Sensitivity of the macroscopic response of elastic microstructures to the insertion of inclusions

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This paper proposes an exact analytical formula for the topological sensitivity of the macroscopic response of elastic microstructures to the insertion of circular inclusions. The macroscopic response is assumed to be predicted by a well-established multi-scale constitutive theory where the macroscopic strain and stress tensors are defined as volume averages of their microscopic counterpart fields over a Representative Volume Element (RVE) of material. The proposed formula – a symmetric fourth order tensor field over the RVE domain – is a topological derivative which measures how the macroscopic elasticity tensor changes when an infinitesimal circular elastic inclusion is introduced within the RVE. In the limits, when the inclusion/matrix phase contrast ratio tends to zero and infinity, the sensitivities to the insertion of a hole and a rigid inclusion, respectively, are rigorously obtained. The derivation relies on the topological asymptotic analysis of the predicted macroscopic elasticity and is presented in detail. The derived fundamental formula is of interest to many areas of applied and computational mechanics. To illustrate its potential applicability, a simple finite element-based example is presented where the topological derivative information is used to automatically generate a bi-material microstructure to meet pre-specified macroscopic properties.

Keywords: Topological derivative, sensitivity analysis, multi-scale modelling, synthesis of microstructures.

1. Introduction

The ability to predict the macroscopic constitutive response of materials from the knowledge of their microstructure has long been a subject of intensive research in applied and computational mechanics circles. The large body of publications currently available in this field ranges from early fundamental work (e.g. Hill (1963); Hashin & Shtrikman (1963); Hill (1965); Mandel (1971); Gurson (1977); Bensoussan *et al.* (1978); Sanchez-Palencia (1980); Germain *et al.* (1983); Suquet (1987)) to more recent numerical simulations mainly based on the finite element method (Michel *et al.* (1999); Miehe *et al.* (1999); Terada *et al.* (2003); Matsui *et al.* (2004); Speirs *et al.* (2008); Giusti *et al.* (2009*a*)).

Among the various applications of such so-called multi-scale constitutive theories, of particular interest is the study of the sensitivity of the macroscopic response to changes in the microstructure. In this context, the use of sensitivity information has been successfully applied in the topological optimisation of microstructures, among others, by Sigmund (1994), Silva *et al.* (1997), Kikuchi *et al.* (1998), Hyun & Torquato (2001) and Guest & Prevost (2006). The approach adopted by these authors relies essentially on the regularisation of the actual RVE topology optimisation problem by introducing a ficticious density field of which the elastic material parameters are assumed to be a function. Throughout the optimisation iterations, voids are assumed to be located wherever the ficticious density field (the design variable in the regularised optimisation problem) falls below a given numerical tolerance. The sensitivity of the macroscopic elastic parameters to topological changes of the RVE (the introduction of voids in this case) is calculated only in an approximate sense. The approximate character of the sensitivity calculation stem from the fact that procedures of this type are based on the conventional concept of derivative and the introdution of topological changes such as voids are inherently singular and do not fit within the conventional notion of differentiability.

In the present paper, we propose an exact analytical formula for the sensitivity of the macroscopic elasticity tensor to topological microstructural changes. The macroscopic elasticity tensor is assumed to be predicted by a well-established multi-scale constitutive theory based on the volume averaging of the stress and strain tensors over the RVE. Within this constitutive framework upper and lower bounds for the elastic behaviour can be obtained by assuming, respectively, linear RVE boundary displacements and minimum RVE kinematical constraint compatible with the strain averaging assumption (and resulting in uniform RVE boundary tractions). In addition, the widely used assumption of periodic RVE boundary displacement fluctuations provides an estimate for the response of periodic media. The topological change considered consists of the insertion of a circular isotropically elastic inclusion within the isotropically elastic RVE matrix. The Young's modulus of the inclusion is assumed to be a scalar multiple of the Young's modulus of the matrix. In the limits when the scalar multiple (the phase contrast parameter) tends to zero and infinity the proposed formula gives the exact topological sensitivity of the macroscopic elasticity tensor to the insertion of a hole and a rigid inclusion, respectively. The derivation of the analytical sensitivity is presented in detail. It relies on the concepts of topological asymptotic expansion and topological derivative (Céa *et al.* (2000); Sokołowski & Żochowski (1999)) which provides the correct mathematical framework for the treatment of singularities of the present type. The derived formula is of great potential use in applied and computational mechanics and its final format is remarkably simple. Its potential applicability is illustrated in a finite element-based example where the topological derivative information is used in a very simple algorithm to automatically generate a bi-material microstucture to meet a pre-specified macroscopic behaviour.

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 with a detailed derivation of the proposed sensitivity formula. The application of the topological derivative to the synthesis of microstructures is shown in Section 4. Finally, some concluding remarks are made in Section 5.

2. Multi-scale constitutive modelling

This section presents a summary of the multi-scale constitutive theory upon which we rely for the estimation of the macroscopic elasticity properties. This family of (now well established) constitutive theories has been formally presented in a rather general setting by Germain *et al.* (1983) and later exploited, among others, by Michel *et al.* (1999) and Miehe *et al.* (1999) in the computational context. When applied to the modelling of linearly elastic periodic media, it coincides with the asymptotic expansion-based theory described by Bensoussan *et al.* (1978) and Sanchez-Palencia (1980).

The starting point of this family of constitutive theories is the assumption that any point $\boldsymbol{x}$ of the macroscopic continuum (refer to Fig. 1) is associated to a local

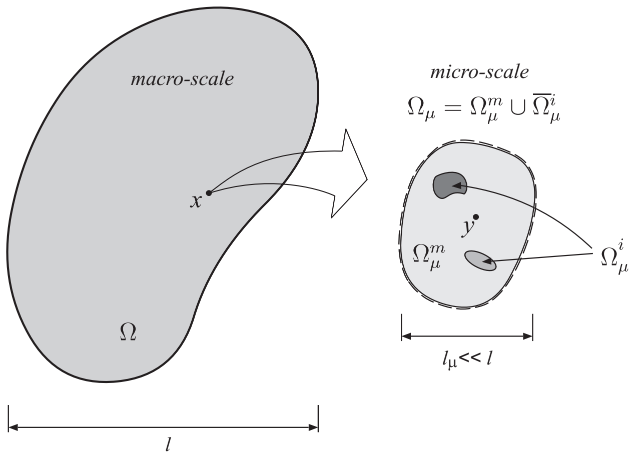


Figure 1. Macroscopic continuum with a locally Representative Volume Element.

RVE whose domain Ω_μ, with 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 consists of a matrix, Ω_μ^m, containing inclusions of different materials occupying a domain Ω_μ^i (see Fig.1).

An axiomatic variational framework for this family of constituive theories is presented in detail by de Souza Neto & Feijóo (2006). Accordingly, the entire theory can be derived from five basic principles: (1) The strain averaging relation; (2) A simple further constraint upon the possible functional sets of kinematically admissible displacement fields of the RVE; (3) The equilibrium of the RVE; (4) The stress averaging relation; (5) The Hill-Mandel Principle of Macro-Homogeneity, which ensures the energy consistency between the so-called micro- and macro-scales of the material. These are briefly stated in the following.

The first basic axiom – the strain averaging relation – states that the macroscopic strain tensor $\mathbf{E}$ at a point $\boldsymbol{x}$ of the macroscopic continuum is the volume average of its microscopic counterpart $\mathbf{E}_\mu$ over the domain of the RVE:

$$\mathbf{E} := \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{E}_\mu, \tag{2.1}$$

where V_μ is a total volume of the RVE and

$$\mathbf{E}_\mu := \nabla^s \mathbf{u}_\mu, \tag{2.2}$$

with $\mathbf{u}_\mu$ denoting the microscopic displacement field of the RVE. Equivalently, in terms of RVE boundary displacements, the homogenised strain (2.1,2.2) can be written as

$$\mathbf{E} = \frac{1}{V_\mu}\int_{\partial\Omega_\mu} \mathbf{u}_\mu \otimes_s \mathbf{n}, \tag{2.3}$$

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

As a result of axiom (2.1) and, in addition, by requiring without loss of generality that the volume average of the microscopic displacement field coincide with the macroscopic displacement $\mathbf{u}$, any chosen set $\mathcal{K}_\mu$ of admissible displacement fields of the RVE must satisfy

$$\mathcal{K}_\mu \subset \mathcal{K}_\mu^* := \left\{ \boldsymbol{v} \in \left[H^1(\Omega_\mu)\right]^2 : \int_{\Omega_\mu} \boldsymbol{v} = V_\mu \mathbf{u}\,, \int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \mathbf{n} = V_\mu\, \mathbf{E},\ [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\Omega_\mu^i \right\}, \tag{2.4}$$

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

$$[\![(\cdot)]\!] := (\cdot)|_m - (\cdot)|_i\,, \tag{2.5}$$

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

Now, without loss of generality, $\mathbf{u}_\mu$ may be decomposed as a sum

$$\mathbf{u}_\mu(\boldsymbol{y}) = \mathbf{u} + \bar{\mathbf{u}}(\boldsymbol{y}) + \tilde{\mathbf{u}}_\mu(\boldsymbol{y})\,, \tag{2.6}$$

of a constant (rigid) RVE displacement coinciding with the macro displacement $\mathbf{u}$, a field $\bar{\mathbf{u}}(\boldsymbol{y}) := \mathbf{E}\,\boldsymbol{y}$, linear in the local RVE coordinate $\boldsymbol{y}$ (whose origin is assumed without loss of generality to be located at the centroid of the RVE) and a fluctuation displacement field $\tilde{\mathbf{u}}_\mu(\boldsymbol{y})$ that, in general, varies with $\boldsymbol{y}$. With the above split, the microscopic strain field (2.2) can be written as a sum

$$\mathbf{E}_\mu = \mathbf{E} + \tilde{\mathbf{E}}_\mu, \tag{2.7}$$

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

The additive split (2.6) allows constraint (2.4) to be expressed in terms of displacement fluctuations alone. It is equivalent to requiring that the (as yet to be defined) set $\tilde{\mathcal{K}}_\mu$ of admissible displacement fluctuations of the RVE be a subset of the *minimally constrained space of displacement fluctuations*, $\tilde{\mathcal{K}}_\mu^*$:

$$\tilde{\mathcal{K}}_\mu \subset \tilde{\mathcal{K}}_\mu^* := \left\{ \boldsymbol{v} \in \left[H^1(\Omega_\mu)\right]^2 : \int_{\Omega_\mu} \boldsymbol{v} = \mathbf{0}, \int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \mathbf{n} = \mathbf{0},\ [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\Omega_\mu^i \right\}. \tag{2.8}$$

At this point we introduce the further assumption that $\tilde{\mathcal{K}}_\mu$ is a *subspace* of $\tilde{\mathcal{K}}^*_\mu$. Then, we have that the space of *virtual displacement* of the RVE, defined as

$$\mathcal{V}_\mu := \left\{ \boldsymbol{\eta} \in \left[H^1(\Omega_\mu)\right]^2 : \boldsymbol{\eta} = \boldsymbol{v}_1 - \boldsymbol{v}_2;\ \forall \boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathcal{K}_\mu \right\}, \tag{2.9}$$

coincides with the space of microscopic displacement fluctuations, i.e.,

$$\mathcal{V}_\mu = \tilde{\mathcal{K}}_\mu. \tag{2.10}$$

The next axiom establishes that the macroscopic stress tensor $\mathbf{T}$ is given by the volume average of the microscopic stress field $\mathbf{T}_\mu$ over the RVE, i.e.,

$$\mathbf{T} := \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{T}_\mu. \tag{2.11}$$

The present paper is focussed on RVEs whose matrix and inclusion materials are described by the classical isotropic linear elastic constitutive law. That is, the microscopic stress tensor field $\mathbf{T}_\mu$ satisfies

$$\mathbf{T}_\mu = \mathbb{C}_\mu \mathbf{E}_\mu, \tag{2.12}$$

where $\mathbb{C}_\mu$ is the fourth order isotropic elasticity tensor:

$$\mathbb{C}_\mu = \frac{E}{1-\nu^2} \left[(1-\nu)\, \mathbb{I} + \nu \left(\mathbf{I} \otimes \mathbf{I} \right) \right], \tag{2.13}$$

with E and ν denoting, respectively, the Young's modulus and the Poisson's ratio. These parameters are given by

$$E := \left\{ \begin{array}{lll} E_m & \text{if} & \boldsymbol{y} \in \Omega_\mu^m \\ E_i & \text{if} & \boldsymbol{y} \in \Omega_\mu^i \end{array} \right. \quad \text{and} \quad \nu := \left\{ \begin{array}{lll} \nu_m & \text{if} & \boldsymbol{y} \in \Omega_\mu^m \\ \nu_i & \text{if} & \boldsymbol{y} \in \Omega_\mu^i \end{array} \right. . \tag{2.14}$$

The parameters E_i and ν_i constant within each inclusion but may in general vary from inclusion to inclusion. In eq.(2.13), we use $\mathbf{I}$ and $\mathbb{I}$ to denote the second and fourth order identity tensors, respectively.

The linearity of (2.12) together with the additive decomposition (2.7) allows the microscopic stress field to be split as

$$\mathbf{T}_\mu = \bar{\mathbf{T}}_\mu + \tilde{\mathbf{T}}_\mu, \tag{2.15}$$

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

A further axiom of the theory is the so-called Hill-Mandel Principle of Macro-Homogeneity (Hill (1965) and Mandel (1971)). This principle establishes that the power of the macroscopic stress tensor at an arbitrary point of the macro-continuum must equal 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. As a consequence of this principle (de Souza Neto & Feijóo (2006)) the RVE body force $\mathbf{b}_\mu$ and external traction field $\mathbf{q}_\mu$ produce no virtual work:

$$\int_{\Omega_\mu} \mathbf{b}_\mu \cdot \boldsymbol{\eta} = 0 \quad \text{and} \quad \int_{\partial\Omega_\mu} \mathbf{q}_\mu \cdot \boldsymbol{\eta} = 0 \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{2.16}$$

That is, the RVE body force and external traction fields 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.

The general theory is completed by a final axiom which establishes that the RVE must in equilibrium. Then, with the introduction of (2.15) and (2.16) into the classical virtual work variational equation, we have that the *RVE mechanical equilibrium problem* consists of finding, for a given macroscopic strain $\mathbf{E}$, a kinematically admissible microscopic displacement fluctuation field $\tilde{\mathbf{u}}_\mu \in \mathcal{V}_\mu$, such that

$$\int_{\Omega_\mu} \tilde{\mathbf{T}}_\mu \cdot \nabla^s \boldsymbol{\eta} = -\int_{\Omega_\mu} \bar{\mathbf{T}}_\mu \cdot \nabla^s \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{2.17}$$

(a) *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 the three classical possible choices:

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

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{L}} := \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}^*_\mu : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}) = \mathbf{0} \ \forall \boldsymbol{y} \in \partial\Omega_\mu \right\}. \tag{2.18}$$

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

- *Periodic boundary fluctuations model.* This class of models is typical of the analysis of periodic media, where the macroscopic continuum is generated by the repetition of the RVE. In this case, the geometry of the RVE must satisfy certain geometrical constraints not needed by the other two classes discussed here. Considering for simplicity the case of polygonal RVE geometries (see fig.2), we have that the boundary $\partial\Omega_\mu$ is composed of a number of pairs of equally-sized subsets $\{\Gamma_i^+, \Gamma_i^-\}$ with normals $\mathbf{n}_i^+ = -\mathbf{n}_i^-$. For each pair $\{\Gamma_i^+, \Gamma_i^-\}$ of sides there is a one-to-one correspondence between points $\boldsymbol{y}^+ \in \Gamma_i^+$ and $\boldsymbol{y}^- \in \Gamma_i^-$. The periodicity of the structure requires that the dis-

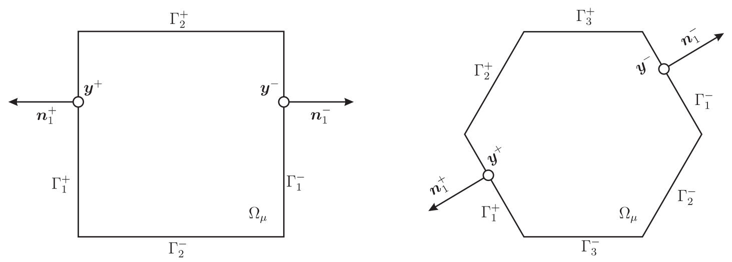


Figure 2. Typical RVE geometries for periodic media.

placement fluctuation at any point $\boldsymbol{y}^+$ coincide with that of the corresponding point $\boldsymbol{y}^-$. Hence, the space of displacement fluctuations is defined as

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{P}} := \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}_\mu^* : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^+) = \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^-) \;\forall \,\text{pairs}\; (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu \right\}. \tag{2.19}$$

Again, only the zero body force field is orthogonal to the chosen space of fluctuations. The reactive external surface traction fields that comply with $(2.16)_2$ are *anti-periodic*, i.e.,

$$\mathbf{q}_\mu(\boldsymbol{y}^+) = -\mathbf{q}_\mu(\boldsymbol{y}^-) \quad \forall \text{ pairs } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu. \tag{2.20}$$

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

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{U}} := \tilde{\mathcal{K}}_\mu^*. \tag{2.21}$$

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 & Feijóo (2006)):

$$\mathbf{q}_\mu\,(\boldsymbol{y}) = \mathbf{T}\mathbf{n}\,(\boldsymbol{y}) \quad \forall \boldsymbol{y} \in \partial\Omega_\mu, \tag{2.22}$$

where $\mathbf{T}$ is the macroscopic stress tensor defined in (2.11).

(*b*) *The homogenised elasticity tensor*

The assumed type of the material response in the microscale implies that the macroscopic response is linear elastic. That is, there is a *homogenised elasticity tensor* $\mathbb{C}$ such that

$$\mathbf{T} = \mathbb{C}\,\mathbf{E}. \tag{2.23}$$

A closed form for the homogenised constitutive tensor can be derived by the approach suggested by Michel *et al.* (1999) and relies on the representation of the RVE equilibrium problem (2.17) as a superposition of linear variational problems associated with the cartesian components of the macroscopic strain tensor. The resulting expression for $\mathbb{C}$ reads

$$\mathbb{C} = \bar{\mathbb{C}} + \tilde{\mathbb{C}}, \tag{2.24}$$

where $\bar{\mathbb{C}}$ is the volume average macroscopic elasticity tensor

$$\bar{\mathbb{C}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu, \tag{2.25}$$

and the contribution $\tilde{\mathbb{C}}$ (generally dependent upon the choice of space $\mathcal{V}_\mu$) is defined as

$$\tilde{\mathbb{C}} := \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\tilde{\mathbf{T}}_{\mu_{kl}})_{ij} \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l)\,, \tag{2.26}$$

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 $\tilde{\mathbf{u}}_{\mu_{ij}} \in \mathcal{V}_\mu$ that solves linear variational problem

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} \cdot \nabla^s \boldsymbol{\eta} = -\int_{\Omega_\mu} \mathbb{C}_\mu (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \nabla^s \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu, \tag{2.27}$$

for $i, j = 1, 2$ (in the two-dimensional case). In the above, $\{\mathbf{e}_i\}$ denotes an orthonormal basis for the two-dimensional Euclidean space.

For a more detailed description on the derivation of expressions (2.24 – 2.27) we refer the reader to Michel *et al.* (1999); de Souza Neto & Feijóo (2006) and Giusti *et al.* (2009*b*).

3. The topological sensitivity of the homogenised elasticity tensor

In this section we present the main result of this paper – a closed formula for the sensitivity of the homogenised elasticity tensor (2.24) to the introduction of an infinitesimal circular inclusion centered at an arbitrary point of the RVE domain.

The proposed formula is obtained by following analogous steps to those presented by Giusti *et al.* (2009*b*) for the sensitivity to the introduction a circular void in the micro-scale, but contains fundamental differences that justify the presentation of the details of its derivation in the following.

We start by providing a brief introduction to the relatively new mathematical concepts of *topological asymptotic expansion* and *topological derivative*. To this end, let ψ be a functional whose value depends on a given domain and let ψ have sufficient regularity so that the following expansion is possible

$$\psi\left(\varepsilon\right)=\psi\left(0\right)+f\left(\varepsilon\right)D_T\psi+o\left(f\left(\varepsilon\right)\right), \tag{3.1}$$

where $\psi(0)$ is the value of the functional for an original (unperturbed) domain and $\psi(\varepsilon)$ denotes the value of the functional for a domain that differs from the original one by a topological perturbation of size ε. Note 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 right hand side of (3.1) is named the *asymptotic topological expansion* of the functional ψ and the term $D_T\psi$ is defined as the *topological derivative* of ψ at the unperturbed RVE domain.

The concept of topological derivative was rigorously introduced by Sokołowski & 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, see for instance, Amstutz *et al.* (2005); Céa *et al.* (2000); Garreau *et al.* (2001); Novotny *et al.* (2007).

(*a*) *Application to the multi-scale elasticity model*

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

$$\psi(\varepsilon) := V_\mu \mathbf{T}^\varepsilon \cdot \mathbf{E}, \quad \Rightarrow \quad \psi(0) = V_\mu \mathbf{T}\cdot\mathbf{E}, \tag{3.2}$$

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

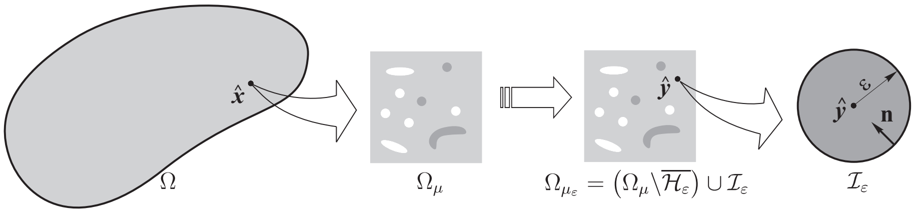


Figure 3. Microstructure perturbed with a inclusion $\mathcal{I}_\varepsilon$.

an arbitrary point $\hat{\boldsymbol{y}} \in \Omega_\mu$. Next, this region is replaced with the circular inclusion $\mathcal{I}_\varepsilon$ made of a different material. Then, the perturbed domain is defined as $\Omega_{\mu_\varepsilon} = \left(\Omega_\mu \backslash \overline{\mathcal{H}_\varepsilon}\right) \cup \mathcal{I}_\varepsilon$ (refer to Fig. 3). Thus, the asymptotic topological expansion of the functional $(3.2)_1$ reads

$$\mathbf{T}^\varepsilon \cdot \mathbf{E} = \mathbf{T} \cdot \mathbf{E} + \frac{1}{V_\mu} f(\varepsilon)\, D_T\psi + o\left(f(\varepsilon)\right). \tag{3.3}$$

(*b*) *Topological derivative calculation*

Our purpose here is to derive the closed formula for the topological sensitivity of the macroscopic elasticity tensor (2.24). Then, we start deriving a closed formula for the associated topological derivative $D_T\psi$, which characterizes the asymptotic expansion (3.3). To this end, we re-define the functional

$$\psi(\varepsilon) := \mathcal{J}_{\Omega_{\mu_\varepsilon}}\left(\mathbf{u}_{\mu_\varepsilon}\right) = \int_{\Omega_{\mu_\varepsilon}} \mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \mathbf{u}_{\mu_\varepsilon}, \tag{3.4}$$

where $\mathbf{T}_{\mu_\varepsilon}$ is the microscopic stress field of the perturbed domain Ω_{μ_ε}. The microscopic stress field $\mathbf{T}_{\mu_\varepsilon}$ is given by

$$\mathbf{T}_{\mu_\varepsilon} = \mathbb{C}^*_\mu \mathbf{E}_{\mu_\varepsilon}, \tag{3.5}$$

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

$$\mathbb{C}^*_\mu = \left\{ \begin{array}{ll} \mathbb{C}_\mu & \forall \boldsymbol{y} \in \Omega_\mu \backslash \overline{\mathcal{H}_\varepsilon} \\ \gamma \mathbb{C}_\mu & \forall \boldsymbol{y} \in \mathcal{I}_\varepsilon \end{array} \right. . \tag{3.6}$$

where $\gamma \in \Re^+$ is the contrast parameter defining the ratio between the properties of the original and new material at the location of the perturbation. Clearly, this type of perturbation allows us to change only the Young's modulus of the phases. Note that we are dealing with the topological asymptotic analysis of the strain energy stored in the RVE. Therefore, concerning the existence of the topological derivative for the energy-shape functional associated to elasticity system, the reader may refer to Sokołowski & Żochowski (1999) and Nazarov & Sokołowski (2003).

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

$$\mathbf{u}_{\mu_\varepsilon} = \mathbf{u} + \mathbf{E}\boldsymbol{y} + \tilde{\mathbf{u}}_{\mu_\varepsilon}, \tag{3.7}$$

where the displacement fluctuation field $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ is the solution of the following variational problem in 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

$$\int_{\Omega_{\mu_\varepsilon}} \tilde{\mathbf{T}}_{\mu_\varepsilon} \cdot \nabla^s \boldsymbol{\eta}_\varepsilon = -\int_{\Omega_{\mu_\varepsilon}} \bar{\mathbf{T}}_\mu^* \cdot \nabla^s \boldsymbol{\eta}_\varepsilon \quad \forall \boldsymbol{\eta}_\varepsilon \in \mathcal{V}_{\mu_\varepsilon}, \tag{3.8}$$

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 Sokołowski & Żochowski (2001) and Novotny *et al.* (2003), whereby the topological derivative is obtained as

$$D_T \psi = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}). \tag{3.9}$$

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 $\mathcal{I}_\varepsilon$.

Proposition 3.1. *Let $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ be the functional defined by (3.4). Then, the derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ with respect to the small parameter ε is given by*

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \boldsymbol{\Sigma}_{\mu_\varepsilon} \cdot \nabla \mathbf{v}, \tag{3.10}$$

where $\mathbf{v}$ is the RVE shape-change velocity field defined in Ω_{μ_ε} and $\boldsymbol{\Sigma}_{\mu_\varepsilon}$ is a generalisation of the classical Eshelby momentum-energy tensor (Eshelby (1975); Gurtin (2000)) of the RVE, given in the present case by

$$\boldsymbol{\Sigma}_{\mu_\varepsilon} = (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon})\mathbf{I} - 2(\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon})^T \mathbf{T}_{\mu_\varepsilon}. \tag{3.11}$$

Proof. By making use of Reynolds' transport theorem (Gurtin (1981); Sokołowski & Zolésio (1992)), we obtain the identity

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \frac{d}{d\varepsilon}(\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) + \mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon} \operatorname{div} \mathbf{v}. \tag{3.12}$$

Next, by using the concept of material derivative of a spatial field, we find that the first term of the above right hand side integral can be written as

$$\frac{d}{d\varepsilon}(\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \dot{\mathbf{E}}_{\mu_\varepsilon}, \tag{3.13}$$

where the superimposed dot denotes the (total) material derivative with respect to ε. Further, note that

$$\mathbf{E}_{\mu_\varepsilon} = \mathbf{E} + \nabla^s \tilde{\mathbf{u}}_{\mu_\varepsilon}, \quad \Rightarrow \quad \dot{\mathbf{E}}_{\mu_\varepsilon} = \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \nabla \mathbf{v})^s. \tag{3.14}$$

Then, by introducing the above expression into (3.13) we obtain

$$\frac{d}{d\varepsilon}(\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon} \cdot (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \nabla \mathbf{v})^s, \tag{3.15}$$

which, substituted in (3.12) gives

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon}\cdot(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon}\nabla\mathbf{v})^s + (\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\mathbf{I}\cdot\nabla\mathbf{v}, \quad (3.16)$$

where we have made use of the identity div $\mathbf{v} = \mathbf{I}\cdot\nabla\mathbf{v}$. Now, note that by definition of the spaces of virtual displacements, we have $\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon}$. This, together with the equilibrium equation (3.8), implies that the first term of (3.16) vanishes. Then, a straightforward rearrangement of the above yields (3.10).

□

Proposition 3.2. *Let $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ be the functional defined by (3.4). Then, the derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ with respect to the small parameter ε can be written as*

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\partial\Omega_\mu}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} + \int_{\partial\Omega_\mu^i}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}, \quad (3.17)$$

where $\mathbf{v}$ is the RVE shape-change velocity field and $\mathbf{\Sigma}_{\mu_\varepsilon}$ is given by (3.11).

Proof. Let us compute the shape derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ using the following version for the Reynolds' transport theorem (Gurtin (1981); Sokołowski & Zolésio (1992)),

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= \int_{\Omega_{\mu_\varepsilon}}\frac{\partial}{\partial\varepsilon}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}) + \int_{\partial\Omega_\mu}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{n}\cdot\mathbf{v}\\ &\quad + \int_{\partial\Omega_\mu^i}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}. \quad (3.18)\end{aligned}$$

Next, by using the concept of spatial derivative and (2.12), we find that the first term of the above right hand side integral can be written as

$$\frac{\partial}{\partial\varepsilon}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}'_{\mu_\varepsilon}, \quad (3.19)$$

where the prime denotes the (partial) spatial derivative with respect to ε. Further, note that the relation (3.14) gives

$$\mathbf{E}'_{\mu_\varepsilon} = \nabla^s\tilde{\mathbf{u}}'_{\mu_\varepsilon} = \nabla^s(\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - \nabla\tilde{\mathbf{u}}_{\mu_\varepsilon}\mathbf{v}). \quad (3.20)$$

Then, by introducing the above expression into (3.19) we obtain

$$\frac{\partial}{\partial\varepsilon}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon}\mathbf{v}). \quad (3.21)$$

With the above result, the sensitivity of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ reads

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= \int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon}\mathbf{v}) + \int_{\partial\Omega_\mu}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{n}\cdot\mathbf{v}\\ &\quad + \int_{\partial\Omega_\mu^i}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}. \quad (3.22)\end{aligned}$$

Now, note that by definition of the spaces of virtual displacements we have $\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon}$. This, together with the equilibrium equation (3.8), implies that the first term of (3.22) vanishes. Then, we obtain

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= -\int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon}\cdot\nabla^s(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon}\mathbf{v}) + \int_{\partial\Omega_\mu}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{v}\cdot\mathbf{n}\\ &\quad + \int_{\partial\Omega_\mu^i}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}. \qquad (3.23)\end{aligned}$$

In view of the tensor relation

$$\operatorname{div}\left(\mathbf{T}_{\mu_\varepsilon}^{\mathrm{T}}\left[(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\,\mathbf{v}\right]\right) = \mathbf{T}_\varepsilon\cdot\nabla^s\left[(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\,\mathbf{v}\right] + \operatorname{div}(\mathbf{T}_{\mu_\varepsilon})\cdot(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\,\mathbf{v}, \qquad (3.24)$$

and the divergence theorem, expression (3.23) can be written as

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= 2\int_{\Omega_{\mu_\varepsilon}}\operatorname{div}\mathbf{T}_{\mu_\varepsilon}\cdot(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\,\mathbf{v} + \int_{\partial\Omega_\mu}[(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{I} - 2\,(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})^{\mathrm{T}}\,\mathbf{T}_{\mu_\varepsilon}]\mathbf{n}\cdot\mathbf{v}\\ &\quad + \int_{\partial\Omega_\mu^i}[\![(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{I} - 2\,(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})^{\mathrm{T}}\,\mathbf{T}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}\\ &\quad + \int_{\partial\mathcal{I}_\varepsilon}[\![(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{I} - 2\,(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})^{\mathrm{T}}\,\mathbf{T}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}. \qquad (3.25)\end{aligned}$$

Finally, since the stress field $\mathbf{T}_{\mu_\varepsilon}$ is in equilibrium, we have that $\operatorname{div}\mathbf{T}_{\mu_\varepsilon} = \mathbf{0}$ in Ω_{μ_ε} so that a straightforward rearrangement of the above yields (3.17). □

Corollary 3.3. *By applying the divergence theorem to the right hand side of (3.10), we obtain*

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= \int_{\partial\Omega_\mu}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} + \int_{\partial\Omega_\mu^i}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{v}\\ &\quad - \int_{\Omega_{\mu_\varepsilon}}\operatorname{div}(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v}\,d\Omega_\mu. \qquad (3.26)\end{aligned}$$

Since (3.17) and (3.26) remain valid for all velocity fields $\mathbf{v}\in\overline{\Omega_{\mu_\varepsilon}}$, *we have*

$$\int_{\Omega_{\mu_\varepsilon}}\operatorname{div}(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v}\,d\Omega_\mu = 0 \quad \forall\mathbf{v}\in\Omega_{\mu_\varepsilon} \quad \Rightarrow \quad \operatorname{div}(\mathbf{\Sigma}_{\mu_\varepsilon}) = \mathbf{0} \ \textit{in}\ \Omega_{\mu_\varepsilon}, \qquad (3.27)$$

i.e. $\mathbf{\Sigma}_{\mu_\varepsilon}$ *is a divergence-free field.* □

From the above corollary it follows that the shape derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$, for the particular case of an uniform expansion of the perturbation – circular inclusion – can be expressed exclusively in terms of an integral over the boundary $\partial\mathcal{I}_\varepsilon$ of the inclusion:

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = -\int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n}. \qquad (3.28)$$

In order to derive an explicit expression for the integrand on the right hand side of (3.28), 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

$$\begin{aligned} \mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} &= \mathrm{T}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n}) + \mathrm{T}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t}) + \mathrm{T}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n}) + \mathrm{T}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}), \\ \mathbf{E}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} &= \mathrm{E}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n}) + \mathrm{E}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t}) + \mathrm{E}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n}) + \mathrm{E}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}). \end{aligned} \tag{3.29}$$

The Neumann boundary condition along $\partial\mathcal{I}_\varepsilon$, together with $(3.29)_1$, gives

$$\begin{aligned} [\![\tilde{\mathbf{T}}_{\mu_\varepsilon}]\!]\mathbf{n}|_{\partial\mathcal{I}_\varepsilon} &= -[\![\bar{\mathbf{T}}^*_\mu]\!]\mathbf{n} \quad\Rightarrow\quad [\![\mathbf{T}_{\mu_\varepsilon}]\!]\mathbf{n}|_{\partial\mathcal{I}_\varepsilon} = \mathbf{0}, \\ &\Rightarrow\quad \mathrm{T}^{nn}_{\mu_\varepsilon}|_m = \mathrm{T}^{nn}_{\mu_\varepsilon}|_i \quad\text{and}\quad \mathrm{T}^{tn}_{\mu_\varepsilon}|_m = \mathrm{T}^{tn}_{\mu_\varepsilon}|_i \quad \text{on} \quad \partial\mathcal{I}_\varepsilon. \end{aligned} \tag{3.30}$$

Similarly to eq. (3.29), the fluctuation displacement field $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ can be decomposed on $\partial\mathcal{I}_\varepsilon$ as

$$\tilde{\mathbf{u}}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} = \tilde{\mathrm{u}}^n_{\mu_\varepsilon}\mathbf{n} + \tilde{\mathrm{u}}^t_{\mu_\varepsilon}\mathbf{t}. \tag{3.31}$$

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

$$[\![\tilde{\mathbf{u}}_{\mu_\varepsilon}]\!]|_{\partial\mathcal{I}_\varepsilon} = \mathbf{0} \quad\Rightarrow\quad \left.\frac{\partial\tilde{\mathbf{u}}_{\mu_\varepsilon}}{\partial t}\right|_m = \left.\frac{\partial\tilde{\mathbf{u}}_{\mu_\varepsilon}}{\partial t}\right|_i \ \text{on}\ \partial\mathcal{I}_\varepsilon. \tag{3.32}$$

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

$$\tilde{\mathrm{E}}^{tt}_{\mu_\varepsilon}|_m = \tilde{\mathrm{E}}^{tt}_{\mu_\varepsilon}|_i. \tag{3.33}$$

In addition, in view of the additive split (2.7), condition (3.33) establishes the continuity of component tt of the strain tensor $\mathbf{E}_{\mu\varepsilon}$, i.e.,

$$\mathrm{E}^{tt}_{\mu_\varepsilon}|_m = \mathrm{E}^{tt}_{\mu_\varepsilon}|_i. \tag{3.34}$$

By taking into account the decompositions (3.29) and (3.31) and the continuity condition (3.30), (3.32) and (3.34), the jump of the Eshelby tensor flux in the normal direction to the boundary of the perturbation $\mathcal{I}_\varepsilon$ can be written as

$$[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = [\![\mathrm{T}^{tt}_{\mu_\varepsilon}]\!]\mathrm{E}^{tt}_{\mu_\varepsilon}|_i - [\![\tilde{\mathrm{E}}^{nn}_{\mu_\varepsilon}]\!]\mathrm{T}^{nn}_{\mu_\varepsilon}|_i - \left[\!\!\left[\frac{\partial\tilde{\mathrm{u}}^t_{\mu_\varepsilon}}{\partial n}\right]\!\!\right]\mathrm{T}^{nt}_{\mu_\varepsilon}|_i. \tag{3.35}$$

Note that, by using the constitutive law (3.5), the jump terms on the right hand side of the above expression satisfy

$$[\![\mathrm{T}^{tt}_{\mu_\varepsilon}]\!] = E(1-\gamma)\mathrm{E}^{tt}_{\mu_\varepsilon}|_i, \tag{3.36}$$

$$[\![\tilde{\mathrm{E}}^{nn}_{\mu_\varepsilon}]\!] = \frac{1-\nu^2}{E}\left(\frac{\gamma-1}{\gamma}\tilde{\mathrm{T}}^{nn}_{\mu_\varepsilon}|_i - [\![\bar{\mathrm{T}}^{nn}_\mu]\!]\right), \tag{3.37}$$

$$\left[\!\!\left[\frac{\partial\tilde{\mathrm{u}}^t_{\mu_\varepsilon}}{\partial n}\right]\!\!\right] = 2\frac{1-\nu}{E}\left(\frac{\gamma-1}{\gamma}\tilde{\mathrm{T}}^{tn}_{\mu_\varepsilon}|_i - [\![\bar{\mathrm{T}}^{tn}_\mu]\!]\right), \tag{3.38}$$

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 $\mathrm{T}^{tn}_{\mu_\varepsilon}$ of the stress tensor $\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon}$ given by $(3.29)_1$.

By introducing the above results into (3.35) and taking into account the additive decomposition of the components of the microscopic stress field $\mathbf{T}_{\mu_\varepsilon}$ we find that the jump of the Eshelby tensor flux in the normal direction to the boundary $\partial\mathcal{I}_\varepsilon$ has the following representation in terms of the solution inside the perturbation $\mathcal{I}_\varepsilon$:

$$[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = \frac{1-\gamma}{\gamma^2 E}\left[\left(\mathrm{T}^{tt}_{\mu_\varepsilon}|_i - \nu\mathrm{T}^{nn}_{\mu_\varepsilon}|_i\right)^2 + \gamma(1-\nu^2)\mathrm{T}^{nn}_{\mu_\varepsilon}|_i^2 + 2\gamma(1+\nu)\mathrm{T}^{tn}_{\mu_\varepsilon}|_i^2\right]. \tag{3.39}$$

In order to obtain an analytical formula for the boundary integral (3.28) we make use of the classical asymptotic analysis for two-dimensional elasticity problems (see Appendix A). Thus, the distribution of the microscopic stress field on boundary $\partial\mathcal{I}_\varepsilon$ can be written as

$$\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{I}_\varepsilon} = \mathbb{L}\bar{\mathbf{T}}_\mu + \mathbb{S}\tilde{\mathbf{T}}_\mu + \mathcal{O}(\varepsilon), \tag{3.40}$$

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

$$\mathbb{L} = \gamma\frac{1-\gamma}{1+\alpha\gamma}\left[\frac{1+\alpha}{1-\gamma}\mathbb{I} + \frac{\beta-\alpha}{2(1+\beta\gamma)}(\mathbf{I}\otimes\mathbf{I})\right], \tag{3.41}$$

$$\mathbb{S} = \frac{\gamma}{(1+\alpha\gamma)(1+\nu)}\left\{4\mathbb{I} + \left[\frac{\beta(1+\alpha\gamma)}{1+\beta\gamma} - 2\right](\mathbf{I}\otimes\mathbf{I})\right\}, \tag{3.42}$$

where the constants α and β are defined as

$$\alpha := \frac{3-\nu}{1+\nu} \quad \text{and} \quad \beta := \frac{1+\nu}{1-\nu}. \tag{3.43}$$

With the stress distribution along the boundary $\partial\mathcal{I}_\varepsilon$ shown in eq. (3.40) and the result (3.39), we can obtain the topological derivative by evaluating the boundary integral (3.28) analytically. This gives

$$\int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}]\!]\mathbf{n}\cdot\mathbf{n} = \frac{2\pi\varepsilon}{E}\left(\frac{1-\gamma}{1+\alpha\gamma}\right)\left[4\mathbf{T}_\mu\cdot\mathbf{T}_\mu + \frac{\gamma(\alpha-2\beta)-1}{1+\beta\gamma}(\mathrm{tr}\mathbf{T}_\mu)^2\right] + o(\varepsilon). \tag{3.44}$$

Finally, by substituting the above in (3.9) and adopting the function $f(\varepsilon)$ as the size (area) of the circular perturbation, we obtain the explicit closed form expression for the topological derivative of ψ:

$$D_T\psi = -\mathbb{H}\mathbf{T}_\mu\cdot\mathbf{T}_\mu. \tag{3.45}$$

where the fourth order tensor $\mathbb{H}$ is defined as

$$\mathbb{H} := \frac{1}{E}\left(\frac{1-\gamma}{1+\alpha\gamma}\right)\left[4\mathbb{I} + \frac{\gamma(\alpha-2\beta)-1}{1+\beta\gamma}(\mathbf{I}\otimes\mathbf{I})\right]. \tag{3.46}$$

(*c*) *The sensitivity of the macroscopic elasticity tensor*

Expressions (3.3) and (3.45) promptly lead to the explicit formula for the topological asymptotic expansion of ψ:

$$\mathbf{T}^\varepsilon\cdot\mathbf{E} = \mathbf{T}\cdot\mathbf{E} - v(\varepsilon)\mathbb{H}\mathbf{T}_\mu\cdot\mathbf{T}_\mu + o(v(\varepsilon)), \tag{3.47}$$

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

The approach used in Section 2(b) to obtain a closed form expression for the macroscopic elasticity tensor $\mathbb{C}$ can be easily extended to derive an analytical formula for its topological sensitivity – the main result of this paper. Accordingly, we write the microscopic strain as a linear combination of the Cartesian components of its macroscopic counterpart:

$$\mathbf{E}_\mu = \mathrm{E}_{ij}\left(\mathbf{e}_i \otimes \mathbf{e}_j + \tilde{\mathbf{E}}_{\mu_{ij}}\right) = \mathrm{E}_{ij}\mathbf{E}_{\mu_{ij}}. \tag{3.48}$$

With the introduction of the above expression in (2.12), the microscopic stress tensor $\mathbf{T}_\mu$ can be written as

$$\mathbf{T}_\mu = \mathrm{E}_{ij}\mathbb{C}_\mu\mathbf{E}_{\mu_{ij}} = (\mathbf{T}_{\mu_{ij}} \otimes \mathbf{e}_i \otimes \mathbf{e}_j)\mathbf{E}, \tag{3.49}$$

where $\mathbf{T}_{\mu_{ij}}$ denotes the microspic stress field associated with each displacement fluctuation field $\tilde{\mathbf{u}}_{\mu_{ij}}$ that solves the variational equation (2.27). Then, by combining (3.45) and (3.49) we obtain the following alternative formula for the topological derivative of ψ

$$D_T\psi = -\mathbb{D}_{T\mu}\mathbf{E} \cdot \mathbf{E}, \tag{3.50}$$

where $\mathbb{D}_{T\mu}$ is the fourth order symmetric tensor field over Ω_μ defined by

$$\mathbb{D}_{T\mu} = \mathbb{H}\mathbf{T}_{\mu_{ij}} \cdot \mathbf{T}_{\mu_{kl}}(\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l), \qquad i,j,k,l = 1,2. \tag{3.51}$$

Our main result – the asymptotic expansion of the macroscopic elasticity tensor and the corresponding sensitivity formula – is presented in the following. From (3.45), (3.47) and (3.50) and by making use of the fact that the macroscopic constitutive response is linear elastic, we obtain

$$\mathbb{C}_\varepsilon\,\mathbf{E} \cdot \mathbf{E} = \mathbb{C}\,\mathbf{E} \cdot \mathbf{E} - v(\varepsilon)\mathbb{D}_{T\mu}\mathbf{E} \cdot \mathbf{E} + o(v(\varepsilon)), \tag{3.52}$$

where $\mathbb{C}_\varepsilon$ is the macroscopic elasticity tensor of the topologically perturbed microstructure, i.e.

$$\mathbf{T}^\varepsilon = \mathbb{C}_\varepsilon\,\mathbf{E}. \tag{3.53}$$

Finally, since (3.52) is valid for any $\mathbf{E}$ we arrive at explicit expression for the topological expansion of the macroscopic elasticity tensor:

$$\mathbb{C}_\varepsilon = \mathbb{C} - v(\varepsilon)\mathbb{D}_{T\mu} + o(v(\varepsilon)). \tag{3.54}$$

Remark: *The topological sensitivity tensor $\mathbb{D}_{T\mu}$ field over Ω_μ, whose explicit expression is given by (3.51), provides a first order accurate measure of how the macroscopic elasticity tensor varies when a topological perturbation (a circular inclusion) is added to the RVE. The value of each Cartesian component $(\mathbb{D}_{T\mu})_{ijkl}$ at an arbitrary point $\boldsymbol{y} \in \Omega_\mu$ 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 $\boldsymbol{y}$. The remarkable simplicity of the closed form sensitivity given by (3.51) is to be noted. Once the vector fields $\tilde{\mathbf{u}}_{\mu_{ij}}$ have been obtained as solutions of (2.27) for the* original *RVE domain, the sensitivity tensor $\mathbb{D}_{T\mu}$ can be trivially assembled.*
Remark: *The topological derivative tensor $\mathbb{D}_{T\mu}$ is dependent upon the contrast parameter γ. This dependency is made explicit in definition (3.46) of the tensor*

$\mathbb{H}$. *Note that the limiting cases* $\gamma \to 0$ *and* $\gamma \to \infty$ *correspond, respectively, to the insertion of a hole (infinitely compliant material) and a rigid inclusion (infinitely stiff material). In such cases, the sensitivity tensor is calculated by means of (3.51) with*

$$\mathbb{H} = \frac{1}{E}[4\mathbb{I} - (\mathbf{I} \otimes \mathbf{I})], \tag{3.55}$$

and

$$\mathbb{H} = -\frac{1}{E\alpha}\left[4\mathbb{I} + \frac{\alpha - 2\beta}{\beta}(\mathbf{I} \otimes \mathbf{I})\right] \tag{3.56}$$

respectively. Expression (3.55) coincides with the result derivated in Giusti et al. *(2009*b*) for the sensitivity of the macroscopic elasticity to the insertion of holes in the microscale.*

4. Example of application. Micro-structure topology synthesis

The explicit formula for the macroscopic elasticity sensitivity derived above is a fundamental result with potential application in different areas of interest. In this section we show what is probably its most intuitive and straightforward application – the finite element-based automatic synthesis of a microstructure to meet a pre-specified macroscopic response.

Crucial to the proposed application is the definition of a measure of distance $d(\mathbb{A}, \mathbb{B})$ between two generic symmetric fourth-order tensors $\mathbb{A}$ and $\mathbb{B}$. Here we shall adopt simply the square of the Euclidean norm of the difference between the two tensors, i.e.

$$d(\mathbb{A}, \mathbb{B}) := \|\mathbb{A} - \mathbb{B}\|^2 = \|\mathbb{A}\|^2 - 2\mathbb{A} \cdot \mathbb{B} + \|\mathbb{B}\|^2 . \tag{4.1}$$

Then, for a pre-specified *target* constitutive tensor $\mathbb{C}^\star$, we conveniently define the functions $\phi(\varepsilon)$ and $\phi(0)$, respectively, as

$$\phi(\varepsilon) := d(\mathbb{C}_\varepsilon, \mathbb{C}^\star) \qquad \text{and} \qquad \phi(0) := d(\mathbb{C}, \mathbb{C}^\star). \tag{4.2}$$

Next, note that by taking into account the asymptotic expansion (3.54) of the homogenized elasticity tensor and definitions (4.1) and (4.2) we obtain the following asymptotic topological expansion of the function $\phi(\varepsilon)$:

$$\begin{aligned} \phi(\varepsilon) = \|\mathbb{C}_\varepsilon - \mathbb{C}^\star\|^2 &= \|[\mathbb{C} - v(\varepsilon)\mathbb{D}_{T\mu} + o(v(\varepsilon))] - \mathbb{C}^\star\|^2 \\ &= \|\mathbb{C} - \mathbb{C}^\star\|^2 - 2v(\varepsilon)\mathbb{D}_{T\mu} \cdot (\mathbb{C} - \mathbb{C}^\star) + o(v(\varepsilon)) \\ &= \phi(0) + D_T\phi + o(v(\varepsilon)), \end{aligned} \tag{4.3}$$

where we have identified the topological derivative of the function ϕ as

$$D_T\phi = -2\mathbb{D}_{T\mu} \cdot (\mathbb{C} - \mathbb{C}^\star). \tag{4.4}$$

Remark: *Note that the topological derivative of* ϕ *has been derived here without the need to perform a full topological asymptotic analysis. Indeed, the derivation has been based on simply introducing (3.54) into (4.2)*$_1$ *and then collecting the terms of same power of* ε*. This procedure can be followed for any function of the macroscopic elasticity tensor which possesses the required degree of regularity.*

(*a*) *A simple microstructural synthesis algorithm*

With the above at hand, we are now ready to devise a simple algorithm to synthesise a bi-material microstructure whose macroscopic response is characterised by $\mathbb{C}^\star$. Our task here is to produce a sequence of changes to a given initial microstructure topology in order to achieve a final topology for which the value of ϕ (a non-negative function) is as close as possible to zero (the zero value obviously corresponds to a perfect match between the target and actual predicted response). A very simple procedure consists in simply requiring at each iteration of the algorithm that a small inclusion be introduced at points $\hat{\boldsymbol{y}}$ of the RVE where the field $D_T\phi$ is most negative. This kind of algorithms has been widely used in the context of topological optimization by using the topological derivative as a feasible descent direction. A detailed development of algorithms of the present type can be found in the work of Giusti *et al.* (2008). For completeness, the algorithm can be summarized in the following:

- **Provide** a complete description of the initial guess (initial topology) of the RVE with domain Ω_μ and the parameter γ defining the phase contrast; a target macroscopic constitutive response $\mathbb{C}^\star$; the maximum number of iterations allowed N and a numerical convergence tolerance ϵ.

- **While** $\phi > \epsilon$ and $j \leq N$, **do**:
  - **Compute** $\mathbb{C}^j$, $\mathbb{D}^j_{T\mu}$ and $D^j_{T\mu}\phi$ in the domain Ω^j_μ.
  - **Change** the material properties of ne finite elements where $D^j_{T\mu}\phi$ is most negative.
  - **Set** $\Omega^{j+1}_\mu = \Omega^j_\mu$ and $j \leftarrow j+1$.

In the above, j denotes the current iteration, Ω^j_μ is the topologically perturbed domain at iteration j, ne is the number of finite elements to be changed their material properties at each iteration j ; and $\mathbb{C}^j$, $\mathbb{D}^j_{T\mu}$ and $D^j_{T\mu}\phi$ are, respectively, the macroscopic elasticity tensor, the topological sensitivity tensor field and the topological derivative field (4.4) evaluated for the domain Ω^j_μ.

(*b*) *Application. Automatic synthesis of a bi-material microstructure*

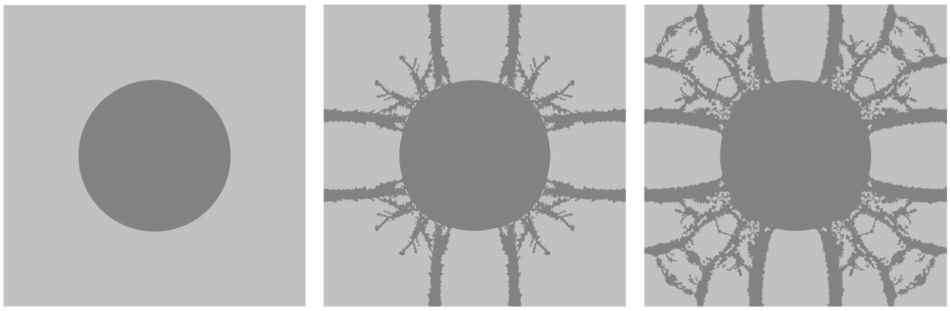
Here the above algorithm is used to generate a two-dimensional bi-material microstructure to meet a pre-specified macroscopic constitutive response under plane stress conditions. The (normalised) Young's modulus of the matrix and inclusion materials are, respectively, $E^m_\mu = 0.01$ and $E^i_\mu = 1.0$, both having Poisson's ratio $\nu = 0.3$. The target two-dimensional elasticity tensor is chosen as

$$\mathbb{C}^\star = \begin{bmatrix} 0.165 & 0.049 & 0 \\ 0.049 & 0.165 & 0 \\ 0 & 0 & 0.013 \end{bmatrix}. \tag{4.5}$$

The starting topology of the RVE consists of a unit square homogeneous matrix with a circular inclusion of diameter 0.50 at the centre of the RVE. In this particular example the widely used periodicity assumption (2.19) is adopted in the prediction of the macroscopic behaviour. The corresponding macroscopic elasticity is

$$\mathbb{C}^0 = \begin{bmatrix} 0.015 & 0.004 & 0 \\ 0.004 & 0.015 & 0 \\ 0 & 0 & 0.005 \end{bmatrix}. \tag{4.6}$$

To solve the set of variational problem at the RVE, we use the finite element strategy proposed by Giusti *et al.* (2009*a*). A fine structured finite element mesh consisting of 93,080 three-noded (linear) triangles is used to discretise the RVE. The mesh is kept constant and only the properties of the elements change (between E_μ^m and E_μ^i) throughout the iterations according to the criterion set out in the definition of the algorithm above. In particular, the parameter ne is chosing as 1% of the total number of elements. Figure 4 illustrates the evolution of the topology during the automatic synthesis procedure. It shows the initial, an intermediate and the final topology. The dark areas correspond to inclusion material and the light coloured areas to matrix material. Figure 5 shows the periodic assemble of the final



(a) (b) (c)

Figure 4. RVE topology evolution. (a) Given initial topology; (b) Intermediate topology at iteration 20, and; (c) Final topology (iteration 100).

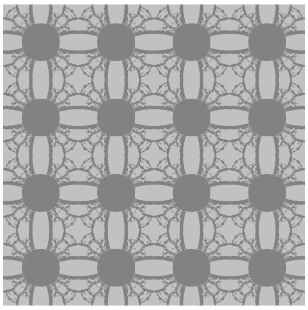
microstructure topology and the corresponding evolution of the distance function ϕ. The final topology has macroscopic elasticity tensor

$$\mathbb{C} = \begin{bmatrix} 0.165 & 0.048 & 0 \\ 0.048 & 0.165 & 0 \\ 0 & 0 & 0.016 \end{bmatrix} \tag{4.7}$$

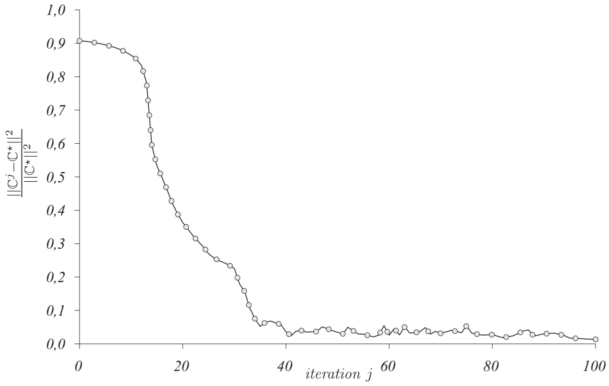
with corresponding normalised value of the distance function $\phi \approx 0.013$. We remark that due to the simplicity of the derived topological derivative formula, the calculations required by the algorithm are straightforward and of easy computational implementation.

5. Conclusions

A fundamental analytical formula for the sensitivity of the two-dimensional macroscopic elasticity tensor to the insertion of circular inclusions has been derived by applying the concept of topological derivative within a well-established multi-scale



(a)



(b)

Figure 5. Final results. (a) Periodic microstructures; (b) Evolution of the relative value of function ϕ.

constitutive modelling framework for linear elasticity. The multi-scale constitutive framework is based on the assumption that the macroscopic strain and stress tensors are defined as volume averages of their microscopic counterparts over an RVE. It allows different predictions of macroscopic behaviour – including an upper and a lower bound for stiffness – to be obtained according to the chosen kinematical constraints imposed upon 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 microscale. This result is fundamental and has potential application in different areas of interest. To illustrate its potential applicability, a very simple algorithm based on the proposed formula and relying on the finite element approximation of the RVE equilibrium problem has been devised to synthesise a microstructure to a prespecified macroscopic response. The numerical results have shown the successful use of the proposed expression in this context. Further use of the present formula in the context of microstructural optimisation is currently under investigation and will be the subject of a forthcoming publication.

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Appendix A. Asymptotic analysis

This appendix presents the derivation of the asymptotic formula used in the topological sensitivity analysis developed in Section 3(b). We start by considering the following expansion of the stress fluctuation field associated with the solution $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ to problem (3.8), see Sokołowski & Żochowski (1999):

$$\tilde{\mathbf{T}}_{\mu_\varepsilon} = \tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon} + o(\varepsilon), \tag{A 1}$$

where $\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon}$ denotes the solution of the elasticity system (3.8) in the infinite domain $\Re^2 \backslash \overline{\mathcal{H}_\varepsilon}$, such that the stresses $\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon}$ tend to a constant value when $\|\boldsymbol{y}\| \to \infty$. Then, the exterior problem can be written as

$$\left\{\begin{array}{llll} \text{div}\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon} & = \mathbf{0} & \text{in} & \Re^2\backslash\overline{\mathcal{H}_\varepsilon} \\ \text{div}\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon} & = \mathbf{0} & \text{in} & \mathcal{I}_\varepsilon \\ \tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon} & \to \tilde{\mathbf{T}}_\mu & \text{at} & \infty \\ [\![\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon}]\!]\mathbf{n} & = -[\![\bar{\mathbf{T}}_\mu]\!]\mathbf{n} & \text{on} & \partial\mathcal{I}_\varepsilon, \end{array}\right. \tag{A 2}$$

where $\mathbf{n}$ denotes the outward unit normal to the boundary $\partial\mathcal{I}_\varepsilon$, $\tilde{\mathbf{T}}_\mu$ is the solution of the unperturbed problem (2.17) and $\bar{\mathbf{T}}_\mu$ is defined in (2.15).

In a polar coordinate system (r,θ) having its origin at the centre of the hole $\mathcal{H}_\varepsilon$ and with the angle θ measured with respect to one of the principal directions of $\tilde{\mathbf{T}}_\mu$, the components of the solution of the partial differential equation (A 2), see Obert & Duvall (1967); Little (1973), are given by

- Exterior solution $(r \geq \varepsilon)$

$$\begin{aligned} (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{rr} &= \bar{S}\tfrac{1}{1+\beta\gamma}\tfrac{\varepsilon^2}{r^2} + \bar{D}\tfrac{1}{1+\alpha\gamma}\tfrac{\varepsilon^2}{r^2}\left(4-3\tfrac{\varepsilon^2}{r^2}\right)\cos 2(\theta+\varphi) \\ &\quad +\tilde{S}\left(1-\tfrac{1-\gamma}{1+\beta\gamma}\tfrac{\varepsilon^2}{r^2}\right) + \tilde{D}\left[1-\tfrac{1-\gamma}{1+\alpha\gamma}\tfrac{\varepsilon^2}{r^2}\left(4-3\tfrac{\varepsilon^2}{r^2}\right)\right]\cos 2\theta, \\ (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{\theta\theta} &= -\bar{S}\tfrac{1}{1+\beta\gamma}\tfrac{\varepsilon^2}{r^2} + \bar{D}\tfrac{3}{1+\alpha\gamma}\tfrac{\varepsilon^4}{r^4}\cos 2(\theta+\varphi) \\ &\quad +\tilde{S}\left(1+\tfrac{1-\gamma}{1+\beta\gamma}\tfrac{\varepsilon^2}{r^2}\right) - \tilde{D}\left(1+3\tfrac{1-\gamma}{1+\alpha\gamma}\tfrac{\varepsilon^4}{r^4}\right)\cos 2\theta, \\ (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{\theta r} &= \bar{D}\tfrac{1}{1+\alpha\gamma}\tfrac{\varepsilon^2}{r^2}\left(2-3\tfrac{\varepsilon^2}{r^2}\right)\sin 2(\theta+\varphi) \\ &\quad -\tilde{D}\left[1+\tfrac{1-\gamma}{1+\alpha\gamma}\tfrac{\varepsilon^2}{r^2}\left(2-3\tfrac{\varepsilon^2}{r^2}\right)\right]\cos 2\theta. \end{aligned} \tag{A 3}$$

- Interior solution $(0 < r < \varepsilon)$

$$\begin{aligned} (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{rr} &= -\tfrac{\beta\gamma}{1+\beta\gamma}\left[\bar{S}-\tfrac{2}{1+\nu_m}\tilde{S}\right] - \tfrac{\alpha\gamma}{1+\alpha\gamma}\left[\bar{D}\cos 2(\theta+\varphi) - \tfrac{4}{3-\nu_m}\tilde{D}\cos 2\theta\right], \\ (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{\theta\theta} &= -\tfrac{\beta\gamma}{1+\beta\gamma}\left[\bar{S}-\tfrac{2}{1+\nu_m}\tilde{S}\right] + \tfrac{\alpha\gamma}{1+\alpha\gamma}\left[\bar{D}\cos 2(\theta+\varphi) - \tfrac{4}{3-\nu_m}\tilde{D}\cos 2\theta\right], \\ (\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon})^{\theta r} &= \tfrac{\alpha\gamma}{1+\alpha\gamma}\left[\bar{D}\sin 2(\theta+\varphi) - \tfrac{4}{3-\nu_m}\tilde{D}\sin 2\theta\right]. \end{aligned} \tag{A 4}$$

where φ indicates the angle between principal stress directions associated to the stress fields $\bar{\mathbf{T}}_\mu$ and $\tilde{\mathbf{T}}_\mu$. In addition, we denote

$$\bar{S} = -(1-\gamma)\frac{\bar{\sigma}_{\mu_1}+\bar{\sigma}_{\mu_2}}{2}, \quad \tilde{S} = \frac{\tilde{\sigma}_{\mu_1}+\tilde{\sigma}_{\mu_2}}{2}, \tag{A 5}$$

$$\bar{D} = -(1-\gamma)\frac{\bar{\sigma}_{\mu_1}-\bar{\sigma}_{\mu_2}}{2}, \quad \tilde{D} = \frac{\tilde{\sigma}_{\mu_1}-\tilde{\sigma}_{\mu_2}}{2}, \tag{A 6}$$

with $\bar{\sigma}_{\mu_{1,2}}$ and $\tilde{\sigma}_{\mu_{1,2}}$ representing the principal stresses associated with the displacement fields $\bar{\mathbf{u}}$ and $\tilde{\mathbf{u}}_\mu$ of the original (unperturbed) domain Ω_μ. The constants α and β used in eqs. (A 3) and (A 4) are given by

$$\alpha = \frac{3-\nu_m}{1+\nu_m} \quad \text{and} \quad \beta = \frac{1+\nu_m}{1-\nu_m}. \tag{A 7}$$

References

Amstutz, S., Horchani, I. & Masmoudi, M. 2005 Crack detection by the topological gradient method. *Control and Cybernetics*, **34**(1), 81–101.

Bensoussan, A., Lions, J. & Papanicolau, G. 1978 *Asymptotic analysis for periodic microstructures*. Amsterdam: North Holland.

Céa, J., Garreau, S., Guillaume, P. & Masmoudi, M. 2000 The shape and topological optimizations connection. *Computer Methods in Applied Mechanics and Engineering*, **188**(4), 713–726.

de Souza Neto, E. & Feijóo, R. 2006 Variational foundations of multi-scale constitutive models of solid: small and large strain kinematical formulation. Tech. Rep. N 16/2006, Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, Brasil.

Eshelby, J. 1975 The elastic energy-momentum tensor. *Journal of Elasticity*, **5**(3-4), 321–335.

Garreau, S., Guillaume, P. & Masmoudi, M. 2001 The topological asymptotic for pde systems: the elasticity case. *SIAM Journal on Control and Optimization*, **39**(6), 1756–1778.

Germain, P., Nguyen, Q. & Suquet, P. 1983 Continuum thermodynamics. *Journal of Applied Mechanics, Transactions of the ASME*, **50**(4), 1010–1020.

Giusti, S., Novotny, A. & Padra, C. 2008 Topological sensitivity analysis of inclusion in two-dimensional linear elasticity. *Engineering Analysis with Boundary Elements*, **32**(11), 926–935.

Giusti, S., Blanco, P., de Souza Neto, E. & Feijóo, R. 2009*a* An assessment of the Gurson yield criterion by a computational multi-scale approach. *Engineering Computations*, **26**(3), 281–301.

Giusti, S., Novotny, A., de Souza Neto, E. & Feijóo, R. 2009*b* Sensitivity of the macroscopic elasticity tensor to topological microstructural changes. *Journal of the Mechanics and Physics of Solids*, **57**(3), 555–570.

Guest, J. & Prevost, J. 2006 Optimizing multifunctional materials: design of microstructures for maximized stiffness and fluid permeability. *International Journal of Solids and Structures*, **43**(22-23), 7028–7047.

Gurson, A. 1977 Continuum theory of ductile rupture by void nucleation and growth: Part i – yield criteria and flow rule for porous ductile media. *Journal Engineering Materials and Technology – Transactions of the ASME*, **99**(1), 2–15.

Gurtin, M. 1981 *An introduction to continuum mechanics*. Mathematics in Science and Engineering vol. 158. New York: Academic Press.

Gurtin, M. 2000 *Configurational forces as basic concept of continuum physics*. Applied Mathematical Sciences vol. 137. New York: Springer-Verlag.

Hashin, Z. & Shtrikman, S. 1963 A variational approach to the theory of the elastic behaviour of multiphase materials. *Jounal of the Mechanics and Physics of Solids*, **11**(2), 127–140.

Hill, R. 1963 Elastic properties of reinforced solids: Some theoretical principles. *Journal of the Mechanics and Physics of Solids*, **11**, 357–372.

Hill, R. 1965 A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, **13**(4), 213–222.

Hyun, S. & Torquato, S. 2001 Designing composite microstructures with targeted properties. *Journal of Materials Research*, **16**(1), 280–285.

Kikuchi, N., Nishiwaki, S., Fonseca, J. & Silva, E. 1998 Design optimization method for compliant mechanics and material microstructure. *Computer Methods in Applied Mechanics and Engineering*, **151**(3-4), 401–417.

Little, R. 1973 *Elasticity.* New Jersey: Prentice-Hall.

Mandel, J. 1971 *Plasticité classique et viscoplasticité.* CISM Lecture Notes. Udine: Springer-Verlag.

Matsui, K., Terada, K. & Yuge, K. 2004 Two-scale finite element analysis of heterogeneous solids with periodic microstructure. *Computer and Structures*, **82**(7-8), 593–606.

Michel, J., Moulinec, H. & Suquet, P. 1999 Effective properties of composite materials with periodic microstructure: a computational approach. *Computer Methods in Applied Mechanics and Engineering*, **172**(1-4), 109–143.

Miehe, C., Schotte, J. & Schröder, J. 1999 Computational micro-macro transitions and overall moduli in the analysis of polycrystals at large strains. *Computational Materials Science*, **16**(1-4), 372–382.

Nazarov, S. & Sokołowski, J. 2003 Asymptotic analysis of shape functionals. *Journal de Mathématiques Pures et Appliquées*, **82**(2), 125–196.

Novotny, A., Feijóo, R., Padra, C. & Taroco, E. 2003 Topological sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, **192**(7-8), 803–829.

Novotny, A., Feijóo, R., Taroco, E. & Padra, C. 2007 Topological sensitivity analysis for three-dimensional linear elasticity problem. *Computer Methods in Applied Mechanics and Engineering*, **196**(41-44), 4354–4364.

Obert, L. & Duvall, W. 1967 *Rock mechanics and the design of structures in rock.* New York: John Wiley & Sons.

Sanchez-Palencia, E. 1980 *Non-homogeneous media and vibration theory*, vol. 127 of *Lecture Notes in Physics 127.* Berlin: Springer-Verlag.

Sigmund, O. 1994 Materials with prescribed constitutive parameters: an inverse homogenization problem. *International Journal Solids and Structures*, **31**(17), 2313–2329.

Silva, E., Fonseca, J. & Kikuchi, N. 1997 Optimal design of periodic microstructures. *Computational Mechanics*, **19**(5), 397–410.

Sokołowski, J. & Żochowski, A. 1999 On the topological derivatives in shape optmization. *SIAM Journal on Control and Optimization*, **37**(4), 1251–1272.

Sokołowski, J. & Żochowski, A. 2001 Topological derivatives of shape functionals for elasticity systems. *Mechanics of Structures and Machines*, **29**(3), 333–351.

Sokołowski, J. & Zolésio, J. 1992 *Introduction to shape optimization - shape sensitivity analysis.* New York: Springer-Verlag.

Speirs, D., de Souza Neto, E. & Perić, D. 2008 An approach to the mechanical constitutive modelling of arterial tissue based on homogenization and optimization. *Journal of Biomechanics*, **41**(12), 2673–2680.

Suquet, P. 1987 *Elements of homogenization for inelastic solid mechanics*, vol. 272 of *Homogenization techniques for composite media, Lecture Notes in Physics 272.* Berlin: Springer-Verlag.

Terada, K., Saiki, I., Matsui, K. & Yamakawa, Y. 2003 Two-scale kinematics and linearization for simultaneous two-scale analysis of periodic heterogeneous solids at finite strains. *Computer Methods in Applied Mechanics and Engineering*, **192**(31-32), 3531–3563.