Topological derivatives of leading-and second-order homogenized coefficients in bi-periodic media

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Abstract We derive the topological derivatives of the homogenized coefficients associated to a periodic material, with respect of the small size of a penetrable inhomogeneity introduced in the unit cell that defines such material. In the context of antiplane elasticity, this work extends existing results to (i) time-harmonic wave equation and (ii) second-order homogenized coefficients, whose contribution reflects the dispersive behavior of the material.

Keywords: homogenization, topological derivatives.

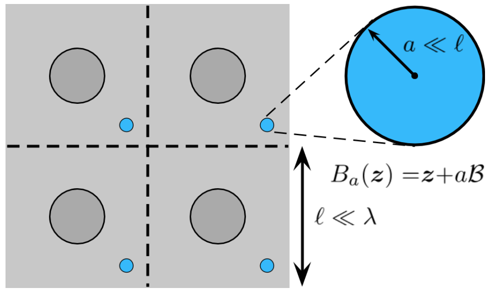

Figure 1: Perturbed periodic material

Introduction Consider an elastic material occupying a 2D domain and characterized by periodic shear modulus μ and density ρ. The unit cell Y has characteristic length ℓ. Under time-harmonic conditions, the antiplane displacement u satisfies the wave equation:

$$\boldsymbol{\nabla} \cdot (\mu \boldsymbol{\nabla} u) + \omega^2 \rho u = 0$$

For long-wavelength configurations (i.e. $\ell \ll \lambda$), two-scale periodic homogenization of this equation in terms of $\varepsilon = \ell/\lambda$ [4] leads to the equation satisfied by the mean field U:

$$\begin{aligned} &\boldsymbol{\mu}^0 : \boldsymbol{\nabla}^2 U + \omega^2 \rho^0 U \\ &\quad = -\varepsilon^2 \left[\boldsymbol{\mu}^2 :: \boldsymbol{\nabla}^4 U + \omega^2 \boldsymbol{\rho}^2 : \boldsymbol{\nabla}^2 U \right] + O(\varepsilon^4), \end{aligned}$$

where the leading-order and second-order homogenized coefficients $(\boldsymbol{\mu}^0, \rho^0, \boldsymbol{\mu}^2, \boldsymbol{\rho}^2)$ are constant tensors and $\boldsymbol{\nabla}^k U$ stands for the k-th gradient of U.

This study considers a periodic perturbation of this material, whereby a penetrable inhomogeneity B_a, of size a and shape $\mathcal{B}$, characterized by contrasts $(\Delta\mu, \Delta\rho)$ is introduced at point $\boldsymbol{z} \in Y$ (Fig. 1). Then, the leading-order expansion coefficients of $(\boldsymbol{\mu}^0, \rho^0, \boldsymbol{\mu}^2, \boldsymbol{\rho}^2)$ w.r.t. a, namely their topological derivatives, are computed, as in [3] for in-plane elastostatics.

Leading-order coefficients Let $\langle \cdot \rangle = \frac{1}{|Y|} \int_Y \cdot$ denote an average on the unit cell. The homogenized density ρ^0 is defined by $\rho^0 = \langle \rho \rangle$, so that the perturbed coefficient ρ^0_a and the topological derivative $\mathcal{D}\rho^0$ are exactly given by:

$$\rho^0_a = \rho^0 + a^2 |Y|^{-1} \mathcal{D}\rho^0; \qquad \mathcal{D}\rho^0 = |\mathcal{B}| \Delta\rho.$$

The homogenized shear modulus $\boldsymbol{\mu}^0$ is defined by $\boldsymbol{\mu}^0 = \langle \mu (\boldsymbol{I} + \boldsymbol{\nabla P}) \rangle^{\mathrm{S}}$, where $\boldsymbol{I}$ is the identity tensor, the first *cell function* $\boldsymbol{P}$ [4] is the Y-periodic and zero-mean vector-valued solution of:

$$\boldsymbol{\nabla} \cdot (\mu (\boldsymbol{I} + \boldsymbol{\nabla P})) = \boldsymbol{0} \tag{1}$$

and the superscript $\cdot^{\mathrm{S}}$ means symmetrization w.r.t. all index permutations. Consequently, $\boldsymbol{\mu}^0_a$ is computed as:

$$\boldsymbol{\mu}^0_a = \boldsymbol{\mu}^0 + \langle \mu \boldsymbol{\nabla p}_a \rangle^{\mathrm{S}} + \langle \chi_{B_a} \Delta\mu (\boldsymbol{I} + \boldsymbol{\nabla P}_a) \rangle^{\mathrm{S}}$$

where $\boldsymbol{p}_a := \boldsymbol{P}_a - \boldsymbol{P}$ is the perturbation of $\boldsymbol{P}$. The analysis of this perturbation is done by reformulating problem (1) and its perturbed counterpart using domain integral equations [2]. With the help of the adjoint state method, it leads to the following leading-order expansion:

$$\boldsymbol{\mu}^0_a = \boldsymbol{\mu}^0 + a^2 |Y|^{-1} \mathcal{D}\boldsymbol{\mu}^0(\boldsymbol{z}) + o(a^2 |Y|^{-1}), \tag{2}$$

with the topological derivative $\mathcal{D}\boldsymbol{\mu}^0$ given by:

$$\mathcal{D}\boldsymbol{\mu}^0(\boldsymbol{z}) = \left[(\boldsymbol{I} + \boldsymbol{\nabla P}) \cdot \boldsymbol{A} \cdot (\boldsymbol{I} + \boldsymbol{\nabla P})^{\mathrm{T}} \right] (\boldsymbol{z})$$

and $\boldsymbol{A}(\boldsymbol{z}) = \boldsymbol{A}(\mathcal{B}, \mu(\boldsymbol{z}), \Delta\mu)$ is the polarization tensor [1] associated to shape $\mathcal{B}$ and moduli $\mu(\boldsymbol{z})$ and $\mu(\boldsymbol{z}) + \Delta\mu$. Under notational adjustments, this result is similar to [3]. For homogeneous background materials, in which case $\boldsymbol{P} = \boldsymbol{0}$, it reduces to $\mathcal{D}\boldsymbol{\mu}^0 = \boldsymbol{A}$ as shown by [1].

Second-order coefficients The second-order homogenized density is defined by $\boldsymbol{\rho}^2 = \langle \rho \boldsymbol{Q} \rangle^{\mathrm{S}}$, where the *second cell function* $\boldsymbol{Q}$ is the Y-periodic, zero-mean, tensor-valued solution of:

$$\begin{aligned}\boldsymbol{\nabla}\cdot(\mu(\boldsymbol{P}\otimes\boldsymbol{I}+\boldsymbol{\nabla}\boldsymbol{Q})) \\ = -\mu(\boldsymbol{I}+\boldsymbol{\nabla}\boldsymbol{P}) + (\rho/\rho^0)\boldsymbol{\mu}^0 \quad (3)\end{aligned}$$

Relying on the same integral equation framework, and with careful analysis of the influence of the source terms involving $\boldsymbol{P}_a$ when adressing the perturbed cell function $\boldsymbol{Q}_a$, we show that $\boldsymbol{\rho}_a^2$ has an expansion of the same form as (2), with its topological derivative $\mathcal{D}\boldsymbol{\rho}^2$ given by:

$$\begin{aligned}\mathcal{D}\boldsymbol{\rho}^2(\boldsymbol{z}) = \Big[&(\boldsymbol{I}+\boldsymbol{\nabla}\boldsymbol{P})\cdot\boldsymbol{A}\cdot\Big(\beta\boldsymbol{I}+\boldsymbol{\nabla}\hat{\boldsymbol{X}}[\beta]\Big)^{\mathrm{T}} \\ &- (\boldsymbol{P}\otimes\boldsymbol{I}+\boldsymbol{\nabla}\boldsymbol{Q})\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla}\beta \\ &- \big(\mathcal{D}\boldsymbol{\mu}^0 - (\mathcal{D}\rho^0/\rho^0)\boldsymbol{\mu}^0\big)\,\langle\rho(\beta/\rho^0)\rangle \\ &- \mathcal{D}\rho^0\,\big((\beta/\rho^0)\boldsymbol{\mu}^0 - \boldsymbol{Q}\big)\Big]^{\mathrm{S}}(\boldsymbol{z}). \quad (4)\end{aligned}$$

The above expression features (i) various combinations of the previously computed cell solutions and topological derivatives and (ii) two new *adjoint fields* β and $\hat{\boldsymbol{X}}[\beta]$ defined as the (Y-periodic, zero-mean) solutions of:

$$\begin{aligned}&\boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\beta) = -(\rho-\rho^0) \\ \text{and}\quad &\boldsymbol{\nabla}\cdot(\mu(\beta\boldsymbol{I}+\boldsymbol{\nabla}\hat{\boldsymbol{X}}[\beta])) = -\mu\boldsymbol{\nabla}\beta.\end{aligned}$$

In particular, all the fields involved in (4) solve problems posed on the *unperturbed* cell.

The second-order homogenized shear modulus is defined by $\boldsymbol{\mu}^2 = \langle \mu(\boldsymbol{Q}\otimes\boldsymbol{I}+\boldsymbol{\nabla}\boldsymbol{R})\rangle^{\mathrm{S}}$ in terms of $\boldsymbol{Q}$ and a third cell function $\boldsymbol{R}$. Once again, an analysis of the problems satisfied by $\boldsymbol{R}$ and $\boldsymbol{R}_a$ is conducted. As a result, $\boldsymbol{\mu}_a^2$ is found to have an expansion similar to (2), and its topological derivative $\mathcal{D}\boldsymbol{\mu}^2$ (not shown here for brevity) is expressed in terms of the cell solutions $(\boldsymbol{P},\boldsymbol{Q},\boldsymbol{R})$ and the previously determined topological derivatives $(\mathcal{D}\rho^0,\mathcal{D}\boldsymbol{\mu}^0,\mathcal{D}\boldsymbol{\rho}^2)$.

Perspectives. The obtained expansions of the homogenized coefficients are useful on their own right, e.g. for computing quickly an approximation of the properties of a perturbed periodic material for several trial inhomogeneity locations $\boldsymbol{z}$ without solving the new cell problems. As an example, an approximation of $\boldsymbol{\mu}_a^0$ is obtained by neglecting the remainder in (2), as illustrated on Fig. 2 for a chessboard-like cell.

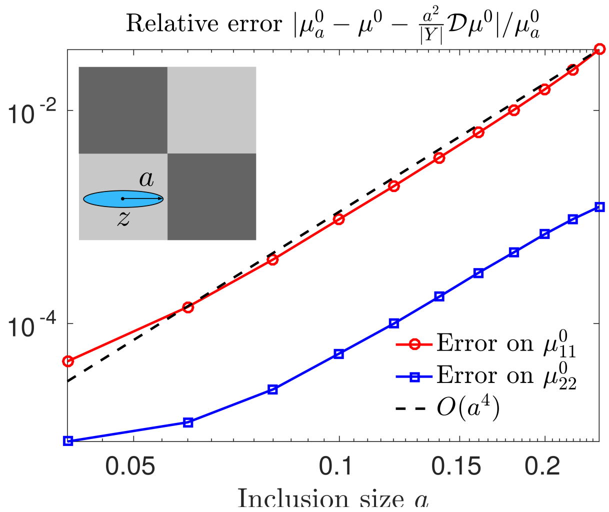

Figure 2: Relative error on shear modulus $\boldsymbol{\mu}_a^0$ approximated by expansion (2) for an ellipsoidal inhomogeneity of semi-axes $(a, 0.2a)$ placed at $\boldsymbol{z} = (0.25, 0.25)$ in a chessboard-like cell $Y = [0,1]^2$. In this case, since the medium is locally homogeneous around $\boldsymbol{z}$, the remainder can be shown to be in $O(a^4)$ as observed.

However, as already intended in [3], the main usefulness of such expansions occurs for optimizing a periodic structure towards some desirable property. Since they address the time-harmonic case and the second-order homogenized coefficients, our results should notably allow to tune the dispersive properties of the homogenized material, in particular the so-called *band-gaps* (forbidden frequencies for which no wave propagates through the structure).

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