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# The topological derivative for homogenized elastic coefficients of periodic microstructures

Anca-Maria Toader
CMAF, Av. Prof. Gama Pinto, 2
1649-003 Lisboa, Portugal
tel. + 351 217904918, fax + 351 217954288
e-mail: amtan@ptmat.fc.ul.pt

**Summary** In the present paper we compute in full mathematical rigor the topological derivative of the elastic homogenized coefficients of periodic microstructures. The expression here proven for the topological derivative was successfully used for optimizing homogenized coefficients in a alternate directions optimization algorithm (jointly with the shape derivative) in [3].

The main ingredients for proving the formula of the topological derivative are a generalized adjoint method and a Dirichlet-to-Neumann operator.

The techniques employed are general and may be adapted to different functionals depending on elliptic PDEs under periodicity conditions.

**Key words** topological derivative, periodic homogenization, optimization of homogenized coefficients

## 1. Introduction

The topological derivative is a very important tool in optimization of structures (microstructures in our context), emerging from the calculus of variations. It measures the variation of a functional depending on a solution of a PDE and on its derivatives when the domain where the PDE is defined varies by removing an infinitesimal part of it (a hole). According to the intention of minimization/maximization of the functional under consideration, the interest is to have a negative/positive value of the topological derivative.

The topological derivative imposed as (proved to be) one of the most powerful tool in optimization of structures jointly with the shape derivative. Although the formal idea goes back to the work in engineering by H. Eschenauer, V. Kobelev, A. Schumacher [7], the rigorous mathematical expression and proof of the topological derivative was accomplished later with the works of J. Sokołowski, A. Żochowski [13], S. Garreau, P. Guillaume, M. Masmoudi [8].

In the present paper we compute in full mathematical rigor the topological derivative of the elastic homogenized coefficients of periodic microstructures. The periodicity notion here used is the most general one in $\mathbb{R}^N$ (subsection 2.1). The techniques employed may treat mixtures of materials but we present the case of mixture between material and void, so called homogenization of porous materials.

According to the homogenization theory, described in subsection 2.2, the macroscopic behaviour of a periodic porous microstructure (a mixture between a base material with elastic tensor $C$ and void) subject to the macroscopic strain $A$ is modeled by the following cellular problem

$$\begin{cases} -\mathrm{div}(Ce(u_A)) = 0 \text{ in } \mathbb{R}^N_{\mathrm{perf}}(T) \\ Ce(u_A)n = 0 \text{ on } \partial T \\ u_A(x) = Ax + \phi_A(x), \quad \phi_A \text{ periodic function.} \end{cases}$$

The homogenized tensor $C^H$ can be defined through

$$\langle C^H A, B\rangle = \frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(u_A), e(u_B)\rangle\, dx.$$

Considering, in particular, the matrices $A$ and $B$ (effective strains) in a basis of the space of symmetric matrices, one obtains each one of the homogenized coefficients, i.e. the entries of the homogenized tensor. In general, for $A$ and $B$ arbitrarily fixed one studies the functional

$$j(Y\setminus T) = \frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(u_A), e(u_B)\rangle\, dx.$$

The above problem is perturbed by creating at a location $x_0$ lying in a zone of material, an infinitesimal hole, typically spherical, whose radius $\rho$ tends to 0, and on the boundary of which homogeneous Neumann conditions are applied. So the domain varies with the parameter $\rho$ and therefore the solution of the cellular problem will depend on $\rho$ (subsection 3.1). These dependencies infer on the functional $j$ and we are interested precisely in its asymptotic expansion in $\rho$ :

$$j(Y\setminus(T\cup \bar{B}(x_0,\rho))) = j(Y\setminus T) + f(\rho)D_T j(x_0) + o(f(\rho)),$$

where $\lim_{\rho\to 0} f(\rho) = 0$, $f(\rho) > 0$.

The second term in the asymptotic expansion involves the so called topological derivative $D_T j$ in $x_0$. When minimizing a certain homogenized coefficient then an infinitesimal hole is created at the location $x_0$ where the topological derivative takes its most negative value. This is the main idea of the optimization algorithm in [3] using the topological derivative as one of the alternate directions. Note however that the theory applies to nucleation of infinitesimal holes only, so when handling variation of existing holes a shape derivative is employed (the other alternate direction of optimization).

The asymptotic development that we obtain in the main result (Theorem 9 in subsection 3.4) for $j(\rho) := j(Y\setminus(T\cup\bar{B}(x_0,\rho))$ is

$$j(\rho) = j(0) + \rho^N \frac{1}{|Y|}\int_{\partial B(x_0,R)} \delta_T u_0 u_0 ds(x) + o(\rho^N)$$

that is the topological derivative has the same expression as in the non-periodic context, see [8], but with the opposite sign. This fact was discussed in the engineering community recently in [14] and is justified along the present paper with special emphasis in Section 4.

The technique used to compute the topological derivative is based on an adjoint method adapted to the periodic context and on the Dirichlet-to-Neumann operator denoted by $\mathcal{T}$. The operator denoted by $\delta_{\mathcal{T}}$ in the above formula represents the second term in the asymptotic development of $\mathcal{T}$ with respect to $\rho$ and was explicitly computed in [8] and [11].

When the cellular problem is written in its strain formulation (see Section 2), a generalized adjoint method is needed (subsections 3.2 and 3.3), which deals with a bilinear form which is coercive only on a subspace of the Hilbert space (subsection 2.4).

The expression of the topological derivative was formally obtained in [2] and already used for optimizing homogenized coefficients in a alternate directions optimization algorithm in [3].

The techniques employed are general and may be adapted to different functionals depending on elliptic PDEs under periodicity conditions.

## 2. Periodic homogenization

Suppose that at each point of a given elastic body the material is obtained by homogenizing a periodic microstructure made of a mixture of material and void (porous microstructure). Then, at that chosen point of the body the homogenized material (more precisely, its homogenized tensor) can be characterized in terms of cellular problems that will be presented below.

**2.1. Generalized periodicity notion.** A general notion of periodicity is introduced in Definition 1 below. According to this general notion of periodicity, a function is periodic if it is invariant to a group of translations. Note that any translation can be identified with a vector in $\mathbb{R}^N$ and the composition of translations corresponds to the sum of the respective vectors, thus any notion of periodicity can be described by an additive subgroup of $\mathbb{R}^N$ with $N$ linearly independent generators (such a subgroup is called a lattice).

**Definition 1.** *Consider $\mathcal{G}$ an additive subgroup of $\mathbb{R}^N$ with $N$ linearly independent generators (a lattice). A function $\varphi : \mathbb{R}^N \to \mathbb{R}^m$ is said to be $\mathcal{G}$-periodic if*

$$\varphi(x + \vec{g}) = \varphi(x), \ \forall x \in \mathbb{R}^N \ \forall \vec{g} \in \mathcal{G}.$$

Note that there is a infinity of different sets of linearly independent generators of the same subgroup $\mathcal{G}$. By applying to a set of $N$ linearly independent generators a change of basis in $\mathbb{R}^N$ by a $N \times N$ matrix with integer entries and having the determinant equal to 1 or $-1$, one obtains another set of $N$ linearly independent generators. However the notion of periodicity depends on $\mathcal{G}$ and not on the chosen set of generators.

Another important notion to clarify is the periodicity cell. Each set of linearly independent generators defines a periodicity cell : Let $\{\vec{g}_1, \vec{g}_2, \ldots, \vec{g}_N\}$ be a set of linearly independent generators of $\mathcal{G}$. Then the periodicity cell is the parallelepiped $\{\sum_{i=1}^N \alpha_i \vec{g}_i \mid 0 \leq \alpha_i \leq 1\}$. For a given subgroup $\mathcal{G}$ the associated periodicity cell is not unique. In fact there exist an infinity of periodicity cells since each set of linearly independent generators defines a periodicity cell. It is natural to restrain the family of periodicity cells by introducing the notion of minimal periodicity cells.

**Definition 2.** *Let $\mathcal{G}$ be an additive subgroup of $\mathbb{R}^N$ with $N$ linearly independent generators. An associated minimal periodicity cell is a parallelepiped $\{\sum_{i=1}^{N} \alpha_i \vec{g}_i \mid 0 \leq \alpha_i \leq 1\}$ where $\{\vec{g}_1, \vec{g}_2, \ldots, \vec{g}_N\}$ is a set of generators of $\mathcal{G}$ having the property that $|\vec{g}_1| + \ldots + |\vec{g}_N|$ is minimum between all possible sets of linearly independent generators.*

However, the above definition does not ensure, for a given $\mathcal{G}$, the uniqueness of the minimal periodicity cell.

Consider the discrete subgroup $\mathcal{G} = \mathbb{Z}^2$ in $\mathbb{R}^2$. In Figure 1, two distinct sets of linearly independent generators are represented, together with the respective periodicity cells : $\{(1,0),(0,1)\}$ defines a minimal cell (in the sense of Definition 2) while $\{(1,0),(1,1)\}$ defines a cell which is not minimal. Nevertheless the periodicity notion behind them is the same (cf. Definition 1) depending only on $\mathcal{G} = \mathbb{Z}^2$.

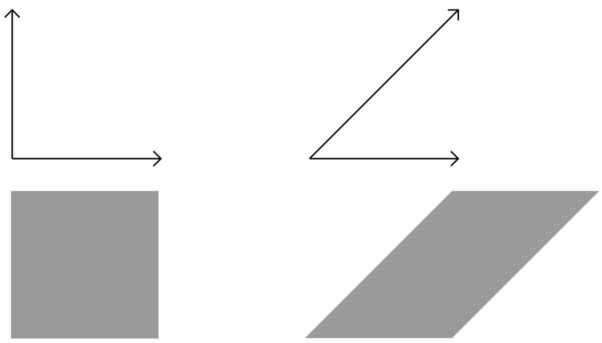

Figure 1. Two sets of generators and respective periodicity cells for the group $\mathbb{Z}^2$.

Note that Definition 1 covers any other notion of periodicity in $\mathbb{R}^N$.

A very popular notion of periodicity in $\mathbb{R}^2$ is the hexagonal periodicity, typical for honeycomb structures, treated by many authors, see for instance [9] and [12]. The hexagonal periodicity is recovered by choosing the subgroup of $\mathbb{R}^2$ generated by $\{(1,0),(\frac{1}{2},\frac{\sqrt{3}}{2})\}$. In Figure 2 two sets of correspondent points are represented, one of them with black balls and the other with gray crosses.

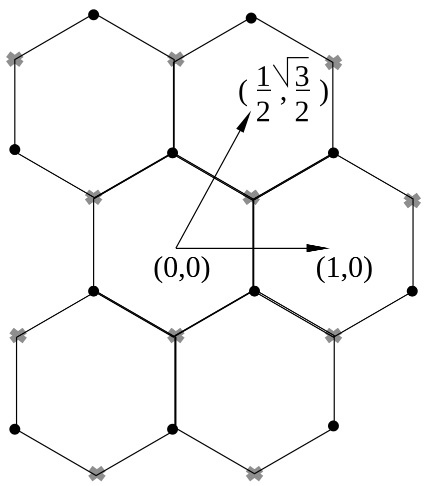


Figure 2. Set of generators for the hexagonal periodicity (honeycomb structure).

Other sets of generators for the same subgroup are $\{(\frac{1}{2}, \frac{\sqrt{3}}{2}), (-\frac{1}{2}, \frac{\sqrt{3}}{2})\}$, $\{(-\frac{1}{2}, \frac{\sqrt{3}}{2}), (-1, 0)\}$, $\{(1, 0), (-\frac{1}{2}, \frac{\sqrt{3}}{2})\}$, $\{(\frac{1}{2}, \frac{\sqrt{3}}{2}), (-1, 0)\}$ and $\{(-\frac{1}{2}, \frac{\sqrt{3}}{2}), (-\frac{1}{2}, -\frac{\sqrt{3}}{2})\}$. The periodicity cells generated by the above sets of linearly independent generators are represented in Figure 3 and each one verifies the criteria from Definition 2. So the hexagonal periodicity may be described by choosing any one of the parallelograms in Figure 3.

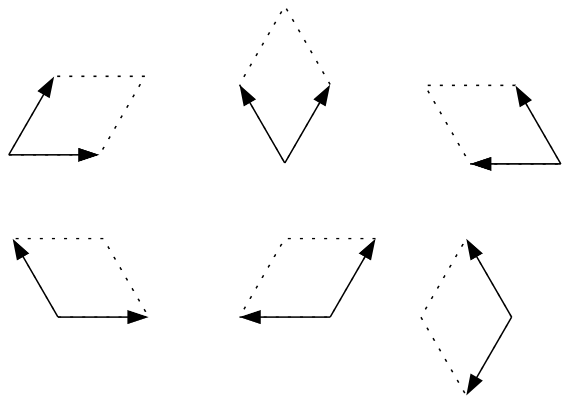

Figure 3. Different sets of linearly independent generators for the hexagonal periodicity and the corresponding minimal periodicity cells.

**2.2. Cellular problem in strong formulation.** Consider in $\mathbb{R}^N$ an additive subgroup $\mathcal{G}$ with $N$ linearly independent generators and let $Y$ be a periodicity cell, not necessarily minimal. Consider $T$ a compact set having Lipschitz boundary and such that $T \subset \overset{\circ}{Y}$ (see subsection 2.3 for a weaker hypothesis). Suppose that in the periodicity cell $Y$ the set $Y \setminus T$ is filled with a material having the elastic tensor $C$ while $T$ corresponds to a hole (there is no material inside $T$). Attending to the $\mathcal{G}$-periodicity, the space $\mathbb{R}^N$ is periodically perforated with holes that are translations of $T$ obtaining

$$\mathbb{R}^N_{\text{perf}}(T) = \mathbb{R}^N \setminus \bigcup_{k \in \mathbb{Z}^N} (T + k_1 \vec{g}_1 + \dots k_N \vec{g}_N). \tag{1}$$

An example of $\mathbb{R}^2_{\text{perf}}(T)$ with a hexagonal periodicity is presented in Figure 4, where the gray zone is occupied by the material $C$ and void is represented in white.

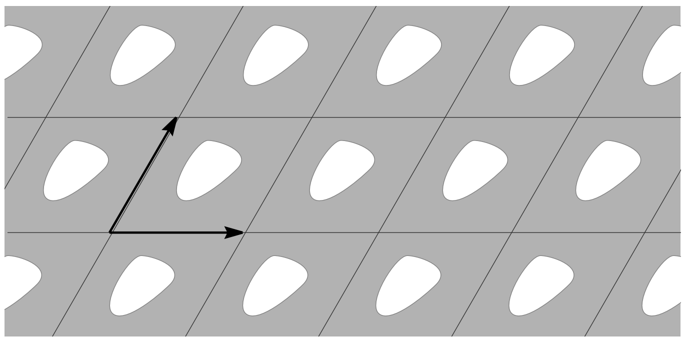

Figure 4. $\mathbb{R}^2_{\text{perf}}(T)$ with hexagonal periodicity.

For a small parameter $\varepsilon > 0$, one makes an $\varepsilon$ zoom of $\mathbb{R}^N_{perf}(T)$ that is a homothety of ratio $\varepsilon$. This new perforated domain is filled with the material of tensor $C$. When the parameter $\varepsilon$ goes to zero, the effective behaviour of the corresponding microstructure is characterized by the homogenized tensor $C^H$. According to the homogenization theory, see the work by D. Cioranescu and J. Saint Jean Paulin [6], and more precisely using the $H$-convergence for perforated domains, see the work by M. Briane, A. Damlamian and P. Donato [4], the homogenized tensor $C^H$ may be characterized in terms of the solution of the cellular problem :

**Theorem 1.** *Given an effective strain $A$, that is a symmetric matrix in $\mathcal{M}^N(\mathbb{R})$ the homogenized tensor $C^H$ is characterized by*

$$C^H A = \frac{1}{|Y|} \int_{Y \setminus T} Ce(u_A) dx \tag{2}$$

*where $u_A$ is the solution of the cellular problem below:*

$$\begin{cases} -div(Ce(u_A)) = 0 \ \ in \ \mathbb{R}^N_{\text{perf}}(T) \\ Ce(u_A)n = 0 \ \ on \ \partial T \\ u_A(x) = Ax + \phi_A(x), \quad \phi_A \ \mathcal{G}\text{-periodic function.} \end{cases} \tag{3}$$

*Another characterization of $C^H$ involving energy type products is*

$$\langle C^H A, B \rangle = \frac{1}{|Y|} \int_{Y \setminus T} \langle Ce(u_A), e(u_B) \rangle dx \, . \tag{4}$$

*where $u_A$ and $u_B$ are solution of the cellular problem (3) for two different effective strains $A$ and $B$.*

For the proof of the above theorem see the works by D. Cioranescu and J. Saint Jean Paulin [6] and by M. Briane, A. Damlamian and P. Donato [4].

Denote by $H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$ the completion in the norm of $H^1(Y \setminus T, \mathbb{R}^N)$ of the space of functions in $C^\infty(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$ which are $\mathcal{G}$-periodic.

Consider $LP(\mathbb{R}^N_{\text{perf}}(T))$ the space of linear plus periodic displacements defined in $\mathbb{R}^N_{\text{perf}}(T)$ :

$$\begin{aligned} LP(\mathbb{R}^N_{\text{perf}}(T)) = \{u : \mathbb{R}^N_{\text{perf}}(T) \to \mathbb{R}^N \mid u(x) = Ax + \varphi(x), \\ A \in \mathcal{M}^s_N(\mathbb{R}), \varphi \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)\}, \end{aligned} \tag{5}$$

where $\mathcal{M}^s_N(\mathbb{R})$ denotes the space of $N \times N$ matrices with real elements. $LP(\mathbb{R}^N_{\text{perf}}(T))$ is a Hilbert space since it is a direct sum between a finite dimensional space and $H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$.

For $A \in \mathcal{M}^s_N(\mathbb{R})$ arbitrarily fixed, denote by $LP_A(\mathbb{R}^N_{\text{perf}}(T))$ the set of linear plus periodic displacements having the linear part $Ax$ :

$$LP_A(\mathbb{R}^N_{\text{perf}}(T)) = \{u : \mathbb{R}^N_{\text{perf}}(T) \to \mathbb{R}^N \mid u(x) = Ax + \varphi(x), \varphi \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)\}. \tag{6}$$

Thus the last equation in (3) is equivalent to $u_A \in LP_A(\mathbb{R}^N_{\text{perf}}(T))$. Note that $LP_0(\mathbb{R}^N_{\text{perf}}(T)) = H^1_{\#}(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$ is a closed subspace of $LP(\mathbb{R}^N_{\text{perf}}(T))$ and for an arbitrary strain $A \in \mathcal{M}^s_N(\mathbb{R})$ the set $LP_A(\mathbb{R}^N_{\text{perf}}(T))$ is a translation of $LP_0(\mathbb{R}^N_{\text{perf}}(T))$: $LP_A(\mathbb{R}^N_{\text{perf}}(T)) = A + LP_0(\mathbb{R}^N_{\text{perf}}(T)) = A + H^1_{\#}(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$. Moreover

$$LP(\mathbb{R}^N_{\text{perf}}(T)) = \bigcup_{A \in \mathcal{M}^s_N(\mathbb{R})} LP_A(\mathbb{R}^N_{\text{perf}}(T)).$$

The cellular problem (3) above may be written in strain formulation as follows (see also [2]) :
Given a strain $A$, that is a symmetric matrix in $\mathcal{M}^s_N(\mathbb{R})$, the function $u_A$ is solution of

$$\begin{cases} u_A \in LP(\mathbb{R}^N_{\text{perf}}(T)) \\ -\text{div}(Ce(u_A)) = 0 \text{ in } \mathbb{R}^N_{\text{perf}}(T) \\ Ce(u_A)n = 0 \text{ on } \partial T \\ \frac{1}{|Y|}\Big(\int_{Y\setminus T} e(u_A)dx - \int_{\partial T} u_A \vee n \, ds(x)\Big) = A \, , \end{cases} \tag{7}$$

where the symbol $\vee$ denotes the symmetric part of the tensor product.

**Theorem 2.** *The cellular problem (3) is equivalent to the cellular problem in the strain formulation (7).*

Proof : Given a strain $A$ in $\mathcal{M}^s_N(\mathbb{R})$, if $u_A$ is solution of (3) then, the function $\phi_A$ verifies

$$\int_{Y\setminus T} \nabla \phi_A dx = \int_{\partial T} \phi_A \otimes n \, ds(x) + \int_{\partial Y} \phi_A \otimes n \, ds(x),$$

and having in mind that $\phi_A$ is $\mathcal{G}$-periodic

$$\int_{Y\setminus T} \nabla \phi_A dx = \int_{\partial T} \phi_A \otimes n \, ds(x).$$

Replacing $\phi_A(x) = u_A(x) - Ax$, and keeping in the lefthandside only the terms that contain $u_A$ the above equality writes :

$$\int_{Y\setminus T} \nabla u_A dx - \int_{\partial T} u_A \otimes n ds(x) = \int_{Y\setminus T} A dx - \int_{\partial T} Ax \otimes n ds(x). \tag{8}$$

The normal $n$ is oriented outwards the domain occupied by the material, points inside the hole $T$; therefore the last integral in the above formula may be written as

$$-\int_{\partial T} Ax \otimes n ds(x) = \int_T \nabla(Ax) dx = \int_T A dx.$$

Replacing the above expression in (7) one obtains

$$\int_{Y\setminus T} \nabla u_A dx - \int_{\partial T} u_A \otimes n ds(x) = \int_{Y\setminus T} A dx + \int_T A dx = \int_Y A dx = |Y| A.$$

By taking the symmetric part of the terms in both sides of the equality, the last condition in problem (7) is obtained.

Conversely, if $u_A$ is solution of (7) then the last condition in (7) allows one to identify the linear part of $u_A$ and therefore $u_A$ is solution of (3).

In stress formulation the cellular problem (3) writes as follows (see also [2]) :
Given a stress $\sigma$, that is a symmetric matrix in $\mathcal{M}_N(\mathbb{R})$, the function $w_\sigma$ is solution of

$$\begin{cases} w_\sigma \in LP(\mathbb{R}^N_{\text{perf}}(T)), \\ -\text{div}(Ce(w_\sigma)) = 0 \text{ in } \mathbb{R}^N_{\text{perf}}(T) \\ Ce(w_\sigma)n = 0 \text{ on } \partial T \\ \frac{1}{|Y|}\int_{Y\setminus T} Ce(w_\sigma)dx = \sigma\,. \end{cases} \tag{9}$$

Note that the formulation in strain (7) of the cellular problem is equivalent to the formulation in stress (9) in the following sense :

**Theorem 3.** *Given a symmetric matrix $A \in \mathcal{M}^N(\mathbb{R})$ the solution $u_A$ of problem (7) is also solution of problem (9) for $\sigma = C^H A$. Conversely, given a symmetric matrix $\sigma \in \mathcal{M}^N(\mathbb{R})$ the solution $w_\sigma$ of problem (9) is also solution of problem (7) for $A = (C^H)^{-1}\sigma$, where $(C^H)^{-1}$ is the inverse of the homogenized $C^H$ tensor, called homogenized compliance tensor.*

A similar result was proven in [2] for the case of periodic homogenization with two materials.

Here is a sketched proof: Consider $u \in LP(\mathbb{R}^N_{\text{perf}}(T))$ solution of (7). Then $u_A$ is also solution of problem (3) (see Theorem 2) and from Theorem 1 it turns out that

$$C^H A = \frac{1}{|Y|}\int_{Y\setminus T} Ce(u_A)dx.$$

Therefore by setting $\sigma = C^H A$, the function $u_A$ is solution of (9).

Conversely, consider $w_\sigma$ solution of (9). From the first three conditions in (9), employing similar arguments to those used in the proof of Theorem 2, it turns out that the linear part of $w_\sigma$ may be identified by

$$\frac{1}{|Y|}\Big(\int_{Y\setminus T} e(w_\sigma)dx - \int_{\partial T} w_\sigma \vee n\, ds(x)\Big) = A.$$

This means that $w_\sigma$ is solution of (7) and therefore is also solution of (3) (by Theorem 2). From Theorem 1 and from the last condition in (9) it turns out that $C^H A = \sigma$, hence $A = (C^H)^{-1}\sigma$.

**2.3. The case $T \not\subset \overset{\circ}{Y}$.** In the context above, the model hole $T$ has been taken such as $T \subset \overset{\circ}{Y}$ in order to simplify the writing. However, this hypothesis is not essential, and can be replaced by the weaker hypothesis

$$T \cap (T + \vec{g}) = \emptyset,\ \forall \vec{g} \in \mathcal{G}, \vec{g} \neq \vec{0} \tag{10}$$

which means that $T$ does not touch any of its $\mathcal{G}$ translations (see Figure 5 for an example with square periodicity). This gives to the hole $T$ the freedom to touch or cross the boundary $\partial Y$ of the periodicity cell $Y$, which is important for computational applications (see [1], [3]).

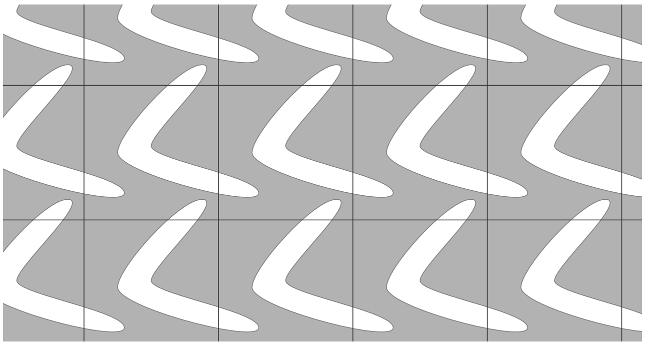

Figure 5. $\mathbb{R}^2_{\text{perf}}(T)$ with a hole that does not fit into any translation of $Y$.

Nevertheless, replacing the hypothesis $T \subset \overset{\circ}{Y}$ by (10) requires some additional work to obtain the strong formulations of the cellular problem. Note that in some cases this can be worked around by simply translating the model hole $T$ in order to bring it inside $\overset{\circ}{Y}$ (see Figures 10, 14 and 20 in [1]), but in many interesting cases this is not possible (see Figures 11, 15 and 24 in [1] and also final designs in Figures 25, 26 and others in [3]) and the condition (10) must be used instead of $T \subset \overset{\circ}{Y}$. The mathematical formulation above introduced can be adapted to deal with the weaker hypothesis (10). In all formulae, the domain $Y \setminus T$ should be replaced by $Y \cap \mathbb{R}^N_{perf}(T)$.

The cellular problem (3) should be understood as a problem on $\mathbb{R}^N_{perf}(T)$ and no longer on a periodicity cell $Y$ as $T$ cannot be confined to any translation of the cell $Y$. The formulation in strain (7) becomes

$$\left\{ \begin{array}{c} u_A \in LP(\mathbb{R}^N_{\text{perf}}(T)) \\ -\text{div}(Ce(u_A)) = 0 \text{ in } \mathbb{R}^N_{\text{perf}}(T) \\ Ce(u_A)n = 0 \text{ on } \partial(\mathbb{R}^N_{perf}(T)) \\ \dfrac{1}{|Y|}\Big(\displaystyle\int_{Y\cap\mathbb{R}^N_{perf}(T)} e(u_A)dx - \int_{Y\cap\partial(\mathbb{R}^N_{perf}(T))} u_A \vee n \, ds(x)\Big) = A\,. \end{array} \right.$$

The proof of Theorem 2 becomes more complicated since one must eliminate from the analysis the part of $\partial Y$ which is outside $\mathbb{R}^N_{perf}(T)$.

The formulation in stress (9) becomes

$$\left\{ \begin{array}{c} w_\sigma \in LP(\mathbb{R}^N_{\text{perf}}(T)), \\ -\text{div}(Ce(w_\sigma)) = 0 \text{ in } \mathbb{R}^N_{\text{perf}}(T) \\ Ce(w_\sigma)n = 0 \text{ on } \partial(\mathbb{R}^N_{perf}(T)) \\ \dfrac{1}{|Y|}\displaystyle\int_{Y\cap\mathbb{R}^N_{perf}(T)} Ce(w_\sigma)dx = \sigma\,. \end{array} \right.$$

For the variational formulation of the cellular problem in the subsection below, the only change to perform is replacing the domain of integration $Y \setminus T$ by $Y \cap \mathbb{R}^N_{perf}(T)$.

Throughout Section 3, the domain of integration $Y \setminus (T \cup \bar{B}(x_0, R))$ should be replaced by $Y \cap \mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R))$.

**2.4. Cellular problem in variational formulation.** An important ingredient for the sequel of the paper is the variational formulation of the cellular problem in both strain and stress forms. Between all variational formulations of problem (7) the following one is chosen since it best fits the subsequent purpose :

$$\begin{cases} u_A \in LP_A(\mathbb{R}^N_{\text{perf}}(T)) \\ \displaystyle\int_{Y\setminus T} \langle Ce(u_A), e(v)\rangle dx = 0 \ \ \forall v \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N), \end{cases} \tag{11}$$

the strain $A$ being given in $\mathcal{M}^s_N(\mathbb{R})$.

The variational formulation (11) of the cellular problem (7) has a slightly different form than the classical theory. The space $H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$ is a closed subspace of the Hilbert space $LP(\mathbb{R}^N_{\text{perf}}(T))$ and the solution $u_A$ belongs to $LP_A(\mathbb{R}^N_{\text{perf}}(T))$ which is the translation with $A$ of $H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N)$. A Lax Milgram type lemma (Lemma 4 below) is needed in order to ensure existence and uniqueness of the solution of the variational formulation (11).

Consider $V$ a fixed Hilbert space, let $V_0$ be a closed subspace of $V$ and let $K = \gamma + V_0$ be a translation of $V_0$ (a closed affine manifold in $V$) where $\gamma$ is a fixed element of $V$.

**Lemma 4.** *Consider $a : V \times V \to \mathbb{R}$ a bilinear, symmetric continuous form on $V$ which is coercive only on $V_0$, and consider $l : V \to \mathbb{R}$ a linear continuous form on $V$. Then the problem*

$$\begin{cases} \textit{find } u \in K \textit{ such that} \\ a(u, v) = l(v) \ \forall v \in V_0, \end{cases} \tag{12}$$

*has a unique solution.*

Applying the above Lemma 4 to the variational formulation (11), $V = LP(\mathbb{R}^N_{\text{perf}}(T))$, $V_0 = H^1_\#(\mathbb{R}^N_{\text{perf}}(T), \mathbb{R}^N))$ and $K = LP_A(\mathbb{R}^N_{\text{perf}}(T))$, it turns out that (11) has a unique solution.

The variational formulation of the cellular problem in stress form (9) is the following

$$\begin{cases} w_\sigma \in LP(\mathbb{R}^N_{\text{perf}}(T)) \\ \displaystyle\int_{Y\setminus T} \langle Ce(w_\sigma), e(v)\rangle dx = \langle \sigma, \int_{Y\setminus T} e(v) dx\rangle, \ \ \forall v \in LP(\mathbb{R}^N_{\text{perf}}(T)), \end{cases} \tag{13}$$

for a given stress $\sigma$ in $\mathcal{M}^s_N(\mathbb{R})$. The classical Lax Milgram Lemma ensures existence and uniqueness of the solution $w_\sigma$.

## 3. The topological derivative

According to Theorem 1, the homogenized material is characterized by the functional

$$j(Y \setminus T) = \langle C^H A, B\rangle = \frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(u_A), e(u_B)\rangle dx\,. \tag{14}$$

where $u_A$ and $u_B$ are solution of the cellular problem (3) for two different effective strains $A$ and $B$. For optimization purposes, it is important to understand how the functional $j$ varies when an infinitesimal hole is nucleated in $Y \setminus T$.

More precisely, consider a small parameter $\rho > 0$ and suppose that at given location $x_0$ of the periodicity cell, $x_0 \in Y\setminus T$, a hole is nucleated : inside $\bar{B}(x_0, \rho)$ the material changes to void. Assume that $\rho$ is small enough to ensure that $T \cap \bar{B}(x_0, \rho) = \emptyset$. The homogenized material corresponding to the periodicity cell $Y \setminus (T \cup \bar{B}(x_0, \rho))$ is characterized by the functional $j(Y\setminus(T\cup\bar{B}(x_0, \rho)))$ and depends on $\rho$. One looks for an asymptotic development of the form

$$j(Y \setminus (T \cup \bar{B}(x_0, \rho))) = j(Y \setminus T) + f(\rho)D_T j(x_0) + o(f(\rho)), \tag{15}$$

where $f(\rho) > 0$ and $f(\rho) \to 0$ when $\rho \to 0$.

Note that it is also possible to nucleate a hole precisely at the boundary of the cell, $x_0 \in \partial Y$; this case can be handled in the spirit of subsection 2.3. Actually, in the code implemented in [1] and [3], the boundary of the cell is not explicitly implemented; a mesh on the torus is used.

Our goal is to prove that the above expansion (15) exists and to compute the topological derivative of $j$ denoted by $D_T j$ together with $f$. Our approach is based on a generalized adjoint method which goes back to the works of J. Cea and that was adapted to the topology optimization context in [8] and [11].

**3.1. Topology perturbation.** The new problem to solve depends on the parameter $\rho$ and represents a perturbation of problem (3) due to the nucleation of the hole $\bar{B}(x_0, \rho)$ :

$$\begin{cases} -\mathrm{div}(Ce(u_A^\rho)) = 0 \text{ in } \mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0, \rho)) \\ Ce(u_A^\rho)n = 0 \text{ on } \partial T \\ Ce(u_A^\rho)n = 0 \text{ on } \partial B(x_0, \rho) \\ u_A^\rho(x) = Ax + \phi_A^\rho(x), \quad \phi_A^\rho \text{ } \mathcal{G}\text{-periodic function.} \end{cases} \tag{16}$$

Consider $R > 0$ such that $\bar{B}(x_0, R) \cap T = \emptyset$. Instead of solving problem (16) above (whose solution is defined on a domain dependent on $\rho$) one may solve the following problem which involves a Dirichlet-to-Neumann $\mathcal{T}_\rho$ operator but whose solution is defined on a fixed space :

$$\begin{cases} -\mathrm{div}(Ce(u_\rho)) = 0 \text{ in } \mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0, R)) \\ Ce(u_\rho)n = 0 \text{ on } \partial T \\ Ce(u_\rho)n = \mathcal{T}_\rho u_\rho \text{ on } \partial B(x_0, R) \\ u_\rho(x) = Ax + \phi_A^R(x), \quad \phi_A^R \text{ } \mathcal{G}\text{-periodic function.} \end{cases} \tag{17}$$

The Dirichlet-to-Neumann operator $\mathcal{T}_\rho$ is defined by

$$\begin{aligned} \mathcal{T}_\rho : H^{1/2}(\partial B(x_0,R))^N \mapsto H^{-1/2}(\partial B(x_0,R))^N, \\ \varphi \mapsto \mathcal{T}_\rho \varphi = Ce(w_\rho^\varphi)n, \end{aligned} \tag{18}$$

In (17) and (18) $n$ denotes the exterior normal to the ball $B(x_0,R)$ and $w_\rho^\varphi$ is solution of the following problem :

$$\begin{cases} -\mathrm{div}(Ce(w_\rho^\varphi)) = 0 \text{ in } B(x_0,R) \setminus \bar{B}(x_0,\rho), \\ w_\rho^\varphi = \varphi \text{ on } \partial B(x_0,R) \\ Ce(w_\rho^\varphi)n = 0 \text{ on } \partial B(x_0,\rho). \end{cases} \tag{19}$$

Note that if $\rho = 0$ there is no nucleation of hole in $x_0$ and $w_0^\varphi$ is solution of the problem

$$\begin{cases} -\mathrm{div}(Ce(w_0^\varphi)) = 0 \text{ in } B(x_0,R), \\ w_0^\varphi = \varphi \text{ on } \partial B(x_0,R). \end{cases}$$

The operator $\mathcal{T}_\rho$, for $\rho \geq 0$, is the same as introduced in [8]. Note that its definition depends only on the differential operator considered, $-\mathrm{div}(Ce(\cdot))$. This is why it can be used in the present context of periodicity conditions.

According to a standard result in PDE theory, the solution $u_A^\rho$ of problem (16) restricted to $\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R))$ is solution of problem (17).

The variational formulation of problem (17) is the following

$$\begin{cases} \text{find } u_\rho \in LP_A(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R))) \text{ such that} \\ a_\rho(u_\rho, v) = 0 \ \forall v \in H^1_\#(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N), \end{cases} \tag{20}$$

where the bilinear form $a_\rho : LP(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R))) \times LP(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R))) \to \mathbb{R}$ is defined by

$$a_\rho(u,v) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u), e(v)\rangle dx + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_\rho u v \, ds(x). \tag{21}$$

The boundary integral above writes as

$$\int_{\partial B(x_0,R)} \mathcal{T}_\rho u v ds(x) = \int_{B(x_0,R)\setminus\bar{B}(x_0,\rho)} \langle Ce(w_\rho^u), e(w_\rho^v)\rangle dx, \tag{22}$$

where $w_\rho^u$ is the solution of (19) with $\varphi = u$ on $\partial B(x_0,R)$ and $w_\rho^v$ is the solution of (19) with $\varphi = v$ on $\partial B(x_0,R)$. Therefore the form $a_\rho$ is symmetric, continuous and coercive on $H^1_\#(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N)$ which is a closed subspace of $LP(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R)))$. Note that $LP_A(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R)))$ is a translation with $A$ of $H^1_\#(\mathbb{R}^N_{\mathrm{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N)$. According to Lemma 4, the above problem (20) has a unique solution.

The functional $j(Y \setminus (T \cup \bar{B}(x_0,\rho)))$ corresponding to the perturbed configuration, will be denoted in the sequel by $j(\rho)$ in order to simplify the notations and writes as

$$j(\rho) := j(Y \setminus (T \cup \bar{B}(x_0,\rho))) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_B^\rho)\rangle dx \tag{23}$$

where $u_A^\rho$ is the solution of problem (16), and consequently

$$j(\rho) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u_A^\rho), e(u_B^\rho)\rangle dx + \frac{1}{|Y|}\int_{B(x_0,R)\setminus\bar{B}(x_0,\rho)} \langle Ce(w_\rho^{u_A^\rho}), e(w_\rho^{u_B^\rho})\rangle dx,$$

where in the first integral term $u_A^\rho$ stands for the solution of problem (17) and $w_\rho^{u_A^\rho}$ in the second integral term stands for the solution of problem (19) with the condition $\varphi = u_A^\rho\,|_{\partial B(x_0,R)}$. By a flux-divergence theorem the second integral term may be written as

$$\int_{B(x_0,R)\setminus\bar{B}(x_0,\rho)} \langle Ce(w_\rho^{u_A^\rho}), e(w_\rho^{u_B^\rho})\rangle dx = \int_{\partial B(x_0,R)} \mathcal{T}_\rho u_A^\rho u_B^\rho ds(x)$$

and therefore the functional has the following form :

$$j(\rho) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u_A^\rho), e(u_B^\rho)\rangle + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_\rho u_A^\rho u_B^\rho ds(x). \tag{24}$$

Note that for $\rho = 0$ the functional $j(0)$ denotes $j(Y\setminus T)$ and writes

$$j(0) := j(Y\setminus T) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u_A^0), e(u_B^0)\rangle + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_0 u_A^0 u_B^0 ds(x), \tag{25}$$

where $u_A^0$ is solution of (17) for $\rho = 0$ and therefore $u_A^0$ is solution of the variational problem (20) for $\rho = 0$.

Observing formula (24), one notices that $j$ has the following form :

$$j(\rho) = \tilde{J}_\rho(u_A^\rho, u_B^\rho),$$

where $u_A^\rho$ and $u_B^\rho$ are solutions of problem (20) for two different effective strain matrices $A$ and $B$, and where $\tilde{J}_\rho : LP(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)))\times LP(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)))\mapsto\mathbb{R}$ is given by

$$\tilde{J}_\rho(u,v) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u), e(v)\rangle + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_\rho u\, v ds(x).$$

The functional $\tilde{J}_\rho$ above is bilinear and due to (22) it is symmetric.

As a consequence of Lemma 5 below, the quantity $\tilde{J}_\rho(u_A^\rho, u_B^\rho)$ depends linearly on $A$ and on $B$ respectively.

**Lemma 5.** *The solution $u_A^\rho$ of problem (20) here restated*

$$\begin{cases} \text{find } u_A^\rho \in LP_A(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R))) \text{ such that} \\ a_\rho(u_A^\rho, v) = 0\ \forall v\in H^1_\#(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)),\mathbb{R}^N), \end{cases}$$

*depends linearly on the strain matrix $A$.*

Proof : It suffices to note that if $u\in LP_A(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)))$ and $v\in LP_B(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)))$ then $u+v \in LP_{A+B}(\mathbb{R}^N_{\text{perf}}(T\cup\bar{B}(x_0,R)))$. Also, if $\alpha\in\mathbb{R}$ and $u\in$

$LP_A(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$, then $\alpha u \in LP_{\alpha A}(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$. The linearity of the equation $a_\rho(u_\rho, v) = 0$ $\forall v \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$ ensures the property in the statement (see also [2]).

Due to the above considerations, the following relation holds :

$$\tilde{J}_\rho(u^\rho_A, u^\rho_B) = \frac{1}{4}\left[\tilde{J}_\rho(u^\rho_{A+B}, u^\rho_{A+B}) - \tilde{J}_\rho(u^\rho_{A-B}, u^\rho_{A-B})\right]. \tag{26}$$

If one knows the derivative with respect to $\rho$ of terms of the type $\tilde{J}(u^\rho_A, u^\rho_A)$ for arbitrary $A$, then using it for $A+B$ and $A-B$, respectively, the derivation of (26) in $\rho$ yields the derivative of $\tilde{J}_\rho(u^\rho_A, u^\rho_B)$ with respect to $\rho$.

**3.2. Outline of the adjoint method.** In fact the problem reduces to the following : obtain the derivative of $j(\rho) = \tilde{J}_\rho(u^\rho_A, u^\rho_A)$, with respect to $\rho$ where $u^\rho_A$ is solution of (20). The dependency of the functional $j(\rho)$ on $\rho$ comes in this case from a functional $J_\rho$ and from $u^\rho_A$, that is $j(\rho) = J_\rho(u^\rho_A)$, where the functional $J_\rho : LP(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R))) \to \mathbb{R}$, is defined by

$$J_\rho(u) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,R))} \langle Ce(u), e(u)\rangle + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_\rho u\, u ds(x). \tag{27}$$

Formally, any variation in $\rho$ of $J_\rho(u^\rho_A)$ writes :

$$\frac{\delta}{\delta\rho}(J_\rho(u^\rho_A)) = \frac{\delta J_\rho}{\delta\rho}(u^\rho_A) + \frac{\delta J_\rho}{\delta u}(u^\rho_A)\frac{\delta u^\rho_A}{\delta\rho},$$

where $u^\rho_A \in LP_A(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$ is solution of the problem

$$a_\rho(u^\rho_A, v) = l_\rho(v), \forall v \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N).$$

By deriving the above problem with respect to $\rho$, and having in mind the linearity of $a_\rho(\cdot, v)$ for a fixed $v$, one obtains that $\dfrac{\delta u^\rho_A}{\delta\rho} \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$ is solution of the following problem :

$$a_\rho(\frac{\delta u^\rho_A}{\delta\rho}, v) = \frac{\delta l_\rho}{\delta\rho}(v) - \frac{\delta a_\rho}{\delta\rho}(u^\rho_A, v), \forall v \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N).$$

By introducing an adjoint state $p_\rho \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$ as solution of the problem

$$a_\rho(w, p_\rho) = -\frac{\delta J_\rho}{\delta u}(u^\rho_A)w, \forall w \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$$

and choosing $w = \frac{\delta u^\rho_A}{\delta\rho}$, the variation of $J_\rho(u^\rho_A)$ may be written as :

$$\delta J_\rho(u^\rho_A) = \frac{\delta J_\rho}{\delta\rho}(u^\rho_A) - a_\rho(\frac{\delta u^\rho_A}{\delta\rho}, p_\rho) = \frac{\delta J_\rho}{\delta\rho}(u^\rho_A) + \frac{\delta a_\rho}{\delta\rho}(u^\rho_A, p_\rho) - \frac{\delta l_\rho}{\delta\rho}(p_\rho).$$

Going back to the works of J. Cea [5], the above idea writes in mathematical rigor as a generalized adjoint method where the bilinear forms are coercive only on a closed subspace.

**3.3. The generalized adjoint method.** Consider a parameter $\rho > 0$ and a family $a_\rho : V \times V \to \mathbb{R}$ of bilinear, symmetric, uniformly continuous forms (with constant $M$), that are coercive only on $V_0$ (with constant $\alpha > 0$) :

$$a_\rho(u, v) \leq M\|u\|\|v\| \ \forall u, v \in V,$$

$$a_\rho(u, v) \geq \alpha\|u\|^2 \ \forall u \in V_0.$$

Consider a family $l_\rho : V \to \mathbb{R}$ of linear uniformly continuous forms (with constant $L > 0$) :

$$|l_\rho(v)| \leq L\|v\| \ \forall v \in V.$$

Assume that there exists a real function $f : \mathbb{R}_+ \to \mathbb{R}_+$ with the property

$$\lim_{\rho \to 0} f(\rho) = 0,$$

such that the following estimates hold

$$\|a_\rho - a_0 - f(\rho)\delta_a\|_{\mathcal{L}^2(V)} = o(f(\rho)), \tag{28}$$

$$\|l_\rho - l_0 - f(\rho)\delta_l\|_{\mathcal{L}(V)} = o(f(\rho)), \tag{29}$$

where $\delta_a : V \times V \to \mathbb{R}$ is a bilinear, symmetric and continuous form, $\delta_l : V \to \mathbb{R}$ is a linear continuous form. $\mathcal{L}(V)$ (respectively $\mathcal{L}^2(V)$) denotes the space of continuous and linear (respectively bilinear) forms on $V$.

According to Lemma 4, for an arbitrarily fixed parameter $\rho > 0$, the problem

$$\begin{cases} \text{find } u_A^\rho \in K \text{ such that} \\ a_\rho(u_A^\rho, v) = l_\rho(v) \ \forall v \in V_0, \end{cases} \tag{30}$$

has a unique solution.

The following lemma describes the behaviour of $u_A^\rho$ in terms of the solution of the non perturbed problem $u_A^0$ :

**Lemma 6.** *If $u_A^\rho$ is the solution of problem (30) above and $u_A^0$ is the solution of*

$$\begin{cases} \textit{find } u_A^0 \in K \textit{ such that} \\ a_0(u_A^0, v) = l_0(v) \ \forall v \in V_0, \end{cases} \tag{31}$$

*one has*

$$\|u_A^\rho - u_A^0\| = O(f(\rho)).$$

The above result is an adaptation of Lemma 2.1 in [8] and the proof follows the same steps, therefore it will not be given in the present paper.

In order to study the minimization problem

$$\min j(\rho) \text{ where } j(\rho) = J_\rho(u_A^\rho),$$

a Lagrangian may be introduced according to [5] in the form : $\mathcal{L}_\rho : V \times V \to \mathbb{R}$.

$$\mathcal{L}_\rho(u, v) = J_\rho(u) + a_\rho(u, v) - l_\rho(v).$$

The main result of the present section is stated below and allows one to compute the derivative of $j(\rho)$ with respect to $\rho$, that is the topological derivative in the current context. This result is a generalization of Theorem 2.2 in [8], in the sense that in [8] $V = V_0 = K$.

**Theorem 7.** *Suppose that there exists $\delta_J : V \to \mathbb{R}$ such that*

$$J_\rho(v) - J_0(u) = DJ(u)(v-u) + f(\rho)\delta_J(u) + o(\|v-u\| + f(\rho)), \text{ for all } u, v \in V, \quad (32)$$

*where $DJ(u)$ is the Gâteaux derivative of $J_0$ with respect to $u$. Then, the functional $j(\rho)$ has the following asymptotic expansion*

$$j(\rho) = j(0) + f(\rho)\delta_{\mathcal{L}}(u_A^0, p_A) + o(f(\rho)), \quad (33)$$

*where $\delta_{\mathcal{L}}$ denotes $\delta_{\mathcal{L}}(u, v) = \delta_J(u) + \delta_a(u, v) - \delta_l(v)$ and the adjoint state $p_A$ is the solution of the adjoint problem*

$$\begin{cases} \text{find } p_A \in V_0 \text{ such that} \\ a_0(w, p_A) = -DJ(u_A^0)w, \ \forall w \in V_0. \end{cases} \quad (34)$$

Proof: Note that from (28) and (29) one obtains

$$\mathcal{L}_\rho(u, v) - \mathcal{L}_0(u, v) = f(\rho)\delta_{\mathcal{L}}(u, v) + o(f(\rho)),$$

Since $u_A^\rho$ is solution of (30) and $u_A^0$ is solution of (31), then $j(\rho) = \mathcal{L}_\rho(u_A^\rho, v), \forall v \in V_0$, and $j(0) = \mathcal{L}_0(u_A^0, v), \forall v \in V_0$.

Then $j(\rho) - j(0) = \mathcal{L}_\rho(u_A^\rho, v) - \mathcal{L}_0(u_A^0, v) = J_\rho(u_A^\rho) - J_0(u_A^0) + a_\rho(u_A^\rho, v) - a_0(u_A^0, v) + l_\rho(v) - l_0(v) = DJ(u_A^0)(u_A^\rho - u_A^0) + a_\rho(u_A^\rho, v) - a_0(u_A^0, v) + f(\rho)(\delta_J(u_A^0) - \delta_l(v)) + o(f(\rho))$, where (32) and the estimation in Lemma 6 were used to obtain the last equality.

Taking $v$ as the adjoint state $v = p_A$ solution of (33) one obtains $j(\rho) - j(0) = -a_0(u_A^\rho - u_A^0, p_A) + a_\rho(u_A^\rho, p_A) - a_0(u_A^0, p_A) + f(\rho)(\delta_J(u_A^0) - \delta_l(p_A)) + o(f(\rho)) = a_\rho(u_A^\rho, p_A) - a_0(u_A^\rho, p_A) + f(\rho)(\delta_J(u_A^0) - \delta_l(p_A)) + o(f(\rho))$, and having in mind (28) and again the estimation in Lemma 6 it turns out that $j(\rho) - j(0) = f(\rho)\delta_a(u_A^\rho, p_A) + f(\rho)(\delta_J(u_A^0) - \delta_l(p_A)) + o(f(\rho)) = f(\rho)\delta_{\mathcal{L}}(u_A^0, p_A) + o(f(\rho))$.

**3.4. Calculation of the topological derivative.** The problem of finding the asymptotic development (15) and consequently the topological derivative fits into the context described in subsection 3.3.

By taking the spaces $V$ and $V_0$ as $V = LP(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$ and $V_0 = H^1_{\#}(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$, the bilinear form $a_\rho$ defined in (21) verifies an estimate like (28) with $a_0 : V \times V \mapsto \mathbb{R}$ ,

$$a_0(u, v) = \frac{1}{|Y|} \int_{Y \setminus (T \cup \bar{B}(x_0, R))} \langle Ce(u), e(v) \rangle dx + \frac{1}{|Y|} \int_{\partial B(x_0, R)} \mathcal{T}_0 uv \, ds(x).$$

Due to the following equality (see (22))

$$\int_{\partial B(x_0, R)} \mathcal{T}_0 uv \, ds(x) = \int_{B(x_0, R)} \langle Ce(w_0^u), e(w_0^v) \rangle dx, \tag{35}$$

the bilinear form $a_0$ writes

$$a_0(u, v) = \frac{1}{|Y|} \int_{Y \setminus T} \langle Ce(u), e(v) \rangle dx. \tag{36}$$

The following estimate holds

$$\| a_\rho - a_0 - \rho^N \delta_a \|_{\mathcal{L}^2(V)} = o(\rho^N), \tag{37}$$

where the bilinear form $\delta_a$ is defined by

$$\delta_a(u, v) = \frac{1}{|Y|} \int_{\partial B(x_0, R)} \delta_{\mathcal{T}} uv ds(x). \tag{38}$$

The operator $\delta_{\mathcal{T}}$ in $\mathcal{L}(H^{1/2}(\partial B(x_0, R))^N, H^{-1/2}(\partial B(x_0, R))^N)$, according to Proposition 4.5 in [8] verifies

$$\| \mathcal{T}_\rho - \mathcal{T}_0 - \rho^N \delta_{\mathcal{T}} \|_{\mathcal{L}(H^{1/2}(\partial B(x_0, R))^N, H^{-1/2}(\partial B(x_0, R))^N)} = o(\rho^N). \tag{39}$$

The linear forms $l_\rho$ and $l_0$ are identically zero and therefore an estimate like (29) is verified with $\delta_l$ equal to zero.

By taking the closed affine manifold $K = LP_A(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$ in $LP(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))$, the estimate in Lemma 6 holds between the solutions $u_\rho$ of (20), for $\rho > 0$, and $u_0$ of (20), for $\rho = 0$, that is

$$\| u_\rho - u_0 \|_{LP(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R)))} = O(\rho^N). \tag{40}$$

In order to apply Theorem 7 with the functional $J_\rho : LP(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0, R))) \to \mathbb{R}$, defined in formula (27) and restated below,

$$J_\rho(u) = \frac{1}{|Y|} \int_{Y \setminus (T \cup \bar{B}(x_0, R))} \langle Ce(u), e(u) \rangle + \frac{1}{|Y|} \int_{\partial B(x_0, R)} \mathcal{T}_\rho u \, u ds(x),$$

an estimation result to guarantee an asymptotic development like (32) is given in Proposition 8. Note that the Gâteaux derivative of $J_0$ is

$$DJ(u)(w) = \frac{2}{|Y|}\int_{Y\setminus T} \langle Ce(u), e(w)\rangle dx. \tag{41}$$

**Proposition 8.** *The functional $J_\rho$ satisfies :*

$$\begin{aligned} J_\rho(v) - J_0(u) \quad = \quad & \frac{2}{|Y|}\int_{Y\setminus T} \langle Ce(u), e(v-u)\rangle dx + \\ + \quad & \rho^N \frac{1}{|Y|}\int_{\partial B(x_0,R)} \delta_{\mathcal{T}} uu ds(x) + o(\|v-u\| + \rho^N). \end{aligned} \tag{42}$$

Proof: The difference

$$J_\rho(v) - J_0(u) - \frac{2}{|Y|}\int_{Y\setminus T} \langle Ce(u), e(w)\rangle dx$$

may be written in the form

$$\frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(v-u), e(v-u)\rangle dx + \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_\rho vv\, ds(x) - \frac{1}{|Y|}\int_{\partial B(x_0,R)} \mathcal{T}_0 vv\, ds(x),$$

which, using estimation (39) becomes

$$\frac{1}{|Y|}\rho^N \int_{\partial B(x_0,R)} \delta_{\mathcal{T}} vv\, ds(x) + o(\|v-u\|^2) + o(\rho^N).$$

Writing $v = u + (v-u)$ and having in mind that $\delta_{\mathcal{T}}$ is linear and continuous the above expression is equal to

$$\frac{1}{|Y|}\rho^N \int_{\partial B(x_0,R)} \delta_{\mathcal{T}} uu\, ds(x) + o(\|v-u\| + \rho^N),$$

which concludes the estimation (42).□

The adjoint problem writes

$$\left\{ \begin{array}{c} \text{find the adjoint state } p \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N) \text{ such that} \\ a_0(w,p) = -DJ(u_0)w \ \forall w \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N). \end{array} \right.$$

Having in mind (40), the definition (36) of $a_0$ and its property of symmetry, the adjoint state satisfies

$$a_0(w,p) = -2a_0(w,u_0) \text{ for all } w \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N).$$

Since $u_0$ is solution of (20) (for $\rho = 0$), it turns out that $a_0(w,p) = 0$ for all $w \in H^1_\#(\mathbb{R}^N_{\text{perf}}(T \cup \bar{B}(x_0,R)), \mathbb{R}^N)$, which implies $p = 0$ (the problem is self-adjoint).

The main result of the paper may now be stated as follows and gives the topological derivative of functionals defined in (23), for the case when the effective stains $A$ and $B$ coincide :

**Theorem 9.** *The functional*

$$j(\rho) = \frac{1}{|Y|} \int_{Y \setminus (T \cup \bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_A^\rho) \rangle dx \tag{43}$$

*has the following asymptotic expansion*

$$j(\rho) = j(0) + \rho^N D_T j(x_0) + o(\rho^N), \tag{44}$$

*where the topological derivative $D_T j$ in $x_0$ writes in terms of the operator $\mathcal{T}$ as*

$$D_T j(x_0) = \frac{1}{|Y|} \int_{\partial B(x_0,R)} \delta_{\mathcal{T}} u_0 u_0 ds(x)$$

*with $u_0$ solution of (11).*

Proof : Theorem 7 may be applied since all its hypotheses are fulfilled. The functional $j$ admits an asymptotic expansion like (33) with $f(\rho) = \rho^N$ and $\delta_{\mathcal{L}}(u_0,p) = \delta_J(u_0) + \delta_a(u_0,p) = \delta_J(u_0)$ since the adjoint state $p = 0$. From Proposition 8 it turns out that $\delta_J(u_0) = \dfrac{1}{|Y|} \displaystyle\int_{\partial B(x_0,R)} \delta_{\mathcal{T}} u_0 u_0 ds(x)$.□

Suppose that the material tensor $C$ in Section 2 corresponds is isotropic with the Lamé constants $\lambda$ and $\mu$. The having in mind formula (26), the following explicit expressions for the topological derivative may be deduced :

**Corollary 10.** *Consider the functional defined in (23)*

$$j(\rho) = \frac{1}{|Y|} \int_{Y \setminus (T \cup \bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_B^\rho) \rangle dx$$

*where $u_A$ and $u_B$ are the corresponding solutions of the cellular problem (11) with the effective strains $A$ and $B$, respectively. Then $j$ admits the asymptotic expansion*

$$j(\rho) = j(0) + \rho^N D_T j(x_0) + o(\rho^N),$$

*where the topological derivative $D_T j$ in $x_0$ for $N = 2$, has the form:*

$$\begin{aligned} D_T j(x_0) = -\frac{\pi}{|Y|} \frac{\lambda + 2\mu}{\lambda + \mu} \Big[ & 4\mu e(u_A(x_0)) e(u_B(x_0)) + \\ & \frac{\lambda^2 + 2\lambda\mu - \mu^2}{\mu} \, tr e(u_A(x_0)) \, tr e(u_B(x_0)) \Big] . \end{aligned} \tag{45}$$

*For $N = 3$ the topological derivative has the form*

$$D_T j(x_0) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{9\lambda+14\mu}\Big[40\mu e(u_A(x_0))e(u_B(x_0))+ \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\, tr e(u_A(x_0))\, tr e(u_B(x_0))\Big]. \tag{46}$$

Proof : According to (26), and applying Theorem 9 with the functionals like (43) with the stains $A+B$ and $A-B$, respectively, and having in mind the linearity of the solutions with respect to the effective stains (see Lemma 5), one obtains

$$D_T j(x_0) = \frac{1}{|Y|}\int_{\partial B(x_0,R)} \delta_{\mathcal{T}} u_A u_B ds(x).$$

The expression of the operator $\delta_{\mathcal{T}}$ is too complicated and will not be reproduced here; see formula (4.17) in [8]. In order to obtain formulas (45) and (46) we shall only need the following property of $\delta_{\mathcal{T}}$ : for an isotropic material tensor $C$, one has

$$\frac{1}{|Y|}\int_{\partial B(x_0,R)} \delta_{\mathcal{T}}\varphi\, \psi ds(x) = -\pi\frac{\lambda+2\mu}{\lambda+\mu}\Big[4\mu e(\varphi(x_0))e(\psi(x_0))+ \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\,\mathrm{tr}\, e(\varphi(x_0))\,\mathrm{tr}\, e(\psi(x_0))\Big], \tag{47}$$

for two dimensions, and

$$\frac{1}{|Y|}\int_{\partial B(x_0,R)} \delta_{\mathcal{T}}\varphi\, \psi ds(x) = -\pi\frac{\lambda+2\mu}{9\lambda+14\mu}\Big[40\mu e(\varphi(x_0))e(\psi(x_0))+ \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\,\mathrm{tr}\, e(\varphi(x_0))\,\mathrm{tr}\, e(\psi(x_0))\Big], \tag{48}$$

for three dimensions (see in [8], Table 3.1, the case of the Neumann boundary condition on the hole). □

## 4. Comments and conclusions

For practical purposes, the formulas in Corollary 10 may be particularized in order to obtain the topological derivative for each of the elastic coefficients of the homogenized tensor $C^H$ (see Theorem 1) as follows

**Corollary 11.** *The topological derivative of each coefficient of the homogenized tensor $C^H$, for $N = 2$, has the form:*

$$D_T\langle C^H f_i, f_j\rangle(x) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\Big[4\mu e(u_{f_i})e(u_{f_j})+ \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\, tr e(u_{f_i})\, tr e(u_{f_j})\Big](x), \tag{49}$$

*where* $(f_i)_{i=1,2,3}$ *is the following basis of symmetric matrices of* $\mathcal{M}_2(\mathbb{R})$*:*

$$f_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} , \; f_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} , \; f_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

*and* $u_{f_i}$ *are the corresponding solutions of the cellular problem (11) with the effective strain* $f_i$*. In three dimensions, the topological derivative of the coefficients of* $C^H$ *has the form*

$$D_T\langle C^H f_i, f_j\rangle(x) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{9\lambda+14\mu}\Big[40\mu e(u_{f_i})e(u_{f_j}) + \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\, tr e(u_{f_i})\, tr e(u_{f_j})\Big](x)\,, \tag{50}$$

*where*

$$f_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} , \; f_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} , \; f_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} ,$$

$$f_4 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} , f_5 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} , f_6 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} .$$

The above result was stated in Theorem 4 from [2], with a more intuitive proof. That proof uses the formulation in stress of the cellular problem (9) and its variational formulation (13). A formal similarity between problem (9) and a pure Neumann problem (see Lemma 3, Remark 3 and Lemma 6 in [2]) allows one to compute the topological derivative of the homogenized compliance tensor, that is of the inverse of the homogenized tensor $C^H$. Then, the topological derivative of $C^H$ presents the opposite sign since it is the derivative of an inverse.

The formulas of the topological derivative of the homogenized coefficients were successfully implemented and used in a alternate directions optimization algorithm, jointly with the shape derivative, and some optimized microstructures were presented in [3].

**Remark 9.** The present paper studies the functional (43)

$$j(\rho) = \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_A^\rho)\rangle dx.$$

This quantity has the nature of an energy (stored elastic energy); recall that $u_A^\rho$ is the solution of problem (16).

It is interesting to compare the behaviour of the functional $j$ with the classical case studied in [8], where the elasticity problem has the form (see (3.2) in [8]) :

$$\begin{cases} u^\rho \in H^1(\Omega\setminus\bar{B}(x_0,\rho)), \\ -div(Ce(u^\rho)) = 0 \text{ in } \Omega\setminus\bar{B}(x_0,\rho), \\ u^\rho = 0 \text{ on } \Gamma_D, \\ C(e(u^\rho))n = g \text{ on } \Gamma_N, \\ C(e(u^\rho))n = \text{ on } \partial B(x_0,\rho). \end{cases} \tag{51}$$

In the above, $\Omega$ is a bounded domain in $\mathbb{R}^N$ and $\partial\Omega = \bar{\Gamma}_D \cup \bar{\Gamma}_N$, $\Gamma_D \cap \Gamma_N = \emptyset$. The stored elastic energy

$$\mathcal{J}(\rho) = \int_{\Omega\setminus\bar{B}(x_0,\rho)} \langle Ce(u^\rho), e(u^\rho)\rangle dx \tag{52}$$

describes the *compliance* of the body. This is very different from the case of the cellular problem, where stored elastic energy $j$ describes the *rigidity* of the microstructure with respect to the imposed macroscopic strain $A$. This difference is due to the different nature of the two elasticity problems : the cellular problem (16) is subject to periodicity conditions which have the nature of a non-homogeneous Dirichlet condition (see Remark 2 in [2]), while problem (51) has only homogeneous Dirichlet conditions, complemented by non-zero Neumann conditions.

With the results in [8], it is a mere exercise to prove that the topological derivative of the compliance

$$D_T\mathcal{J} = -\int_{\Gamma_R} \delta_{\mathcal{T}} uud\gamma(x),$$

where $\delta_{\mathcal{T}}$ is the same operator as introduced in (39) and $u$ is the solution of an elasticity problem like (51) but with no hole ($\rho = 0$). Due to the properties (47) and (48) of $\delta_{\mathcal{T}}$, the above topological derivative of the compliance has positive values.

The different behaviours of the stored elastic energy in the two contexts is reflected in the final formulas of their topological derivatives. The topological derivative of $\mathcal{J}$ is always positive, which means that drilling a hole in the body will increase its compliance (by increasing the stored elastic energy) for a fixed applied force $g$ in (51). On the other hand, the topological derivative of $j$, computed in the present paper (Theorem 9) has the same formula with opposite sign, so it is always negative, which means that drilling a hole in the periodicity cell will decrease the rigidity of the homogenized material (by decreasing the stored elastic energy) for a fixed macroscopic strain $A$ in (16).

The communication [14] and the discussion which followed it motivated the above comments and the whole paper actually.

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