Struct Multidisc Optim (2010) 40:381–391
DOI 10.1007/s00158-009-0378-0

RESEARCH PAPER

Shape and topology optimization for periodic problems

Part I: The shape and the topological derivative

Cristian Barbarosie · Anca-Maria Toader

Received: 3 December 2008 / Revised: 17 February 2009 / Accepted: 4 March 2009 / Published online: 23 April 2009

Abstract In the present paper we deduce formulae for the shape and topological derivatives for elliptic problems in unbounded domains subject to periodicity conditions. Note that the known formulae of shape and topological derivatives for elliptic problems in bounded domains do not apply to the periodic framework. We consider a general notion of periodicity, allowing for an arbitrary parallelepiped as periodicity cell. Our calculations are useful for optimizing periodic composite materials by gradient type methods using the topological derivative jointly with the shape derivative for periodic problems. Important particular cases of functionals to minimize/maximize are presented. A numerical algorithm for optimizing periodic composites using the topological and shape derivatives is the subject of a second paper (Barbarosie and Toader, Struct Multidiscipl Optim, 2009).

Keywords Optimization of microstructures · Shape derivative · Topological derivative · Periodic homogenization · Porous materials

1 Introduction

The main motivation of the present paper comes from the study of periodic microstructures and optimization of their macroscopic properties, in the context of linearized elasticity. A periodic microstructure is a body whose material coefficients vary at a microscopic scale, according to a periodic pattern. Homogenization theory allows one to accurately describe the macroscopic behaviour of such a microstructure by means of so-called cellular problems, which are elliptic PDEs subject to periodicity conditions. Porous materials, that is, bodies with periodic infinitesimal perforations, can be described in a similar manner.

This is the first of a series of two papers; it contains the theoretical background about shape and topology derivatives in the periodic framework; the second paper (Barbarosie and Toader 2009) presents a numerical implementation and results of an optimization method for periodic microstructures. This paper is self contained and therefore independent from Part II (Barbarosie and Toader 2009); the formulae presented for the shape and topological derivatives can be used for different numerical implementations. Some preliminary results were presented in Toader (2008).

In Section 2 some notations and mathematical tools for periodic functions are introduced. Section 3 states two different formulations of the cellular problem for mixtures of materials; in one of the problems the unknown is the strain while in the other the unknown is the stress. Each formulation has its own importance for the calculations in Sections 5 and 6.

For practical purposes, porous materials have special relevance. Section 4 presents the cellular problems in strain and stress formulation describing the behaviour of porous materials (which are different from the ones presented in Section 3 for mixtures of materials).

Section 5 is devoted to the computation of the topological derivative of the homogenized elastic coefficients, while in Section 6 the shape derivative of the same homogenized coefficients is computed. The

C. Barbarosie (✉) · A.-M. Toader
CMAF, Av. Prof. Gama Pinto, 2, 1649-003, Lisbon, Portugal
e-mail: barbaros@ptmat.fc.ul.pt

A.-M. Toader
e-mail: amtan@ptmat.fc.ul.pt

formulae obtained are specific for the periodic case and different from the topological and shape derivatives of energy type terms (e.g. compliance) for problems defined on bounded domains.

A list of examples of optimization problems for periodic microstructure is presented in Section 7, together with references to Part II (Barbarosie and Toader 2009) for specific numerical results. The most common functionals like bulk modulus, shear response are presented as linear combinations of certain homogenized coefficients. Also a functional used to minimize the Poisson coefficient is studied, with the goal of obtaining auxetic materials.

2 Preliminaries on periodic functions

We shall consider a parallelepiped Y in $\mathbb{R}^n$ (a parallelogram in $\mathbb{R}^2$) which defines the periodicity of the microstructures. Often Y is taken to be the unit cube for the sake of simplicity.

Consider the set of *linear plus periodic* functions denoted by

$$LP = \big\{\mathbf{u} : \mathbb{R}^n \mapsto \mathbb{R}^n \mid \mathbf{u}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \boldsymbol{\varphi}(\mathbf{x}), \mathsf{A} \in \mathscr{M}_n(\mathbb{R}),$$
$$\boldsymbol{\varphi} \in H^1_{loc}(\mathbb{R}^n; \mathbb{R}^n) \text{ and } Y-\text{periodic}\big\},$$

where $\mathscr{M}_n(\mathbb{R})$ is the set of $n \times n$ real matrices. Here $H^1_{loc}(\mathbb{R}^n; \mathbb{R}^n)$ represents the space of vector fields which are locally square-integrable and whose weak partial derivatives of order one have the same property.

The following properties of periodic functions will be used in the sequel:

Lemma 1 *Let $\boldsymbol{\varphi}$ in $H^1_{loc}(\mathbb{R}^n; \mathbb{R}^n)$ be a Y - periodic function. Then:*

1) $\displaystyle\int_{\partial Y} \varphi_i n_j = 0$, *where* $\mathbf{n}$ *is the unit normal to* ∂Y *(pointing outwards).*
2) $\displaystyle\int_Y \nabla\boldsymbol{\varphi} = \mathsf{0}.$

Proof The first assertion is a consequence of $\boldsymbol{\varphi}$ having equal values on opposite faces of the parallelogram Y while $\mathbf{n}$ (since it points outwards) has opposite values on opposite faces of Y. In order to prove the second assertion, apply the flux divergence theorem and use the first part. □

As a consequence of the above Lemma 1, the linear part of a function $\mathbf{u}$ in LP can be identified by

$$\mathsf{A} = \fint \nabla\mathbf{u},$$

where in general by $\fint \mathbf{h}$ we shall denote the average of $\mathbf{h}$ in Y, that is,

$$\fint \mathbf{h} = \frac{1}{|Y|}\int_Y \mathbf{h}(\mathbf{x})d\mathbf{x}\,.$$

In the case when A is symmetric one has

$$\mathsf{A} = \fint \mathsf{e}(\mathbf{u})$$

where $\mathsf{e}(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + \nabla^T\mathbf{u})$ is the strain associated to $\mathbf{u}$.

Lemma 2 *Let* $\mathbf{u}$ *in* LP.

1) *If* $\mathsf{A} = \fint \nabla\mathbf{u}$ *then* $\mathbf{u}$ *can be represented by*

$$\mathbf{u}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \boldsymbol{\varphi}(\mathbf{x}), \textit{ with } \boldsymbol{\varphi} \quad Y-\textit{periodic};$$

2) *If* $\mathsf{A} = \fint \mathsf{e}(\mathbf{u})$ *then* $\mathbf{u}$ *can be represented, up to a rigid rotation, by*

$$\mathbf{u}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \boldsymbol{\varphi}(\mathbf{x}), \textit{ with } \boldsymbol{\varphi} \quad Y-\textit{periodic}.$$

3 Strain and stress formulations of the cellular problem

Consider a periodic elliptic problem

$$\begin{cases} -\mathrm{div}(\mathsf{Ce}(\mathbf{u}_\mathsf{A})) = \mathbf{0} \text{ in } \mathbb{R}^n \\ \mathbf{u}_\mathsf{A}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \phi_\mathsf{A}(\mathbf{x}), \quad \text{with } \phi_\mathsf{A} \quad Y-\text{periodic.} \end{cases} \tag{1}$$

where A is a given symmetric matrix and the elastic tensor C is Y-periodic on $\mathbb{R}^n$. Problem (1) above is known in homogenization theory as *cellular problem*.

Problem (1) models the microscopic behaviour of a microstructure whose elastic coefficients vary according to the periodic pattern tensor field C and subject to the macroscopic strain A. Typically, but not necessarily, the pattern tensor field C takes only two values, modeling a periodic mixture between two given component materials (see Fig. 1).

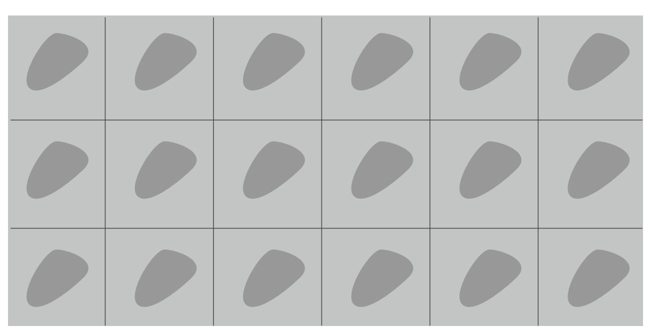

Fig. 1 Periodic mixture of two materials

The homogenized elastic tensor C^H, describing the effective (macroscopic) behaviour of this microstructure, will be defined in the sequel with the aid of the cellular problem (1).

The solution $\mathbf{u}_\mathsf{A}$ of problem (1) has the property that its average strain is equal to A:

$$\fint \nabla \mathbf{u}_\mathsf{A} = \fint \mathsf{e}(\mathbf{u}_\mathsf{A}) = \mathsf{A} \tag{2}$$

(see the consequences of Lemma 1).

Thus, the cellular problem (1) may be written in strain formulation as follows:

$$\begin{cases} \mathbf{u}_\mathsf{A} \in LP \\ -\mathrm{div}(\mathsf{Ce}(\mathbf{u}_\mathsf{A})) = \mathbf{0} \text{ in } \mathbb{R}^n \\ \fint \mathsf{e}(\mathbf{u}_\mathsf{A}) = \mathsf{A}\,, \end{cases} \tag{3}$$

where $\mathsf{A} \in \mathscr{M}_n(\mathbb{R})$ is a given symmetric matrix.

From the homogenization theory, it is known that the homogenized elastic tensor C^H relates the average strain A with the average stress associated to $\mathbf{u}_\mathsf{A}$:

$$\fint \mathsf{Ce}(\mathbf{u}_\mathsf{A}) = \mathsf{C}^H \mathsf{A}\,,$$

while the energy type product $\langle \mathsf{C}^H\mathsf{A}, \mathsf{B}\rangle$ may be expressed as

$$\fint \mathsf{Ce}(\mathbf{u}_\mathsf{A})\mathsf{e}(\mathbf{u}_\mathsf{B}) = \langle \mathsf{C}^H\mathsf{A}, \mathsf{B}\rangle.$$

For homogenization theory of periodic composites we refer to Allaire (1992) where the cellular problem is stated in a slightly different way.

Remark 1 The average strain A can also be expressed as a boundary integral. It suffices to apply the flux divergence theorem to the above formula (2) in order to obtain

$$\mathsf{A} = \frac{1}{|Y|}\int_{\partial Y} \mathbf{u}_\mathsf{A} \otimes \mathbf{n} = \frac{1}{|Y|}\int_{\partial Y} \mathbf{u}_\mathsf{A} \vee \mathbf{n}\,, \tag{4}$$

where $\mathbf{n}$ denotes the unit normal to ∂Y (pointing outwards), $\otimes$ denotes the tensor product

$$(\mathbf{u}_\mathsf{A} \otimes \mathbf{n})_{ij} = (u_\mathsf{A})_i n_j$$

and $\vee$ denotes the symmetrized tensor product:

$$(\mathbf{u}_\mathsf{A} \vee \mathbf{n})_{ij} = \frac{1}{2}\big((u_\mathsf{A})_i n_j + (u_\mathsf{A})_j n_i\big)\,.$$

For a rectangular cell, it suffices to compute averages on specific faces of Y. More precisely, let S_j^+ and S_j^- be the two parallel sides of Y orthogonal to $\mathbf{e}_j$, where $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ is the canonical basis of $\mathbb{R}^n$. Denote by h_j the height of the cell (the distance between S_j^+ and S_j^-). Recall that $|S_j^+| = |S_j^-|$ and $h_j|S_j^+| = |Y|$. In this case, formula (4) can be written as

$$\begin{aligned} \mathsf{A}_{ij} &= \frac{1}{|Y|}\left(\int_{S_j^+}(u_\mathsf{A})_i - \int_{S_j^-}(u_\mathsf{A})_i\right) \\ &= \frac{1}{h_j}\left(\frac{1}{|S_j^+|}\int_{S_j^+}(u_\mathsf{A})_i - \frac{1}{|S_j^-|}\int_{S_j^-}(u_\mathsf{A})_i\right)\,. \end{aligned}$$

Remark 2 Condition $\fint \mathsf{e}(\mathbf{u}_\mathsf{A}) = \mathsf{A}$ may be viewed as a Dirichlet condition: by Lemma 2, $\mathbf{u}_\mathsf{A}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \phi_\mathsf{A}(\mathbf{x})$, with $\phi_\mathsf{A} \in H^1_{loc}(\mathbb{R}^n;\mathbb{R}^n)$ and Y-periodic. Hence,

$$\mathbf{u}_\mathsf{A}(\mathbf{x} + h_i\mathbf{e}_i) - \mathbf{u}_\mathsf{A}(\mathbf{x}) = \mathsf{A}\,h_i\mathbf{e}_i$$

that is, the difference between the values of $\mathbf{u}_\mathsf{A}$ on opposite faces is prescribed. This condition has the same nature as a non-homogeneous Dirichlet boundary condition.

In the above, a rectangular cell was considered, being $h_i\mathbf{e}_i$ its generators. However, this remark holds for any parallelepiped Y, replacing $h_i\mathbf{e}_i$ by an arbitrary set of n generator vectors $\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_n$.

In the following another formulation of the above cellular problem will be useful: the formulation in stress.

Given a symmetric matrix $\sigma \in \mathscr{M}_n(\mathbb{R})$ representing an effective stress, one looks for the solution $\mathbf{w}_\sigma$ of:

$$\begin{cases} \mathbf{w}_\sigma \in LP, \\ -\mathrm{div}(\mathsf{Ce}(\mathbf{w}_\sigma)) = \mathbf{0} \text{ in } \mathbb{R}^n \\ \fint \mathsf{Ce}(\mathbf{w}_\sigma) = \sigma\,. \end{cases} \tag{5}$$

In this context, the average strain satisfies

$$\fint \mathsf{e}(\mathbf{w}_\sigma) = (\mathsf{C}^H)^{-1}\sigma$$

and, for an arbitrary symmetric matrix η,

$$\fint \mathsf{Ce}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\eta) = \big\langle (\mathsf{C}^H)^{-1}\sigma, \eta\big\rangle.$$

The above problem (5) is the same as problem (5) in Suquet (1982) used for deducing corrector formulae.

The cellular problem in its stress formulation (5) may be viewed as a Neumann problem due to the following:

Lemma 3 *For a rectangular cell, condition* $\fint \mathsf{Ce}(\mathbf{w}_\sigma) = \sigma$ *is equivalent to*

$$\frac{1}{|S_i^+|}\int_{S_i^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n} = \sigma\mathbf{e}_i, \quad i = 1, \ldots, n\,. \tag{6}$$

Proof On S_i^+ we have $x_i = h_i$ and the outwards normal to Y is $\mathbf{e}_i$ while on S_i^- we have $x_i = 0$ and the outwards normal to Y is $-\mathbf{e}_i$.

Then

$$\int_Y \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{e}_i = \int_Y \mathsf{Ce}(\mathbf{w}_\sigma)\nabla x_i = \int_{\partial Y} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n}x_i,$$

where the flux divergence theorem and the condition

$-\mathrm{div}(\mathsf{Ce}(\mathbf{w}_\sigma)) = \mathbf{0}$ in Y

were applied in order to deduce the last equality. The above integral on the boundary of Y writes

$$\begin{aligned}
&\int_{\partial Y} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n}x_i \\
&= \sum_{j=1}^{n}\left[\int_{S_j^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n}x_i + \int_{S_j^-} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n}x_i\right] \\
&= \int_{S_i^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n} + \sum_{i\neq j}\left[\int_{S_j^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{e}_j x_i - \int_{S_j^-} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{e}_j x_i\right] \\
&= h_i \int_{S_i^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n}\,,
\end{aligned}$$

where to obtain the last equality one uses the periodic character of $\mathsf{Ce}(\mathbf{w}_\sigma)x_i$ with respect to $h_j\mathbf{e}_j$ (for $i \neq j$). Using the hypothesis $\fint \mathsf{Ce}(\mathbf{w}_\sigma) = \sigma$ and having in mind that $|Y| = h_i|S_i^+|$ for any i, formula (6) is obtained. □

Remark 3 Condition (6) can be viewed as an averaged Neumann condition on each face of the periodicity cell Y.

Remark 4 Lemma 3 above holds also for an arbitrary parallelogram cell, although the proof is more intricate. For a cell Y generated by vectors $\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_n$, formula (6) becomes

$$\frac{1}{|S_i^+|}\int_{S_i^+} \mathsf{Ce}(\mathbf{w}_\sigma)\mathbf{n} = \sigma\mathbf{n}_i, \quad i = 1, \ldots, n\,.$$

where $\mathbf{n}_i$ is the unit normal vector to the face S_i^+.

Remark 5 The cellular problem (1) has a solution which is unique up to translations. Cellular problems (3) and (5) have solutions unique up to a rigid body displacement.

Denote by D^H the inverse of the homogenized tensor, called also homogenized compliance tensor: $\mathsf{D}^H = (\mathsf{C}^H)^{-1}$. The two formulations of the cellular problem (3) and (5) are equivalent as stated in the following:

Theorem 1 *Given a symmetric matrix $\mathsf{A} \in \mathscr{M}^n(\mathbb{R})$ the solution $\mathbf{u}_\mathsf{A}$ of problem (3) is also solution of problem (5) for $\sigma = \mathsf{C}^H\mathsf{A}$. Conversely, given a symmetric matrix $\sigma \in \mathscr{M}^n(\mathbb{R})$ the solution $\mathbf{w}_\sigma$ of problem (5) is also solution of problem (3) for $\mathsf{A} = \mathsf{D}^\mathsf{H}\sigma$.*

Proof In fact, for arbitrary $\mathbf{u} \in LP$ satisfying the state equation $-\mathrm{div}(\mathsf{Ce}(\mathbf{u})) = \mathbf{0}$, by defining $A = \fint \mathsf{e}(u)$ one obtains a cellular problem in the strain formulation (3). The same solution is obtained by defining $\sigma = \fint \mathsf{Ce}(\mathbf{u})$ and solving the cellular problem in stress formulation (5). This is similar to a Dirichlet to Neumann operator (or to a Neumann to Dirichlet operator, respectively). □

The solution of the cellular problem has the following linearity property:

Lemma 4 *The solution $\mathbf{u}_\mathsf{A}$ of problem (3) depends linearly on the matrix A, that is, given two symmetric matrices $\mathsf{A}, \mathsf{B} \in \mathscr{M}_\mathsf{n}(\mathbb{R})$ and given $\alpha, \beta \in \mathbb{R}$, one has $\mathbf{u}_{\alpha\mathsf{A}+\beta\mathsf{B}} = \alpha\mathbf{u}_\mathsf{A} + \beta\mathbf{u}_\mathsf{B}$ up to a rigid body displacement. The solution $\mathbf{w}_\sigma$ of problem (5) depends also linearly on the symmetric matrix σ.*

The proof is straightforward having in mind the linear character of problems (3) and (5), respectively.

4 Porous materials

The case of porous materials, that is, bodies having periodic infinitesimal perforations, can be treated in a similar way. We shall consider a model hole, which is a compact set $T \subset Y$ (see Fig. 2), where Y is the periodicity cell. The cellular problem describing the behaviour of this perforated material is quite similar to the one described in the previous section, except now the domain of the problem is the perforated space denoted by $\mathbb{R}^n_{\mathrm{perf}}$ and a Neumann boundary condition is imposed on the boundary of the model hole.

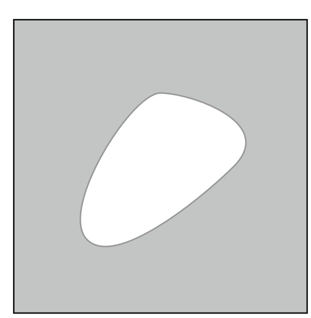

Fig. 2 Periodicity cell with model hole (zoomed)

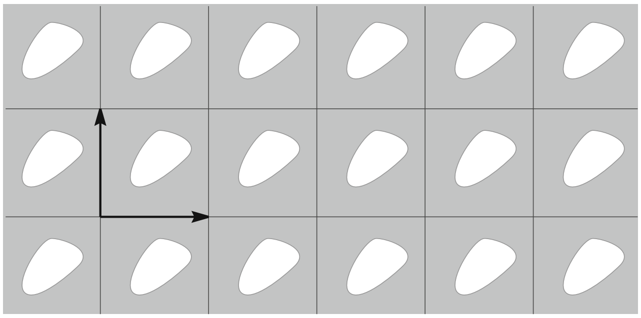

Fig. 3 Periodically perforated plane $\mathbb{R}^2_{\mathrm{perf}}$

The perforated space is obtained from $\mathbb{R}^n$ by removing translations of the model hole. For a cubic cell Y, one has (see Fig. 3)

$$\mathbb{R}^n_{\mathrm{perf}} = \mathbb{R}^n \setminus \bigcup_{\mathbf{k}\in\mathbb{Z}^n} (T + \mathbf{k}) \tag{7}$$

For an arbitrary parallelepiped Y generated by vectors $\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_n$, one has (see Fig. 4)

$$\mathbb{R}^n_{\mathrm{perf}} = \mathbb{R}^n \setminus \bigcup_{\mathbf{k}\in\mathbb{Z}^n} (T + k_1\mathbf{g}_1 + k_2\mathbf{g}_2 + \cdots + k_n\mathbf{g}_n) \tag{8}$$

Remark 6 Note that the same microstructure can be viewed as being generated by different periodicity cells. Figures 3 and 5 show a microstructure which can be built by using a square cell and a 45° parallelogram cell, respectively.

However, parallelogram cells have their own importance since there are microstructures which cannot be obtained with square periodicity cells. The microstructure shown in Fig. 4 was generated by a 60° parallelogram cell and cannot be produced with a square periodicity cell. We conjecture that the class of microstructures generated with general cells is wider than the class of microstructures generated with square cells. The examples given in Subsection 6.5 in Part II (Barbarosie and Toader 2009) illustrate this fact.

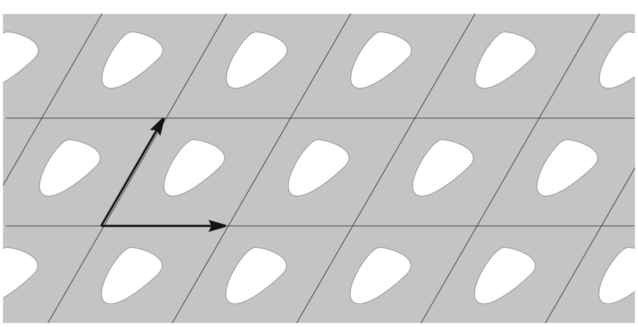

Fig. 4 Periodically perforated plane $\mathbb{R}^2_{\mathrm{perf}}$ for another cell

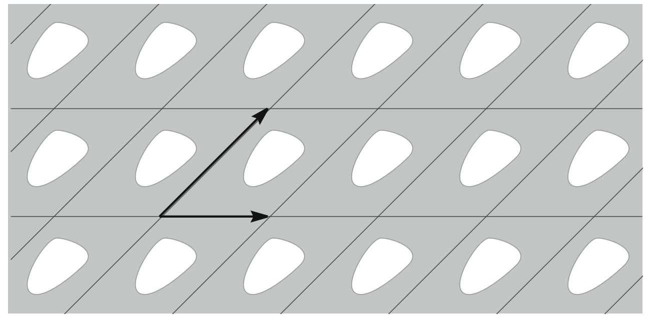

Fig. 5 The same structure as in Fig. 3 generated by a different cell

The direct generalization of the cellular problem (1) for porous materials is:

$$\begin{cases} -\mathrm{div}(\mathsf{Ce}(\mathbf{u}_\mathsf{A})) = \mathbf{0} \text{ in } \mathbb{R}^n_{\mathrm{perf}} \\ \mathsf{Ce}(\mathbf{u}_\mathsf{A})\mathbf{n} = \mathbf{0} \text{ on } \partial T \\ \mathbf{u}_\mathsf{A}(\mathbf{x}) = \mathsf{A}\mathbf{x} + \phi_\mathsf{A}(\mathbf{x}), \quad \phi_\mathsf{A} \text{ periodic function.} \end{cases} \tag{9}$$

Re-writing the above periodicity condition in terms of average strain like in (3) is more complicated in the presence of holes. The following result presents the strain formulation of the cellular problem for porous materials:

Lemma 5 *The cellular problem (9) is equivalent to*

$$\begin{cases} \mathbf{u}_\mathsf{A} \in LP_{perf} \\ -div(\mathsf{Ce}(\mathbf{u}_\mathsf{A})) = \mathbf{0} \textit{ in } \mathbb{R}^n_{perf} \\ \mathsf{Ce}(\mathbf{u}_\mathsf{A})\mathbf{n} = \mathbf{0} \textit{ on } \partial\mathsf{T} \\ \dfrac{1}{|Y|}\left(\displaystyle\int_{Y\setminus T} \mathsf{e}(\mathbf{u}_\mathsf{A}) + \int_{\partial\mathsf{T}} \mathbf{u}_\mathsf{A} \vee \mathbf{n}\right) = \mathsf{A}\,, \end{cases} \tag{10}$$

where LP_{perf} is the space of linear plus periodic *functions defined in $\mathbb{R}^n_{perf}$, $\mathbf{n}$ denotes the unit normal vector to ∂T pointing outwards $\mathbb{R}^n_{perf}$ (i.e., pointing into the hole T).*

Proof We shall justify the integral condition in (10) (the last equation), all other points being straightforward. Note that the first part of Lemma 1 in Section 2 still holds for periodic functions defined on $\mathbb{R}^n_{\mathrm{perf}}$ (while the second part makes no sense as the function is not defined in the whole Y). Thus, $\int_{\partial Y} \phi \otimes \mathbf{n} = 0$ (we shall omit the subscript A in order to simplify the notations). Then, the flux divergence theorem for ϕ implies that

$$\int_{Y\setminus T} \phi_{k,i} = \int_{\partial T} \phi_k n_i\,, \quad \forall\, i, k = 1, 2, \ldots, n,$$

where the subscript $_{,i}$ denotes the partial derivative with respect to the variable x_i. Replacing ϕ by $\mathbf{u}(x) - \mathsf{A}\mathbf{x}$ one obtains

$$\int_{Y\setminus T} (\mathbf{u}(\mathbf{x}) - \mathsf{A}\mathbf{x})_{k,i} = \int_{\partial T} (u_k(\mathbf{x}) - \mathsf{A}_{kj}x_j)n_i$$

that is,

$$\int_{Y\setminus T} u_{k,i} - \int_{\partial T} u_k n_i = \int_{Y\setminus T} \mathsf{A}_{ki} - \int_{\partial T} \mathsf{A}_{kj}x_j n_i \tag{11}$$

Since $\mathbf{n}$ is the outward normal to the domain occupied by the material, it is the opposite of the normal exterior to the hole T. Therefore,

$$-\int_{\partial T} \mathsf{A}_{kj}x_j n_i = \int_T (\mathsf{A}_{kj}x_j)_{,i} = \int_T \mathsf{A}_{ki} = |T|\mathsf{A}_{ki}$$

From (11) one obtains

$$\int_{Y\setminus T} \nabla \mathbf{u}_\mathsf{A} - \int_{\partial T} \mathbf{u}_\mathsf{A} \otimes \mathbf{n} = |Y|\mathsf{A}$$

which (having in mind that A is symmetric) is equivalent to the last condition in (10). □

Note that the average strain A can still be expressed as integrals on ∂Y, that is, formula (4) in Remark 1, Section 3, holds unchanged for porous materials. Note also that the last condition in (9), $\mathbf{u}_\mathsf{A} = \mathsf{A}\mathbf{x} + \phi_\mathsf{A}(\mathbf{x})$, which is equivalent to the integral condition in (10), can be viewed as a Dirichlet condition like in the case of mixtures (see Remark 2 in Section 3).

Similarly to the previous section, the homogenized tensor C^H can be defined through

$$\mathsf{C}^H\mathsf{A} = \frac{1}{|Y|}\int_{Y\setminus T} \mathsf{C}e(\mathbf{u}_\mathsf{A}) \tag{12}$$

or

$$\langle \mathsf{C}^H\mathsf{A}, \mathsf{B}\rangle = \frac{1}{|Y|}\int_{Y\setminus T} \langle \mathsf{C}e(\mathbf{u}_\mathsf{A}), e(\mathbf{u}_\mathsf{B})\rangle\,. \tag{13}$$

The stress formulation of the cellular problem, stated in Theorem 2 below, completes the setting.

Theorem 2 *The cellular problem (9) is equivalent to*

$$\begin{cases} \mathbf{w}_\sigma \in LP_{perf}, \\ -div(\mathsf{C}e(\mathbf{w}_\sigma)) = \mathbf{0} \text{ in } \mathbb{R}^n_{perf} \\ \mathsf{C}e(\mathbf{w}_\sigma)\mathbf{n} = \mathbf{0} \text{ on } \partial\mathrm{T} \\ \dfrac{1}{|Y|}\displaystyle\int_{Y\setminus T} \mathsf{C}e(\mathbf{w}_\sigma) = \sigma\,. \end{cases} \tag{14}$$

The proof of Theorem 2 is similar to that of Theorem 1.

An alternative expression of the last equality of (14) can be given, in the spirit of Lemma 3 and Remark 4:

Lemma 6 *Condition* $\frac{1}{|Y|}\int_{Y\setminus T} \mathsf{C}e(\mathbf{w}_\sigma) = \sigma$ *is equivalent to*

$$\frac{1}{|S_i^+|}\int_{S_i^+} \mathsf{C}e(\mathbf{w}_\sigma)\mathbf{n} = \sigma\mathbf{n}_i, \quad i = 1,\ldots,n\,.$$

The above assertion is proven by computations similar to those used in the proof of Lemma 5. An integral on ∂T appears, like in formula (11), but it vanishes due to the Neumann condition.

Remark 7 Although these equations are valid for any periodic tensor field C, we shall focus on the case where C is a constant elastic tensor (not depending on $x \in \mathbb{R}^n_{\text{perf}}$) corresponding to an isotropic material with Lamé coefficients μ and λ: $\mathsf{C}\xi = 2\mu\xi + \lambda(\text{tr}\xi)I$. Thus, the homogenized coefficients (the components of C^H) will depend essentially on the shape of the model hole T.

Remark 8 Note that, through careful interpretation, problems (9) and (14) make sense even if the model hole T exits partially the periodicity cell Y, as long as it does not touch any of its translations $T + \mathbf{k}$, $\mathbf{k} \in \mathbb{Z}^n$, $\mathbf{k} \neq \mathbf{0}$, see Fig. 6. For problem (10), the boundary integral needs to be re-defined in an appropriate manner. This is important since, in the optimization process, the model hole often crosses the boundary of Y; see Section 4 in Part II (Barbarosie and Toader 2009).

Remark 9 In Figs. 2 through 6, the model hole T was chosen to be connected. But there is no difficulty in considering a model hole with several connected components. Section 6 in Part II (Barbarosie and Toader

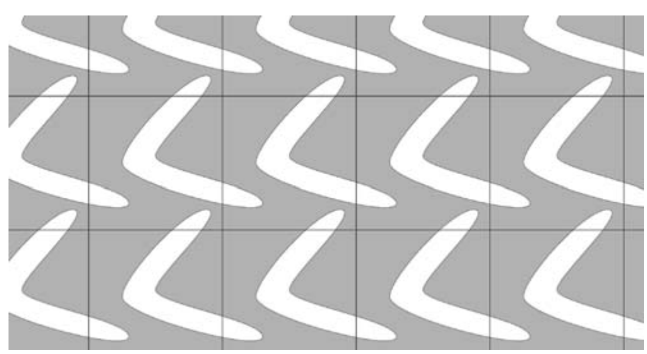

Fig. 6 General hole T not touching its translations, see Remark 8

2009) presents many examples obtained with a periodicity cell having two or three perforations.

5 The topological derivative

As stated in the Introduction, the main goal of the present work is to optimize macroscopic properties of periodic microstructures, more precisely, to minimize or maximize functionals depending on the homogenized elastic coefficients. The optimization process relies on two distinct tools: the shape derivative and the topological derivative. The present section is devoted to the latter.

The so-called bubble method (see Eschenauer et al. 1994) is the early precursor of the topological derivative, described in Garreau et al. (2001) and Sokołowski and Żochowski (2001). The idea is to evaluate whether it is convenient or not to introduce a new hole at a certain location in the domain. In the bubble method, an ad-hoc criterion is used for choosing the location of the new hole: the minimum points of the energy density are chosen. In Garreau et al. (2001) and Sokołowski and Żochowski (2001) a rigorous approach is proposed: the optimality of such a topology variation is tested by drilling an infinitesimal circular hole and imposing zero Neumann condition on the newly created boundary. In the framework of structural optimization, consider the compliance

$$J(\Omega) = \int_{\Omega} \mathsf{E}e(\mathbf{u})\mathsf{E}(\mathbf{u})d\mathbf{x} \tag{15}$$

of a body occupying a domain $\Omega \subset \mathbb{R}^n$ and made of a linear isotropic elastic material with Hooke's law (ξ being an arbitrary symmetric matrix):

$$\mathsf{E}\xi = 2\mu\xi + \lambda(\mathrm{tr}\xi)I\,.$$

The displacement field $\mathbf{u}$ is the solution of the linearized elasticity system

$$\begin{cases} -\mathrm{div}(\mathsf{E}e(\mathbf{u})) = \mathbf{0} & \text{in } \Omega \\ \mathbf{u} = \mathbf{0} & \text{on } \Gamma_D \\ (\mathsf{E}e(\mathbf{u}))\mathbf{n} = \mathbf{g} & \text{on } \Gamma_N \end{cases}$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$ (if $\Gamma_D = \emptyset$, equilibrium conditions should be imposed on g).

Consider that, at a point $\mathbf{x}_0 \in \Omega$, a hole $\omega_\rho = \mathbf{x}_0 + \rho\omega$ is inserted, where $\rho \geq 0$ is a small parameter and $\omega \subset \mathbb{R}^n$ is a model hole, typically the unit ball. Consider the elliptic problem in the perforated domain $\Omega_\rho = \Omega \setminus \omega_\rho$:

$$\begin{cases} -\mathrm{div}(\mathsf{E}e(\mathbf{u}_\rho)) = \mathbf{0} & \text{in } \Omega_\rho \\ \mathbf{u}_\rho = \mathbf{0} & \text{on } \Gamma_D \\ (\mathsf{E}e(\mathbf{u}_\rho))\mathbf{n} = \mathbf{g} & \text{on } \Gamma_N \\ (\mathsf{E}e(\mathbf{u}_\rho))\mathbf{n} = \mathbf{0} & \text{on } \partial\omega_\rho \end{cases}$$

Note that we put Neumann boundary conditions on $\partial\omega_\rho$.

Then, the asymptotic expansion of a general objective function writes as

$$J(\Omega_\rho) = J(\Omega) + \rho^n D_T J(x_0) + o(\rho^n)$$

where $J(\omega_\rho)$ is computed with the elastic displacement $\mathbf{u}_\rho$.

The following result gives the expressions of the topological derivative for the compliance, when a spherical hole is nucleated at an arbitrary point $\mathbf{x} \in \Omega$.

Theorem 3 *Suppose that* $\mathbf{g} \in H^2(\Omega)^N$ *and* $\mathbf{u} \in H^2(\Omega)^N$. *Then, for any* $\mathbf{x} \in \Omega$, *the topological derivative of the compliance* (15) *is, for* $n = 2$,

$$D_T J(\mathbf{x}) = \frac{\pi(\lambda + 2\mu)}{2\mu(\lambda + \mu)}\big\{4\mu\mathsf{E}e(\mathbf{u}) \cdot e(\mathbf{u}) + (\lambda - \mu)tr(\mathsf{E}e(\mathbf{u}))tr(e(\mathbf{u}))\big\}(x) \tag{16}$$

and for $n = 3$

$$D_T J(\mathbf{x}) = \frac{\pi(\lambda+2\mu)}{\mu(9\lambda+14\mu)}\big\{20\mu\mathsf{E}e(\mathbf{u}) \cdot e(\mathbf{u}) + (3\lambda-2\mu)tr(\mathsf{E}e(\mathbf{u}))tr(e(\mathbf{u}))\big\}(x) \tag{17}$$

See Garreau et al. (2001) for the proof of the above result.

Remark 10 The topological derivative has positive values, which means that for compliance minimization there is no interest in nucleating holes if there is no volume constraint.

In the periodic context under consideration, one evaluates whether it is convenient or not to introduce a new hole at a certain location in the periodicity cell. Note that the cellular problem is an elliptic partial differential system of equations defined on the periodicity cell Y with unusual boundary conditions (periodicity conditions) or, to be more rigorous, defined on the torus. This problem is perturbed by introducing only one infinitesimal hole at some location in the cell, which is equivalent to introducing one infinitesimal hole at some location in the torus. This should not be viewed as a large number of infinitesimal holes appearing simultaneously in the macroscopic domain since the microstructure has already been homogenized (the usual small parameter ε has already converged to 0).

A direct application of formulae (16) and (17) in the periodic context is wrong when the strain formulation (3) is employed, since this formulation involves non-homogeneous Dirichlet conditions (see Remark 2). Incidentally, the correct formula has opposite sign as we shall prove in the rest of this Section, see Theorem 4.

On the other hand, the cellular problem in stress formulation (5) can be viewed as a Neumann problem due to Lemma 3. Therefore, the formulae in Theorem 3 may be used for computing the topological derivative of the functional

$$\langle \mathsf{D}^H \sigma, \sigma\rangle = \fint \mathsf{C}\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\sigma) \tag{18}$$

which is a compliance-like quantity similar to (15). If σ belongs to a basis of symmetric matrices, the expression $\langle \mathsf{D}^H\sigma, \sigma\rangle$ represents a diagonal coefficient of the homogenized compliance tensor D^H.

Lemma 7 *The topological derivative of functional (18) has the form, for $n = 2$:*

$$D_T\langle \mathsf{D}^H\sigma, \sigma\rangle(x) = \frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\left[4\mu\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\sigma) + \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\right](x) \tag{19}$$

and for $n = 3$:

$$D_T\langle \mathsf{D}^H\sigma, \sigma\rangle(x) = \frac{\pi}{|Y|}\frac{\lambda+2\mu}{9\lambda+14\mu}\left[40\mu\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\sigma) + \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\right](x), \tag{20}$$

where $\mathbf{w}_\sigma$ is solution of (5).

Proof Formulae (19) and (20) are direct consequences of formulae (16) and (17), respectively, and of Hooke's law $\mathsf{C}\xi = 2\mu\xi + \lambda(\mathrm{tr}\xi)I$ for isotropic elastic material with Lamé coefficients μ and λ. □

The other coefficients of the tensor D^H can be recovered by choosing two different elements of the basis of symmetric matrices:

Lemma 8 *Given σ and η two symmetric matrices in $\mathscr{M}_n(\mathbb{R})$, the topological derivative of the functional*

$$\langle \mathsf{D}^H\sigma, \eta\rangle = \fint \mathsf{C}\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\eta) \tag{21}$$

is given, for $n = 2$, by

$$D_T\langle \mathsf{D}^H\sigma, \eta\rangle(x) = \frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\left[4\mu\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\eta) + \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\, tr\,\mathsf{e}(\mathbf{w}_\eta)\right](x), \tag{22}$$

where $\mathbf{w}_\sigma$ and $\mathbf{w}_\eta$ are solution of cellular problems (5) with effective stress σ and η, respectively. For $n = 3$, the topological derivative of (21) is given by

$$D_T\langle \mathsf{D}^H\sigma, \eta\rangle(x) = \frac{\pi}{|Y|}\frac{9\lambda+14\mu}{\lambda+\mu}\left[40\mu\mathsf{e}(\mathbf{w}_\sigma)\mathsf{e}(\mathbf{w}_\eta) + \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\, tr\,\mathsf{e}(\mathbf{w}_\sigma)\, tr\,\mathsf{e}(\mathbf{w}_\eta)\right](x), \tag{23}$$

Proof It suffices to write

$$\langle \mathsf{D}^H\sigma, \eta\rangle = \frac{1}{4}\left[\langle \mathsf{D}^H(\sigma+\eta), \sigma+\eta\rangle - \langle \mathsf{D}^H(\sigma-\eta), \sigma-\eta\rangle\right]$$

and to apply Lemma 7 together with Lemma 4. □

Theorem 4 *The topological derivative of each coefficient of the homogenized tensor C^H, for $n = 2$, has the form:*

$$D_T\langle \mathsf{C}^H\mathsf{f}_i, \mathsf{f}_j\rangle(x) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\left[4\mu\mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\mathsf{e}(\mathbf{u}_{\mathsf{f}_j}) + \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\, tr\,\mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\, tr\,\mathsf{e}(\mathbf{u}_{\mathsf{f}_j})\right](x), \tag{24}$$

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

$$\mathsf{f}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \ \mathsf{f}_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \ \mathsf{f}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and $\mathbf{u}_{\mathsf{f}_i}$ *are the corresponding solutions of the cellular problem* (3) *with the effective strain* f_i*. In three dimensions, the topological derivative of the coefficients of* C^H *has the form*

$$D_T\langle \mathsf{C}^H \mathsf{f}_i, \mathsf{f}_j\rangle(x) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{9\lambda+14\mu}\Bigg[40\mu \mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\mathsf{e}(\mathbf{u}_{\mathsf{f}_j}) + \frac{9\lambda^2+20\lambda\mu-4\mu^2}{\mu}\, tr\, \mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\, tr\, \mathsf{e}(\mathbf{u}_{\mathsf{f}_j})\Bigg](x), \tag{25}$$

where

$$\mathsf{f}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \ \mathsf{f}_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \ \mathsf{f}_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathsf{f}_4 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \mathsf{f}_5 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathsf{f}_6 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

Proof We shall use Einstein's convention of repeated indices. Denote $\mathsf{C}^H_{ij} = \langle \mathsf{C}^H \mathsf{f}_i, \mathsf{f}_j\rangle$ and $\mathsf{D}^H_{ij} = \langle \mathsf{D}^H \mathsf{f}_i, \mathsf{f}_j\rangle$. Since $\mathsf{D}^H = (\mathsf{C}^H)^{-1}$, one has

$$\mathsf{C}^H_{ij}\mathsf{D}^H_{jk} = \delta_{ik}\,. \tag{26}$$

By applying the topological derivative to (26), one obtains

$$D_T\mathsf{C}^H_{ij}\,\mathsf{D}^H_{jk} + \mathsf{C}^H_{ij}\,D_T\mathsf{D}^H_{jk} = 0\,,\ i,k = 1,2,3$$

and therefore

$$D_T\mathsf{C}^H_{il} = -\mathsf{C}^H_{ij}\,D_T\mathsf{D}^H_{jk}\,\mathsf{C}^H_{kl}\,,\ i,l = 1,2,3\,. \tag{27}$$

From Lemma 8 for $\sigma = \mathsf{f}_j$ and $\eta = \mathsf{f}_k$ it turns out that

$$D_T\mathsf{D}^H_{jk}(x) = \frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\Bigg[4\mu \mathsf{e}(\mathbf{w}_{\mathsf{f}_j})\mathsf{e}(\mathbf{w}_{\mathsf{f}_k}) + \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\,\mathrm{tr}\,\mathsf{e}(\mathbf{w}_{\mathsf{f}_j})\,\mathrm{tr}\,\mathsf{e}(\mathbf{w}_{\mathsf{f}_k})\Bigg](x), \tag{28}$$

where $\mathbf{w}_{\mathsf{f}_j}$ and $\mathbf{w}_{\mathsf{f}_k}$ are solutions of the cellular problem (5) with the effective stress f_j and f_k, respectively. From Theorem 1 one concludes that $\mathbf{w}_\sigma = \mathbf{u}_{\mathsf{D}^H\sigma}$ (up to a rigid body displacement) for any symmetric matrix σ. In particular, $\mathbf{w}_{\mathsf{f}_j} = \mathbf{u}_{\mathsf{D}^H\mathsf{f}_j} = \mathbf{u}_{\mathsf{D}^H_{ji}\mathsf{f}_i} = \mathsf{D}^H_{ji}\mathbf{u}_{\mathsf{f}_i}$, where the last equality is a consequence of Lemma 4. Hence, replacing $\mathbf{w}_{\mathsf{f}_j}$ and $\mathbf{w}_{\mathsf{f}_k}$ by $\mathsf{D}^H_{ji}\mathbf{u}_{\mathsf{f}_i}$ and $\mathsf{D}^H_{kl}\mathbf{u}_{\mathsf{f}_l}$ in (28), one obtains:

$$D_T\mathsf{D}^H_{jk}(x) = \frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\Bigg[4\mu \mathsf{D}^H_{ji}\mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\mathsf{D}^H_{kl}\mathsf{e}(\mathbf{u}_{\mathsf{f}_l}) + \frac{\lambda^2+2\lambda\mu-\mu^2}{\mu}\,\mathsf{D}^H_{ji}\mathrm{tr}\,\mathsf{e}(\mathbf{u}_{\mathsf{f}_i})\,\mathsf{D}^H_{kl}\mathrm{tr}\,\mathsf{e}(\mathbf{u}_{\mathsf{f}_l})\Bigg](x), \tag{29}$$

Combining formulae (27) and (29) and having in mind that $\mathsf{D}^H = (\mathsf{C}^H)^{-1}$, one obtains the expression of the topological derivative (24). The proof of (25) is similar. □

Remark 11 Although the homogenized elastic coefficients $\mathsf{C}^H_{ij} = \langle \mathsf{C}^H \mathsf{f}_i, \mathsf{f}_j\rangle$ can be expressed as energy-like quantities, see formula (13), their topological derivative are different from the derivative of the compliance for bounded domains, given in Theorem 3. In fact, one obtains an opposite sign. This happens because of the boundary conditions. In Theorem 3, one has zero Dirichlet boundary conditions on a part of $\partial\Omega$ and non-zero Neumann conditions on the rest of $\partial\Omega$. In the cellular problem, the periodicity conditions have the same nature as a non-zero Dirichlet boundary condition (see Remark 2).

In applications, for penalization of the volume, the topological derivative of the volume percentage of material

$$V = \frac{|Y \setminus T|}{|Y|} = 1 - \frac{|T|}{|Y|}$$

is needed. This is straightforward to compute, and the result is

$$D_T V = -\frac{|B(0,1)|}{|Y|}\,, \tag{30}$$

where $|B(0,1)|$ is the volume of the unit ball in $\mathbb{R}^n$. In two dimensions, $D_T V = -\pi/|Y|$, while in three dimensions $D_T V = -\frac{4\pi}{3|Y|}$.

6 The shape derivative

Besides creating new holes, one should find the best shape of existing holes. The shape derivative describes the variation of a certain objective functional when an infinitesimal deformation is applied to a given geometry. Consider $\theta : \mathbb{R}^n \to \mathbb{R}^n$ a vector field defining the deformation; note that θ itself should be periodic in order to preserve the periodic character of the microstructure under study. Then the variation induced by this deformation in the quantity $\langle \mathsf{C}^H \mathsf{A}, \mathsf{B}\rangle$ is

$$D_S\langle \mathsf{C}^H \mathsf{A}, \mathsf{B}\rangle = \frac{1}{|Y|}\int_{\partial T} \langle \mathsf{C}\mathsf{e}(\mathbf{u}_\mathsf{A}), \mathsf{e}(\mathbf{u}_\mathsf{B})\rangle\, \theta\cdot\mathbf{n} \tag{31}$$

where $\mathbf{n}$ is the unit normal to the boundary of the hole T and pointing inside T. Assuming that C is a linear isotropic elastic tensor, $\mathsf{C}\xi = 2\mu\xi + \lambda(\mathrm{tr}\xi)I$, the above formula becomes

$$D_S\langle \mathsf{C}^H \mathsf{A}, \mathsf{B}\rangle = \frac{1}{|Y|}\int_{\partial T} \big[2\mu\langle \mathsf{e}(\mathbf{u}_\mathsf{A}), \mathsf{e}(\mathbf{u}_\mathsf{B})\rangle + \lambda \mathrm{tr}(\mathsf{e}(\mathbf{u}_\mathsf{A}))\mathrm{tr}(\mathsf{e}(\mathbf{u}_\mathsf{B}))\big]\,\theta\cdot\mathbf{n} \tag{32}$$

In particular, this gives the shape derivative of the homogenized coefficients:

Theorem 5 *The shape derivative of each coefficient of the homogenized tensor* C^H *has the form:*

$$D_S\langle \mathsf{C}^H \mathsf{f}_i, \mathsf{f}_j\rangle = \frac{1}{|Y|}\int_{\partial T} \big[2\mu\langle \mathsf{e}(\mathbf{u}_{\mathsf{f}_i}), \mathsf{e}(\mathbf{u}_{\mathsf{f}_j})\rangle + \lambda\, tr(\mathsf{e}(\mathbf{u}_{\mathsf{f}_i}))tr(\mathsf{e}(\mathbf{u}_{\mathsf{f}_j}))\big]\,\theta\cdot\mathbf{n} \tag{33}$$

Formula (32) has been obtained by direct computation in Barbarosie (2003). Note that, for mixtures of two or more materials, an analogous formula holds with an integrand involving jumps of the derivatives of $\mathbf{u}_\mathsf{A}$ and $\mathbf{u}_\mathsf{B}$ across the interface, see Barbarosie (2002).

Formula (32) can alternatively be obtained by applying Theorem 6 below to the stress formulation of the cellular problem (14). Thus, one differentiates quantities of the form $\langle \mathsf{D}^H\sigma, \eta\rangle$ involving the inverse elastic tensor D^H and then goes back to the components of the tensor C^H. We do not present these computations here; a similar development has been presented in detail in the previous section for the topological derivative.

We state here the main result in classical shape optimization, for which we refer to Murat and Simon (1976), Sokołowski and Zolezio (1992), Allaire et al. (2004).

Theorem 6 *For Ω a smooth bounded open set in $\mathbb{R}^n$, consider a partition of its boundary $\partial\Omega = \Gamma_D \cup \Gamma_{opt} \cup \Gamma_N$, where Γ_{opt} represents the part of the boundary to be optimized. Let* $\mathbf{u}$ *be the solution of*

$$\begin{cases} -div(\mathsf{E}\mathsf{e}(\mathbf{u})) = \mathbf{0} & in \quad \Omega \\ \mathbf{u} = \mathbf{0} & on \quad \Gamma_D \\ (\mathsf{E}\mathsf{e}(\mathbf{u}))\mathbf{n} = \mathbf{0} & on \quad \Gamma_{opt} \\ (\mathsf{E}\mathsf{e}(\mathbf{u}))\mathbf{n} = \mathbf{g} & on \quad \Gamma_N \end{cases}$$

Then the shape derivative of

$$J(\Omega) = \int_\Omega \langle \mathsf{E}\mathsf{e}(\mathbf{u}), \mathsf{e}(\mathbf{u})\rangle = \int_{\Gamma_N}\langle \mathbf{g}, \mathbf{u}\rangle$$

is

$$J'(\Omega)(\theta) = -2\int_{\Gamma_{opt}} \langle \mathsf{E}\mathsf{e}(\mathbf{u}), \mathsf{e}(\mathbf{u})\rangle\langle\theta, \mathbf{n}\rangle\,,$$

where $\theta : \mathbb{R}^n \to \mathbb{R}^n$ is a vector field defining an (infinitesimal) deformation of the domain Ω such that $\theta = \mathbf{0}$ on $\Gamma_D \cup \Gamma_N$.

The shape derivative of the volume percentage of material $V = |Y \setminus T|/|Y|$ is needed in applications for penalization purposes. Straightforward computations show that

$$D_S V = \frac{1}{|Y|}\int_{\partial T} \theta\cdot\mathbf{n}\,. \tag{34}$$

7 Examples

In Sections 5 and 6 above, the shape derivative and the topological derivative have been computed for the coefficients of the homogenized elastic tensor C^H. These derivatives are to be used in an optimization process whose goal is to optimize properties of the homogenized material, under a constraint on the volume percentage of material. Typical examples include: maximization of the bulk modulus, maximization of the shear response, search for negative Poisson coefficient. See Section 6 of Part II (Barbarosie and Toader 2009) for numerical results.

For maximization of the bulk modulus of C^H, one chooses the matrix

$$\mathsf{A} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

which is a pure compression strain, and maximizes

$$\langle \mathsf{C}^H \mathsf{A}, \mathsf{A}\rangle = \mathsf{C}^H_{1111} + 2\mathsf{C}^H_{1122} + \mathsf{C}^H_{2222}$$

This case is treated in Subsection 6.2 of Part II (Barbarosie and Toader 2009).

For maximization of the shear response of C^H, one chooses the matrix

$$\mathsf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

which is a pure shear strain, and maximizes

$$\langle \mathsf{C}^H \mathsf{A}, \mathsf{A} \rangle = 4\mathsf{C}^H_{1212}$$

Numerical results for this example are presented in Subsection 6.5 of Part II (Barbarosie and Toader 2009).

Searching for a homogenized tensor C^H having a negative Poisson coefficient is more delicate. Recall that, for an anisotropic elastic tensor C^H, the behaviour of the mixture is characterized through two Poisson-like coefficients defined by:

$$-\frac{\mathsf{D}^H_{2211}}{\mathsf{D}^H_{1111}} \quad \text{or} \quad -\frac{\mathsf{D}^H_{2211}}{\mathsf{D}^H_{2222}}$$

where D^H is the inverse tensor of C^H However, in order to avoid computing the derivative of the above fraction, we have chosen a different approach: take two different strains

$$\mathsf{A} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathsf{B} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

and minimize

$$\langle \mathsf{C}^H \mathsf{A}, \mathsf{B} \rangle = \mathsf{C}^H_{1122}$$

This is of course not equivalent to minimizing the Poisson coefficient itself, but it goes in the right direction, as mechanical intuition suggests and numerical experiences confirm, see Subsection 6.6 of Part II (Barbarosie and Toader 2009).

8 Conclusions

Periodic composites, as well as periodic porous materials, are described in terms of a cellular problem. Different formulations of the cellular problem are given, namely a formulation in strain and one in stress. The topological derivative and the shape derivative of the homogenized elastic coefficients are computed.

A second paper (Barbarosie and Toader 2009) deals with the implementation of an optimization algorithm which applies alternately shape and topology optimization.

Acknowledgements This work was partially supported by Fundação para a Ciência e a Tecnologia, Financiamento Base 2008 - ISFL/1/209 and by the project "Análise Assimptótica aplicada à Mecânica dos Meios Contínuos", PPCDT/MAT/60587/2004.

References

Allaire G (1992) Homogenization and two-scale convergence. SIAM J Math Anal 23(6):1482–1518

Allaire G, Jouve F, Toader A-M (2004) Structural optimization using sensitivity analysis and a level set method. J Comput Phys 194:363–393

Barbarosie C (2002) Optimização de forma aplicada a materiais compósitos. In: Goicolea JM, Mota Soares C, Pastor M, Bugeda G (eds) Métodos Numéricos en Ingenieria V, SEMNI, Sociedad Española de Métodos Numéricos en Ingenieria, p 369

Barbarosie C (2003) Shape optimization of periodic structures. Comput Mech 30:235–246

Barbarosie C, Toader A-M (2009) Shape and topology optimization for periodic problems, part II, optimization algorithm and numerical examples. Struct Multidiscipl Optim. doi:10.1007/s00158-009-0377-1

Eschenauer H, Kobelev V, Schumacher A (1994) Bubble method for topology and shape optimization of structures. Struct Optim 8:42–51

Garreau S, Guillaume P, Masmoudi M (2001) The topological asymptotic for PDE systems: the elasticity case. SIAM J Control Optim 39:1756–1778

Murat F, Simon J (1976) Etudes de problèmes d'optimal design. Lecture notes in computer science, vol 41. Springer, Berlin, pp 54–62

Sokołowski J, Żochowski A (2001) Topological derivatives of shape functionals for elasticity systems. Mech Struct Mach 29:331–349

Sokołowski A, Zolezio JP (1992) Introduction to shape optimization: shape sensitivity analysis. Springer series in computational mathematics, vol 10. Springer, Berlin

Suquet PM (1982) Une méthode duale en homogénéisation: application aux milieux élastiques. J Méc Théor Appl 79–98 (Numéro spécial)

Toader A-M (2008) Optimization of periodic microstructures using shape and topology derivatives. Communication at WCCM8, ECCOMAS 2008, Venice, July 2008