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 $U$:

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

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

$$\begin{align*}
\rho^0_a & = \rho^0 + a^2 |Y|^{-1} \mathcal{D} \rho^0; \quad \mathcal{D} \rho^0 = |B| \Delta \rho.
\end{align*}$$

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

$$\nabla \cdot (\mu (I + \nabla P)) = 0$$

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

$$\mu^0_a = \mu^0 + \langle \mu \nabla p_a \rangle^S + \langle \chi_{B_a} \Delta \mu (I + \nabla P_a) \rangle^S$$

where $p_a := P_a - P$ is the perturbation of $P$. The analysis of this perturbation is done by re-formulating 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:

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

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

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

and $A(z) = A(B, \mu(z), \Delta \mu)$ is the polarization tensor [1] associated to shape $B$ 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 $P = 0$, it reduces to $\mathcal{D} \mu^0 = A$ 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:

\[
\nabla \cdot (\mu (P \otimes I + \nabla Q)) = -\mu (I + \nabla P) + (\rho/\rho^0) \mu^0 \quad (3)
\]

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 \( \rho^2_a \) has an expansion of the same form as (2), with its topological derivative \( \mathcal{D} \rho^2 \) given by:

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

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

\[
\nabla \cdot (\mu \nabla \beta) = -\langle \rho - \rho^0 \rangle
\]
\[
\text{and} \quad \nabla \cdot (\mu (\beta I + \nabla X[\beta])) = -\mu \nabla \beta.
\]

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 \(|\mu_a^0 - \mu^0 - \frac{\bar{a}^2}{\bar{Y}} \mathcal{D} \mu^0/\mu_a^0|\) 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).

References


