in the normal direction through of the boundary of the perturbation $\mathcal{I}_\varepsilon$ can be written as

$$[\![\boldsymbol{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = [\![\mathrm{T}^{tt}_{\mu_\varepsilon}]\!]\mathrm{E}^{tt}_{\mu_\varepsilon}|_i - [\![\tilde{\mathrm{E}}^{nn}_{\mu_\varepsilon}]\!]\mathrm{T}^{nn}_{\mu_\varepsilon}|_i - \left[\!\!\left[\frac{\partial\tilde{\mathrm{u}}^t_{\mu_\varepsilon}}{\partial n}\right]\!\!\right]\mathrm{T}^{nt}_{\mu_\varepsilon}|_i. \tag{42}$$

Observe that, using the constitutive law given by eq. (30), the jump terms to the right of the above expressions satisfy

$$[\![\mathrm{T}^{tt}_{\mu_\varepsilon}]\!] = E(1-\gamma)\mathrm{E}^{tt}_{\mu_\varepsilon}|_i, \tag{43}$$

$$[\![\tilde{\mathrm{E}}^{nn}_{\mu_\varepsilon}]\!] = \frac{1-\nu^2}{E}\left(\frac{\gamma-1}{\gamma}\tilde{\mathrm{T}}^{nn}_{\mu_\varepsilon}|_i - [\![\bar{\mathrm{T}}^{nn}_\mu]\!]\right), \tag{44}$$

$$\left[\!\!\left[\frac{\partial\tilde{\mathrm{u}}^t_{\mu_\varepsilon}}{\partial n}\right]\!\!\right] = 2\frac{1-\nu}{E}\left(\frac{\gamma-1}{\gamma}\tilde{\mathrm{T}}^{tn}_{\mu_\varepsilon}|_i - [\![\bar{\mathrm{T}}^{tn}_\mu]\!]\right), \tag{45}$$

where $\bar{\mathrm{T}}^{nn}_{\mu}$, $\bar{\mathrm{T}}^{tn}_{\mu}$, $\tilde{\mathrm{T}}^{nn}_{\mu_\varepsilon}$ and $\tilde{\mathrm{T}}^{tn}_{\mu_\varepsilon}$ are the constant and fluctuation part of components $\mathrm{T}^{nn}_{\mu_\varepsilon}$ and $\mathrm{T}^{tn}_{\mu_\varepsilon}$, respectively, of the stress tensor $\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon}$, eq.(36)$_1$.

Therefore, introducing the above results into (42) and tacking into account the additive decomposition of the components of the microscopic stress field $\mathbf{T}_{\mu_\varepsilon}$, the jump of the Eshelby tensor flux in the normal direction through of the boundary $\partial\mathcal{I}_\varepsilon$ satisfy the following representation in terms of the solution inside of the perturbation $\mathcal{I}_\varepsilon$:

$$[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = \frac{1-\gamma}{\gamma^2 E}\left[\left(\mathrm{T}^{tt}_{\mu_\varepsilon}|_i - \nu\mathrm{T}^{nn}_{\mu_\varepsilon}|_i\right)^2 + \gamma(1-\nu^2)\mathrm{T}^{nn}_{\mu_\varepsilon}|_i^2 + 2\gamma(1+\nu)\mathrm{T}^{tn}_{\mu_\varepsilon}|_i^2\right]. \tag{46}$$

In order to obtain an analytical formula for the boundary integral (35) we make use of the classical asymptotic analysis for the two-dimensional elasticity problems, see Little (1973). Thus, the distribution of the microscopic stress field on boundary $\partial\mathcal{I}_\varepsilon$ is written as

$$\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} = \mathbb{L}\bar{\mathbf{T}}_\mu + \mathbb{S}\tilde{\mathbf{T}}_\mu + \mathcal{O}(\varepsilon), \tag{47}$$

with $\mathcal{O}(\varepsilon)\to 0$ as $\varepsilon\to 0$ and the fourth order tensors $\mathbb{L}$ and $\mathbb{S}$ are given by

$$\mathbb{L} = \gamma\frac{1-\gamma}{1+\alpha\gamma}\left[\frac{1+\alpha}{1-\gamma}\mathbb{I} + \frac{\beta-\alpha}{2(1+\beta\gamma)}(\mathbf{I}\otimes\mathbf{I})\right], \quad \mathbb{S} = \frac{\gamma}{(1+\alpha\gamma)(1+\nu)}\left\{4\mathbb{I} + \left[\frac{\beta(1+\alpha\gamma)}{1+\beta\gamma} - 2\right](\mathbf{I}\otimes\mathbf{I})\right\}, \tag{48}$$

being that the constants α and β are defined as

$$\alpha = \frac{3-\nu}{1+\nu} \quad \text{and} \quad \beta = \frac{1+\nu}{1-\nu}. \tag{49}$$

With the stress distribution along the boundary $\partial\mathcal{I}_\varepsilon$, shown in eq. (47), and the result (46), it is possible to obtain the topological derivative evaluating analytically the boundary integral (35). In fact,

$$\int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = \frac{2\pi\varepsilon}{E}\left(\frac{1-\gamma}{1+\alpha\gamma}\right)\left[4\mathbf{T}_\mu\cdot\mathbf{T}_\mu + \frac{\gamma(\alpha-2\beta)-1}{1+\beta\gamma}(\mathrm{tr}\mathbf{T}_\mu)^2\right] + o(\varepsilon). \tag{50}$$

Substituting the previous result in (34) and adopting the function $f(\varepsilon)$ as th size of the circular perturbation, finally, we obtain the explicit closed form expression for the topological derivative of ψ:

$$D_T\psi = -\mathbb{H}\mathbf{T}_\mu\cdot\mathbf{T}_\mu, \quad \text{with} \quad \mathbb{H} := \frac{1}{E}\left(\frac{1-\gamma}{1+\alpha\gamma}\right)\left[4\mathbb{I} + \frac{\gamma(\alpha-2\beta)-1}{1+\beta\gamma}(\mathbf{I}\otimes\mathbf{I})\right]. \tag{51}$$

3.2 The sensitivity of the macroscopic elasticity tensor

With the result of the topological sensitivity analysis at hand, eq.(51), we have the explicit expression for the topological asymptotic expansion of ψ:

$$\mathbf{T}^\varepsilon\cdot\mathbf{E} = \mathbf{T}\cdot\mathbf{E} - v(\varepsilon)\mathbb{H}\mathbf{T}_\mu\cdot\mathbf{T}_\mu + o(v(\varepsilon)), \tag{52}$$

where $v(\varepsilon) := \pi\varepsilon^2/V_\mu$ is the RVE volume fraction occupied by the perturbation.

The concepts used in Section 2.5, in order to write a closed expression for the macroscopic constitutive tensor $\mathbb{C}$, can be easily extended to derive a analytical formulae for the topological sensitivity of the elasticity tensor. In this sense, we write the microscopic strain and stress as a linear combination of the Cartesian components of the macroscopic strain as:

$$\mathbf{E}_\mu = (\mathbf{E})_{ij}\left(\mathbf{e}_i\otimes\mathbf{e}_j + \tilde{\mathbf{E}}_{\mu_{ij}}\right) = (\mathbf{E})_{ij}\,\mathbf{E}_{\mu_{ij}}, \quad \Rightarrow \quad \mathbf{T}_\mu = (\mathbf{E})_{ij}\,\mathbb{C}_\mu\mathbf{E}_{\mu_{ij}} = (\mathbf{T}_{\mu_{ij}}\otimes\mathbf{e}_i\otimes\mathbf{e}_j)\mathbf{E}, \tag{53}$$

where $\mathbf{T}_{\mu_{ij}}$ denotes the microspic stress field associated with each displacement fluctuation field $\tilde{\mathbf{u}}_{\mu_{ij}}$, solutions of the set of variational equations (25).

Tacking into account the above expressions, we see that the topological derivative of ψ given by (51) can be represented as (with $i,j,k,l = 1,2$)

$$D_T\psi = -\mathbb{D}_{T\mu}\mathbf{E}\cdot\mathbf{E}, \quad \text{with} \quad \mathbb{D}_{T\mu} = \mathbb{H}\mathbf{T}_{\mu_{ij}}\cdot\mathbf{T}_{\mu_{kl}}(\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k\otimes\mathbf{e}_l). \tag{54}$$

From (52), (54)$_2$ and assuming a linear elastic constitutive response for the macroscopic stress tensor, we have that the explicit expression for the topological expansion of the macroscopic elasticity tensor satisfies:

$$\mathbb{C}_\varepsilon = \mathbb{C} - v(\varepsilon)\mathbb{D}_{T\mu} + o(v(\varepsilon)). \tag{55}$$

The topological sensitivity tensor (54)$_2$ provides a first order accurate measure of how the macroscopic elasticity tensor varies when a topological perturbation is added to the RVE. Each Cartesian component $(\mathbb{D}_{T\mu})_{ijkl}$ represents the derivative of the component $ijkl$ of the macroscopic elasticity tensor with respect to the volume fraction $v(\varepsilon)$ of a circular inclusion of radius ε inserted at an arbitrary point $\boldsymbol{y}$ of the RVE. The remarkable simplicity of the closed form sensitivity given by (54)$_2$ is to be noted. Once the vector fields $\tilde{\mathbf{u}}_{\mu_{ij}}$ have been obtained as solutions of (25) for the *original* RVE domain, the sensitivity tensor $\mathbb{D}_{T\mu}$can be trivially assembled.

Remark 1 *The topological derivative tensor $\mathbb{D}_{T\mu}$ have a explicit dependency with the contrast parameter γ. Then, through the tensor $\mathbb{H}$, its possible analyse the limit cases of the topological sensitivity tensor, wich are:*

– *Hole ($\gamma \to 0$):*

$$\mathbb{H} = \frac{1}{E}[4\mathbb{I} - (\mathbf{I} \otimes \mathbf{I})], \tag{56}$$

– *Rigid inclusion ($\gamma \to \infty$):*

$$\mathbb{H} = -\frac{1}{E\alpha}\left[4\mathbb{I} + \frac{\alpha - 2\beta}{\beta}(\mathbf{I} \otimes \mathbf{I})\right]. \tag{57}$$

Note that, the result of the final expression (54)$_2$ for the case ($\gamma \to 0$) coincides with the result derivated in Giusti et al. (2009) for topological perturbation characterized by a small circular hole instead of an inclusion.

4. Conclusions

By making use the concept of topological derivative, applied within a variational multi-scale constitutive model for linear elasticity, an analytical formula for the sensitivity of the two-dimensional macroscopic elasticity tensor has been proposed in this work. The used multi-scale constitutive framework is based on the assumption that the macroscopic strain and stress tensor at each point of the macroscopic continuum are defined as volume averages of their microscopic counterparts over a Representative Volume Element of material associated with that point. The adopted model for the estimation of the macroscopic response allows different predictions of macroscopic behavior to be obtained according to the constraints imposed upon the chosen functional space displacement fluctuations of the RVE. The derived sensitivity – a symmetric fourth order tensor field over the RVE domain – measures how the estimated macroscopic elasticity tensor changes when a small circular inclusion is introduced at the micro-scale. The formula presented here can be potentially used in a number of applications of practical interest such as, for instance, the design and optimization of microstructures to achieve a specified macroscopic behavior. Finally, it is worth emphasizing that this methodology makes possible that the topological derivative for a vast class of shape functionals to be promptly obtained.

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