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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.

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:

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

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 :

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

where the leading-order and second-order homogenized coefficients $(\mu^0, \rho^0, \mu^2, \rho^2)$ are constant tensors and $\nabla^k U$ 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 $z \in Y$ (Fig. 1). Then, the leading-order expansion coefficients of $(\mu^0, \rho^0, \mu^2, \rho^2)$ 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

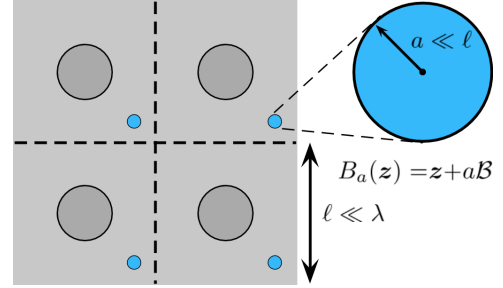


Figure 1: Perturbed periodic material

the perturbed coefficient ρ_a^0 and the topological derivative $\mathcal{D}\rho^0$ are exactly given by:

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

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

$$\nabla \cdot (\mu(\mathbf{I} + \nabla \mathbf{P})) = \mathbf{0} \quad (1)$$

and the superscript \cdot^S means symmetrization w.r.t. all index permutations. Consequently, μ_a^0 is computed as:

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

where $\mathbf{p}_a := \mathbf{P}_a - \mathbf{P}$ is the perturbation of \mathbf{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:

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

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

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

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

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

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

Relying on the same integral equation framework, and with careful analysis of the influence of the source terms involving \mathbf{P}_a when addressing the perturbed cell function \mathbf{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:

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

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

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

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

The second-order homogenized shear modulus is defined by $\boldsymbol{\mu}^2 = \langle \mu(\mathbf{Q} \otimes \mathbf{I} + \nabla \mathbf{R}) \rangle^S$ in terms of \mathbf{Q} and a third cell function \mathbf{R} . Once again, an analysis of the problems satisfied by \mathbf{R} and \mathbf{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 $(\mathbf{P}, \mathbf{Q}, \mathbf{R})$ 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 \mathbf{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.

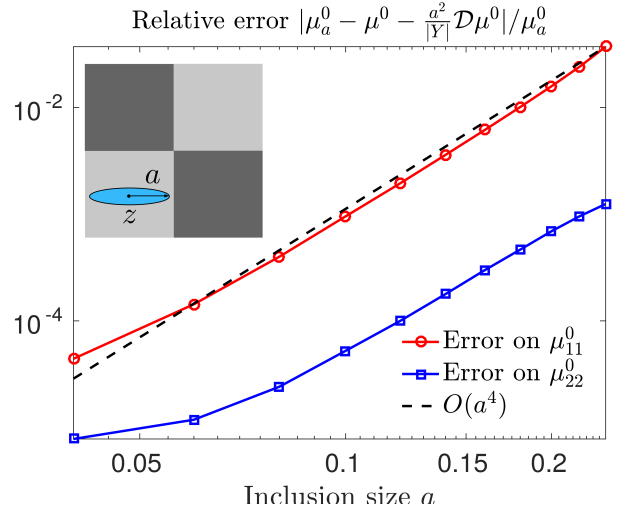


Figure 2: Relative error on shear modulus $\boldsymbol{\mu}_a^0$ approximated by expansion (2) for an ellipsoidal inhomogeneity of semi-axes $(a, 0.2a)$ placed at $\mathbf{z} = (0.25, 0.25)$ in a chessboard-like cell $Y = [0, 1]^2$. In this case, since the medium is locally homogeneous around \mathbf{z}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