SENSITIVITY OF THE MACROSCOPIC ELASTICITY TENSOR TO TOPOLOGICAL MICROSTRUCTURAL CHANGES

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ABSTRACT. A remarkably simple analytical expression for the sensitivity of the two-dimensional macroscopic elasticity tensor to topological microstructural changes of the underlying material is proposed. The derivation of the proposed formula relies on the concept of topological derivative, applied within a variational multi-scale constitutive framework where the macroscopic strain and stress at each point of the macroscopic continuum are volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material associated with that point. The derived sensitivity – a symmetric fourth order tensor field over the RVE domain – measures how the estimated two-dimensional macroscopic elasticity tensor changes when a small circular hole is introduced at the micro-scale level. This information has potential use in the design and optimisation of microsctructures.

1. INTRODUCTION

Composite materials have become one of the most important classes of engineering materials. Their macroscopic mechanical behavior is of paramount importance in the design of load bearing components for a vast number of applications in civil, mechanical, aerospace, biomedical and nuclear industries. 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. For example, changes in shape of graphite inclusions in a cast iron matrix may produce dramatic changes in the corresponding macroscopic properties of this material. 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 [1, 30, 31] by means of a relaxation-based technique in the design of microstructural topologies that produce negative macroscopic Poisson's ratio. This type of approach relies on the use of a fictitious material density field and mimics, in a regularised sense, the introduction of localised topological microstructural changes (voids) wherever the artificial density is sufficiently close to zero (refer, for instance, to the fundamental papers [9, 53]).

In contrast to the heuristic, regularised approach, this paper proposes a general *exact* analytical expression for the 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 [19, 37] 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 constants estimated within the multi-scale framework changes when a small circular void is introduced at the micro-scale. Its analytical formula is derived by making use of the concepts of *topological asymptotic expansion* and *topological derivative* [50, 12] within a variational formulation of the adopted multi-scale theory. The (relatively new) mathematical notions of topological asymptotic expansion and topological derivative allow the closed form exact calculation of the sensitivity of a given shape functional with respect

Key words and phrases. Elasticity tensor, topological derivative, sensitivity analysis, multi-scale modelling.

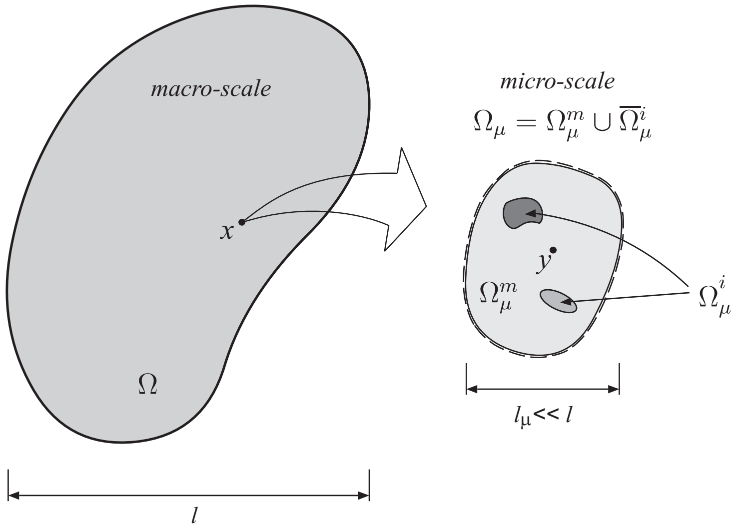


FIGURE 1. Macroscopic continuum with a locally attached microstructure.

to infinitesimal domain perturbations such as the insertion of voids, inclusions or source terms. Their use in the context of solid mechanics, topological optimisation of load bearing structures and inverse problems is reported in a number of recent publications [18, 33, 43, 44, 10, 26]. In the present context, the variational setting for the multi-scale modelling methodology as described in [14] is found to be particularly well-suited for the application of the topological derivative formalism. 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. Section 2 briefly describes the multi-scale constitutive framework adopted in the estimation of the macroscopic elasticity tensor. The modelling approach is cast within the variational setting described in [14]. The main contribution of the paper – the closed formula for the sensitivity of the macroscopic elasticity tensor to topological microstructural perturbations – is presented in Section 3. Here, an overview of the topological derivative concept is given, followed by its application to the problem in question. This leads to the identification of the required sensitivity tensor field. Numerical confirmation of the derived analytical formula is provided by means a simple finite element-based example. Finally, some concluding remarks are made in Section 4.

2. Multi-scale modelling

This section describes a homogenisation-based variational multi-scale framework for classical elasticity problems which allows the macroscopic elasticity tensor to be estimates from the given geometrical and elastic properties of a local Representative Volume Element (RVE) of material. This constitutive modelling approach has been proposed by Germain *et al.* [19] and has been exploited in the computational context, among others, by Michel *et al.* [37] and Miehe *et al.* [38]. Its variational structure is described in detail in [14]. For related multi-scale approaches based on asymptotic analysis, the reader may refer to [3, 48].

The starting point of the multi-scale constitutive theory adopted to estimate the macroscopic elastic properties of the continuum is the assumption that any material point $\boldsymbol{x}$ of the macroscopic continuum (refer to Fig. 1) is associated to a local Representative Volume Element (RVE) whose domain Ω_μ has characteristic length l_μ, much smaller than the characteristic length l of the macro-continuum domain, Ω. For the purposes of the analysis conducted in this paper, we shall consider the RVE to consist of a matrix, denoted by domain Ω_μ^m, containing inclusions of different materials occupying a domain Ω_μ^i, see Fig. 1.

Crucial to the present approach is the assumption 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:

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

where V_μ is a total volume of the RVE, i.e. $V_\mu = V_\mu^m + V_\mu^i$, with V_μ^m and V_μ^i denoting the matrix and inclusion volume of the RVE and

$$\mathbf{E}_\mu \equiv \nabla^s \mathbf{u}_\mu (\boldsymbol{y}), \tag{2.2}$$

with $\mathbf{u}_\mu$ denoting the microscopic displacement field of the RVE. The use of Green's Theorem in definition (2.1,2.2) gives the following equivalent expression for $\mathbf{E}$

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

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

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

$$\mathbf{u}_\mu (\boldsymbol{y}) = \mathbf{u} (\boldsymbol{x}) + \mathbf{E}\, \boldsymbol{y} + \tilde{\mathbf{u}}_\mu (\boldsymbol{y}), \tag{2.4}$$

of a constant (rigid) RVE displacement coinciding with the macro displacement $\mathbf{u}(\boldsymbol{x})$, a homogeneous strain displacement field, linear in $\boldsymbol{y}$, and a *displacement fluctuation* field $\tilde{\mathbf{u}}_\mu (\boldsymbol{y})$.

Following (2.4) the microscopic strain field (2.2) can be expressed as a sum

$$\mathbf{E}_\mu = \mathbf{E} + \nabla^s \tilde{\mathbf{u}}_\mu, \tag{2.5}$$

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

2.1. **Admissible and virtual microscopic displacement fields.** Assumption (2.1, 2.2) places a constraint on the admissible displacement fields of the RVE. That is, only fields $\mathbf{u}_\mu$ that satisfy (2.1, 2.2) can be said to be kinematically admissible. This condition can be formally expressed by requiring the (as yet not defined) set $\mathcal{K}_\mu$ of kinematically admissible displacements of the RVE to satisfy

$$\begin{aligned} \mathcal{K}_\mu \subset \mathcal{K}_\mu^* \equiv \Big\{ \boldsymbol{v} \in \left[H^1(\Omega_\mu)\right]^2 : & \textstyle\int_{\Omega_\mu} \boldsymbol{v} d\Omega_\mu = V_\mu \mathbf{u}, \\ & \textstyle\int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \mathbf{n}\, d\partial\Omega_\mu = V_\mu \mathbf{E},\ [\![\boldsymbol{v}]\!] = \mathbf{0} \text{ on } \partial\Omega_\mu^i \Big\}, \end{aligned} \tag{2.6}$$

where $\mathcal{K}_\mu^*$ is named the *minimally constrained set of kinematically admissible RVE displacement fields* – the most general set of microscopic displacement fields compatible with the strain averaging assumption – and $[\![\boldsymbol{v}]\!]$ denotes the *jump* of function $\boldsymbol{v}$ across the matrix/inclusion interface $\partial\Omega_\mu^i$:

$$[\![(\cdot)]\!] \equiv (\cdot)|_m - (\cdot)|_i, \tag{2.7}$$

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

In view of (2.4) and assuming that the origin of the coordinate system coincides with the centroid of the RVE, constraint (2.6) can, without loss of generality, be made equivalent to 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*, $\tilde{\mathcal{K}}_\mu^*$:

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

Trivially, we have that the space of virtual displacement of the RVE, defined as

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

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

2.2. **Macroscopic stress and the Hill-Mandel Principle.** Similarly to the macroscopic strain tensor (2.1), the macroscopic stress tensor, $\mathbf{T}$, is defined as the volume average of the microscopic stress field $\mathbf{T}_\mu$, over the RVE:

$$\mathbf{T} \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{T}_\mu d\Omega_\mu. \tag{2.10}$$

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 $\partial\Omega_\mu$. The Hill-Mandel Principle of Macro-Homogeneity [27, 35] establishes that the power of the macroscopic stress tensor at an arbitrary point of the macro-continuum must 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. As shown in [14], as a consequence of the the Hill-Mandel principle, $\mathbf{b}_\mu$ and $\mathbf{q}_\mu$ must satisfy the variational equations

$$\int_{\Omega_\mu} \mathbf{b}_\mu \cdot \boldsymbol{\eta} d\Omega_\mu = 0 \quad \text{and} \quad \int_{\partial\Omega_\mu} \mathbf{q}_\mu \cdot \boldsymbol{\eta} d\partial\Omega_\mu = 0 \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{2.11}$$

That is, 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, embedded in the choice of $\mathcal{V}_\mu$ (or $\mathcal{K}_\mu$). Hence, once the space $\mathcal{V}_\mu$ of microscopic displacement fluctuations is chosen, the space of admissible body force and external traction fields is automatically defined so that these fields cannot be independently prescribed [14].

2.3. **The RVE equilibrium problem.** In the present analysis, we shall assume the materials of the RVE matrix and inclusions to satisfy the classical linear elastic constitutive law:

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

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

$$\mathbb{C}_\mu = \mathbb{C}_\mu(\boldsymbol{y}) = \begin{cases} \mathbb{C}_m & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^m \\ \mathbb{C}_i & \text{if} \quad \boldsymbol{y} \in \Omega_\mu^i, \end{cases} \tag{2.13}$$

with $\mathbb{C}_m$ and $\mathbb{C}_i$ denoting, respectively, the elasticity constitutive tensors of the matrix and inclusion parts of the RVE:

$$\mathbb{C}_m = \frac{E_m}{1-\nu_m^2}\left[(1-\nu_m)\,\mathbf{I\!I} + \nu_m\,(\mathbf{I}\otimes\mathbf{I})\right], \quad \mathbb{C}_i = \frac{E_i}{1-\nu_i^2}\left[(1-\nu_i)\,\mathbf{I\!I} + \nu_i(\mathbf{I}\otimes\mathbf{I})\right]. \tag{2.14}$$

In the above, we have assumed the matrix and inclusion materials to be isotropic. The parameters E_m and E_i are the Young's moduli of the matrix and inclusions, ν_m and ν_i the corresponding Poisson's ratios and $\mathbf{I}$ and $\mathbf{I\!I}$ are the second and fourth order identity tensors, respectively. If the RVE has more than one inclusion, the parameters E_i and ν_i are constant within each inclusion, but may differ between inclusions.

The linearity of (2.12) together with the additive decomposition (2.5), allows the microscopic stress field to be split as

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

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

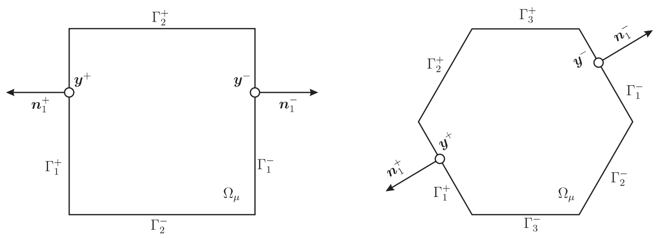


FIGURE 2. RVE geometries for periodic media. Square and hexagonal cells.

Tacking into account (2.15) and in view of (2.11), this leads to the definition of the *RVE equilibrium problem* which 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

$$\int_{\Omega_\mu} \tilde{\mathbf{T}}_\mu(\tilde{\mathbf{u}}_\mu) \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu = -\int_{\Omega_\mu} \mathbb{C}_\mu \mathbf{E} \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu \qquad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{2.16}$$

By means of standard arguments, it can be shown that the above variational form leads to the following Euler-Lagrange equations

$$\left\{ \begin{array}{rlll} \operatorname{div}\tilde{\mathbf{T}}_\mu(\tilde{\mathbf{u}}_\mu) & = \mathbf{0} & \text{in} & \Omega_\mu \\ \tilde{\mathbf{T}}_\mu(\tilde{\mathbf{u}}_\mu) & = \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_\mu & \text{in} & \Omega_\mu \\ \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu & = \mathbf{0} & & \\ \int_{\partial\Omega_\mu} \tilde{\mathbf{u}}_\mu \otimes_s \mathbf{n} \, d\partial\Omega_\mu & = \mathbf{0} & & \\ [\![\tilde{\mathbf{u}}_\mu]\!] & = \mathbf{0} & \text{on} & \partial\Omega_\mu^i \\ [\![\tilde{\mathbf{T}}_\mu(\tilde{\mathbf{u}}_\mu)\,\mathbf{n}]\!] & = -[\![(\mathbb{C}_\mu \mathbf{E})\mathbf{n}]\!] & \text{on} & \partial\Omega_\mu^i. \end{array} \right. \tag{2.17}$$

Remark 1. *Condition (2.17)$_4$ is naturally satisfied due to the choice of space $\tilde{\mathcal{K}}_\mu$ according to (2.8). Also note that, trivially, the mean value of the right hand side of (2.17)$_6$ vanishes. Then from (2.17)$_3$ and the Lax-Milgram Lemma we have that there exists an unique solution for (2.16).*

2.4. **Classes of multi-scale constitutive models .** To completely define a constitutive model of the present type, the choice of a space $\mathcal{V}_\mu \subset \tilde{\mathcal{K}}_\mu^*$ of variations of admissible displacement must be made. We list below four classical possible choices:

(a) *Taylor model* or *Rule of Mixtures* (homogeneous strain over the RVE). This class of models is obtained by simply defining

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{T}} \equiv \{\mathbf{0}\}. \tag{2.18}$$

In this case, the strain is homogeneous over the RVE, i.e. $\mathbf{E}_\mu = \mathbf{E}$ in Ω_μ. The reactive RVE body force and external traction fields, $(\mathbf{q}_\mu, \mathbf{b}_\mu) \in \left(\mathcal{V}_\mu^{\mathcal{T}}\right)^\perp$, may be arbitrary functions.

(b) *Linear boundary displacement model* . For this class of models the choice is

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{L}} \equiv \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}) = \mathbf{0} \ \forall \boldsymbol{y} \in \partial\Omega_\mu \right\}. \tag{2.19}$$

The only possible reactive body force over Ω_μ orthogonal to $\mathcal{V}_\mu^{\mathcal{L}}$ is $\mathbf{b}_\mu = \mathbf{0}$. That is, only a zero microscopic body force is compatible with this class of models. 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.

(c) *Periodic boundary fluctuations model* . This class of constitutive models is appropriated to represent the behavior of materials with periodic microstructure. Typical examples of periodic RVEs in two dimensions are square and hexagonal cells (see Figure 2). In this case the RVE boundary is composed for N pairs of equally sized sets of sides

$$\partial\Omega_\mu = \bigcup_{j=1}^{N} \left(\Gamma_j^+, \Gamma_j^-\right), \tag{2.20}$$

such that, each point $\boldsymbol{y}^+ \in \Gamma_j^+$ has a corresponding point $\boldsymbol{y}^- \in \Gamma_j^-$, and that the normal vectors to the sides (Γ_j^+, Γ_j^-) at the points $(\boldsymbol{y}^+, \boldsymbol{y}^-)$ satisfy

$$\mathbf{n}_j^+ = -\mathbf{n}_j^-. \tag{2.21}$$

The space of displacement fluctuations is defined as

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{P}} \equiv \left\{ \tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^+) = \tilde{\mathbf{u}}_\mu(\boldsymbol{y}^-) \ \forall \text{pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu \right\}. \tag{2.22}$$

Again, only the zero body force field is orthogonal to the chosen space of fluctuations. The external traction fields – in this case orthogonal to $\mathcal{V}_\mu^{\mathcal{P}}$ – satisfy

$$\mathbf{q}_\mu(\boldsymbol{y}^+) = -\mathbf{q}_\mu(\boldsymbol{y}^-) \quad \forall \text{pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu. \tag{2.23}$$

That is, the external traction is *anti-periodic.*

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

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{U}} \equiv \tilde{\mathcal{K}}_\mu^*. \tag{2.24}$$

Again only the zero body force field is orthogonal to the chosen space. The boundary traction orthogonal to the space of fluctuations in this case can be shown (refer to [14], for instance) to satisfy the *uniform boundary traction condition*:

$$\mathbf{q}_\mu(\boldsymbol{y}) = \mathbf{T}\mathbf{n}(\boldsymbol{y}) \quad \forall \boldsymbol{y} \in \partial\Omega_\mu, \tag{2.25}$$

where $\mathbf{T}$ is the macroscopic stress tensor (2.10) at point $\boldsymbol{x}$ of the macro-continuum.

Note that the spaces of displacement fluctuations (and virtual displacement) listed above satisfy

$$\mathcal{V}_\mu^{\mathcal{T}} \subset \mathcal{V}_\mu^{\mathcal{L}} \subset \mathcal{V}_\mu^{\mathcal{P}} \subset \mathcal{V}_\mu^{\mathcal{U}}. \tag{2.26}$$

The variational framework adopted in the estimation of the macroscopic response allows different predictions (including an upper and a lower bound) of macroscopic behavior to be obtained according to the constraints imposed upon the chosen functional space displacement fluctuations of the RVE.

2.5. **The homogenised elasticity tensor .** Crucial to the developments presented in Section 3, which form the main contribution of the present paper, is the derivation of formulae for the macroscopic elasticity tensors obtained by means of the multi-scale modelling procedure discussed in the above. This is addressed in the following.

With the notation introduced in (2.12), the variational problem defined by (2.16) can be equivalently written as

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_\mu \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu = -\int_{\Omega_\mu} \mathbb{C}_\mu \mathbf{E} \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu \qquad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu. \tag{2.27}$$

To derive a compact expression of the macroscopic elasticity tensor it is convenient to re-write (2.27) as a superposition of linear problems associated with the individual Cartesian components of the macroscopic strain tensor as suggested by Michel *et al.* [37]. We start by writing the macroscopic strain in Cartesian component form:

$$\mathbf{E} = (\mathbf{E})_{ij} \mathbf{e}_i \otimes \mathbf{e}_j, \tag{2.28}$$

where $\{\mathbf{e}_i\}$ is an orthonormal basis of the two-dimensional Euclidean space and the scalars $(\mathbf{E})_{ij}$ are the corresponding Cartesian components of the macroscopic strain, i.e. $(\mathbf{E})_{ij} = \mathbf{E} \cdot (\mathbf{e}_i \otimes \mathbf{e}_j)$. Since (2.27) is linear, its solution $\tilde{\mathbf{u}}_\mu \in \mathcal{V}_\mu$ can be constructed as a linear combination of the components of the macroscopic strain, $(\mathbf{E})_{ij}$, as

$$\tilde{\mathbf{u}}_\mu = (\mathbf{E})_{ij} \, \tilde{\mathbf{u}}_{\mu_{ij}}, \tag{2.29}$$

where the vector fields $\tilde{\mathbf{u}}_{\mu_{ij}} \in \mathcal{V}_\mu$ are the solutions to the linear variational equations

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu = -\int_{\Omega_\mu} \mathbb{C}_\mu (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \nabla^s \boldsymbol{\eta} d\Omega_\mu \qquad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu, \tag{2.30}$$

for $i, j = 1, 2$ (in the two-dimensional case). The above equation is obtained by combining (2.27), (2.28) and (2.29).

By combining (2.5), (2.28) and (2.29) we can write the microscopic strain as a linear combination of the Cartesian components of the macroscopic strain

$$\mathbf{E}_{\mu} = (\mathbf{E})_{ij} \left(\mathbf{e}_i \otimes \mathbf{e}_j + \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} \right) = (\mathbf{E})_{ij} \, \mathbf{E}_{\mu_{ij}}. \tag{2.31}$$

Then we can define the canonical stress and strain tensors as

$$\mathbf{T}_{\mu_{ij}} = \mathbb{C}_{\mu} \mathbf{E}_{\mu_{ij}} \qquad \text{with} \qquad \mathbf{E}_{\mu_{ij}} = \mathbf{e}_i \otimes \mathbf{e}_j + \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}}. \tag{2.32}$$

With the introduction of the additive decomposition (2.15) and the constitutive law (2.12) into (2.10) and by making use of (2.29), the macroscopic stress tensor $\mathbf{T}$ can be written as

$$\mathbf{T} = \mathbb{C}^{\mathcal{T}} \mathbf{E} + \left(\frac{1}{V_{\mu}} \int_{\Omega_{\mu}} \mathbb{C}_{\mu} \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} d\Omega_{\mu} \right) (\mathbf{E})_{ij} \,, \tag{2.33}$$

where $\mathbb{C}^{\mathcal{T}}$ is the homogenised (volume average) macroscopic elasticity tensor associated with the Taylor model, given by

$$\mathbb{C}^{\mathcal{T}} = \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} \mathbb{C}_{\mu} d\Omega_{\mu}. \tag{2.34}$$

Now, note that the second order tensor $\mathbb{C}_{\mu} \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}}$ can be expressed as

$$\mathbb{C}_{\mu} \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} = (\mathbb{C}_{\mu})_{klpq} \, (\nabla^s \tilde{\mathbf{u}}_{\mu_{ij}})_{pq} \, (\mathbf{e}_k \otimes \mathbf{e}_l) \,. \tag{2.35}$$

Also, let us assume that, at the macroscopic level, the constitutive law for linear elasticity reads

$$\mathbf{T} = \mathbb{C}^{\mathcal{H}} \mathbf{E}, \tag{2.36}$$

where $\mathbb{C}^{\mathcal{H}}$ can be recognized as the homogenised elasticity tensor. In fact, by replacing the above into (2.33), we obtain

$$\mathbb{C}^{\mathcal{H}} \mathbf{E} = \mathbb{C}^{\mathcal{T}} \mathbf{E} + \tilde{\mathbb{C}} \mathbf{E}, \tag{2.37}$$

where $\tilde{\mathbb{C}}$ is given by

$$\tilde{\mathbb{C}} \equiv \left[\frac{1}{V_{\mu}} \int_{\Omega_{\mu}} (\mathbb{C}_{\mu})_{ijpq} \, (\nabla^s \tilde{\mathbf{u}}_{\mu_{kl}})_{pq} d\Omega_{\mu} \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l) \tag{2.38}$$

Finally, with the above at hand, we arrive at the following compact canonical mathematical expression for the homogenised elasticity tensor

$$\mathbb{C}^{\mathcal{H}} = \mathbb{C}^{\mathcal{T}} + \tilde{\mathbb{C}}. \tag{2.39}$$

Note that only the contribution of $\tilde{\mathbb{C}}$ depends on the choice of space $\mathcal{V}_{\mu}$ (the solutions $\tilde{\mathbf{u}}_{\mu_{ij}}$ of (2.30) taking part in (2.38) depend of this choice). Obviously, under Taylor assumption $\tilde{\mathbf{u}}_{\mu_{ij}} = \mathbf{0}$ for all i, j. In this case, $\tilde{\mathbb{C}} = \mathbf{0}$ and $\mathbb{C}^{\mathcal{H}} = \mathbb{C}^{\mathcal{T}}$.

3. The topological sensitivity of the homogenised elasticity tensor

This section presents the main result of this paper. Here, we derive a closed formula for the sensitivity of the homogenised elasticity tensor (2.39) to the introduction of a circular hole centered at an arbitrary point of the RVE domain.

The result is valid for two-dimensional problems. The sensitivity in the present case is the fourth order tensor *field* over Ω_{μ} (the *original* domain of the RVE, without the hole) given by

$$\mathbb{S}(\boldsymbol{y}) = -\frac{1}{E(\boldsymbol{y})} \left(\mathbb{H} \mathbf{T}_{\mu_{ij}} \cdot \mathbf{T}_{\mu_{kl}} \right) \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \quad \forall \boldsymbol{y} \in \Omega_{\mu}, \tag{3.1}$$

where $\mathbf{T}_{\mu_{ij}}$ is defined in $(2.32)_1$ and $\mathbb{H}$ is the fourth order tensor

$$\mathbb{H} = 4\mathbf{I\!I} - \mathbf{I} \otimes \mathbf{I}. \tag{3.2}$$

The tensor $\mathbb{S}(\boldsymbol{y})$ is the (topological) sensitivity of the macroscopic elasticity tensor $\mathbb{C}^{\mathcal{H}}$ with respect to the topological change of the RVE produced by the introduction of a hole centered at point $\boldsymbol{y} \in \Omega_\mu$.

To gain some insight into the meaning of $\mathbb{S}$, let $\delta\mathbb{C}^{\mathcal{H}}_\varepsilon$ denote the difference

$$\delta\mathbb{C}^{\mathcal{H}}_\varepsilon = \mathbb{C}^{\mathcal{H}}_\varepsilon - \mathbb{C}^{\mathcal{H}}, \tag{3.3}$$

between the homogenised elasticity tensor $\mathbb{C}^{\mathcal{H}}_\varepsilon$ of the RVE topologically perturbed by the introduction of a hole of radius ε and the elasticity tensor $\mathbb{C}^{\mathcal{H}}$ of the unperturbed (original) RVE. The approximation to $\delta\mathbb{C}^{\mathcal{H}}_\varepsilon$ linear in the volume fraction $\pi\varepsilon^2/V_\mu$ of perturbation is given by

$$\delta\mathbb{C}^{\mathcal{H}}_\varepsilon = \frac{\pi\varepsilon^2}{V_\mu}\,\mathbb{S} + o\left(\varepsilon^2\right). \tag{3.4}$$

The sensitivity tensor (3.1) provides a first order sensitivity of how the macroscopic elasticity tensor varies when a topological perturbation is added to the RVE. Each Cartesian component $\mathbb{S}_{ijkl}(\boldsymbol{y})$ represents the derivative of the component $ijkl$ of the macroscopic elasticity tensor with respect to the volume fraction $\pi\varepsilon^2/V_\mu$ of a circular hole of radius ε inserted at an arbitrary point $\boldsymbol{y}$ of the RVE.

Remark 2. *The remarkable simplicity of the closed form sensitivity given by (3.1) is to be noted. Once the vector fields $\tilde{\mathbf{u}}_{\mu_{ij}}$ have been obtained as solutions of (2.30) for the* original *RVE domain, the sensitivity tensor can be trivially assembled. The information provided by (3.1) can be potentially used in a number of practical applications such as, for example, the design of microstructures to match a specified macroscopic constitutive response.* □

The derivation of (3.1)–(3.4) is based on the mathematical concept of *topological derivative* [50, 12, 18, 40, 43] and is presented in detail in Sections 3.3–3.5. Before proceeding to the derivation, however, we find convenient to present below some background material on this relatively new topic which should be particularly helpful to those unfamiliar with the topological derivative concept.

3.1. **Topological derivative. Preliminaries.** Let ψ be a functional that depends on a given domain and let it have sufficient regularity so that the following expansion is possible

$$\psi\left(\varepsilon\right) = \psi\left(0\right) + f\left(\varepsilon\right) D_T\psi + o\left(f\left(\varepsilon\right)\right), \tag{3.5}$$

where $\psi(0)$ is the functional evaluated for the given original domain and $\psi(\varepsilon)$ denotes the functional evaluated for a domain obtained by introducing a topological perturbation in the original domain. The parameter ε is a small positive scalar defining 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

$$\lim_{\varepsilon\to 0^+} f(\varepsilon) = 0, \tag{3.6}$$

and $o\left(f\left(\varepsilon\right)\right)$ contains all terms of higher order in $f(\varepsilon)$.

Expression (3.5) is named the *topological asymptotic expansion* of ψ. The term $D_T\psi$ is defined as the *topological derivative* of ψ at the unperturbed (original) RVE domain. The term $f(\varepsilon)D_T\psi$ is a *correction of first order in* $f(\varepsilon)$ to the functional $\psi(0)$, evaluated for the original domain, to obtain $\psi(\varepsilon)$ – the functional value for the perturbed domain. Analogously to (3.3) let $\delta\psi_\varepsilon$ denote the difference

$$\delta\psi_\varepsilon = \psi(\varepsilon) - \psi(0), \tag{3.7}$$

then, similar to (3.4), we have the linear approximation

$$\delta\psi_\varepsilon = f(\varepsilon)\, D_T\psi + o\left(f\left(\varepsilon\right)\right). \tag{3.8}$$

The concept of topological derivative is an extension of the classical notion of derivative. It has been rigorously introduced in 1999 by Sokolowski & Zochowski [50] in the context of shape optimisation for two-dimensional heat conduction and elasticity problems (for an introduction to the shape optimisation concept see [39, 52]). In their pioneering paper, these authors have considered domains topologically perturbed by the introduction of a hole subjected to homogeneous Neumann boundary condition. 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 (Céa *et al.* [12], Garreau *et al.* [18], Guillaume & Sid Idris [22], Novotny *et al.* [43], Feijóo *et al.* [17], Nazarov & Sokolowski [40], Lewinski & Sokolowski [33], Samet *et al.* [47], Sokolowski [49], Guillaume & Sid Idris [23], Burger *et al.* [11], Nazarov & Sokolowski [41], Feijóo [16], Amstutz [4], Amstutz *et al.* [6], Sokolowski & Zochowski [51], Hintermüller [28], Masmoudi *et al.* [36], Amstutz & Andrä [5], Bonnet [10], Auroux *et al.* [7]). More recent developments include the use of the topological derivative in two- and three-dimensional optimisation of elastic structures [45, 21], image processing [8, 32] with application to breast cancer diagnosis [26] and the extension of the original concept to the definition of a second order topological derivative [13].

3.2. **Application to the multi-scale elasticity model.** Our purpose here is to derive the closed formula for the topological sensitivity of the macroscopic elasticity tensor. To this end, it is appropriate to define the following functional

$$\psi(\varepsilon) \equiv V_\mu \mathbf{T}^\varepsilon \cdot \mathbf{E}, \quad \Rightarrow \quad \psi(0) = V_\mu \mathbf{T} \cdot \mathbf{E}, \tag{3.9}$$

where $\mathbf{T}^\varepsilon$ denotes the macroscopic stress tensor resulting from a macroscopic strain $\mathbf{E}$ at a point of the macro-continuum associated with a RVE topologically perturbed by a small hole defined by $\mathcal{H}_\varepsilon$ and $\mathbf{T}$ denotes the macroscopic stress tensor associated to the original (unperturbed) domain Ω_μ. More precisely, the perturbed RVE domain Ω_{μ_ε} is defined as follows (refer to Fig. 3). The hole $\mathcal{H}_\varepsilon$ of radius ε is introduced at an arbitrary point $\hat{\boldsymbol{y}} \in \Omega_\mu$ of the original RVE

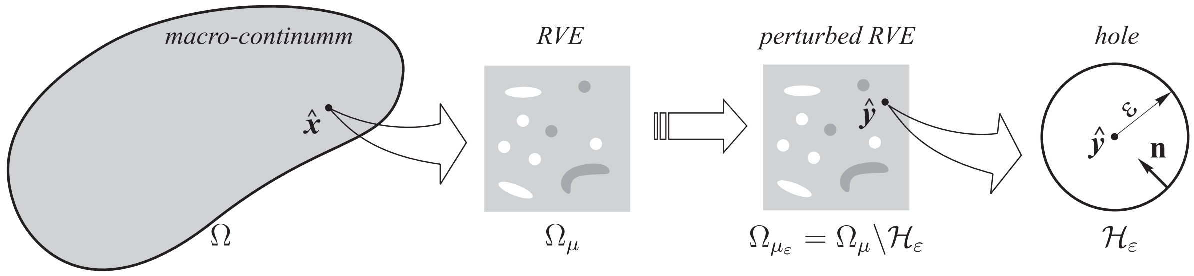


FIGURE 3. Microstructure perturbed with a hole $\mathcal{H}_\varepsilon$.

domain $\Omega_\mu = \Omega_\mu^m \cup \overline{\Omega}_\mu^i$ of Section 2. The topologically perturbed domain is then defined as

$$\Omega_{\mu_\varepsilon} = \Omega_\mu \backslash \overline{\mathcal{H}}_\varepsilon. \tag{3.10}$$

The asymptotic topological expansion of the functional (3.9) reads

$$\mathbf{T}^\varepsilon \cdot \mathbf{E} = \mathbf{T} \cdot \mathbf{E} + \frac{1}{V_\mu} f(\varepsilon) D_T \psi + o(f(\varepsilon)), \tag{3.11}$$

or, equivalently, by making use of the macroscopic constitutive law used in Section 2.5 ($\mathbf{T}^\varepsilon = \mathbb{C}_\varepsilon^{\mathcal{H}} \mathbf{E}$, $\mathbf{T} = \mathbb{C}^{\mathcal{H}} \mathbf{E}$) and definition (3.3),

$$\delta \mathbb{C}_\varepsilon^{\mathcal{H}} \mathbf{E} \cdot \mathbf{E} = \frac{1}{V_\mu} f(\varepsilon) D_T \psi + o(f(\varepsilon)). \tag{3.12}$$

The sensitivity tensor will be determined as follows. Once the asymptotic expansion of ψ leading to an explicit closed form for (3.12) has been carried out, the sensitivity tensor will be identified by comparing the resulting expression with (3.4).

3.3. **Topological derivative calculation .** In order to obtain a closed form expression of the asymptotic expansion (3.11), we start here by deriving a closed formula for the associated topological derivative $D_T\psi$. To this end, we define the functional

$$\psi(\varepsilon) \equiv \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \mathbf{T}_{\mu_\varepsilon}(\mathbf{u}_{\mu_\varepsilon}) \cdot \nabla^s \mathbf{u}_{\mu_\varepsilon} d\Omega_\mu, \tag{3.13}$$

where

$$\mathbf{u}_{\mu_\varepsilon} = \mathbf{u} + \mathbf{E}\boldsymbol{y} + \tilde{\mathbf{u}}_{\mu_\varepsilon}, \tag{3.14}$$

is the microscopic displacement field that solves the equilibrium problem for the perturbed RVE, $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ is the corresponding displacement fluctuation and $\mathbf{T}_{\mu_\varepsilon}$ – also a functional of $\mathbf{u}_{\mu_\varepsilon}$ – is the microscopic stress field, that is

$$\mathbf{T}_{\mu_\varepsilon} = \mathbb{C}_\mu \mathbf{E}_{\mu_\varepsilon} \qquad \text{with} \qquad \mathbf{E}_{\mu_\varepsilon} = \nabla^s \mathbf{u}_{\mu_\varepsilon}. \tag{3.15}$$

In particular, $\tilde{\mathbf{u}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon}$ is the solution of the following variational equation:

$$\int_{\Omega_{\mu_\varepsilon}} \tilde{\mathbf{T}}_{\mu_\varepsilon}(\tilde{\mathbf{u}}_{\mu_\varepsilon}) \cdot \nabla^s \boldsymbol{\eta}_\varepsilon d\Omega_\mu = -\int_{\Omega_{\mu_\varepsilon}} \mathbb{C}_\mu \mathbf{E} \cdot \nabla^s \boldsymbol{\eta}_\varepsilon d\Omega_\mu \quad \forall \boldsymbol{\eta}_\varepsilon \in \mathcal{V}_{\mu_\varepsilon}, \tag{3.16}$$

where $\mathcal{V}_{\mu_\varepsilon} = \mathcal{V}_\mu(\Omega_{\mu_\varepsilon})$ is the chosen space of kinematically admissible displacement fluctuations of the perturbed RVE.

The Euler-Lagrange equation associated with the variational form (3.16) is given by the following boundary value problem,

$$\left\{ \begin{array}{rll} \operatorname{div} \tilde{\mathbf{T}}_{\mu_\varepsilon}(\tilde{\mathbf{u}}_{\mu_\varepsilon}) & = \mathbf{0} & \text{in} \quad \Omega_\mu \backslash \overline{\mathcal{H}}_\varepsilon \\ \tilde{\mathbf{T}}_{\mu_\varepsilon}(\tilde{\mathbf{u}}_{\mu_\varepsilon}) & = \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_\varepsilon} & \text{in} \quad \Omega_\mu \backslash \overline{\mathcal{H}}_\varepsilon \\ \int_{\Omega_{\mu_\varepsilon}} \tilde{\mathbf{u}}_{\mu_\varepsilon} d\Omega_\mu & = \mathbf{0} & \\ \int_{\partial\Omega_\mu} \tilde{\mathbf{u}}_{\mu_\varepsilon} \otimes_s \mathbf{n} d\partial\Omega_\mu & = \mathbf{0} & \\ [\![\tilde{\mathbf{u}}_{\mu_\varepsilon}]\!] & = \mathbf{0} & \text{on} \quad \partial\Omega_\mu^i \\ [\![\tilde{\mathbf{T}}_{\mu_\varepsilon}(\tilde{\mathbf{u}}_{\mu_\varepsilon}) \mathbf{n}]\!] & = -[\![(\mathbb{C}_\mu \mathbf{E}) \mathbf{n}]\!] & \text{on} \quad \partial\Omega_\mu^i \\ \tilde{\mathbf{T}}_{\mu_\varepsilon}(\tilde{\mathbf{u}}_{\mu_\varepsilon}) \mathbf{n} & = -(\mathbb{C}_\mu \mathbf{E}) \mathbf{n} & \text{on} \quad \partial\mathcal{H}_\varepsilon. \end{array} \right. \tag{3.17}$$

Remark 3. *Once again (refer to Remark 1), condition (3.17)$_4$ is naturally satisfied by the choice of the space $\mathcal{V}_{\mu_\varepsilon}$, compatible with the choice for $\mathcal{V}_\mu$. In addition, since the mean value of the right hand sides of (3.17)$_{6,7}$ vanish, from (3.17)$_3$ and the Lax-Milgram Lemma we have that there exists an unique solution for (3.16). Finally, from the coercivity of the left-hand side of (2.16) and (3.16) we have that the following estimate holds for the two-dimensional case under analysis* [2, 4, 51]

$$\|\tilde{\mathbf{u}}_{\mu_\varepsilon} - \tilde{\mathbf{u}}_\mu\|_{\mathcal{V}_{\mu_\varepsilon}} = \mathcal{O}(\varepsilon). \tag{3.18}$$

It should be noted that the functional (3.13) depends explicitly and implicitly on the domain Ω_{μ_ε}. Its implicit dependence stems from the fact that the displacement fluctuation field $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ is the solution of the RVE equilibrium problem (3.16), for the *perturbed* RVE domain.

Among the methods for calculation of the topological derivative currently available in the literature, here we shall adopt the methodology proposed by Sokolowski & Zochowski [51] and further developed by Novotny *et al.* [43], whereby the topological derivative is obtained as the limit

$$D_T\psi = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}). \tag{3.19}$$

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 [39], to the change in shape produced by a uniform expansion of the hole. Accordingly, we define a sufficiently regular *shape change velocity field*, $\mathbf{v}$, over Ω_{μ_ε}, such that

$$\left\{ \begin{array}{ll} \mathbf{v} = \mathbf{0}, & \text{on } \partial\Omega_\mu \\ \mathbf{v} = -\mathbf{n}, & \text{on } \partial\mathcal{H}_\varepsilon. \end{array} \right. \tag{3.20}$$

3.3.1. *Rule of mixtures.* Let us start by dealing with the simplest class of multi-scale models described in Section 2.4 – the rule of mixtures (or Taylor) model. In this case, we combine (3.13) and the result presented in the Case (a) of Section 2.4 for the perturbed RVE to derive

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= \frac{d}{d\varepsilon}\int_{\Omega_{\mu_\varepsilon}} \bar{\mathbf{T}}_\mu \cdot \mathbf{E}_{\mu_\varepsilon} d\Omega_\mu \\ &= \frac{d}{d\varepsilon}\int_{\Omega_\mu \setminus \mathcal{H}_\varepsilon} \bar{\mathbf{T}}_\mu \cdot \mathbf{E} d\Omega_\mu \\ &= \bar{\mathbf{T}}_\mu \cdot \mathbf{E}\int_{\partial\Omega_\mu} (\mathbf{v}\cdot\mathbf{n}) d\partial\Omega_\mu + \bar{\mathbf{T}}_\mu \cdot \mathbf{E}\int_{\partial\mathcal{H}_\varepsilon} (\mathbf{v}\cdot\mathbf{n}) d\partial\mathcal{H}_\varepsilon \\ &= -2\pi\varepsilon\bar{\mathbf{T}}_\mu \cdot \mathbf{E}.\end{aligned} \tag{3.21}$$

By substituting (3.21) into definition (3.19) of the topological derivative and identifying function $f(\varepsilon)$ as

$$f(\varepsilon) = \pi\varepsilon^2, \tag{3.22}$$

we find that, for the rule of mixtures model,

$$D_T^{\mathcal{T}}\psi = -\bar{\mathbf{T}}_\mu \cdot \mathbf{E}. \tag{3.23}$$

Note that $f(\varepsilon)$ represents the hole area.

3.3.2. *Other classes of multi-scale models.* The derivation presented in the above is relatively simple due to the trivial definition (2.18) of the space of variations of admissible displacement fields for the rule of mixtures model. For the other models of Section 2.4, the derivation is considerably more elaborated as due account needs to be taken of the fact that $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ is the solution of the variational equilibrium problem (3.16) for the perturbed RVE domain.

In order to proceed, it is convenient to introduce an analogy to classical continuum mechanics [24] whereby the RVE shape change velocity field (3.20) is identified with the classical velocity field of a deforming continuum and ε is identified as a time parameter (refer to [42, 52] for analogies of this type in the context of shape sensitivity analysis).

Proposition 4. *Let $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$ be the functional defined by (3.13). 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*

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \mathbf{\Sigma}_{\mu_\varepsilon} \cdot \nabla\mathbf{v} d\Omega_\mu, \tag{3.24}$$

where $\mathbf{v}$ is the RVE shape change velocity field defined in Ω_{μ_ε} and $\mathbf{\Sigma}_{\mu_\varepsilon}$ is a generalisation of the classical Eshelby momentum-energy tensor [15, 25] *of the RVE, given by*

$$\mathbf{\Sigma}_{\mu_\varepsilon} = (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon})\mathbf{I} - 2(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})^T\,\mathbf{T}_{\mu_\varepsilon}. \tag{3.25}$$

Proof. By making use of Reynolds' Transport Theorem [24, 52], we obtain the identity

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \frac{d}{d\varepsilon}(\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) + \mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon} \mathrm{div}\mathbf{v} d\Omega_\mu. \tag{3.26}$$

Next, by using the concept of material derivative of a spatial field [24, 52], we find that the first term of the above right hand side integral can be written as

$$\frac{d}{d\varepsilon}(\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \dot{\mathbf{E}}_{\mu_\varepsilon}, \tag{3.27}$$

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

$$\mathbf{E}_{\mu_\varepsilon} = \mathbf{E} + \nabla^s\tilde{\mathbf{u}}_{\mu_\varepsilon}, \tag{3.28}$$

gives

$$\dot{\mathbf{E}}_{\mu_\varepsilon} = (\nabla^s\tilde{\mathbf{u}}_{\mu_\varepsilon})^{\cdot}, \tag{3.29}$$

which, after some manipulations exploring the relations between the material derivatives of spatial quantities and their gradients, results in

$$\dot{\mathbf{E}}_{\mu_\varepsilon} = \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \nabla \mathbf{v})^s . \tag{3.30}$$

Then, by introducing the above expression into (3.27) we obtain

$$\frac{d}{d\varepsilon} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon} \cdot (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \nabla \mathbf{v})^s , \tag{3.31}$$

which, substituted in (3.26) gives

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon} \cdot (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \nabla \mathbf{v})^s + (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) \mathbf{I} \cdot \nabla \mathbf{v} d\Omega_\mu . \tag{3.32}$$

where we have made use of the identity, $\operatorname{div} \mathbf{v} = \mathbf{I} \cdot \nabla \mathbf{v}$. Now, note that by definition of the spaces of displacement variations, we have $\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon}$. This, together with the equilibrium equation (3.16), implies that the first term of (3.32) vanishes. □ □

Proposition 5. *Let $\mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon})$ be the functional defined by (3.13). 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*

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon}) = \int_{\partial\Omega_{\mu_\varepsilon}} \mathbf{\Sigma}_{\mu_\varepsilon} \mathbf{n} \cdot \mathbf{v} d\partial\Omega_\mu , \tag{3.33}$$

where $\mathbf{v}$ is the RVE shape change velocity field and $\mathbf{\Sigma}_{\mu_\varepsilon}$ is given by (3.25).

Proof. Let us compute the shape derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ using the following version for the Reynolds' Transport Theorem [24, 52],

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \frac{\partial}{\partial\varepsilon} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) d\Omega_\mu + \int_{\partial\Omega_{\mu_\varepsilon}} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) \mathbf{v} \cdot \mathbf{n} d\partial\Omega_\mu . \tag{3.34}$$

Next, by using the concept of spatial derivative [24, 52] and (2.12), we find that the first term of the above right hand side integral can be written as

$$\frac{\partial}{\partial\varepsilon} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}'_{\mu_\varepsilon} . \tag{3.35}$$

where the prime denotes the (partial) spatial derivative with respect to ε. Further, note that the relation (3.28) gives

$$\mathbf{E}'_{\mu_\varepsilon} = \nabla^s \tilde{\mathbf{u}}'_{\mu_\varepsilon} = \nabla^s [\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - \nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \mathbf{v}] . \tag{3.36}$$

Then, by introducing the above expression into (3.35) we obtain

$$\frac{\partial}{\partial\varepsilon} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) = 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} - 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \mathbf{v}) . \tag{3.37}$$

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

$$\begin{aligned} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon}) &= 2 \int_{\Omega_{\mu_\varepsilon}} \mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s \dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} d\Omega_\mu - \int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \mathbf{v}) d\Omega_\mu \\ &\quad + \int_{\partial\Omega_{\mu_\varepsilon}} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) \mathbf{v} \cdot \mathbf{n} d\partial\Omega_\mu . \end{aligned} \tag{3.38}$$

Now, note that by definition of the spaces of displacement variations, we have $\dot{\tilde{\mathbf{u}}}_{\mu_\varepsilon} \in \mathcal{V}_{\mu_\varepsilon}$. This, together with the equilibrium equation (3.16), implies that the first term of (3.38) vanishes. Then, we obtain

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}} (\mathbf{u}_{\mu_\varepsilon}) = - \int_{\Omega_{\mu_\varepsilon}} 2\mathbf{T}_{\mu_\varepsilon} \cdot \nabla^s (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon} \mathbf{v}) d\Omega_\mu + \int_{\partial\Omega_{\mu_\varepsilon}} (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon}) \mathbf{v} \cdot \mathbf{n} d\partial\Omega_\mu . \tag{3.39}$$

Using the tensor relation

$$\operatorname{div} \left(\mathbf{T}^{\mathrm{T}}_{\mu_\varepsilon} [(\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon}) \mathbf{v}] \right) = \mathbf{T}_\varepsilon \cdot \nabla^s [(\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon}) \mathbf{v}] + \operatorname{div} (\mathbf{T}_{\mu_\varepsilon}) \cdot (\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon}) \mathbf{v} , \tag{3.40}$$

and the divergence theorem, the expression (3.39) can be written as

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) &= 2\int_{\Omega_{\mu_\varepsilon}} \mathrm{div}\mathbf{T}_{\mu_\varepsilon}\cdot(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\,\mathbf{v}d\Omega_\mu - 2\int_{\partial\Omega_{\mu_\varepsilon}}(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})^{\mathrm{T}}\,\mathbf{T}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v}d\partial\Omega_\mu \\ &\quad+\int_{\partial\Omega_{\mu_\varepsilon}}(\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})\,\mathbf{v}\cdot\mathbf{n}d\partial\Omega_\mu. \end{aligned}\tag{3.41}$$

Since the stress field $\mathbf{T}_{\mu_\varepsilon}$ is in equilibrium, from Euler-Lagrange equation $(3.17)_1$, we have that $\mathrm{div}\mathbf{T}_{\mu_\varepsilon}=\mathbf{0}$ in Ω_{μ_ε}. Therefore, a straightforward rearrangement of the above yields (3.33). □ □

Corollary 6. *By applying the divergence theorem to the right hand side of (3.24), we obtain*

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\partial\Omega_{\mu_\varepsilon}}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v}d\partial\Omega_\mu - \int_{\Omega_{\mu_\varepsilon}}\mathrm{div}\,(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v}d\Omega_\mu. \tag{3.42}$$

Since (3.33) and (3.42) remain valid for all velocity fields $\mathbf{v}$ *of* $\overline{\Omega}_{\mu_\varepsilon}$, *we have that*

$$\int_{\Omega_{\mu_\varepsilon}}\mathrm{div}\,(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v}d\Omega_\mu = 0 \quad \forall\mathbf{v}\in\Omega_{\mu_\varepsilon} \quad\Rightarrow\quad \mathrm{div}\,(\mathbf{\Sigma}_{\mu_\varepsilon})=\mathbf{0} \textit{ in } \Omega_{\mu_\varepsilon}, \tag{3.43}$$

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

Then, from the result (3.33) and taking definition (3.20) into account, together with the definition of $\partial\Omega_{\mu_\varepsilon}$, we finally arrive at the following expression for the sensitivity of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ exclusively in terms of integrals over the boundary $\partial\mathcal{H}_\varepsilon$ of the hole

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = -\int_{\partial\mathcal{H}_\varepsilon}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{n}d\partial\mathcal{H}_\varepsilon. \tag{3.44}$$

We now proceed to derive an explicit expression for the integrand on the right hand side of (3.44). Then, consider a curvilinear coordinate system n–t along $\partial\mathcal{H}_\varepsilon$, characterised by the orthonormal vectors $\mathbf{n}$ and $\mathbf{t}$. For convenience we decompose the stress tensor $\mathbf{T}_{\mu_\varepsilon}(\mathbf{u}_{\mu_\varepsilon})$ and the strain tensor $\mathbf{E}_{\mu_\varepsilon}(\mathbf{u}_{\mu_\varepsilon})$ on the boundary $\partial\mathcal{H}_\varepsilon$ as follows

$$\begin{aligned}\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{H}_\varepsilon} &= \mathrm{T}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n})+\mathrm{T}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t})+\mathrm{T}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n})+\mathrm{T}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}),\\ \mathbf{E}_{\mu_\varepsilon}|_{\partial\mathcal{H}_\varepsilon} &= \mathrm{E}^{nn}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{n})+\mathrm{E}^{nt}_{\mu_\varepsilon}(\mathbf{n}\otimes\mathbf{t})+\mathrm{E}^{tn}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{n})+\mathrm{E}^{tt}_{\mu_\varepsilon}(\mathbf{t}\otimes\mathbf{t}).\end{aligned}\tag{3.45}$$

Now note that the Neumann condition along $\partial\mathcal{H}_\varepsilon$ gives

$$\tilde{\mathbf{T}}_{\mu_\varepsilon}\mathbf{n}|_{\partial\mathcal{H}_\varepsilon} = -\bar{\mathbf{T}}_\mu\mathbf{n} \quad\Rightarrow\quad \mathbf{T}_{\mu_\varepsilon}\mathbf{n}|_{\partial\mathcal{H}_\varepsilon}=\mathbf{0}, \tag{3.46}$$

so that decomposition $(3.45)_1$ reads

$$\mathbf{T}_{\mu_\varepsilon}\mathbf{n}|_{\partial\mathcal{H}_\varepsilon} = \mathrm{T}^{nn}_{\mu_\varepsilon}\mathbf{n}+\mathrm{T}^{tn}_{\mu_\varepsilon}\mathbf{t}=\mathbf{0} \quad\Rightarrow\quad \mathrm{T}^{nn}_{\mu_\varepsilon}=\mathrm{T}^{tn}_{\mu_\varepsilon}=0 \text{ on } \partial\mathcal{H}_\varepsilon. \tag{3.47}$$

With decomposition (3.45) and boundary condition (3.47), the normal flux of the Eshelby tensor (3.25) through $\partial\mathcal{H}_\varepsilon$ can be written as

$$\begin{aligned}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{n} &= (\mathbf{T}_{\mu_\varepsilon}\cdot\mathbf{E}_{\mu_\varepsilon})-2\mathbf{T}_{\mu_\varepsilon}\mathbf{n}\cdot(\nabla\tilde{\mathbf{u}}_{\mu_\varepsilon})\mathbf{n}\\ &= \mathrm{T}^{nn}_{\mu_\varepsilon}\mathrm{E}^{nn}_{\mu_\varepsilon}+2\mathrm{T}^{nt}_{\mu_\varepsilon}\mathrm{E}^{nt}_{\mu_\varepsilon}+\mathrm{T}^{tt}_{\mu_\varepsilon}\mathrm{E}^{tt}_{\mu_\varepsilon}\\ &= \mathrm{T}^{tt}_{\mu_\varepsilon}\mathrm{E}^{tt}_{\mu_\varepsilon},\end{aligned}\tag{3.48}$$

or, equivalently (using the inverse constitutive relation),

$$\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{n} = \frac{1}{E(\boldsymbol{y})}\mathrm{T}^{tt}_{\mu_\varepsilon}(\mathrm{T}^{tt}_{\mu_\varepsilon}-\nu(\boldsymbol{y})\mathrm{T}^{nn}_{\mu_\varepsilon}) = \frac{1}{E(\boldsymbol{y})}(\bar{\mathrm{T}}^{tt}_{\mu}+\tilde{\mathrm{T}}^{tt}_{\mu_\varepsilon})^2, \tag{3.49}$$

where $\bar{\mathrm{T}}^{tt}_{\mu}$ and $\tilde{\mathrm{T}}^{tt}_{\mu_\varepsilon}$ are the constant and fluctuation part, respectively, of component $\mathrm{T}^{tt}_{\mu_\varepsilon}$ of the stress tensor $\mathbf{T}_{\mu_\varepsilon}|_{\partial\mathcal{H}_\varepsilon}$, and the parameters $E(\boldsymbol{y})$ and $\nu(\boldsymbol{y})$ are defined as

$$E(\boldsymbol{y}) = \left\{\begin{array}{ll} E_m & \text{if} \quad \boldsymbol{y}\in\Omega^m_\mu \\ E_i & \text{if} \quad \boldsymbol{y}\in\Omega^i_\mu\end{array}\right. , \quad \nu(\boldsymbol{y}) = \left\{\begin{array}{ll} \nu_m & \text{if} \quad \boldsymbol{y}\in\Omega^m_\mu \\ \nu_i & \text{if} \quad \boldsymbol{y}\in\Omega^i_\mu\end{array}\right. . \tag{3.50}$$

In order to obtain an analytical formula for the boundary integral of (3.44) we make use of a polar coordinate system (r, θ) centered at point $\hat{\boldsymbol{y}}$ and the classical asymptotic analysis described in Appendix A, see for instance [2, 29]. The substitution of (A.4), into (3.49) and then into (3.44) allows the integral of the normal flux of the Eshelby tensor across $\partial\mathcal{H}_\varepsilon$ to be analytically integrated, resulting in

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = -\frac{2\pi\varepsilon}{E(\hat{\boldsymbol{y}})}\left[4\mathbf{T}_\mu \cdot \mathbf{T}_\mu - (\mathrm{tr}\mathbf{T}_\mu)^2\right] + o(\varepsilon), \tag{3.51}$$

where $\mathrm{tr}(\cdot)$ denotes the trace of $(\cdot)$.

The substitution of the above expression for the derivative of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ into (3.19) allows the function $f(\varepsilon)$ to be promptly identified in the same way as (3.22). Finally, by taking the limit of the resulting formula for $\varepsilon \to 0$, we obtain the explicit closed form expression for the topological derivative of ψ:

$$D_T\psi = -\frac{1}{E(\hat{\boldsymbol{y}})}\mathbb{H}\mathbf{T}_\mu \cdot \mathbf{T}_\mu, \tag{3.52}$$

where $\mathbb{H}$ is given by (3.2).

Remark 7. *The topological derivative of ψ given by (3.52) is a scalar field over Ω_μ that depends only on the material properties of matrix (or inclusions) and on the solution $\mathbf{u}_\mu$ for the original* unperturbed *domain Ω_μ. The striking simplicity of the exact formula (3.52) is to be noted.* □

3.4. **Numerical verification.** In direct analogy with classical finite difference-based methods for the numerical approximation of the derivative of a generic function, a first order *topological finite difference* formula based on (3.8) to approximate numerically the value of $D_T\psi$ at the unperturbed RVE configuration can be defined as

$$d_T\psi_\varepsilon \equiv \frac{\psi(\varepsilon) - \psi(0)}{f(\varepsilon)}, \tag{3.53}$$

with finite ε. The above satisfies

$$\lim_{\varepsilon \to 0} d_T\psi_\varepsilon = D_T\psi. \tag{3.54}$$

If for a given RVE we calculate $\psi(0)$ and its perturbed counterpart $\psi(\varepsilon)$ for a sequence of decreasing (sufficiently small) inclusion radii ε, the use of formula (3.53) will provide an asymptotic approximation to the analytical value of $D_T\psi$ given by (3.52). Here such a procedure is used to provide a numerical validation of (3.52). The required values of the function ψ are computed numerically by means of a finite element procedure specially suited to handle the kinematical constraints of the present multi-scale theory (refer, for instance, to [20]). The unperturbed RVE considered (refer to Fig. 4) consists of a unit square containing a circular inclusion of radius 0.1 centred at the point with coordinates (0.35,0.75) – with the origin of the Cartesian coordinate system located at the bottom left hand corner of the RVE. For the computation of the values of $\psi(\varepsilon)$, a sequence of finite element analyses are carried out for perturbed RVEs obtained by introducing in the original RVE a circular hole of radii

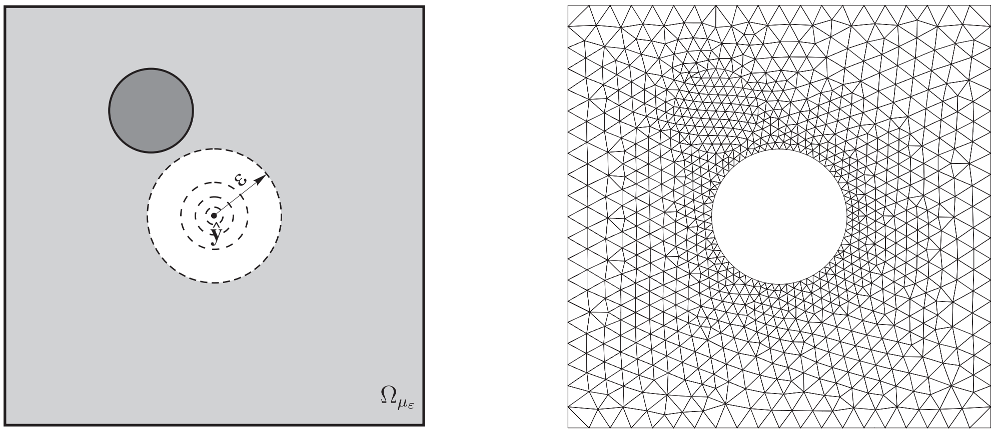
$$\varepsilon \in \{0.160, 0.080, 0.040, 0.020, 0.010, 0.005\}, \tag{3.55}$$

centred at $\hat{\boldsymbol{y}} = (0.5, 0.5)$. Finite element meshes of six-noded isoparametric triangles are used to discretise the perturbed domains. All meshes are built such that the hole boundary of radius ε has 80 elements. For example, the mesh with $\varepsilon = 0.16$ (shown in Fig. 4(b)) contains 1864 elements with a total number of 5593 nodes. The macroscopic strain tensor (which can be chosen arbitrarily) considered to compute ψ in the analyses is

$$\mathbf{E} = \begin{bmatrix} 1.00 & 0.05 \\ 0.05 & 2.00 \end{bmatrix}. \tag{3.56}$$

The study is conducted for two different sets of material properties for the matrix and inclusion:

- Case A: $E_m = 50.0$, $\nu_m = 1/3$, $E_i = 5.0$ and $\nu_i = 1/3$.
- Case B: $E_m = 50.0$, $\nu_m = 1/5$, $E_i = 5.0$ and $\nu_i = 1/5$.



(a) (b)

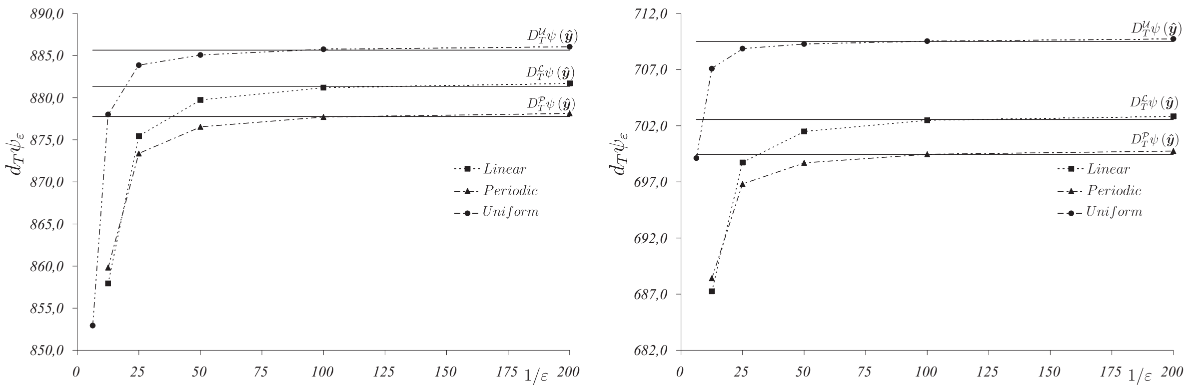
FIGURE 4. Numerical verification. (a) RVE geometry, and; (b) Finite element mesh for $\varepsilon = 0.16$.

In each case, the numerical verification is carried out under the assumptions of:

(a) Linear boundary displacement;
(b) Periodic boundary displacement fluctuations, and;
(c) Uniform boundary traction.

The rule of mixtures (or Taylor) model is not considered. For this model, the solution is trivial and does not require a finite element analysis. If one insisted in undertaking the present verification for the rule of mixtures model, the only difference between the exact topological derivative (3.23), which does not depend on ε, and its numerical counterpart would be the result of the geometrical approximation of the inclusion domain by the relevant assembly of finite element subdomains.

The results of the analyses are plotted in Fig. 5. They show the analytical topological derivative and the corresponding numerical approximation for each value of ε for all classes of multiscale model considered. The convergence of the numerical topological derivatives to



(a) Case A. (b) Case B.

FIGURE 5. Numerical verification. Convergence of numerical topological derivative to analytical value.

their corresponding analytical values with decreasing ε is obvious in all cases and confirms the estimate (3.18) and also the correctness of formula (3.52).

3.5. **The sensitivity of the macroscopic elasticity tensor .** From (3.52) and (3.11) we have the explicit expression for the topological expansion of ψ:

$$\mathbf{T}^{\varepsilon} \cdot \mathbf{E} = \mathbf{T} \cdot \mathbf{E} - \frac{v(\varepsilon)}{E(\hat{\boldsymbol{y}})} \mathbb{H} \mathbf{T}_{\mu} \cdot \mathbf{T}_{\mu} + o(\varepsilon^2). \tag{3.57}$$

where

$$v(\varepsilon) = \pi\varepsilon^2 / V_{\mu}, \tag{3.58}$$

is the RVE volume fraction occupied by the perturbation.

Introducing (2.31) into (2.12), the microscopic stress tensor $\mathbf{T}_{\mu}$ can be written as

$$\mathbf{T}_{\mu} = (\mathbf{E})_{ij} \, \mathbb{C}_{\mu} \mathbf{E}_{\mu_{ij}} = (\mathbf{T}_{\mu_{ij}} \otimes \mathbf{e}_i \otimes \mathbf{e}_j) \mathbf{E}, \tag{3.59}$$

where $\mathbf{T}_{\mu_{ij}}$ is defined in $(2.32)_1$.

With the above expressions at hand, we see after straightforward manipulations that the topological derivative of ψ given by (3.52) can be represented as

$$D_T \psi = -\mathbb{D}_{T\mu} \mathbf{E} \cdot \mathbf{E}, \tag{3.60}$$

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

$$\mathbb{D}_{T\mu} = \frac{1}{E(\hat{\boldsymbol{y}})} \left(\mathbb{H} \mathbf{T}_{\mu_{ij}} \cdot \mathbf{T}_{\mu_{kl}} \right) \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l, \tag{3.61}$$

with $i, j, k, l = 1, 2$.

Then, by replacing (3.60,3.61) and (3.22) into (3.12) we obtain the explicit form

$$\delta \mathbb{C}^{\mathcal{H}}_{\varepsilon} \mathbf{E} \cdot \mathbf{E} = -\frac{\pi\varepsilon^2}{V_{\mu}} \mathbb{D}_{T\mu} \mathbf{E} \cdot \mathbf{E} + o(\varepsilon^2). \tag{3.62}$$

Finally, the sensitivity tensor (3.1),

$$\mathbb{S} = -\mathbb{D}_{T_{\mu}}, \tag{3.63}$$

can be promptly identified by comparing (3.62) with the linear approximation (3.4) that defines the sensitivity.

4. Conclusion

An analytical expression for the sensitivity of the two-dimensional macroscopic elasticity tensor to topological microstructural changes of the underlying material has been proposed in this paper. The derivation of the proposed fundamental formula relied on the concept of topological derivative, applied within a variational multi-scale constitutive framework for linear elasticity problems where the macroscopic strain and stress 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 derived sensitivity – a symmetric fourth order tensor field over the RVE domain – measures how the estimated macroscopic elasticity tensor changes when a small circular hole is introduced at the micro-scale. This crucial information can be potentially used in a number of applications of practical interest such as, for instance, the design and optimisation of microstructures to achieve a specified macroscopic behavior. The successful application of analogous ideas in the context of design and optimisation of load bearing (macroscopic) structures is reported in references [45, 21], for instance. Finally, we remark that the derivation of analogous formulae for the three-dimensional case as well as for the sensitivity to the introduction of inclusions in the RVE is currently under way and should be the subject of a future publication.

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References

[1] R.F. Almgreen. An isotropic three-dimensional structure with poisson's ratio -1. *Journal of Elasticity*, 15(4):427–430, 1985.

[2] H. Ammari and H. Kang. *Reconstruction of small inhomogeneities from boundary measurements.* Lectures Notes in Mathematics vol. 1846. Springer-Verlag, Berlin, 2004.

[3] H. Ammari and H. Kang. *Polarization and moment tensors with applications to inverse problems and effective medium theory.* Applied Mathematical Sciences vol. 162. Springer-Verlag, New York, 2007.

[4] S. Amstutz. Sensitivity analysis with respect to a local perturbation of the material property. *Asymptotic Analysis*, 49(1-2):87–108, 2006.

[5] S. Amstutz and H. Andrä. A new algorithm for topology optimization using a level-set method. *Journal of Computational Physics*, 216(2):573–588, 2006.

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

[7] D. Auroux, M. Masmoudi, and L. Belaid. Image restoration and classification by topological asymptotic expansion. In *Variational formulations in mechanics: theory and applications*, Barcelona, 2007.

[8] L.J. Belaid, M. Jaoua, M. Masmoudi, and L. Siala. Application of the topological gradient to image restoration and edge detection. *Engineering Analysis with Boundary Element*, 32(11):891–899, 2008.

[9] M.P. Bendsøe and N. Kikuchi. Generating optimal topologies in structural design using an homogenization method. *Computer Methods in Applied Mechanics and Engineering*, 71(2):197–224, 1988.

[10] M. Bonnet. Topological sensitivity for 3d elastodynamic and acoustic inverse scattering in the time domain. *Computer Methods in Applied Mechanics and Engineering*, 195(37-40):5239–5254, 2006.

[11] M. Burger and R. Stainko. Phase-field relaxation of topology optimization with local stress constraints. *SIAM Journal on Control Optimization*, 45(4):1447–1466, 2006.

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

[13] J. Rocha de Faria, R.A. Feijóo, A.A. Novotny, E. Taroco, and C. Padra. Second order topologial sensitivity analysis. *International Journal of Solids and Structures*, 44(14-15):4958–4977, 2007.

[14] E.A. de Souza Neto and R.A. Feijóo. Variational foundations of multi-scale constitutive models of solid: Small and large strain kinematical formulation. Technical Report N 16/2006, Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, Brasil, 2006.

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

[16] G.R. Feijóo. A new method in inverse scattering based on the topological derivative. *Inverse Problems*, 20(6):1819–1840, 2004.

[17] R.A. Feijóo, A.A. Novotny, E. Taroco, and C. Padra. The topological derivative for the poisson's problem. *Mathematical Models and Methods in Applied Sciences*, 13(12):1825–1844, 2003.

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

[19] P. Germain, Q.S. Nguyen, and P. Suquet. Continuum thermodynamics. *Journal of Applied Mechanics, Transactions of the ASME*, 50(4):1010–1020, 1983.

[20] S.M. Giusti, P.J. Blanco, E.A. de Souza Neto, and R.A. Feijóo. An assessment of the gurson yield criterion by a computational multi-scale approach. Technical Report N 27/2007, Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, Brasil, 2007.

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

[22] P. Guillaume and K. Sid Idris. The topological asymptotic expansion for the dirichlet problem. *SIAM Journal on Control and Optimization*, 41(4):1042–1072, 2002.

[23] P. Guillaume and K. Sid Idris. Topological sensitivity and shape optimization for the stokes equations. *SIAM Journal on Control and Optimization*, 43(1):1–31, 2004.

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

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

[26] B.B. Guzina and I. Chikichev. From imaging to material identification: a generalized concept of topological sensitivity. *Journal of the Mechanics and Physics of Solids*, 55(2):245–279, 2007.

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

[28] M. Hintermüller. Fast level set based algorithms usind shape and topological sensitivity. *Control and Cybernetics*, 34(1):305–324, 2005.

[29] V.A. Kozlov, W.G. Maz'ya, and A.B. Movchan. *Asymptotic analysis of fields in multi-structures.* Clarendon Press, Oxford, 1999.

[30] R. Lakes. Foam structures with negative poisson's ratio. *Science, AAAS*, 235(4792):1038–1040, 1987.

[31] R. Lakes. Negative poisson's ratio materials. *Science, AAAS*, 238(4826):551, 1987.
[32] I. Larrabide, R.A. Feijóo, A.A. Novotny, and E. Taroco. Topological derivative: A tool for image processing. *Computers & Structures*, 86(13-14):1386–1403, 2008.
[33] T. Lewinski and J. Sokołowski. Energy change due to the appearance of cavities in elastic solids. *International Journal of Solids and Structures*, 40(7):1765–1803, 2003.
[34] R.W. Little. *Elasticity*. Prentice-Hall, New Jersey, 1973.
[35] J. Mandel. *Plasticité Classique et Viscoplasticité*. CISM Lecture Notes. Springer-Verlag, Udine, 1971.
[36] M. Masmoudi, J. Pommier, and B. Samet. The topological asymptotic expansion for the maxwell equations and some applications. *Inverse Problems*, 21(2):547–564, 2005.
[37] J.C. Michel, H. Moulinec, and P. Suquet. Effective properties of composite materials with periodic microstructure: a computational approach. *Computer Methods in Applied Mechanics and Engineering*, 172(1-4):109–143, 1999.
[38] C. Miehe, J. Schotte, and J. Schröder. Computational micro-macro transitions and overall moduli in the analysis of polycrystals at large strains. *Computational Materials Science*, 16(1-4):372–382, 1999.
[39] F. Murat and J. Simon. *Sur le Contrôle par un Domaine Géométrique*. Phd thesis, Université Pierre et Marie Curie, Paris, France, 1976.
[40] S.A. Nazarov and J. Sokołowski. Asymptotic analysis of shape functionals. *Journal de Mathématiques Pures et Appliquées*, 82(2):125–196, 2003.
[41] S.A. Nazarov and J. Sokołowski. Self-adjoint extensions for the neumann laplacian and applications. *Acta Mathematicae Applicatae Sinica*, 22(3):879–906, 2006.
[42] E.J. Hauga nd K.K. Choi and V.Komkov. *Desing sensitivity analysis of structural systems*. Academic Press, New York, 1986.
[43] A.A. Novotny, R.A. Feijóo, C. Padra, and E. Taroco. Topological sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, 192(7-8):803–829, 2003.
[44] A.A. Novotny, R.A. Feijóo, C. Padra, and E. Taroco. Topological derivative for linear elastic plate bending problems. *Control and Cybernetics*, 34(1):339–361, 2005.
[45] A.A. Novotny, R.A. Feijóo, E. Taroco, and C. Padra. Topological sensitivity analysis for three-dimensional linear elasticity problem. *Computer Methods in Applied Mechanics and Engineering*, 196(41-44):4354–4364, 2007.
[46] L. Obert and W.I. Duvall. *Rock mechanics and the design of structures in rock*. John Wiley & Sons, New York, 1967.
[47] B. Samet, S. Amstutz, and M. Masmoudi. The topological asymptotic for the helmholtz equation. *SIAM Journal on Control and Optimization*, 42(5):1523–1544, 2003.
[48] E. Sanchez-Palencia. *Non-Homogeneous Media and Vibration Theory*, volume 127 of *Lecture Notes in Physics 127*. Springer-Verlag, Berlin, 1980.
[49] J. Sokołowski. Optimality conditions for simultaneous topology and shape optimization. *SIAM Journal on Control and Optimization*, 42(4):1198–1221, 2003.
[50] J. Sokołowski and A. Żochowski. On the topological derivatives in shape optmization. *SIAM Journal on Control and Optimization*, 37(4):1251–1272, 1999.
[51] J. Sokołowski and A. Żochowski. Topological derivatives of shape functionals for elasticity systems. *Mechanics of Structures and Machines*, 29(3):333–351, 2001.
[52] J. Sokołowski and J.P. Zolésio. *Introduction to Shape Optimization - Shape Sensitivity Analysis*. Springer-Verlag, New York, 1992.
[53] A. Żochowski. Optimal perforation design in 2-dimensional elasticity. *Mechanics of Structures and Machines*, 16(1):17–33, 1988.

Appendix A. Asymptotic analysis

This appendix presents the derivation of the asymptotic formula used in the topological sensitivity analysis developed in Section 3.3. We start by considering the following expansion of the stress fluctuation field associated with the solution $\tilde{\mathbf{u}}_{\mu_\varepsilon}$ to problem (3.17), see [50]:

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

where $\tilde{\mathbf{T}}^{\infty}_{\mu_\varepsilon}$ denotes the solution of the elasticity system (3.17) 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

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

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

In a polar coordinate system (r,θ) having its origin at the center 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 [46, 34], are given by

$$
\begin{aligned}
(\tilde{\mathbf{T}}^\infty_{\mu_\varepsilon})^{rr} &= \tilde{S}\left(1-\frac{\varepsilon^2}{r^2}\right)-\bar{S}\frac{\varepsilon^2}{r^2}+\tilde{D}\left(1-4\frac{\varepsilon^2}{r^2}+3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta \\
&\quad +\bar{D}\left(3\frac{\varepsilon^4}{r^4}-4\frac{\varepsilon^2}{r^2}\right)\cos 2(\theta+\varphi), && \text{(A.3)}\\
(\tilde{\mathbf{T}}^\infty_{\mu_\varepsilon})^{\theta\theta} &= \bar{S}\frac{\varepsilon^2}{r^2}+\tilde{S}\left(1+\frac{\varepsilon^2}{r^2}\right)-\tilde{D}\left(1+3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta \\
&\quad -3\bar{D}\frac{\varepsilon^4}{r^4}\cos 2(\theta+\varphi), && \text{(A.4)}\\
(\tilde{\mathbf{T}}^\infty_{\mu_\varepsilon})^{r\theta} &= -\tilde{D}\left(1+2\frac{\varepsilon^2}{r^2}-3\frac{\varepsilon^4}{r^4}\right)\sin 2\theta+\bar{D}\left(3\frac{\varepsilon^4}{r^4}-2\frac{\varepsilon^2}{r^2}\right)\sin 2(\theta+\varphi), && \text{(A.5)}
\end{aligned}
$$

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

$$
\begin{aligned}
\bar{S} &= \frac{\bar{\sigma}_{\mu_1}(\bar{\mathbf{u}})+\bar{\sigma}_{\mu_2}(\bar{\mathbf{u}})}{2}, \quad \bar{D}=\frac{\bar{\sigma}_{\mu_1}(\bar{\mathbf{u}})-\bar{\sigma}_{\mu_2}(\bar{\mathbf{u}})}{2}, && \text{(A.6)}\\
\tilde{S} &= \frac{\tilde{\sigma}_{\mu_1}(\tilde{\mathbf{u}}_\mu)+\tilde{\sigma}_{\mu_2}(\tilde{\mathbf{u}}_\mu)}{2}, \quad \tilde{D}=\frac{\tilde{\sigma}_{\mu_1}(\tilde{\mathbf{u}}_\mu)-\tilde{\sigma}_{\mu_2}(\tilde{\mathbf{u}}_\mu)}{2}, && \text{(A.7)}
\end{aligned}
$$

where $\bar{\sigma}_{\mu_{1,2}}(\bar{\mathbf{u}})$ and $\tilde{\sigma}_{\mu_{1,2}}(\tilde{\mathbf{u}}_\mu)$ are the principal stresses associated with the displacement fields $\bar{\mathbf{u}}$ and $\tilde{\mathbf{u}}_\mu$ of the original (unperturbed) domain Ω_μ.

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