SYNTHESIS OF MICROSTRUCTURES USING TOPOLOGICAL SENSITIVITY ANALYSIS

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Abstract. This work addresses the topological asymptotic analysis of the two-dimensional macroscopic elasticity tensor to topological microstructural changes of the underlying material. In particular, the microstructure is topologically perturbed by the nucleation of a small circular inclusion. Using the topological derivative concept, applied within a variational multi-scale constitutive framework, a simple analytical expression for the sensitivity is proposed. In the multi-scale modelling, 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 (RVE) of material associated with that point. These mathematical concepts allow the closed form calculation of the sensitivity, whose value depends on the solution of a set of equations over the original (unperturbed) domain, of a given shape functional with respect to an infinitesimal domain perturbation. The main result – a symmetric fourth order tensor field over the RVE domain – measures how the macroscopic elasticity tensor estimated within the multi-scale framework change when a small circular inclusion is introduced at the micro-scale level. The final format of the proposed analytical formula is strikingly simple and can be used in applications such as the synthesis and optimal design of microstructures to meet a specified macroscopic behaviour. In order to show this feature we present several numerical examples using the obtained result together with a level-set based algorithm.

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

1. Introduction

Composite materials have become one of the most important classes of engineering materials. In a broad sense, one can argue that much of material science is about improving macroscopic material properties by means of topological and shape changes at a microstructural level. In this context, the ability to accurately predict the macroscopic mechanical behavior from the corresponding microscopic properties as well as its sensitivity to changes in microstructure becomes essential in the analysis and potential purpose-design and optimisation of heterogeneous media. Such concepts have been successfully used, for instance, by Kikuchi et al. (1998); Sigmund (1994) and Silva et al. (1997); by means of a relaxation-based technique in the design of periodic microstructural topologies. This paper proposes a general exact analytical expression for the topological sensitivity of the two-dimensional macroscopic elasticity tensor to topological changes of the microstructure of the underlying material. The macroscopic linear elastic response is estimated by means of a well-established homogenisation-based multi-scale constitutive theory for elasticity problems, see Germain et al. (1983) and Michel et al. (1999), where the macroscopic strain and stress tensors at each point of the macroscopic continuum are defined as the volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material associated with that point. The proposed sensitivity is a symmetric fourth order tensor field over the RVE that measures how the macroscopic elasticity parameters estimated within the multi-scale framework change when a small circular inclusion is introduced at the micro-scale. Its analytical formula is derived by making use of the concepts of topological asymptotic expansion and topological derivative, Céa et al. (2000) and Sokółowski and Żochowski (1999), within a variational formulation of the adopted multi-scale theory. The final format of the proposed analytical formula is strikingly simple and can be potentially used in applications such as the synthesis and optimal design of microstructures to meet a specified macroscopic behavior. The paper is organised as follows. The multi-scale constitutive framework adopted in the estimation of the macroscopic elasticity tensor is briefly described in Section 2. The main contribution of the paper is presented in Section 3. Here, an overview of the topological derivative concept is given. Finally, the application of the topological derivative to the synthesis of microstructures is shown in Section 4, together with some numerical experiments presented in Section 4.1.
2. Multi-scale modelling

In this section we present a summary of the multi-scale constitutive theory upon which we rely for the estimation of the macroscopic elasticity properties. This family of 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. The starting point of this family of constitutive theories is the assumption that any point \( x \) of the macroscopic continuum (refer to Fig. 1) is associated to a local RVE whose domain \( \Omega_{\mu} \), with boundary \( \partial \Omega_{\mu} \), has characteristic length \( L_{\mu} \), much smaller than the characteristic length \( L \) of the macro-continuum domain, \( \Omega \).

For simplicity, we consider that the RVE domain consists of a matrix, \( \Omega_{\mu} \), containing inclusions of different materials occupying a domain \( \Omega_{\mu}^i \). An axiomatic variational framework for this family of constitutive theories was presented in detail by de Souza Neto and 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 of the RVE; (3) The equilibrium of the RVE; (4) The stress averaging relation and (5) The Hill-Mandel Principle of Macro-Homogeneity (Hill (1965); Mandel (1971)), which ensures the energy consistency between the so-called micro- and macro -scales of the material. For a more detailed description on the derivation of the present multi-scale constitutive model we refer the reader to de Souza Neto and Feijóo (2006) and Michel et al. (1999).

\[ C_{\mu} = \frac{E_{\mu}}{1 - \nu_{\mu}^2} \left[I + \nu_{\mu} (I \otimes I)\right], \quad C_{\mu} = \begin{cases} E_{\mu}^m & \text{if } y \in \Omega_{\mu}^m \\ E_{\mu}^s & \text{if } y \in \Omega_{\mu}^s \end{cases}, \quad \nu_{\mu} = \begin{cases} \nu_{\mu}^m & \text{if } y \in \Omega_{\mu}^m \\ \nu_{\mu}^s & \text{if } y \in \Omega_{\mu}^s \end{cases}, \]

with \( E_{\mu} \) and \( \nu_{\mu} \), denoting, respectively, the Young’s moduli and the Poisson’s ratio of the domain \( \Omega_{\mu} \). If the RVE has more than one inclusion, the parameters \( E_{\mu}^m \) and \( \nu_{\mu}^m \) are considered piecewise constant. In addition, in (2), we use \( I \) and \( \otimes \) to denote the second and fourth order identity tensors, respectively.

As previously mentioned at the beginning of this section, using the concept of homogenization the macroscopic strain and stress tensors, respectively denoted by \( \varepsilon \) and \( \sigma \), at a point \( x \) of the macroscopic continuum are obtained as the volume average of their microscopic counterpart over the domain of the RVE:

\[ \varepsilon := \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} \nabla^s u_{\mu} = \frac{1}{V_{\mu}} \int_{\partial \Omega_{\mu}} u_{\mu} \otimes_s n \quad \text{and} \quad \sigma := \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} \sigma_{\mu}(u_{\mu}) , \]

where \( V_{\mu} \) is the total volume of the RVE, \( n \) represent the outward unit normal to the boundary \( \partial \Omega_{\mu} \) and \( \otimes_s \) denotes the symmetric tensor product of vectors. The description of the equilibrium problem (1) is completed with the definition of the space of virtual displacement fluctuation of the RVE:

\[ U_{\mu} \ni \{ \eta \in [H^1(\Omega_{\mu})]^2 : \eta = v_1 - v_2 ; \forall v_1, v_2 \in V_{\mu} \} , \]

where \( V_{\mu} \) is the set of kinematically admissible displacements of the RVE and \( V_{\mu}^s \) the minimally constrained set of kinematically admissible RVE displacement fields. In particular, the periodicity boundary condition at the micro-scale level can be expressed by requiring that the space \( U_{\mu} \) be defined as

\[ U_{\mu}^P = \{ u_{\mu} \in U_{\mu} : u_{\mu}(y^+) = u_{\mu}(y^-) \forall (y^+, y^-) \in P \} . \]
where \( P \) is the set of pairs of opposite points on the boundary \( \partial \Omega_p \).

In the constitutive multi-scale model previously introduced, it was presented how to use the macroscopic information (strain tensor \( \varepsilon \)) to obtain the macroscopic displacement field \( u_p \). In the same way, by using the above concepts it is possible to obtain a closed form of the macroscopic constitutive response, in our case, the homogenized elasticity tensor \( \mathbb{C} \). This methodology was suggested by Michel et al. (1999) and is based on re-writing the problem (1) as a superposition of linear problems associated with the individual Cartesian components of the macroscopic strain tensor. Then, the macroscopic (homogenized) tensor \( \mathbb{C} \) can be constructed as a sum of an homogenized (volume average) macroscopic elasticity tensor \( \mathbb{C} \) and a contribution \( \tilde{\mathbb{C}} \) associated to the space \( U_p \):

\[
\mathbb{C} = \mathbb{C} + \tilde{\mathbb{C}}, \quad \text{with} \quad \mathbb{C} = \frac{1}{V_p} \int_{\Omega_p} C_{\mu} \quad \text{and} \quad \tilde{\mathbb{C}} := \left[ \frac{1}{V_p} \int_{\Omega_p} (\sigma_{\mu}(\tilde{u}_{\mu}))_{ij} \right] (e_i \otimes e_j \otimes e_k \otimes e_l),
\]

where \( (\sigma_{\mu}(\tilde{u}_{\mu}))_{ij} \) is the \( ij \)-th component of the fluctuation stress field associated with the fluctuation displacement field \( \tilde{u}_{\mu} \), being the vector fields \( \tilde{u}_{\mu} \in U_p \) the solutions of the linear variational equations

\[
\int_{\Omega_p} \sigma_{\mu}(\tilde{u}_{\mu}) \cdot \nabla \eta = - \int_{\Omega_p} C_{\mu}(e_k \otimes e_l) \cdot \nabla \eta \quad \forall \eta \in U_p,
\]

for \( k, l = 1, 2 \) (in the two-dimensional case). In the above expressions the elements \( \{e_i\} \) are the orthonormal basis of the two-dimensional Euclidean space.

### 3. The topological sensitivity of the homogenised elasticity tensor

A closed formula for the sensitivity of the homogenised elasticity tensor (7) to the introduction of a circular inclusion centered at an arbitrary point of the RVE domain is presented in this section. To derive this sensitivity we will use the concepts of topological asymptotic expansion and topological derivative. In this context, the concept of topological derivative was rigorously introduced by Sokolowski and Zochowski (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 Amstutz et al. (2005); Céa et al. (2000); Garreau et al. (2001); Nazarov and Sokolowski (2003); Novotny et al. (2007).

In order to introduce this concepts, let \( \psi \) be a functional that depends on a given domain and let it have sufficient regularity so that the following expansion is possible

\[
\psi (\rho) = \psi (0) + f (\rho) D_T \psi + o (f (\rho)),
\]

where \( \psi (0) \) is the functional evaluated in the original domain and \( \psi (\rho) \) denotes the functional for a topologically perturbed domain. The parameter \( \rho \) defines the size of the topological perturbation, so that the original domain is retrieved when \( \rho = 0 \). In addition, \( f (\rho) \) is a function such that \( f (\rho) \to 0 \) with \( \rho \to 0^+ \) and \( o (f (\rho)) \) contains all terms of higher order in \( f (\rho) \). The term \( D_T \psi \) of (9) is defined as the topological derivative of \( \psi \) at the unperturbed (original) RVE domain.

To begin the topological sensitivity analysis, it is appropriate to define the RVE topologically perturbed by a small inclusion of radius \( \rho \) represented by \( I_\rho \). More precisely, the perturbed domain is obtained when a circular hole \( H_\rho \) of radius \( \rho \) is introduced at an arbitrary point \( \hat{y} \in \Omega_p \). Next, this region is replaced with the circular inclusion \( I_\rho \) with different material property. Then, the perturbed domain is defined as \( \Omega_{\mu,\rho} = (\Omega_\mu \setminus H_\rho) \cup I_\rho \) (refer to Fig. 2).

![Figure 2. Topological perturbation at the microscopic level.](image)

In the presence of the inclusion above described, and for a given contrast parameter \( \gamma \in \mathbb{R} \), the microscopic constitutive tensor and the effective microscopic stress in \( \Omega_{\mu,\rho} \) are defined by

\[
C_{\mu,\rho} = \left\{ \begin{array}{ll} C_{\mu} & \text{in} \ \Omega_\mu \setminus H_\rho \\
\gamma C_{\mu} & \text{in} \ \mathcal{I}_\rho \end{array} \right., \quad \Rightarrow \quad \sigma_{\mu,\rho} = \mathbb{C}^\rho_{\mu,\rho} \nabla \xi = \left\{ \begin{array}{ll} \sigma_{\mu}(\xi) & \text{in} \ \Omega_\mu \setminus H_\rho \\
\gamma \sigma_{\mu}(\xi) & \text{in} \ \mathcal{I}_\rho \end{array} \right.,
\]

Based on these definitions and in view of the homogenization procedure introduced in the previous section, we have that the macroscopic elasticity tensor of the topologically perturbed RVE can be obtained as

\[
C_{ijkl}^\rho = \frac{1}{V_p} \int_{\Omega_p} (\sigma_{\mu}^\rho (u^\rho_{\mu}))_{ij} \in \mathbb{R},
\]
where the microscopic displacement field \( u^{\rho}_{\mu i} \) satisfies the variational equation
\[
\int_{\Omega_\mu} \sigma_\mu^\rho (u^{\rho}_{\mu i}) \cdot \nabla \eta = 0 \quad \forall \eta \in \mathcal{U}_\mu ,
\]
with \( u^{\rho}_{\mu i}(y) = u + (e_k \otimes e_l) y + \bar{u}^{\rho}_{\mu i}(y) \quad \forall \bar{u}^{\rho}_{\mu i} \in \mathcal{U}_\mu .
\]
(12)

As mentioned before, our interest here is the complete characterization of the asymptotic expansion of the homogenized constitutive response \( C \). Then, this asymptotic expansion can be written as:
\[
C = C^\rho + \frac{f(\rho)}{\nu} D_T C + o(\nu^2).
\]
(13)

where \( D_T C \) represents the topological derivative of the tensor \( C \). Finally, after performing the topological asymptotic analysis the components of the topological derivative tensor are given by
\[
D_T C_{ijkl} = H_\gamma \sigma_\mu (u^{\rho}_{\mu j}) \cdot \sigma_\mu (u^{\rho}_{\mu i}) ,
\]
with \( H_\gamma := -\frac{1}{E_\mu} \left( \frac{1 - \gamma}{1 + \alpha \gamma} \right) \left[ 4I - \frac{1 - \gamma (\alpha - 2\beta)}{1 + \beta \gamma} (I \otimes I) \right] \).
(14)

Remark 1 Note that the above expression (for \( \gamma \to 0 \)) coincides with the result derived in Giusti et al. (2009) for topological perturbation characterized by a small circular hole instead of an inclusion.

4. A micro-structure topology optimization algorithm

In this section we present a topology design algorithm based on the topological asymptotic expansion of the homogenized elasticity tensor \( C \). The optimization problem that we shall solve is stated as:

Minimize \( J(\Omega^m) = h(C(\Omega^m)) + \lambda \frac{\| \Omega^m \|}{V_\mu} \),
(15)

where \( h(C) \) is a function of the homogenized elasticity tensor \( C \) given by (7) and \( \lambda \) is a fixed Lagrange multiplier associated to a volume constraint. Since the topological sensitivity is a derivative with respect to the volume fraction of the perturbation, then, we can apply directly the rules of differential calculus. Thus, according to the topological asymptotic expansion of the homogenised elasticity tensor given by (13), the topological derivative of the cost function \( J(\Omega^m) \) can be obtained by using the chain rule. Therefore, it comes
\[
D_T J = \langle Dh(C), D_T C \rangle + \lambda ,
\]
(16)

where the term \( \langle Dh(C), D_T C \rangle \) should be understood as the derivative of the function \( h(C) \) with respect to the tensor \( C \) in the direction of \( D_T C \). The problem given by (15) is solved by using a level-set-based algorithm devised in Amstutz and Andrä (2006).

4.1 Numerical examples

Here we will apply the algorithm presented in the previous Section to the synthesis of microstructures in order to meet a specified macroscopic behavior. Due to the symmetry relations, the homogenized fourth order elasticity tensor \( C \) can be written in the matricial form as
\[
C = \begin{pmatrix}
(C)_{1111} & (C)_{1112} & (C)_{1112} \\
(C)_{1122} & (C)_{2222} & (C)_{2212} \\
(C)_{1212} & (C)_{2212} & (C)_{1212}
\end{pmatrix}
\]
(17)

and, for an orthotropic constitutive behavior, the effective material properties, namely, Young modulus, bulk modulus, shear modulus and Poisson ratio, can be extracted directly from the coefficients \((C^{-1})_{ijkl}\) of the tensor \(C^{-1}\).

We start by fixing the RVE geometry, which is represented by the unity square \( \Omega_\mu = (0,1) \times (0,1) \). The Young modulus and the Poisson ratio associated to the micro-cell are respectively given by \( E^{m}_\mu = 1, E^{l}_\mu = 0.01 \) and \( \nu^{m}_\mu = \nu^{l}_\mu = 0.3 \). The level-set initialization is given by a circular disc centered at point \((0.5,0.5)\) with radius \( r = 0.25 \). We use a structured initial mesh of three-noded triangular elements with a total of 3281 nodes.

(a) Horizontal rigidity maximization. For this first example, we maximize the horizontal rigidity of the micro-cell. In addition we fix \( \lambda = 10 \). The obtained result is shown in fig. (3(a)).

(b) Bulk modulus maximization. By using \( \lambda = 20 \), the obtained result for the bulk modulus maximization is shown in fig. (3(b)).

(c) Shear modulus maximization. In this case, we consider that the Lagrange multiplier is given by \( \lambda = 50 \). The obtained result is shown in fig. (3(c)).
(d) Minimization of a modified Poisson ratio. Here, the Lagrange multiplier associated to the volume constraint is \( \lambda = 0 \). The obtained result is shown in fig. (4). The matricial representation of the obtained homogenised elasticity tensor at the end of the optimization process is presented to the right of fig.(4), which results in a negative Poisson ratio, namely, \( \nu = -0.3740 \). This topology reproduce the classical microstructure characterized by the auxetic behavior of the star-shaped encapsulated inclusions, analyzed by, among others, Theocaris et al. (1997) and Stavroulakis (2005). This type of micro cells are also know as nonconvex-shaped or re-entrant corner microstructures.

(e) Maximization of the Poisson ratio Finally, by choosing \( \lambda = 0 \), the obtained results for the maximization of the Poisson ratio is shown in fig. (5). The matricial representation of the homogenised elasticity tensor obtained at the end of the optimization process is presented to the right of fig.(5), which results in a near one Poisson ratio, namely, \( \nu = 0.8711 \).

\[
C = \begin{pmatrix}
0.0825 & -0.0308 & 0 \\
-0.0308 & 0.0825 & 0 \\
0 & 0 & 0.0105
\end{pmatrix}
\]

Figure 4. Minimization of a modified Poisson ratio.

\[
C = \begin{pmatrix}
0.1565 & 0.1363 & 0 \\
0.1363 & 0.1565 & 0 \\
0 & 0 & 0.1162
\end{pmatrix}
\]

Figure 5. Maximization of the Poisson ratio.
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6. References


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