SENSITIVITY OF THE MACROSCOPIC THERMAL CONDUCTIVITY TENSOR TO TOPOLOGICAL MICROSTRUCTURAL CHANGES

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Abstract. This paper proposes a closed form expression for the sensitivity of the macroscopic heat conductivity tensor for two-dimensional problems to topological microstructural changes of the underlying material. The sensitivity formula is remarkably simple. It is derived by applying the concept of topological derivative within a variational multi-scale framework for steady-state heat conduction where the macroscopic temperature gradient and heat flux are defined as volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material. The classical Fourier law is assumed to hold at the scale referred to as microscopic (the RVE). The derived sensitivity – a symmetric second order tensor field over the RVE domain – measures how the estimated macroscopic conductivity tensor changes when a small circular inclusion is introduced at the micro-scale. The proposed formula finds potential application in the design and optimisation of heat conducting materials.

1. Introduction

The macroscopic (or effective) heat conductivity of materials is a physical property of paramount importance in the design of mechanical, thermal and electronic components for a vast number of applications in civil, aerospace, biomedical, nuclear and electronics industries. In many circumstances, this property dictates the design approach and any improvements in component performance can only be achieved by means of suitable changes in the conductivity behaviour of the adopted materials. In this context, the ability to accurately predict the macroscopic conductivity from the corresponding microstructural properties becomes essential in the analysis and potential purpose-design and optimisation of the underlying heterogeneous medium. Methods for estimation of effective conductivity have been proposed and investigated, among others, by Germain *et al.* [19], Auriault [5], Auriault and Royer [6], Ostoja-Starzewski and Schulte [43], Yin *et al.* [51], Wang *et al.* [50] and Jiang and Sousa [28]. Of crucial importance to the potential optimisation of the conductive medium in this case, is the sensitivity of the effective conductivity to changes in the microstructure – and whose calculation, to the authors knowledge, has not been reported in the literature.

This paper proposes a general analytical expression for the sensitivity of the two-dimensional macroscopic heat conductivity tensor to topological changes of the underlying micro-structure. The macroscopic conductivity is estimated by means of a homogenisation-based multi-scale constitutive theory for steady-state heat conduction problems where, following closely the ideas of Germain *et al.* [19], the macroscopic temperature gradient and heat flux vectors 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. In this context, the estimated effective conductivity for a given microstructure depends on the choice of constraints imposed upon the admissible temperature fields of the RVE, and the upper and lower bounds established by Ostoja-Starzewski and Schulte [43] can be obtained by suitable choices of constraints. Within this homogenisation framework, the classical Fourier law is assumed to hold at the scale referred to as the microscopic scale. Hence, the minimum RVE size that can be considered must be such that this assumption can still provide an adequate description of steady-state heat conduction. The proposed sensitivity is a symmetric second order

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

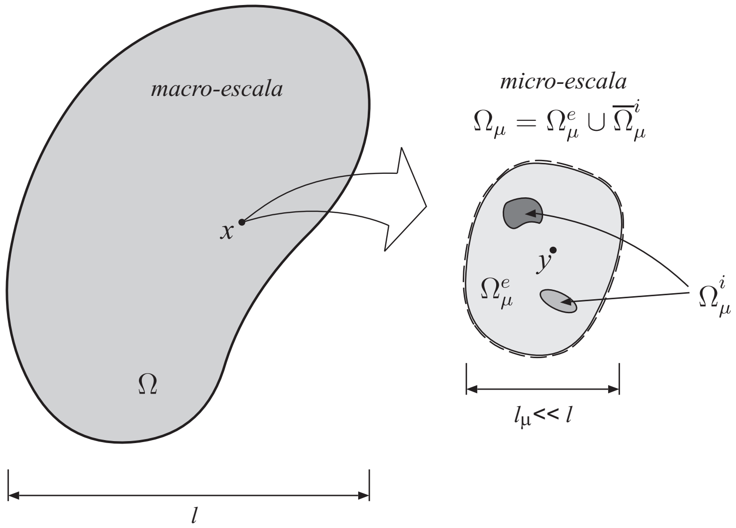


FIGURE 1. Macroscopic continuum with a locally attached microstructure.

tensor field over the RVE that measures how the macroscopic conductivity estimated within the multi-scale framework changes when a small circular inclusion is introduced at the micro-scale. Its analytical formula is derived by making use of the concepts of *topological asymptotic expansion* and *topological derivative* [11, 46] within the adopted multi-scale theory. These relatively new mathematical concepts allow the closed form calculation of the sensitivity of a given shape functional with respect to infinitesimal domain perturbations such as those produced by the insertion of holes, inclusions, cracks or source terms. The value of the sensitivity depends on the solution of a set of equations over the original (unperturbed) domain. The use of such concepts in the context of solid mechanics, topological optimisation of load bearing structures and inverse problems is reported in a number of recent publications [18, 31, 40, 41, 9, 25]. In the present context, the variational setting in which the underlying multi-scale theory is cast is found to be particularly suitable for use in conjunction with the notion of topological derivative. The final format of the proposed analytical formula is remarkably simple. It may be potentially used in applications such as, for example, the sythesis and optimal design of microstructures to meet a specified effective conductivity.

The paper is organised as follows. Section 2 describes the multi-scale constitutive modelling approach adopted in the estimation of the macroscopic heat conductivity tensor. A clear variational foundation of the theory is established which is essential for the main developments to be presented later. The main result of the paper – the closed formula for the sensitivity of the macroscopic conductivity to topological microstructural perturbations – is presented in Section 3. Here, a brief description of the topological derivative concept is initially given. This is followed by its application to the problem in question which leads to the identification of the required sensitivity tensor. A simple finite element-based numerical example is also provided for the numerical verification of the analytically derived topological derivative formula. The paper ends in Section 4 where concluding remarks are presented.

2. Multi-scale heat conduction theory

The present multi-scale constitutive modelling approach for the estimation of the effective heat conductivity tensor follows closely the methodology proposed by Germain *et al.* [19] and is analogous to the theory presented, among others, by Suquet [49], Miehe *et al.* [35] and Michel *et al.* [34] in the context of solid mechanics problems – and whose variational structure is discussed in detail by de Souza Neto & Feijóo [14]. The starting point of the theory is the assumption that any material point $\boldsymbol{x}$ of the macroscopic continuum (refer to Fig. 1) is associated to a local 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 that form the main body of this paper, we shall consider the RVE to consist of a matrix, with domain Ω_μ^m, containing inclusions of different materials[1] occupying a domain Ω_μ^i:

$$\Omega_\mu = \Omega_\mu^m \cup \overline{\Omega}_\mu^i; \qquad \partial\Omega_\mu^m = \partial\Omega_\mu \cup \partial\Omega_\mu^i, \tag{2.1}$$

where $\overline{(\cdot)}$ denotes the closure of the set $(\cdot)$. To simplify the formulation we shall consider here only inclusions that do not intersect the boundary $\partial\Omega_\mu$ of the RVE:

$$\partial\Omega_\mu \cap \overline{\Omega}_\mu^i = \emptyset. \tag{2.2}$$

A crucial concept in the present context is the assumption that at any arbitrary point $\boldsymbol{x} \in \Omega$, the macroscopic temperature gradient ∇u is the volume average of the microscopic temperature gradient ∇u_μ:

$$\nabla u(\boldsymbol{x}) = \frac{1}{V_\mu} \int_{\Omega_\mu} \nabla u_\mu(\boldsymbol{y}), \tag{2.3}$$

where u and u_μ denote, respectively, the macroscopic and microscopic absolute temperature fields and V_μ is the volume of the RVE. In addition, we also assume that

$$u(\boldsymbol{x}) = \frac{1}{V_\mu} \int_{\Omega_\mu} u_\mu(\boldsymbol{y}). \tag{2.4}$$

2.1. **Admissible and virtual microscopic temperature fields.** By making use of Green's theorem, we can promptly establish that the averaging relation (2.3) is equivalent to the following constraint on the temperature fields of the RVE:

$$\int_{\partial\Omega_\mu} u_\mu \, \mathbf{n} = V_\mu \, \nabla u, \tag{2.5}$$

where $\mathbf{n}$ denotes the outward unit normal to the boundary of the RVE. Hence, the temperature gradient averaging relation (2.3) together with the additional constraint (2.4) require the (as yet not defined) set $\mathcal{K}_\mu$ of admissible temperature fields of the RVE to be a subset of the *minimally constrained set of admissible temperature fields*[2], $\mathcal{K}_\mu^*$:

$$\mathcal{K}_\mu \subset \mathcal{K}_\mu^* \equiv \left\{ v \in H^1(\Omega_\mu) : \int_{\Omega_\mu} v = V_\mu \, u, \ \int_{\partial\Omega_\mu} v \, \mathbf{n} = V_\mu \, \nabla u, \ [\![v]\!] = 0 \text{ on } \partial\Omega_\mu^i \right\}, \tag{2.6}$$

where $[\![(\cdot)]\!]$ denotes the *jump* of function $(\cdot)$ accross 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. Without loss of generality, u_μ can be split into a sum

$$u_\mu(\boldsymbol{y}) = u(\boldsymbol{x}) + \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} + \tilde{u}_\mu(\boldsymbol{y}), \tag{2.8}$$

of a constant temperature field (coinciding with the macrosopic temperature u at $\boldsymbol{x}$), a homogeneous gradient temperature field, $\nabla u \cdot \boldsymbol{y}$ (linear in $\boldsymbol{y}$), and a *temperature fluctuation* field, $\tilde{u}_\mu$. Now, from expressions (2.8) and (2.4), we have that

$$\int_{\Omega_\mu} \tilde{u}_\mu(\boldsymbol{y}) = -\int_{\Omega_\mu} \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y}. \tag{2.9}$$

[1]The formulation is completely analogous to the one presented here if the RVE contains voids instead.

[2]The set $\mathcal{K}_\mu^*$ is the largest admissible set of temperature fields of the RVE compatible with the averaging relations (2.3) and (2.4).

In terms of the split (2.8), constraints (2.3,2.9) can be enforced by requiring that the space $\tilde{\mathcal{K}}_\mu$ of admissible temperature fluctuations of the RVE be a subspace of the *minimally constrained space of temperature fluctuations*, $\tilde{\mathcal{K}}^*_\mu$, defined as

$$\tilde{\mathcal{K}}_\mu \subset \tilde{\mathcal{K}}^*_\mu \equiv \left\{ v \in H^1(\Omega_\mu) : \int_{\Omega_\mu} v = -\nabla u\,(\boldsymbol{x}) \cdot \int_{\Omega_\mu} \boldsymbol{y},\ \int_{\partial\Omega_\mu} v\,\mathbf{n} = \mathbf{0},\quad [\![v]\!] = 0 \ \text{ on } \ \partial\Omega^i_\mu \right\}. \tag{2.10}$$

Remark 1. *Without loss of generality, we can place the origin of the coordinate system at the centroid of the RVE. Thus, restriction (2.9) over the temperature fluctuation field $\tilde{u}_\mu\,(\boldsymbol{y})$ reduces to*

$$\int_{\Omega_\mu} \tilde{u}_\mu\,(\boldsymbol{y}) = 0. \tag{2.11}$$

□

The resulting space of virtual temperatures of the RVE, to be used below in the variational statement of the RVE thermal equilibrium, is defined as

$$\mathcal{V}_\mu \equiv \left\{ \eta \in H^1(\Omega_\mu) : \eta = v_1 - v_2;\ v_1, v_2 \in \mathcal{K}_\mu \right\}. \tag{2.12}$$

Note that this space coincides with the space of microscopic temperature fluctuations:

$$\mathcal{V}_\mu = \tilde{\mathcal{K}}_\mu. \tag{2.13}$$

Following the split (2.8), the microscopic temperature gradient can be expressed as a sum

$$\nabla u_\mu\,(\boldsymbol{y}) = \nabla u\,(\boldsymbol{x}) + \nabla \tilde{u}_\mu\,(\boldsymbol{y}), \tag{2.14}$$

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

2.2. **Thermal equilibrium of the RVE.** Let us consider a generic RVE with heat source field $b = b(\boldsymbol{y})$ in Ω_μ and normal heat flux $q = q(\boldsymbol{y})$ across $\partial\Omega_\mu$. The RVE is in thermal equilibrium if and only if the heat flux field $\boldsymbol{q}_\mu = \boldsymbol{q}_\mu(\boldsymbol{y})$ in Ω_μ satisfies the classical variational equation

$$\int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla\eta + \int_{\Omega_\mu} b\eta - \int_{\partial\Omega_\mu} q\eta = 0 \qquad \forall \eta \in \mathcal{V}_\mu. \tag{2.15}$$

2.3. **Macroscopic heat flux and the Hill-Mandel Principle.** Also crucial to the present class of theories is the assumption that the macroscopic heat flux vector, $\boldsymbol{q}$, is the volume average of the microscopic heat flux field, $\boldsymbol{q}_\mu$, over the RVE:

$$\boldsymbol{q}(\boldsymbol{x}) \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{q}_\mu(\boldsymbol{y}). \tag{2.16}$$

Another fundamental concept underlying multi-scale models of the present type is the heat conduction version of the *Hill-Mandel Principle of Macro-homogeneity* for solids [26, 32]. In the context of homogenisation in solid mechanics problems, the Hill-Mandel Principle establishes that the power of the macroscopic stress tensor at an arbitrary point of the macro-continuum must equal the volume average of the power of the microscopic stress over the RVE associated with that point for any kinematically admissible motion of the RVE. Here, we shall assume the analogous relation

$$\boldsymbol{q} \cdot \nabla u = \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla u_\mu, \tag{2.17}$$

to hold for any admissible microscopic temperature field, $u_\mu \in \mathcal{K}_\mu$.

Equation (2.17) plays a crucial role in the formulation of heat conduction constitutive models within the present framework. Its main consequence is the orthogonality between the functional spaces of virtual temperatures (which coincides with the space of admissible temperature fluctuations) and heat source and boundary normal heat flux fields of the RVE. This relation can be derived as follows. By introducing the split (2.14) into (2.17) and making use of the averaging relation (2.16), we obtain the following

$$\int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla \tilde{u}_\mu = 0 \qquad \forall\, \tilde{u}_\mu \in \mathcal{V}_\mu. \tag{2.18}$$

Further, by introducing the above equation into the thermal equilibrium statement (2.15) and making use of the corresponding Euler-Lagrange equations together with the fact that $\mathcal{V}_\mu$ is a vector space, we finally find that version (2.17) of the Hill-Mandel Principle for heat conduction problems implies

$$\int_{\Omega_\mu} b\,\eta = 0\,; \qquad \int_{\partial\Omega_\mu} q\,\eta = 0 \qquad \forall\, \eta \in \mathcal{V}_\mu. \tag{2.19}$$

The above relations impose a constraint upon the possible heat source and normal boundary heat flux fields of the RVE. Formally, they require b and q to be orthogonal to the chosen space $\mathcal{V}_\mu$ (or set $\mathcal{K}_\mu$) – they are reactions to the chosen temperature constraints of the RVE – so that these fields cannot be prescribed independently. This is in complete analogy with the homogenisation-based multi-scale approach to constitutive modelling in solid mechanics as described in [14].

Remark 2. *Equation (2.17) is at variance with Germain* et al. [19] *who postulated the following micro-macro dissipation equivalence relation:*

$$\boldsymbol{q} \cdot \frac{\nabla u}{u} = \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \frac{\nabla u_\mu}{u_\mu}, \tag{2.20}$$

as the heat conduction counterpart of the original mechanical Hill-Mandel Macro-homogeneity Principle. We remark, however, that the use of (2.17) can be justified as follows. Firstly, recall that the basic requirement of positive thermal dissipation at the macro-scale, imposed by the second law of thermodynamics, is expressed by

$$-\boldsymbol{q} \cdot \frac{\nabla u}{u} \geq 0. \tag{2.21}$$

Analogously, at the micro-scale, the inequality

$$-\boldsymbol{q}_\mu \cdot \frac{\nabla u_\mu}{u_\mu} \geq 0, \tag{2.22}$$

must hold point-wise. If (2.22) indeed holds point-wise at the RVE level, then, trivially, since u_μ is positive,

$$-\boldsymbol{q}_\mu \cdot \nabla u_\mu \geq 0. \tag{2.23}$$

The use of (2.17) ensures, in turn, that

$$-\boldsymbol{q} \cdot \nabla u \geq 0, \tag{2.24}$$

so that the macroscopic dissipation inequality (2.21) holds at the corresponding macro-continuum point. In summary, if positive dissipation is assured point-wise at the RVE level, then version (2.17) of the Hill-Mandel Principle of Macro-homogeneity for heat conduction problems ensures positive dissipation at the macroscopic level. □

2.4. **The RVE thermal equilibrium problem.** In the present analysis, we shall assume the materials of the RVE matrix and inclusions to satisfy the classical Fourier constitutive law:[3]

$$\boldsymbol{q}_\mu(\boldsymbol{y}) = -\mathbb{K}_\mu(\boldsymbol{y})\, \nabla u_\mu(\boldsymbol{y}). \tag{2.25}$$

[3]This assumption poses a restriction on the minimum size of the RVE. That is, within the present family of multi-scale theories, the RVE must be large enough so that the Fourier law can provide an accurate description of heat conduction.

In addition, for simplicity, we shall model the matrix and inclusions as two distinct homogenoeus isotropic materials:

$$\mathbb{K}_\mu(\boldsymbol{y}) = k(\boldsymbol{y})\,\boldsymbol{I} = \begin{cases} k^m \boldsymbol{I} & \forall \boldsymbol{y} \in \Omega_\mu^m \\ k^i \boldsymbol{I} & \forall \boldsymbol{y} \in \Omega_\mu^i, \end{cases} \tag{2.26}$$

where k^m and k^i denote, respectively, the heat conductivity coefficients of the matrix and inclusions.

By introducing decomposition (2.14) into the thermal equilibrium equation (2.15) and taking (2.19), (2.25) and (2.26) into account, we obtain the *RVE thermal equilibrium problem* of finding, for a given macroscopic temperature gradient ∇u, an admissible microscopic temperature fluctuation field $\tilde{u}_\mu \in \mathcal{V}_\mu$, such that

$$\int_{\Omega_\mu} k \nabla \tilde{u}_\mu \cdot \nabla \eta = - \int_{\Omega_\mu} k \nabla u \cdot \nabla \eta \qquad \forall \eta \in \mathcal{V}_\mu. \tag{2.27}$$

2.5. **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 temperatures must be made. By following a reasoning completely analogous to that adopted in the definition of classical homogenisation-based constitutive models for solid mechanics problems within a variationnal multi-scale framework [14], we list below four possible choices:

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

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{T}} \equiv \{\mathbf{0}\}. \tag{2.28}$$

In this case, the temperature gradient is homogeneous over the RVE:

$$\nabla u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \qquad \forall\, \boldsymbol{y} \in \Omega_\mu. \tag{2.29}$$

The reactive RVE heat source and normal boundary heat flux fields

$$(q, b) \in \left(\mathcal{V}_\mu^{\mathcal{T}}\right)^\perp, \tag{2.30}$$

may be arbitrary functions.

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

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{L}} \equiv \left\{ \tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu^* : \tilde{u}_\mu(\boldsymbol{y}) = 0 \ \forall \boldsymbol{y} \in \partial\Omega_\mu \right\}. \tag{2.31}$$

In this case, the temperature distribution on the boundary of the RVE reads

$$u_\mu(\boldsymbol{y}) = u(\boldsymbol{x}) + \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} \qquad \forall \boldsymbol{y} \in \partial\Omega_\mu. \tag{2.32}$$

The only possible reactive heat source over Ω_μ orthogonal to $\mathcal{V}_\mu^{\mathcal{L}}$ is

$$b = 0. \tag{2.33}$$

That is, only a zero microscopic heat source is compatible with this class of models. On $\partial\Omega_\mu$, the resulting reactive normal heat flux

$$q \in \left(\mathcal{V}_\mu^{\mathcal{L}}\right)^\perp, \tag{2.34}$$

may be any function.

(c) *Periodic boundary fluctuations model* . The assumption of periodic boundary fluctuations is widely used in the definition of multi-scale constitutive models for solid mechanics problems [34] in the analysis of media with periodic micro-structures. A completely analogous approach is followed in the present context of heat conduction problems. The macro-continuum, in this case, is assumed to be generated by the periodic repetition of the RVE, so that the RVE geometry must satisfy certain constraints. The description here will be focussed on two-dimensional problems (to which the present paper is restricted) and we shall follow closely the notation adopted by Miehe *et al.* [35] in the context of solid mechanics problems. Consider, for example, square or hexagonal RVEs as illustrated in Fig. 2. In this case, each pair j of sides consists of equally sized subsets

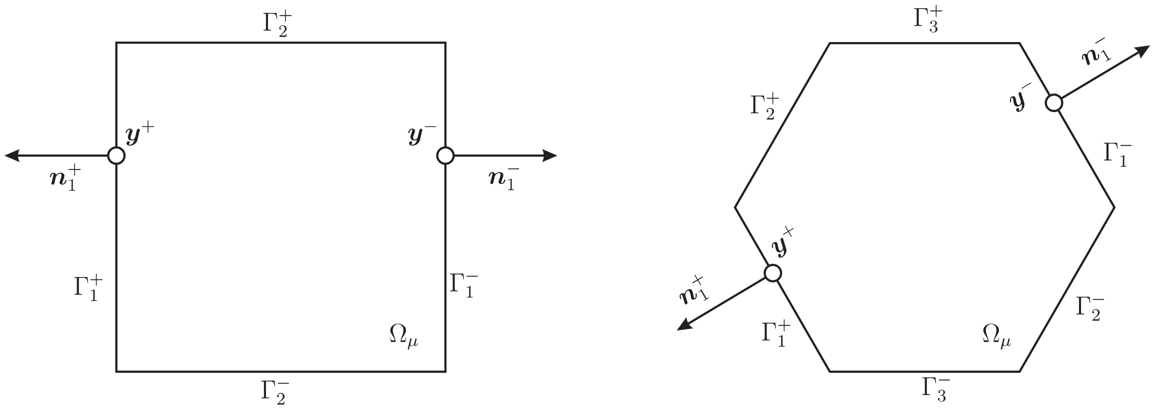


FIGURE 2. RVE geometries for periodic media. Square and hexagonal cells.

$$\Gamma_j^+ \quad \text{and} \quad \Gamma_j^-, \tag{2.35}$$

of $\partial\Omega_\mu$, with respective unit normals

$$\mathbf{n}_j^+ \quad \text{and} \quad \mathbf{n}_j^-, \tag{2.36}$$

such that

$$\mathbf{n}_j^- = -\mathbf{n}_j^+. \tag{2.37}$$

A one-to-one correspondence exists between the points of Γ_j^+ and Γ_j^-. That is, each point $\boldsymbol{y}^+ \in \Gamma_j^+$ has a corresponding point $\boldsymbol{y}^- \in \Gamma_j^-$. The key constraint over the admissible temperature fields for this class of models is that the temperature fluctuation must be periodic on the boundary of the RVE. That is, for each pair $(\boldsymbol{y}^+, \boldsymbol{y}^-)$ of boundary material points we have

$$\tilde{u}_\mu(\boldsymbol{y}^+) = \tilde{u}_\mu(\boldsymbol{y}^-). \tag{2.38}$$

Accordingly, the space of temperature fluctuations is defined as

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{P}} \equiv \left\{ \tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu^* : \tilde{u}_\mu(\boldsymbol{y}^+) = \tilde{u}_\mu(\boldsymbol{y}^-) \ \forall \text{ pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu \right\}. \tag{2.39}$$

Again, only the zero heat source field is orthogonal to the chosen space of fluctuations so that (2.33) must hold for this class of models. The normal boundary heat flux fields – in this case orthogonal to $\mathcal{V}_\mu^{\mathcal{P}}$ – satisfy

$$q(\boldsymbol{y}^+) = -q(\boldsymbol{y}^-) \quad \forall \text{ pair } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu. \tag{2.40}$$

That is, the normal boundary heat flux is *anti-periodic.*

(d) *Minimally constrained* or *Uniform normal boundary heat flux model.* In this case, we choose,

$$\mathcal{V}_\mu = \mathcal{V}_\mu^{\mathcal{U}} \equiv \tilde{\mathcal{K}}_\mu^*. \tag{2.41}$$

Again only the zero heat source field is orthogonal to the chosen space. The normal boundary heat flux orthogonal to the space of fluctuations in this case can be shown to satisfy the *uniform boundary flux condition*:

$$q\,(\boldsymbol{y}) = \boldsymbol{q}\,(\boldsymbol{x}) \cdot \mathbf{n}\,(\boldsymbol{y}) \quad \forall \boldsymbol{y} \in \partial\Omega_\mu, \tag{2.42}$$

where $\boldsymbol{q}(\boldsymbol{x})$ is the macroscopic heat flux vector at the point $\boldsymbol{x}$ of the macro-continuum associated with the RVE in question.

Note that the spaces of temperature fluctuations (and virtual temperatures) listed in the above satisfy

$$\mathcal{V}_\mu^{\mathcal{T}} \subset \mathcal{V}_\mu^{\mathcal{L}} \subset \mathcal{V}_\mu^{\mathcal{P}} \subset \mathcal{V}_\mu^{\mathcal{U}}. \tag{2.43}$$

The rule of mixtures and uniform boundary heat flux models correspond, respectively, to the choices of most and least constrained spaces of RVE temperature fields. It should be said that the rule of mixtures is of little practical use as it is expected, in general, to greatly overestimate the macroscopic conductivity. It has been listed above mainly for the sake of completeness as it can be retrieved within the present framework by the trivial selection of space $\mathcal{V}_\mu$. In general, for a given RVE, each choice of space $\mathcal{V}_\mu$ will produce a different estimate of the corresponding macroscopic conductivity. Ostoja-Starzewski and Schulte [43] show that the RVE boundary conditions imposed upon the linear boundary temperature and uniform boundary flux models lead, respectively, to an upper and lower bound for the macroscopic conductivity tensor and, as such, provide extremely useful estimates of the overall heat conduction property of the material.

2.6. **The homogenised heat conductivity 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 heat conductivity 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 (2.26), the variational problem defined by (2.27) can be equivalently written as

$$\int_{\Omega_\mu} \mathbb{K}_\mu \nabla \tilde{u}_\mu \cdot \nabla \eta = -\int_{\Omega_\mu} \mathbb{K}_\mu \nabla u \cdot \nabla \eta \qquad \forall \eta \in \mathcal{V}_\mu. \tag{2.44}$$

Clearly, the above variational problem is linear. A compact expression for the macroscopic heat conductivity tensor can be obtained by writing the original linear problem as a superposition of linear problems associated with the individual Cartesian components of the macroscopic temperature gradient vector. The procedure is completely analogous to that followed by Michel *et al.* [34] in the context of solid mechanics problems. We start by writing the macroscopic temperature gradient in Cartesian component form:

$$\nabla u = (\nabla u)_i \, \mathbf{e}_i, \tag{2.45}$$

where the vectors $\{\mathbf{e}_i\}$ are an orthonormal basis of the two-dimensional Euclidean space and the scalars $(\nabla u)_i$ are the corresponding Cartesian components. In addition, let the scalar field $\tilde{u}_{\mu_i} \in \mathcal{V}_\mu$ be the solution of the variational problem

$$\int_{\Omega_\mu} \mathbb{K}_\mu \nabla \tilde{u}_{\mu_i} \cdot \nabla \eta = -\int_{\Omega_\mu} \mathbb{K}_\mu \mathbf{e}_i \cdot \nabla \eta \qquad \forall \eta \in \mathcal{V}_\mu. \tag{2.46}$$

The fields $\tilde{u}_{\mu_i}$ will be referred to as *tangential temperature fluctuations*. Each $\tilde{u}_{\mu_i}$ represents the derivative of the temperature fluctuation field of the RVE with respect to the macroscopic temperature gradient component in the direction of the basis vector $\mathbf{e}_i$. Since (2.44) is linear, its solution $\tilde{u}_\mu \in \mathcal{V}_\mu$ can be constructed by the superposition of the tangential temperature fluctuations linearly combined as

$$\tilde{u}_\mu = (\nabla u)_i \, \tilde{u}_{\mu_i}. \tag{2.47}$$

At the macroscopic level, the Fourier law reads

$$\boldsymbol{q} = -\mathbb{K}^{\mathcal{H}} \, \nabla u, \tag{2.48}$$

where $\mathbb{K}^{\mathcal{H}}$ is the homogenised macroscopic heat conductivity tensor – whose closed form representation in terms of tangential fluctuations is the main purpose of this section. In view of definition (2.16) and the microscopic Fourier law (2.25), the above is equivalent to

$$\mathbb{K}^{\mathcal{H}} \, \nabla u = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{K}_\mu \nabla u_\mu (\boldsymbol{y}) \, . \tag{2.49}$$

With the introduction of the additive decomposition (2.14) of the microscopic temperature gradient along with expression (2.47) into (2.49), we have

$$\begin{aligned} \mathbb{K}^{\mathcal{H}} \, \nabla u &= \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{K}_\mu \nabla u + \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{K}_\mu \nabla \tilde{u}_\mu \\ &= \mathbb{K}^{\mathcal{T}} \nabla u + \left(\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{K}_\mu \nabla \tilde{u}_{\mu_i} \right) (\nabla u)_i \, , \end{aligned} \tag{2.50}$$

where

$$\mathbb{K}^{\mathcal{T}} \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{K}_\mu, \tag{2.51}$$

is the volume average of the microscopic conductivity tensor which, as we shall see, corresponds to the macroscopic conductivity tensor predicted by the Taylor (or rule of mixtures) model.

Now, note that the product $\mathbb{K}_\mu \nabla \tilde{u}_{\mu_i}$ can be expressed as

$$\mathbb{K}_\mu \nabla \tilde{u}_{\mu_i} = (\mathbb{K}_\mu)_{jk} (\mathbf{e}_j \otimes \mathbf{e}_k) (\nabla \tilde{u}_{\mu_i})_k \mathbf{e}_k = (\mathbb{K}_\mu)_{jk} (\nabla \tilde{u}_{\mu_i})_k \mathbf{e}_j. \tag{2.52}$$

By substituting (2.52) into (2.50) we obtain

$$\begin{aligned} \mathbb{K}^{\mathcal{H}} \nabla u &= \mathbb{K}^{\mathcal{T}} \nabla u + \left(\frac{1}{V_\mu} \int_{\Omega_\mu} (\mathbb{K}_\mu)_{jl} (\nabla \tilde{u}_{\mu_i})_l \mathbf{e}_j \right) \nabla u \cdot \mathbf{e}_i \\ &= \left(\mathbb{K}^{\mathcal{T}} + \tilde{\mathbb{K}} \right) \nabla u, \end{aligned} \tag{2.53}$$

where

$$\tilde{\mathbb{K}} \equiv \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\mathbb{K}_\mu)_{ik} \left(\nabla \tilde{u}_{\mu_j} \right)_k \right] \mathbf{e}_i \otimes \mathbf{e}_j. \tag{2.54}$$

From the above, we finally have

$$\mathbb{K}^{\mathcal{H}} = \mathbb{K}^{\mathcal{T}} + \tilde{\mathbb{K}}. \tag{2.55}$$

Remark 3. *The homogenised heat conductivity tensor can be represented as a sum of two contributions: (i) the volume average $\mathbb{K}^{\mathcal{T}}$ of the microscopic conductivity; and (ii) a contribution $\tilde{\mathbb{K}}$ that depends solely on the tangential fluctuations $\tilde{u}_{\mu_i}$ which, in turn, depend in general on the choice of space $\mathcal{V}_\mu$. Both contributions are independent of the macroscopic temperature gradient. Note, for example, that for the rule of mixtures, corresponding to the choice (2.28), we have $\tilde{u}_{\mu_i} = 0$ for all directions i. In this case, $\tilde{\mathbb{K}} = \mathbf{0}$ and $\mathbb{K}^{\mathcal{H}} = \mathbb{K}^{\mathcal{T}}$. That is, as mentioned earlier, $\mathbb{K}^{\mathcal{T}}$ is indeed the homogenised conductivity predicted by the rule of mixtures.* □

3. The topological sensitivity of the homogenised conductivity tensor

This section presents the main result of this paper – a closed formula for the sensitivity of the homogenised conductivity tensor (2.55) to the introduction of an arbitrarily positioned topological perturbation (a circular inclusion)[4] in the RVE. The derived formula is valid for two-dimensional problems. The original (unperturbed) RVE comprises a matrix of conductivity k^m with embedded inclusions of conductivity k^i. Both matrix and inclusions are thermally isotropic. The (isotropic) conductivity of the perturbation is assumed to be

$$k^*(\hat{\boldsymbol{y}}) = \begin{cases} k^i = \gamma k^m & \text{if } \hat{\boldsymbol{y}} \in \Omega_\mu^m \\ k^m = \gamma k^i & \text{if } \hat{\boldsymbol{y}} \in \Omega_\mu^i, \end{cases} \tag{3.1}$$

where $\hat{\boldsymbol{y}} \in \Omega_\mu$ denotes the position of the centre of the circular perturbation and $\gamma \in \Re^+$ defines the ratio between the conductivities of the matrix (or inclusion) and the perturbation.

We remark that the derivation of the analytical sensitivity formula is rather lengthy. Hence, we shall choose here to firstly present the closed formula and proceed to its derivation only later in this section. This should be particularly convenient to readers not interested in the details of the mathematical derivation. The sensitivity of the macroscopic conductivity tensor to the topological change produced by the introduction of a circular perturbation is the second-order tensor field over Ω_μ with closed form representation

$$\mathbb{S}(\hat{\boldsymbol{y}}) = -2k(\hat{\boldsymbol{y}}) \frac{1-\gamma}{1+\gamma} \left[\nabla u_{\mu_i}(\hat{\boldsymbol{y}}) \cdot \nabla u_{\mu_j}(\hat{\boldsymbol{y}}) \right] \mathbf{e}_i \otimes \mathbf{e}_j \quad \forall \hat{\boldsymbol{y}} \in \Omega_\mu, \tag{3.2}$$

[4]Topological sensitivity analysis accounting for arbitraryly shaped inclusions and simultaneous nucleation of holes, in different contexts, can be found respectively in [37, 2]

with $i, j = 1, 2$ and

$$\nabla u_{\mu_i} = \mathbf{e}_i + \nabla \tilde{u}_{\mu_i}, \tag{3.3}$$

where $\tilde{u}_{\mu_i}$ denote the solutions of the variational problems defined by (2.46).

The physical meaning of the field $\mathbb{S}$ can be made clear by considering the difference

$$\delta \mathbb{K}_\varepsilon^{\mathcal{H}}(\hat{\boldsymbol{y}}) = \mathbb{K}_\varepsilon^{\mathcal{H}}(\hat{\boldsymbol{y}}) - \mathbb{K}^{\mathcal{H}}, \tag{3.4}$$

between the homogenised conductivity $\mathbb{K}_\varepsilon^{\mathcal{H}}(\hat{\boldsymbol{y}})$, of the RVE with a perturbation of radius ε centred at an arbitrary point $\hat{\boldsymbol{y}} \in \Omega_\mu$, and the homogenised conductivity tensor $\mathbb{K}^{\mathcal{H}}$ of the unperturbed (original) RVE. The approximation to $\delta\mathbb{K}_\varepsilon^{\mathcal{H}}$ linear in the volume fraction $\pi\varepsilon^2/V_\mu$ of perturbation is given by

$$\delta \mathbb{K}_\varepsilon^{\mathcal{H}}(\hat{\boldsymbol{y}}) = \frac{\pi\varepsilon^2}{V_\mu}\,\mathbb{S}(\hat{\boldsymbol{y}}) + o(\varepsilon^2). \tag{3.5}$$

That is, the sensitivity tensor $\mathbb{S}(\hat{\boldsymbol{y}})$ provides the linear approximation, in the volume fraction $\pi\varepsilon^2/V_\mu$ of perturbation, to the change in the homogenised conductivity tensor $\mathbb{K}^{\mathcal{H}}$ resulting from the insertion of a perturbation of radius ε centred at $\hat{\boldsymbol{y}}$. Each component $\mathbb{S}_{ij}(\hat{\boldsymbol{y}})$ is the (topological) derivative of the component ij of the macroscopic conductivity tensor with respect to the RVE volume fraction occupied by the circular perturbation.

Remark 4. *The remarkable simplicity of the closed form sensitivity given by (3.2) is to be noted. Once the tangential fluctuation fields $\tilde{u}_{\mu_i}$ have been obtained as solutions of (2.46) for the* original *RVE domain, the sensitivity tensor can be trivially assembled. The information provided by (3.2) 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 (3.2)–(3.5) is based on the mathematical notion of *topological derivative* and is presented in detail in Sections 3.2–3.5. Before proceding 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

$$\psi(\varepsilon) = \psi(0) + f(\varepsilon)\, D_T\psi + o(f(\varepsilon)), \tag{3.6}$$

where $\psi(0)$ is the value of the functional for the given original domain and $\psi(\varepsilon)$ denotes the value of the functional 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

$$\lim_{\varepsilon \to 0^+} f(\varepsilon) = 0, \tag{3.7}$$

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

Expression (3.6) is named the *topological asymptotic expansion* of ψ. The term $D_T\psi$ is defined as the *topological derivative of first order* 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 (3.4) let $\delta\psi_\varepsilon$ denote the difference

$$\delta\psi_\varepsilon = \psi(\varepsilon) - \psi(0), \tag{3.8}$$

then, similar to (3.5), we have the linear approximation

$$\delta\psi_\varepsilon = f(\varepsilon)\, D_T\psi + o(f(\varepsilon)). \tag{3.9}$$

The concept of topological derivative is an extension of the classical notion of derivative. It has been rigorously introduced in 1999 by Sokołowski & Zochowski [46] in the context of shape optimisation for two-dimensional heat conduction and elasticity problems (for an introduction in the shape optimisation concept see [36, 48]). 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.* [11], Garreau *et al.* [18], Guillaume & Sid Idris [21], Novotny *et al.* [40], Feijóo *et al.* [17], Nazarov & Sokolowski [37], Lewinski & Sokolowski [31], Samet *et al.* [44], Sokolowski [45], Guillaume & Sid Idris [22], Burger *et al.* [10], Nazarov & Sokolowski [38], Feijóo [16], Amstutz [2], Amstutz *et al.* [4], Sokolowski & Zochowski [47], Hintermüller [27], Masmoudi *et al.* [33], Amstutz & Andrä [3], Bonnet [9], Auroux *et al.* [7]). More recent developments include the use of the topological derivative in two- and three-dimensional optimisation of elastic structures [42, 20], image processing [8, 30] with application to breast cancer diagnosis [25] and the extension of the original concept to the definition of a second order topological derivative [13].

3.2. **Application to the multi-scale heat conductivity model.** The first step in the application of the topological derivative concept is the definition of the functional whose topological asymptotic expansion is required. Here, our purpose is to derive the closed formula (3.2) for the sensitivity of the macroscopic heat conductivity tensor. To this end, it is appropriate to define the following functional

$$\psi(\varepsilon) \equiv V_\mu \boldsymbol{q}^\varepsilon \cdot \nabla u, \quad \Rightarrow \quad \psi(0) = V_\mu \boldsymbol{q} \cdot \nabla u, \tag{3.10}$$

where $\boldsymbol{q}^\varepsilon$ denotes the macroscopic heat flux vector resulting from a macroscopic temperature gradient ∇u at a point of the macro-continuum associated with a RVE defined by Ω_{μ_ε} containing a small perturbation and $\boldsymbol{q}$ denotes the macroscopic heat flux vector 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). At an arbitrary point $\hat{\boldsymbol{y}} \in \Omega_\mu^m$ of the matrix of the original RVE domain

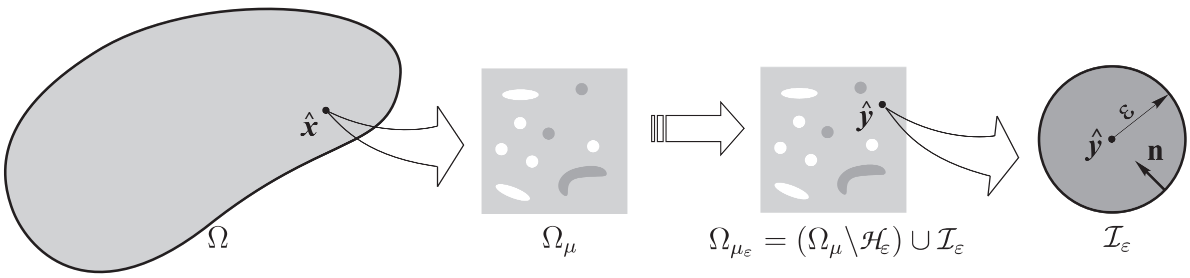


FIGURE 3. Microstructure with a perturbation $\mathcal{I}_\varepsilon$.

$\Omega_\mu = \Omega_\mu^m \cup \overline{\Omega}_\mu^i$ of Section 2, a circular portion $\mathcal{H}_\varepsilon$ of radius ε of matrix material (with isotropic conductivity k^m)[5] is replaced with the circular perturbation $\mathcal{I}_\varepsilon$ of isotropic conductivity k^i. The topologically perturbed domain is then defined as

$$\Omega_{\mu_\varepsilon} = (\Omega_\mu \backslash \mathcal{H}_\varepsilon) \cup \mathcal{I}_\varepsilon. \tag{3.11}$$

The asymptotic topological expansion of the functional (3.10) reads

$$\boldsymbol{q}^\varepsilon \cdot \nabla u = \boldsymbol{q} \cdot \nabla u + \frac{1}{V_\mu} f(\varepsilon)\, D_T\psi + o\left(f(\varepsilon)\right), \tag{3.12}$$

or, equivalently, by making use of the macroscopic Fourier law ($\boldsymbol{q}^\varepsilon = -\mathbb{K}_\varepsilon^{\mathcal{H}} \nabla u$, $\boldsymbol{q} = -\mathbb{K}^{\mathcal{H}} \nabla u$) and definition (3.4),

$$-\delta \mathbb{K}_\varepsilon^{\mathcal{H}} \nabla u \cdot \nabla u = \frac{1}{V_\mu} f(\varepsilon)\, D_T\psi + o\left(f(\varepsilon)\right). \tag{3.13}$$

[5]The derivation for the case where the perturbation is introduced at a point of the RVE containing an inclusion is completely analogous.

The sensitiviy tensor will be determined as follows. Once the asymptotic expansion of ψ leading to an explicit closed form for (3.13) has been carried out, the sensitivity tensor will be identified[6] by comparing the resulting expression with (3.5).

3.3. **Topological derivative calculation .** In order to obtain a closed form expression of the asymptotic expansion (3.12), we start here by deriving a closed formula for the associated topological derivative $D_T\psi$. To this end, we define the functional

$$\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) \equiv \psi(\varepsilon) = \int_{\Omega_{\mu_\varepsilon}} \boldsymbol{q}_{\mu_\varepsilon} \cdot \nabla u_{\mu_\varepsilon}. \tag{3.14}$$

The last right hand side of (3.14) is obtained from definition (3.10) by making use of the Hill-Mandel relation (2.17). In the above,

$$u_{\mu_\varepsilon}(\boldsymbol{y}) = u(\boldsymbol{x}) + \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} + \tilde{u}_{\mu_\varepsilon}(\boldsymbol{y}), \tag{3.15}$$

is the microscopic temperatute field that solves the thermal equilibrium problem for the perturbed RVE, $\tilde{u}_{\mu_\varepsilon}$ is the corresponding temperature fluctuation and $\boldsymbol{q}_{\mu_\varepsilon}$ – also a functional of u_{μ_ε} – is the microscopic heat flux field. In particular, $\tilde{u}_{\mu_\varepsilon}$ solves the following variational problem: Find $\tilde{u}_{\mu_\varepsilon} \in \tilde{\mathcal{K}}_{\mu_\varepsilon} = \{v \in \tilde{\mathcal{K}}_\mu : [\![v]\!]|_{\partial\mathcal{I}_\varepsilon} = 0\}$ such that

$$\int_{\Omega_{\mu_\varepsilon}} k^* \left(\nabla u \cdot \nabla \eta + \nabla \tilde{u}_{\mu_\varepsilon} \cdot \nabla \eta\right) = 0 \quad \forall \eta \in \mathcal{V}_{\mu_\varepsilon} = \{\xi \in \mathcal{V}_\mu : [\![\xi]\!]|_{\partial\mathcal{I}_\varepsilon} = 0\}, \tag{3.16}$$

where, similarly to (2.26), the isotropic conductivity within the perturbed RVE reads

$$k^*(\boldsymbol{y}) = \begin{cases} k^m & \forall \boldsymbol{y} \in \Omega_\mu^m \backslash \mathcal{H}_\varepsilon \\ k^i & \forall \boldsymbol{y} \in \Omega_\mu^i \cup \mathcal{I}_\varepsilon. \end{cases} \tag{3.17}$$

It should be noted that the functional (3.14) depends explicitly and implicitly on the domain Ω_{μ_ε}. Its implicit dependence stems from the fact that the temperature fluctuation field $\tilde{u}_{\mu_\varepsilon}$ is the solution of the RVE thermal equilibrium problem (3.16), for the *perturbed* RVE domain.

Among the methods for calculation of the topological derivative currenlty available in the literature, here we shall adopt the approach presented in [47, 40], whereby the topological derivative is obtained as the limit

$$D_T\psi = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}). \tag{3.18}$$

The derivative of the functional $\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon})$ with respect to the perturbation parameter ε can be seen as the sentitivity of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$, in the classical sense [36], to the change in shape produced by a uniform expansion of the perturbation. Accordingly, we define a sufficiently regular *shape change velocity field*, $\mathbf{v}$, over Ω_{μ_ε}, such that

$$\begin{cases} \mathbf{v} = \mathbf{0}, & \text{on } \partial\Omega_\mu \\ \mathbf{v} = -\mathbf{n}, & \text{on } \partial\mathcal{I}_\varepsilon. \end{cases} \tag{3.19}$$

3.3.1. *Rule of mixtures.* Let us start by dealing with the simplest class of multi-scale models described in Section 2.5 – the rule of mixtures (or Taylor) model. In this case, we combine

[6]This identification is possible due to the symmetry of $\delta\mathbb{K}_\varepsilon^{\mathcal{H}}$.

(3.14), (2.29) and the Fourier law for the perturbed RVE to derive

$$
\begin{aligned}
\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) &= \frac{d}{d\varepsilon}\int_{\Omega_{\mu_\varepsilon}} \boldsymbol{q}_{\mu_\varepsilon}\cdot\nabla u_{\mu_\varepsilon} \\
&= -\frac{d}{d\varepsilon}\int_{\Omega_{\mu_\varepsilon}} k^*\nabla u\cdot\nabla u \\
&= -\frac{d}{d\varepsilon}\left(\int_{\Omega_\mu\setminus\mathcal{H}_\varepsilon} k|\nabla u|^2 + \int_{\mathcal{I}_\varepsilon} k^i|\nabla u|^2\right) \\
&= -k^m|\nabla u|^2\int_{\partial\Omega_\mu}(\mathbf{v}\cdot\mathbf{n}) - k^m|\nabla u|^2\int_{\partial\mathcal{H}_\varepsilon}(\mathbf{v}\cdot\mathbf{n}) + k^i|\nabla u|^2\int_{\partial\mathcal{I}_\varepsilon}(\mathbf{v}\cdot\mathbf{n}) \\
&= 2\pi\varepsilon\left(k^m-k^i\right)|\nabla u|^2.
\end{aligned}
\tag{3.20}
$$

By substituting (3.20) into definition (3.18) of the topological derivative and identifying function $f(\varepsilon)$ as

$$f(\varepsilon) = \pi\varepsilon^2, \tag{3.21}$$

i.e., the perturbation area, we find that, for the rule of mixtures model,

$$D_T^{\mathcal{T}}\psi = \left(k^m - k^i\right)|\nabla u|^2, \tag{3.22}$$

or, equivalently,

$$D_T^{\mathcal{T}}\psi(\hat{\boldsymbol{y}}) = k(\hat{\boldsymbol{y}})(1-\gamma)|\nabla u|^2 \qquad \forall\hat{\boldsymbol{y}}\in\Omega_\mu, \tag{3.23}$$

where we recall that the contrast γ is defined by (3.1).

3.3.2. *Other classes of multi-scale models.* The derivation presented in the above is relatively simple due to the trivial definition (2.28) of the space of variations of admissible temperature fields for the rule of mixtures model. For the other models of Section 2.5, the derivation is considerably more elaborate as due account needs to be taken of the fact that $\tilde{u}_{\mu_\varepsilon}$ is the solution of the variational thermal equilibrium problem (3.16) for the perturbed RVE domain.

In order to proceed, it is convenient to introduce an analogy to classical continuum mechanics [23] whereby the RVE shape change velocity field (3.19) is identified with the classical velocity field of a deforming continuum and ε is identified as a time parameter (refer to [39] for analogies of this type in the context of shape sensitivity analysis). Then, by making use of Reynolds' Transport Theorem [23, 24], we obtain the identity

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = -\int_{\Omega_{\mu_\varepsilon}} k^*\left(\frac{d}{d\varepsilon}|\nabla u_{\mu_\varepsilon}|^2 + |\nabla u_{\mu_\varepsilon}|^2\,\mathrm{div}\,\mathbf{v}\right). \tag{3.24}$$

Next, by using the concept of material derivative of a spatial field [23], we find that the first term of the above right hand side integral can be written as

$$\frac{d}{d\varepsilon}|\nabla u_{\mu_\varepsilon}|^2 = 2\nabla u_{\mu_\varepsilon}\cdot(\nabla u_{\mu_\varepsilon})^{\cdot}, \tag{3.25}$$

where $(\cdot)^{\cdot}$ denotes the (total) material derivative of $(\cdot)$ with respect to ε. Further, note that the relation

$$\nabla u_{\mu_\varepsilon} = \nabla u + \nabla\tilde{u}_{\mu_\varepsilon}, \tag{3.26}$$

gives

$$(\nabla u_{\mu_\varepsilon})^{\cdot} = (\nabla\tilde{u}_{\mu_\varepsilon})^{\cdot}, \tag{3.27}$$

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

$$(\nabla u_{\mu_\varepsilon})^{\cdot} = \nabla\dot{\tilde{u}}_{\mu_\varepsilon} - (\nabla\mathbf{v})^T\nabla\tilde{u}_{\mu_\varepsilon}, \tag{3.28}$$

where $\dot{\tilde{u}}_{\mu_\varepsilon}$ denotes the (total) material derivative of the microscopic temperature fluctation field $\tilde{u}_{\mu_\varepsilon}$ with respect to ε. Then, by introducing the above expression into (3.25) we obtain

$$\frac{d}{d\varepsilon}|\nabla u_{\mu_\varepsilon}|^2 = 2\left[\nabla u\cdot\nabla\dot{\tilde{u}}_{\mu_\varepsilon} + \nabla\tilde{u}_{\mu_\varepsilon}\cdot\nabla\dot{\tilde{u}}_{\mu_\varepsilon} - (\nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla u + \nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla\tilde{u}_{\mu_\varepsilon})\cdot\nabla\mathbf{v}\right], \tag{3.29}$$

which, substituted in (3.24) gives

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = -\int_{\Omega_{\mu_\varepsilon}} \Big\{ 2k^*\Big[&\nabla u\cdot\nabla\dot{\tilde{u}}_{\mu_\varepsilon} + \nabla\tilde{u}_{\mu_\varepsilon}\cdot\nabla\dot{\tilde{u}}_{\mu_\varepsilon} \\ &- (\nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla u + \nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla\tilde{u}_{\mu_\varepsilon})\cdot\nabla\mathbf{v}\Big] \\ &+ k^*\left(|\nabla u|^2 + 2\nabla u\cdot\nabla\tilde{u}_{\mu_\varepsilon} + |\nabla\tilde{u}_{\mu_\varepsilon}|^2\right)\,\mathbf{I}\cdot\nabla\mathbf{v}\Big\},\end{aligned} \tag{3.30}$$

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 temperature variations, we have $\dot{\tilde{u}}_{\mu_\varepsilon}\in\mathcal{V}_{\mu_\varepsilon}$. This, together with the thermal equilibrium equation (3.16), implies that the first two terms within the square brackets of (3.30) vanish. Then, we obtain

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \mathbf{\Sigma}_{\mu_\varepsilon}\cdot\nabla\mathbf{v}, \tag{3.31}$$

where $\mathbf{\Sigma}_{\mu_\varepsilon}$ is the generalised Eshelby momentum-energy tensor [15] of the RVE, here given by

$$\begin{aligned}\mathbf{\Sigma}_{\mu_\varepsilon} &= -k^*\left(|\nabla u|^2 + 2\nabla u\cdot\nabla\tilde{u}_{\mu_\varepsilon} + |\nabla\tilde{u}_{\mu_\varepsilon}|^2\right)\mathbf{I} \\ &\qquad + 2k^*\left(\nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla u + \nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla\tilde{u}_{\mu_\varepsilon}\right) \\ &= -k^*\left[|\nabla u_{\mu_\varepsilon}|^2\mathbf{I} - 2\left(\nabla\tilde{u}_{\mu_\varepsilon}\otimes\nabla u_{\mu_\varepsilon}\right)\right].\end{aligned} \tag{3.32}$$

By applying the divergence theorem to the right hand side of (3.31), we obtain

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) &= \int_{\partial\Omega_\mu}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} - \int_{\Omega_{\mu_\varepsilon}}\operatorname{div}(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v} \\ &\qquad + \int_{\partial\mathcal{I}_\varepsilon}\mathbf{\Sigma}^m_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} - \int_{\partial\mathcal{I}_\varepsilon}\mathbf{\Sigma}^i_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} \\ &= \int_{\partial\Omega_{\mu_\varepsilon}}\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{v} - \int_{\Omega_{\mu_\varepsilon}}\operatorname{div}(\mathbf{\Sigma}_{\mu_\varepsilon})\cdot\mathbf{v} + \int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}]\!]\cdot\mathbf{v}.\end{aligned} \tag{3.33}$$

Then, by taking definition (3.19) into account, together with the fact that $\mathbf{\Sigma}_{\mu_\varepsilon}$ is a divergence-free field[7], we finally arrive at the following expression for the sensitivity of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ exclusively in terms of integrals over the boundary $\partial\mathcal{I}_\varepsilon$

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = -\int_{\partial\mathcal{I}_\varepsilon}[\![\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}]\!]\cdot\mathbf{n}. \tag{3.34}$$

We now proceed to derive an explicit expression for the integrand on the right hand side of (3.34). Then, consider a curvilinear coordinate system n–t along $\partial\mathcal{I}_\varepsilon$, characterised by the orthonormal vectors $\mathbf{n}$ and $\mathbf{t}$. The normal flux of the Eshelby tensor (3.32) can be written as

$$\mathbf{\Sigma}_{\mu_\varepsilon}\mathbf{n}\cdot\mathbf{n} = -k^*\left[|\nabla u|^2 + 2\frac{\partial\tilde{u}_{\mu_\varepsilon}}{\partial t}(\nabla u\cdot\mathbf{t}) - \left(\frac{\partial\tilde{u}_{\mu_\varepsilon}}{\partial n}\right)^2 + \left(\frac{\partial\tilde{u}_{\mu_\varepsilon}}{\partial t}\right)^2\right]. \tag{3.35}$$

In addition, note that the required continuity of the temperature fluctuation $\tilde{u}_{\mu_\varepsilon}$ along $\partial\mathcal{I}_\varepsilon$, enforced in the definition of $\mathcal{V}_{\mu_\varepsilon}$:

$$[\![\tilde{u}_{\mu_\varepsilon}]\!]|_{\partial\mathcal{I}_\varepsilon} = 0, \tag{3.36}$$

[7]The proof that $\mathbf{\Sigma}_{\mu_\varepsilon}$ is a divergence-free field follows completely analogous steps to those shown in [17, 40].

gives

$$\left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_m - \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_i = 0, \tag{3.37}$$

and

$$k^m \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i = -\left(k^m - k^i\right) \nabla u \cdot \mathbf{n}, \tag{3.38}$$

or, equivalently,

$$\left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_m = -\frac{k^m - k^i}{k^m} \nabla u \cdot \mathbf{n} + \frac{k^i}{k^m} \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i . \tag{3.39}$$

With the above relations at hand and definition (3.17) of k^*, we find that the following identities hold on the boundary of the perturbation

$$\begin{aligned}
[\![k^* |\nabla u|^2]\!] &= \left(k^m - k^i\right) |\nabla u|^2, \\
[\![k^* \left(\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right)^2]\!] &= \left(k^m - k^i\right) \left(\left.\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_i \right)^2, \\
[\![k^* \left(\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right)^2]\!] &= k^i \tfrac{k^m - k^i}{k^m} \left[\tfrac{k^m - k^i}{k^i} \left(\nabla u \cdot \mathbf{n}\right)^2 - 2 \left(\nabla u \cdot \mathbf{n}\right) \left.\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i - \left(\left.\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i \right)^2 \right], \\
[\![k^* \tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t} \left(\nabla u \cdot \mathbf{t}\right)]\!] &= \left(k^m - k^i\right) \left(\nabla u \cdot \mathbf{t}\right) \left.\tfrac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_i .
\end{aligned} \tag{3.40}$$

With the above results, the jump of the normal flux of the Eshelby tensor across the boundary of the perturbation can be finally expressed in terms of the solution within the interior of the perturbation $\mathcal{I}_\varepsilon$ as

$$\begin{aligned}
[\![\boldsymbol{\Sigma}_{\mu_\varepsilon} \mathbf{n}]\!] \cdot \mathbf{n} = & -\left(k^m - k^i\right) \Bigg\{ |\nabla u|^2 + \left(\left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_i \right)^2 \\
& + 2 \left(\nabla u \cdot \mathbf{t}\right) \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial t}\right|_i - \frac{k^i}{k^m} \left[\frac{k^m - k^i}{k^i} \left(\nabla u \cdot \mathbf{n}\right)^2 \right. \\
& \left. - 2 \left(\nabla u \cdot \mathbf{n}\right) \left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i - \left(\left.\frac{\partial \tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i \right)^2 \right] \Bigg\} .
\end{aligned} \tag{3.41}$$

In order to obtain an analytical formula for the boundary integral of (3.34) we first make use of classical asymptotic analysis (refer to (A.16) in the appendix) and derive the following expression for the interior solution $\tilde{u}_{\mu_\varepsilon}|_{\mathcal{I}_\varepsilon}$ of the perturbed RVE

$$\tilde{u}_{\mu_\varepsilon}(\boldsymbol{y})|_{\mathcal{I}_\varepsilon} = \tilde{u}_\mu(\boldsymbol{y}) + \frac{k^m - k^i}{k^m + k^i} \left[\nabla u + \nabla \tilde{u}_\mu \left(\hat{\boldsymbol{y}}\right) \right] \cdot \left(\boldsymbol{y} - \hat{\boldsymbol{y}}\right) + o\left(\varepsilon\right), \tag{3.42}$$

where $\tilde{u}_\mu(\boldsymbol{y})$ is the solution to the thermal equilibrium problem of the original (unperturbed) RVE, $\nabla \tilde{u}_\mu(\hat{\boldsymbol{y}})$ is the corresponding gradient evaluated at point $\hat{\boldsymbol{y}}$ (the centre of the circular perturbation) and $o\left(\varepsilon\right)$ contains the higher order terms in ε. This results in the following expansion for the gradient of the temperature fluctuation field in $\mathcal{I}_\varepsilon$

$$\nabla \tilde{u}_{\mu_\varepsilon}\left(\boldsymbol{y}\right)|_{\mathcal{I}_\varepsilon} = \nabla \tilde{u}_\mu\left(\boldsymbol{y}\right) + \frac{k^m - k^i}{k^m + k^i} \left[\nabla u + \nabla \tilde{u}_\mu \left(\hat{\boldsymbol{y}}\right) \right] + o\left(\varepsilon\right). \tag{3.43}$$

On the other hand, by assuming a sufficient degree of regularity of $\tilde{u}_\mu$ in $\mathcal{I}_\varepsilon$ and performing its Taylor series expansion about point $\hat{\boldsymbol{y}}$, we obtain

$$\begin{aligned}
\nabla \tilde{u}_\mu\left(\boldsymbol{y}\right) &= \nabla \tilde{u}_\mu\left(\hat{\boldsymbol{y}}\right) + D\left(\nabla \tilde{u}_\mu\left(\boldsymbol{\xi}\right)\right)\left(\boldsymbol{y} - \hat{\boldsymbol{y}}\right) \\
&= \nabla \tilde{u}_\mu\left(\hat{\boldsymbol{y}}\right) - \varepsilon D\left(\nabla \tilde{u}_\mu\left(\boldsymbol{\xi}\right)\right)\mathbf{n},
\end{aligned} \tag{3.44}$$

where $\boldsymbol{\xi} \in (\boldsymbol{y}, \hat{\boldsymbol{y}})$ and use has been made of the identity $(\boldsymbol{y} - \hat{\boldsymbol{y}}) = -\varepsilon\, \mathbf{n}$ on $\partial \mathcal{I}_\varepsilon$. This gives the following expressions for the normal and tangential derivatives of $\tilde{u}_\mu$ on $\partial \mathcal{I}_\varepsilon$

$$\left.\frac{\partial}{\partial n} \tilde{u}_\mu\left(\boldsymbol{y}\right)\right|_{\partial \mathcal{I}_\varepsilon} = \nabla \tilde{u}_\mu\left(\hat{\boldsymbol{y}}\right) \cdot \mathbf{n} + \mathcal{O}\left(\varepsilon\right); \quad \left.\frac{\partial}{\partial t} \tilde{u}_\mu\left(\boldsymbol{y}\right)\right|_{\partial \mathcal{I}_\varepsilon} = \nabla \tilde{u}_\mu\left(\hat{\boldsymbol{y}}\right) \cdot \mathbf{t} + \mathcal{O}\left(\varepsilon\right), \tag{3.45}$$

with $\mathcal{O}(\varepsilon) \to 0$ as $\varepsilon \to 0$, which substituted into (3.42) and then into (3.43) allows the integral of the jump of the Eshelby tensor across $\partial\mathcal{I}_\varepsilon$ to be analytically integrated, resulting in

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = 4\pi\varepsilon\frac{k^m - k^i}{k^m + k^i}k^m\left[|\nabla u|^2 + 2\left(\nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})\cdot\nabla u\right) + |\nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})|^2\right] + o(\varepsilon). \tag{3.46}$$

The substitution of the above expression for the derivative of $\mathcal{J}_{\Omega_{\mu_\varepsilon}}$ into (3.18) allows the function $f(\varepsilon)$ to be promptly identified as that of (3.21). And, 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:

$$D_T\psi = 2k^m\frac{k^m - k^i}{k^m + k^i}\left[|\nabla u|^2 + 2\left(\nabla\tilde{u}_\mu\cdot\nabla u\right) + |\nabla\tilde{u}_\mu|^2\right]. \tag{3.47}$$

Equivalently, by taking the additive decomposition (3.26) and the definition of the contrast γ into account (3.1), we have

$$D_T\psi(\hat{\boldsymbol{y}}) \quad = \quad 2k(\hat{\boldsymbol{y}})\frac{1-\gamma}{1+\gamma}|\nabla u_\mu(\hat{\boldsymbol{y}})|^2 \qquad \forall\hat{\boldsymbol{y}}\in\Omega_\mu. \tag{3.48}$$

Remark 5. *The topological derivative of ψ given by (3.48) is a scalar field over Ω_μ that depends only on the conductivity parameters of matrix and inclusion and on the solution u_μ of the thermal equilibrium problem for the original* unperturbed *domain Ω_μ. The striking simplicity of the exact formula (3.48) is to be noted.* □

Remark 6. *The final expression (3.48) for the topological derivative of function ψ for constitutive multi-scale heat conductivity models has the same structure that the classical result associated with the Poisson equation at the macroscopic level, see reference* [40]. *In the present context, as we shall see later, it is possible to identify from this expression a second order tensor that represents the topological sensitivity of the macroscopic conductivity tensor to the introduction of a small perturbation within the RVE.* □

3.4. **Numerical verification.** As an extension of the classical finite difference methods for the approximate calculation of the derivative of a generic function, a *topological finite difference* formula of first order based on (3.9), that approximates the topological derivative $D_T\psi$ at the unperturbed RVE configuration, is defined as

$$d_T\psi_\varepsilon \equiv \frac{\psi(\varepsilon) - \psi(0)}{f(\varepsilon)}, \tag{3.49}$$

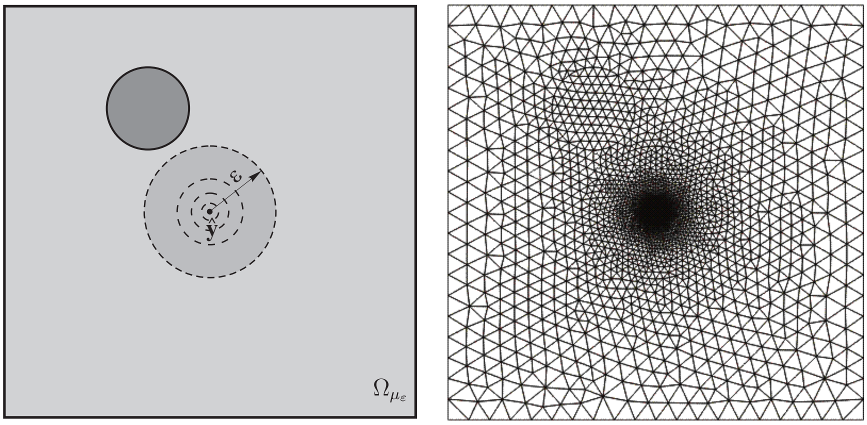
with finite ε. The following limit holds for the above approximation

$$\lim_{\varepsilon\to 0} d_T\psi_\varepsilon = D_T\psi. \tag{3.50}$$

An asymptotic sequence of numerical approximations to the exact value (3.48) of $D_T\psi$ can be obtained by calculating the function $\psi(0)$ as well as its perturbed counterparts $\psi(\varepsilon)$ for a sequence of decreasing values of ε and then using (3.49) to compute the corresponding estimates $d_T\psi$ for $D_T\psi$. This procedure is employed here to validate numerically the analytical expression (3.48). The corresponding values of the function ψ are computed numerically by means of a standard finite element procedure for steady-state heat conduction problems. The unperturbed RVE considered in the verification (refer to Fig. 4(a)) is a unit square with matrix of conductivity $k^m = 2$, containing a circular inclusion of conductivity $k^i = \gamma k^m$ and radius 0.1 centred at the point of coordinates (0.35,0.75) – with the origin of the Cartesian coordinate system located at the bottom left hand corner of the RVE. A sequence of finite element analyses is then carried out with perturbed RVEs obtained by introducing in the unperturbed RVE further circular inclusions of conductivity $k^i = \gamma k^m$ and radii

$$\varepsilon \in \{0.160, 0.080, 0.040, 0.020, 0.010, 0.005\}, \tag{3.51}$$

centred at $\hat{\boldsymbol{y}} = (0.5, 0.5)$. The finite element mesh used to discretise the perturbed RVEs is shown in Fig. 4(b). It contains a total number of 6636 six-noded (quadratic) triangular isoparametric elements and 13353 nodes. The discretization is built such that each inclusion boundary of



(a) RVE geometry (b) Finite element mesh

FIGURE 4. Numerical verification. RVE geometry and finite element mesh.

radius ε has 80 elements and the mesh associated to the internal disk with $\varepsilon = 0.005$ is uniform. The macroscopic temperature gradient considered in the analyses is

$$\nabla u\,(\boldsymbol{x}) = [1, 2]^{\mathrm{T}}. \tag{3.52}$$

The study is conducted for two values of contrast: $\gamma = 0.1$ and $\gamma = 10$. In each case, numerical verification is carried out for the models based on the assumptions of:

(a) Linear boundary temperature;
(b) Periodic boundary temperature fluctuations, and;
(c) Uniform boundary heat flux.

The rule of mixtures model is not considered. Its solution is trivial and does not require a finite element analysis. The results of the analyses are plotted in Fig. 5, where the analytical topological derivative and the numerical approximations for each value of ε are shown for all multiscale models considered. It can be clearly seen that, as expected, the numerical topological derivatives converge to the corresponding analytical values for all models. This confirms the validity of the proposed formula (3.48).

3.5. **The sensitivity of the macroscopic conductivity tensor .** From (3.48) and (3.12) we have the following explicit expression for the topological expansion of ψ:

$$\boldsymbol{q}^{\varepsilon} \cdot \nabla u = \boldsymbol{q} \cdot \nabla u + 2v(\varepsilon)k\frac{1-\gamma}{1+\gamma}\,|\nabla u_\mu|^2 + o(\varepsilon^2), \tag{3.53}$$

where

$$v(\varepsilon) = \pi\varepsilon^2/V_\mu, \tag{3.54}$$

is the RVE volume fraction occupied by the perturbation.

By combining (2.14), (2.45) and (2.47) the gradient of the microscopic temperature can be written as a linear combination of the Cartesian components of the macroscopic temperature gradient as follows

$$\nabla u_\mu = (\nabla u)_i\,(\mathbf{e}_i + \nabla\tilde{u}_{\mu_i}) = (\nabla u)_i\,\nabla u_{\mu_i}, \tag{3.55}$$

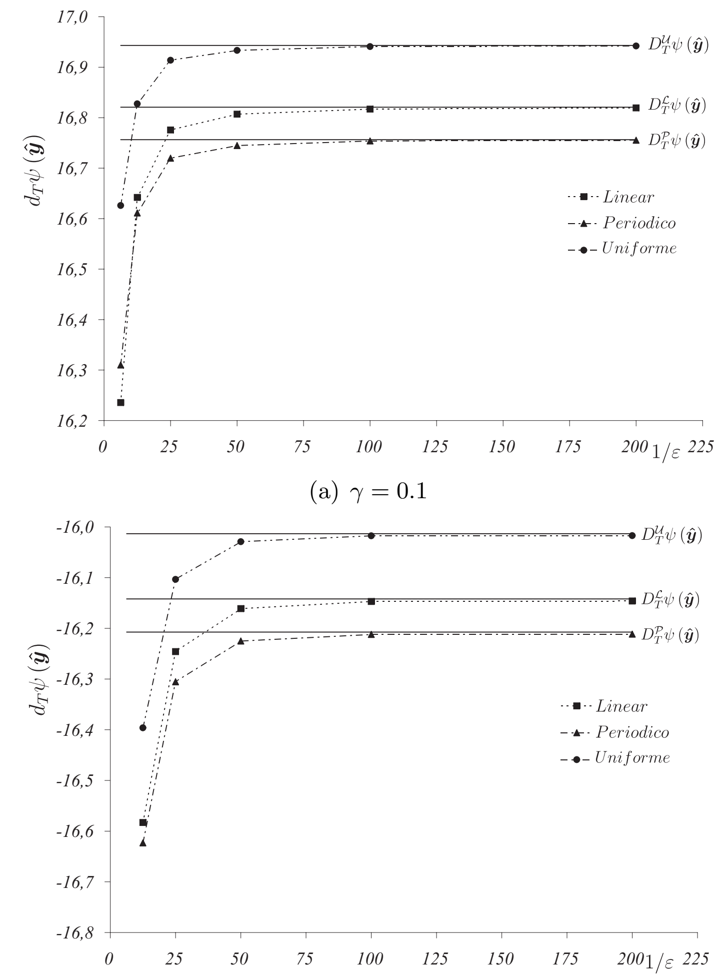
where ∇u_{μ_i} was previously defined in (3.3).

After straightforward manipulations with the above expressions, the topological derivative of ψ given by (3.48) can be represented as

$$D_T\psi = \mathbb{D}_{T\mu}\nabla u \cdot \nabla u, \tag{3.56}$$

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

$$\mathbb{D}_{T\mu} = 2k\frac{1-\gamma}{1+\gamma}\left(\nabla u_{\mu_i} \cdot \nabla u_{\mu_j}\right)\mathbf{e}_i \otimes \mathbf{e}_j, \tag{3.57}$$



(a) $\gamma = 0.1$

(b) $\gamma = 10$

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

with $i, j = 1, 2$.

Then, by replacing (3.56,3.57) and (3.21) into (3.13) we obtain the explicit form

$$-\delta\mathbb{K}_\varepsilon^{\mathcal{H}}\nabla u \cdot \nabla u = \frac{\pi\varepsilon^2}{V_\mu}\,\mathbb{D}_{T\mu}\nabla u \cdot \nabla u + o(\varepsilon^2). \tag{3.58}$$

Finally, the sensitivity tensor (3.2),

$$\mathbb{S} = -\mathbb{D}_{T_\mu}, \tag{3.59}$$

can be easily identified by comparing (3.58) with the expression (3.5) that defines the sensitivity tensor field.

4. Conclusion

A simple analytical expression for the sensitivity of the two-dimensional macroscopic heat conductivity tensor to topological microstructural changes of the underlying material has been proposed in this paper. The proposed formula has been derived by employing the concept of topological sensitivity analysis within a homogenisation-based variational multi-scale constitutive framework for steady-state heat conduction. Within the adopted framework, the temperature gradient and the heat flux at each point of the macroscopic continuum are defined as volume averages of their microscopic counterparts over a Representative Volume Element and different estimates (including an upper and a lower bound) of effective heat conductivity can be obtained according to the choice of functional space of virtual temperatures of the RVE. The derived sensitivity – a symmetric second order tensor field over the RVE domain – measures how the estimated macroscopic conductivity tensor changes when a perturbation in the form of a small circular inclusion is introduced at the micro-scale. This information may be of potential use in a large number of applications such as, for instance, the design and optimisation of heat conducting microstructures to achieve a specified effective behaviour. In fact, the obtained sensitivity field can provide an indication of the best location for the introduction of a perturbation within the RVE in order to produce a desired change in the macroscopic constitutive response. The application of analogous ideas in the context of design and optimisation of elastic load bearing structures is reported in references [41, 20, 42]. Finally, we remark that the present results can be extended, as they stand, for application in the context of seepage flow problems, as their associated classical equations possess the same mathematical structure as the problem studied here.

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Appendix A. Asymptotic analysis

Let $\tilde{u}_{\mu_\varepsilon}$ be the solution of the variational equilibrium equation (3.16) for the perturbed RVE domain, with corresponding strong form

$$\left\{\begin{array}{rlll} -k\Delta\tilde{u}_{\mu_\varepsilon} & = 0 & \text{in} & \Omega_\mu\backslash\mathcal{H}_\varepsilon \\ -k^i\Delta\tilde{u}_{\mu_\varepsilon} & = 0 & \text{in} & \mathcal{I}_\varepsilon \\ \int_{\partial\Omega_\mu}\tilde{u}_{\mu_\varepsilon}\mathbf{n} & = \mathbf{0} & & \\ \int_{\Omega_{\mu_\varepsilon}}\tilde{u}_{\mu_\varepsilon} & = -\nabla u\cdot\int_{\Omega_{\mu_\varepsilon}}\boldsymbol{y} & & \\ [\![\tilde{u}_{\mu_\varepsilon}]\!] & = 0 & \text{on} & \partial\Omega_\mu^i\cup\partial\mathcal{I}_\varepsilon \\ k^m\left.\frac{\partial\tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i\left.\frac{\partial\tilde{u}_{\mu_\varepsilon}}{\partial n}\right|_i & = -\left(k^m-k^i\right)\nabla u\cdot\mathbf{n} & \text{on} & \partial\Omega_\mu^i\cup\partial\mathcal{I}_\varepsilon, \end{array}\right. \tag{A.1}$$

where k is defined in (2.26) and we assume that the origin of the coordinate system coincides with $\hat{\boldsymbol{y}}$. In addition, let the field $\tilde{u}_\mu$ be the solution of the equilibrium problem (2.27) of the unperturbed RVE domain. Now, we propose the following asymptotic expansion of $\tilde{u}_{\mu_\varepsilon}$:

$$\tilde{u}_{\mu_\varepsilon}(\boldsymbol{y}) = \tilde{u}_\mu(\boldsymbol{y}) + \tilde{w}_{\mu_\varepsilon}(\boldsymbol{y}/\varepsilon) + \tilde{v}_{\mu_\varepsilon}(\boldsymbol{y}). \tag{A.2}$$

With the help of the Taylor series expansion of the solution $\tilde{u}_\mu(\boldsymbol{y})$ about a point $\hat{\boldsymbol{y}}$, its normal derivative on the boundary $\partial\mathcal{I}_\varepsilon$ can be written as

$$\left.\frac{\partial}{\partial n}\tilde{u}_\mu(\boldsymbol{y})\right|_{\partial\mathcal{I}_\varepsilon} = \nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})\cdot\mathbf{n} - \varepsilon D(\nabla\tilde{u}_\mu(\boldsymbol{\xi}))(\mathbf{n})^2, \tag{A.3}$$

where $\boldsymbol{\xi}$ is a point of the interval $(\boldsymbol{y},\hat{\boldsymbol{y}})$. By introducing the variable transformation $\boldsymbol{y}=\varepsilon\boldsymbol{z}$ and taking into account that $(\boldsymbol{y}-\hat{\boldsymbol{y}})=-\varepsilon\mathbf{n}$, function $\tilde{w}_{\mu_\varepsilon}(\boldsymbol{z})$ is defined as the solution to the exterior problem: Find $\tilde{w}_{\mu_\varepsilon}$ such that

$$\left\{\begin{array}{rlll} -k\Delta\tilde{w}_{\mu_\varepsilon} & = 0 & \text{in} & \Re^2\backslash\mathcal{H}_1 \\ -k^i\Delta\tilde{w}_{\mu_\varepsilon} & = 0 & \text{in} & \mathcal{I}_1 \\ \tilde{w}_{\mu_\varepsilon} & \to 0 & \text{at} & \infty \\ \tilde{w}_{\mu_\varepsilon}|_m - \tilde{w}_{\mu_\varepsilon}|_i & = 0 & \text{on} & \partial\mathcal{I}_1 \\ k^m\left.\frac{\partial\tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i\left.\frac{\partial\tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_i & = -\varepsilon\left(k^m-k^i\right)\left(\nabla u+\nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})\right)\cdot\mathbf{n} & \text{on} & \partial\mathcal{I}_1. \end{array}\right. \tag{A.4}$$

The discrepancy introduced by the term $\varepsilon D(\nabla\tilde{u}_\mu(\boldsymbol{\xi}))(\mathbf{n})^2$ on $\partial\mathcal{I}_\varepsilon$ and by function $\tilde{w}_{\mu_\varepsilon}$ on $\partial\Omega_\mu$ and $\partial\Omega_\mu^i$ must be balanced by the remaining term $\tilde{v}_{\mu_\varepsilon}(\boldsymbol{y})$. Hence, $\tilde{v}_{\mu_\varepsilon}(\boldsymbol{y})$ must be the solution of the following boundary value problem: Find $\tilde{v}_{\mu_\varepsilon}$ such that

$$\left\{\begin{array}{rlll} -k\Delta\tilde{v}_{\mu_\varepsilon} & = 0 & \text{in} & \Omega_\mu\backslash\mathcal{H}_\varepsilon \\ -k^i\Delta\tilde{v}_{\mu_\varepsilon} & = 0 & \text{in} & \mathcal{I}_\varepsilon \\ \int_{\partial\Omega_\mu}\tilde{v}_{\mu_\varepsilon}\mathbf{n} & = -\int_{\partial\Omega_\mu}\tilde{w}_{\mu_\varepsilon}\mathbf{n} & & \\ \int_{\Omega_{\mu_\varepsilon}}\tilde{v}_{\mu_\varepsilon} & = -\int_{\Omega_{\mu_\varepsilon}}\tilde{w}_{\mu_\varepsilon} & & \\ \tilde{v}_{\mu_\varepsilon}|_m - \tilde{v}_{\mu_\varepsilon}|_i & = 0 & \text{on} & \partial\Omega_\mu^i\cup\partial\mathcal{I}_\varepsilon \\ k^m\left.\frac{\partial\tilde{v}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i\left.\frac{\partial\tilde{v}_{\mu_\varepsilon}}{\partial n}\right|_i & = -\left(k^m\left.\frac{\partial\tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i\left.\frac{\partial\tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_i\right) & \text{on} & \partial\Omega_\mu^i \\ k^m\left.\frac{\partial\tilde{v}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i\left.\frac{\partial\tilde{v}_{\mu_\varepsilon}}{\partial n}\right|_i & = \varepsilon\left(k^m-k^i\right)D^2\tilde{u}_\mu(\boldsymbol{\xi})(\mathbf{n})^2 & \text{on} & \partial\mathcal{I}_\varepsilon. \end{array}\right. \tag{A.5}$$

At this point, it should be noted that problem (A.4) can be solved explicitly by introducing a separation of variables and making use of a Fourier series expansion of the solution $\tilde{w}_{\mu_\varepsilon}$. Indeed, the exterior and interior solutions $\tilde{w}_{\mu_\varepsilon}|_m$ and $\tilde{w}_{\mu_\varepsilon}|_i$ are given, respectively, by

$$\tilde{w}_{\mu_\varepsilon}(\boldsymbol{y})|_m = \frac{k^m - k^i}{k^m + k^i}\frac{\varepsilon^2}{\|\boldsymbol{y}-\hat{\boldsymbol{y}}\|^2}\left(\nabla u + \nabla \tilde{u}_\mu(\hat{\boldsymbol{y}})\right)\cdot(\boldsymbol{y}-\hat{\boldsymbol{y}}), \tag{A.6}$$

$$\tilde{w}_{\mu_\varepsilon}(\boldsymbol{y})|_i = \frac{k^m - k^i}{k^m + k^i}\left(\nabla u + \nabla \tilde{u}_\mu(\hat{\boldsymbol{y}})\right)\cdot(\boldsymbol{y}-\hat{\boldsymbol{y}}). \tag{A.7}$$

For the remaining term, $\tilde{v}_{\mu_\varepsilon}$, we have the following estimate.

Proposition 7. *Let $\tilde{v}_{\mu_\varepsilon}$ be the solution to the boundary value problem (A.5). Then, there exists a constant C, independent of ε, such that*

$$|\tilde{v}_{\mu_\varepsilon}|_{H^1(\Omega_{\mu_\varepsilon})} \leq C\varepsilon^2. \tag{A.8}$$

Proof. By considering (A.6), we note that

$$\int_{\partial\Omega_\mu} \tilde{w}_{\mu_\varepsilon}\mathbf{n} = \varepsilon^2 g(\boldsymbol{y}), \tag{A.9}$$

$$\int_{\Omega_{\mu_\varepsilon}} \tilde{w}_{\mu_\varepsilon} = 0 \tag{A.10}$$

$$\left(k^m \left.\frac{\partial \tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_m - k^i \left.\frac{\partial \tilde{w}_{\mu_\varepsilon}}{\partial n}\right|_i\right) = \varepsilon^2 h(\boldsymbol{y}), \tag{A.11}$$

$$\varepsilon\left(k^m - k^i\right) D^2\tilde{u}_\mu(\boldsymbol{\xi})(\mathbf{n})^2 = \varepsilon p(\boldsymbol{y}), \tag{A.12}$$

where the functions $g(\boldsymbol{y})$, $h(\boldsymbol{y})$ and $p(\boldsymbol{y})$ are independent of ε. Then, we have the following auxiliary boundary value problem: Find $\varphi_{\mu_\varepsilon}$, such that

$$\left\{\begin{array}{rlll} -k\Delta\varphi_{\mu_\varepsilon} & = 0 & \text{in} & \Omega_\mu\backslash\mathcal{H}_\varepsilon \\ -k^i\Delta\varphi_{\mu_\varepsilon} & = 0 & \text{in} & \mathcal{I}_\varepsilon \\ \int_{\partial\Omega_\mu}\varphi_{\mu_\varepsilon}\mathbf{n} & = \varepsilon g(\boldsymbol{y}) & & \\ \int_{\Omega_{\mu_\varepsilon}}\varphi_{\mu_\varepsilon} & = 0 & & \\ \varphi_{\mu_\varepsilon}|_m - \varphi_{\mu_\varepsilon}|_i & = 0 & \text{on} & \partial\Omega_\mu^i \cup \partial\mathcal{I}_\varepsilon \\ k^m \left.\frac{\partial\varphi_{\mu_\varepsilon}}{\partial n}\right|_m - k^i \left.\frac{\partial\varphi_{\mu_\varepsilon}}{\partial n}\right|_i & = \varepsilon h(\boldsymbol{y}) & \text{on} & \partial\Omega_\mu^i \\ k^m \left.\frac{\partial\varphi_{\mu_\varepsilon}}{\partial n}\right|_m - k^i \left.\frac{\partial\varphi_{\mu_\varepsilon}}{\partial n}\right|_i & = p(\boldsymbol{y}) & \text{on} & \partial\mathcal{I}_\varepsilon. \end{array}\right. \tag{A.13}$$

As the above problem is well-posed, up to an arbitrary constant, then exists a constant C, independent of ε, such that [1, 12, 29]

$$|\varphi_{\mu_\varepsilon}|_{H^1(\Omega_{\mu_\varepsilon})} \leq \varepsilon C. \tag{A.14}$$

Hence, from the linearity of problem (A.5) we have that $\tilde{v}_{\mu_\varepsilon} = \varepsilon\varphi_{\mu_\varepsilon}$, and the proof is complete. □

Remark 8. *In order to guarantee the well-posedness of the problems defined in the perturbed domain Ω_{μ_ε}, in the systems (A.1), (A.5) and (A.13) it should be added the boundary condition associated to the space $\mathcal{V}_{\mu_\varepsilon}$, according to the choice of each multi-scale constitutive model.* □

Finally, with expressions (A.6) and (A.7) and Proposition 7 we have that the asymptotic expansion of the solution $\tilde{u}_{\mu_\varepsilon}$ to problem (A.1) in the neighbourhood of the inclusion $\mathcal{I}_\varepsilon$ is given by

$$\tilde{u}_{\mu_\varepsilon}(\boldsymbol{y})|_{\Omega_\mu\backslash\mathcal{H}_\varepsilon} = \tilde{u}_\mu(\boldsymbol{y}) + \frac{k^m - k^i}{k^m + k^i}\frac{\varepsilon^2}{\|\boldsymbol{y}-\hat{\boldsymbol{y}}\|^2}\left[\nabla u + \nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})\right]\cdot(\boldsymbol{y}-\hat{\boldsymbol{y}}) + \tilde{v}_{\mu_\varepsilon}(\boldsymbol{y}), \tag{A.15}$$

and

$$\tilde{u}_{\mu_\varepsilon}(\boldsymbol{y})|_{\mathcal{I}_\varepsilon} = \tilde{u}_\mu(\boldsymbol{y}) + \frac{k^m - k^i}{k^m + k^i}\left[\nabla u + \nabla\tilde{u}_\mu(\hat{\boldsymbol{y}})\right]\cdot(\boldsymbol{y}-\hat{\boldsymbol{y}}) + \tilde{v}_{\mu_\varepsilon}(\boldsymbol{y}). \tag{A.16}$$

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