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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  $\mu$  and density  $\rho$ . The unit cell Y has characteristic length  $\ell$ . 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:

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

where the leading-order and second-order homogenized coefficients  $(\boldsymbol{\mu}^0, \rho^0, \boldsymbol{\mu}^2, \boldsymbol{\rho}^2)$  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  $\rho^0$  is defined by  $\rho^0 = \langle \rho \rangle$ , so that

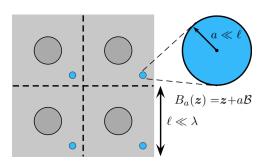


Figure 1: Perturbed periodic material

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

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

The homogenized shear modulus  $\mu^0$  is defined by  $\mu^0 = \langle \mu(\mathbf{I} + \nabla \mathbf{P}) \rangle^{\mathrm{S}}$ , 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:

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

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

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

where  $p_a := P_a - P$  is the perturbation of 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:

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

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

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

and  $\mathbf{A}(\mathbf{z}) = \mathbf{A}(\mathcal{B}, \mu(\mathbf{z}), \Delta \mu)$  is the polarization tensor [1] associated to shape  $\mathcal{B}$  and moduli  $\mu(\mathbf{z})$  and  $\mu(\mathbf{z}) + \Delta \mu$ . 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  $\rho^2 = \langle \rho Q \rangle^{S}$ , where the *second cell function* Q is the Y-periodic, zero-mean, tensor-valued solution of:

$$\nabla \cdot (\mu(\boldsymbol{P} \otimes \boldsymbol{I} + \nabla \boldsymbol{Q}))$$

$$= -\mu(\boldsymbol{I} + \nabla \boldsymbol{P}) + (\rho/\rho^0)\boldsymbol{\mu}^0 \quad (3)$$

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

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

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

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

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

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

**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 z without solving the new cell problems. As an example, an approximation of  $\mu_a^0$  is obtained by neglecting the remainder in (2), as illustrated on Fig. 2 for a chessboard-like cell.

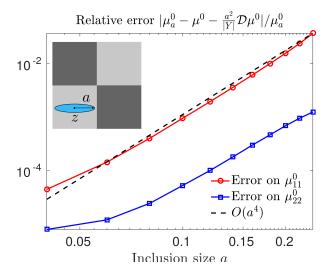


Figure 2: Relative error on shear modulus  $\mu_a^0$  approximated by expansion (2) for an ellipsoidal inhomogeneity of semi-axes (a, 0.2a) placed at z = (0.25, 0.25) in a chessboard-like cell  $Y = [0, 1]^2$ . In this case, since the medium is locally homogeneous around z, the remainder can be shown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