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Micropolar modelling of periodic Cauchy materials based on asymptotic homogenization

Maria Laura De Bellis, Andrea Bacigalupo, Giorgio Zavarise

*Academia is a wide world with a lot of colleagues, some coworkers, and few friends. We have had the privilege to have Peter as a great friend.
Hence, thanks Peter, for all we learned from you and for your friendship.*

Abstract A micropolar-based asymptotic homogenization approach for the analysis of composite materials with periodic microstructure is proposed. The macro descriptors are directly linked to both suitable perturbation functions, obtained via asymptotic homogenization scheme, and micropolar two-dimensional deformation modes. A properly conceived energy equivalence between the macroscopic point and a microscopic representative portion of the periodic composite material is introduced to derive the overall micropolar constitutive tensors. The resulting constitutive tensors are not affected by the choice of the periodic cell.

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1 Introduction

Periodic manufactured composites are widely adopted in many engineering fields. In this context, it is crucial to accurately reproduce the material response in a synthetic, but accurate way. To this aim the study of multi-scale homogenization techniques is a very interesting and debated topic in literature [1, 2, 3]. Homogenization approaches, based on Cauchy continua at both the microscopic and macroscopic scales, may reveal ineffective since are not able to describe size effects as well as the dispersion properties of periodic heterogeneous materials. To overcome these drawbacks, non-local homogenization schemes can be effectively exploited.

In this framework, a micropolar macroscopic modelling of periodic Cauchy materials based on asymptotic homogenization approach is here proposed. In Section 2 the governing equations at both microscopic and macroscopic scales are recalled. Section 3 is devoted to define the micro-macro kinematic relations and the asymptotic expansion of the microscopic governing equations. The upscaling relations and a properly defined kinematic map are, then, fully developed in Section 4. The generalized macro-homogeneity condition is, then, derived in Section 5. An illustrative application is, finally, proposed in Section 6.

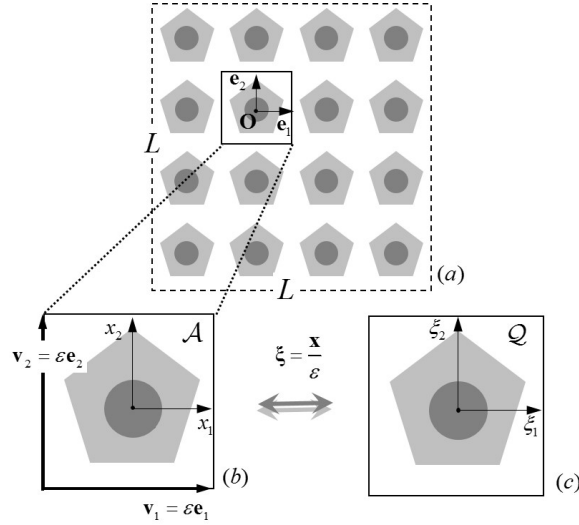


Fig. 1 Heterogeneous material at the microscopic level. (a) Cluster of periodic cells with structural dimensions L ; (b) Periodic Cell \mathcal{A} with characteristic size ε ; (c) unit cell Q .

2 Microscopic and macroscopic governing equations

Focus is on a 2D periodic heterogeneous composite material,, as in Figure 1(a), in the framework of linearised kinematics. A Cauchy continuum, subject to stresses induced by periodic body forces, is adopted. The periodic cell $\mathcal{A} = [-\varepsilon/2, \varepsilon/2] \times [-\varepsilon/2, \varepsilon/2]$, whose characteristic size is ε , is shown in Figure 1(b) together with the corresponding unit cell Q in Figure 1(c) characterized by periodicity vectors $\mathbf{v}_1, \mathbf{v}_2$. The governing equations at the microscopic scale read

$$\nabla \cdot \left(\mathbb{C}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \mathbf{u}(\mathbf{x}) \right) + \mathbf{b}(\mathbf{x}) = \mathbf{0}, \quad (1)$$

where \mathbb{C}^m is the Q -periodic elasticity tensor, \mathbf{b} are the zero-mean-value \mathcal{L} -periodic body force, with $\mathcal{L} = [-L/2; L/2] \times [-L/2; -L/2]$, for $L \gg \varepsilon$. It follows that the microscopic displacement field \mathbf{u} explicitly depends on both \mathbf{x} and $\xi = \mathbf{x}/\varepsilon$.

At the macroscopic scale a micropolar continuum [4] is considered with governing equations

$$\begin{aligned} \nabla \cdot \left[\mathbb{G}^M (\nabla \mathbf{U}(\mathbf{x}) + \epsilon_{3hk} (\mathbf{e}_h \otimes \mathbf{e}_k) \Phi(\mathbf{x})) \right] + \nabla \cdot \left(\mathbf{Y}^M \nabla \Phi(\mathbf{x}) \right) + \mathbf{b}(\mathbf{x}) &= \mathbf{0}, \\ \nabla \cdot \left[\mathbf{Y}^{M^T} (\nabla \mathbf{U}(\mathbf{x}) + \epsilon_{3hk} (\mathbf{e}_h \otimes \mathbf{e}_k) \Phi(\mathbf{x})) \right] + \nabla \cdot \left(\mathbf{S}^M \nabla \Phi(\mathbf{x}) \right) + \\ - \epsilon_{3ij} (\mathbf{e}_i \otimes \mathbf{e}_j) : \left[\mathbb{G}^M (\nabla \mathbf{U}(\mathbf{x}) + \epsilon_{3hk} (\mathbf{e}_h \otimes \mathbf{e}_k) \Phi(\mathbf{x})) + \mathbf{Y}^M \nabla \Phi(\mathbf{x}) \right] + c_3(\mathbf{x}) &= 0, \end{aligned} \quad (2)$$

where $\mathbb{G}^M, \mathbf{Y}^M$ and \mathbf{S}^M are the constitutive tensors, \mathbf{b}, c_3 are the generalized body forces, $\mathbf{U}(\mathbf{x})$ and $\Phi(\mathbf{x})$, are the macro-displacement and micropolar rotation field, respectively.

In what follows a procedure aimed at identifying the macroscopic constitutive tensors, characterizing the equivalent micropolar continuum, are derived from the mechanical properties available at the microscopic scale.

3 Micro-macro kinematic relations and asymptotic expansion of the microscopic governing equations

In line with the asymptotic homogenization scheme (see i.e. [5]), the following asymptotic expansion of the microscopic displacement field is taken

$$u_i \left(\mathbf{x}, \xi = \frac{\mathbf{x}}{\varepsilon} \right) = \left(U_i(\mathbf{x}) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} N_{ijq}^{(l)}(\xi) \frac{\partial^{|q|}}{\partial x_q} U_j(\mathbf{x}) \right) \Bigg|_{\xi = \frac{\mathbf{x}}{\varepsilon}}, \quad (3)$$

where U_i are macro-displacement components, $N_{k p q_1}^{(l)}$ are zero-mean-value Q -periodic perturbation functions and q a multi-index of length l . The equation (3) can

be plug into the microscopic governing equation (1). After suitable manipulations, by collecting the terms with equal power ε , and imposing the so-called solvability condition in the class of Q -periodic functions, a hierarchical sequence of partial differential problems, known as *cell problems*, is obtained as in [6]. More specifically, the perturbation functions at order ε^0 , ε^1 and ε^2 , i.e. $N_{hpq_1}^{(1)}$, $N_{hpq_1q_2}^{(2)}$ and $N_{hpq_1q_2q_3}^{(3)}$ are determined, together with the overall first order constitutive tensor components

$$C_{iq_2pq_1} = \int_Q C_{rjkl}^m \left(N_{riq_2,j}^{(1)} + \delta_{ir} \delta_{jq_2} \right) \left(N_{kpq_1,l}^{(1)} + \delta_{pk} \delta_{lq_1} \right) d\xi, \quad (4)$$

that are key elements intervening in the micropolar homogenization scheme, detailed in the following sections.

4 Upscaling relations and third order polynomial kinematic map

Accordingly with the procedure detailed in [7], the upscaling relations, linking the generalized macro-displacement field, depending on both $\mathbf{U}(\mathbf{x})$ and $\Phi(\mathbf{x})$, to the displacement field at the microscopic level $\mathbf{u}(\mathbf{x})$, are here discussed. In particular for $W_{ij} = -\epsilon_{3ij} \Phi$ a minimization procedure over the unit cell Q is proposed as follows

$$\begin{aligned} U_1(\mathbf{x}) &= \int_Q u_1(\mathbf{x}, \xi) d\xi, & U_2(\mathbf{x}) &= \int_Q u_2(\mathbf{x}, \xi) d\xi, \\ \min_{W_{ij}} \mathcal{F} \left[\omega_{ij}^*(W_{ij}) \right] &= \min_{W_{ij}} \int_Q \left(\|\omega_{ij}(\mathbf{x}, \xi) - \omega_{ij}^*(\mathbf{x}, \xi)\|_2 \right)^2 d\xi, \end{aligned} \quad (5)$$

where ω_{ij} are the components of the micro infinitesimal rotation tensor and ω_{ij}^* are the components of a properly defined skew-symmetric tensor expressed in the form

$$\omega_{ij}^* = W_{ij} + \sum_{l=1}^{+\infty} \sum_{\substack{|q|=l \\ |r|=l}} \frac{1}{2} \left(N_{ijq,r}^{(l)} - N_{jiq,r}^{(l)} \right) \tilde{W}_{qr}. \quad (6)$$

By plugging (6) truncated at the first order into (5) c, after solving the minimization problem, the components of the micropolar rotation tensor are obtained as

$$W_{ij}(\mathbf{x}) = \frac{\int_Q M_{ijpq_1}(\xi) \omega_{pq_1}(\mathbf{x}, \xi) d\xi}{\int_Q \delta_{pr} \delta_{q_1s_1} M_{hkpq_1}(\xi) M_{hkr s_1}(\xi) d\xi}, \quad (7)$$

with $M_{ijpq_1} = \delta_{ip} \delta_{jq_1} + \frac{1}{2} \left(N_{ijp,q_1}^{(1)} - N_{jip,q_1}^{(1)} \right)$.

The upscaling relations are now particularized by truncating the microscopic dis-

placement field at the third order, i.e.

$$\begin{aligned} u_i^{III}(\mathbf{x}, \boldsymbol{\xi}) = & U_i(\mathbf{x}) + \varepsilon N_{ijq_1}^{(1)}(\boldsymbol{\xi}) H_{jq_1}(\mathbf{x}) + \\ & + \varepsilon^2 N_{ijq_1q_2}^{(2)}(\boldsymbol{\xi}) \kappa_{jq_1q_2}(\mathbf{x}) + \varepsilon^3 N_{ijq_1q_2q_3}^{(3)}(\boldsymbol{\xi}) \kappa_{jq_1q_2q_3}(\mathbf{x}), \end{aligned} \quad (8)$$

where $U_i(\mathbf{x})$ is the macroscopic displacement field and $H_{jq_1}(\mathbf{x})$, $\kappa_{jq_1q_2}(\mathbf{x})$ and $\kappa_{jq_1q_2q_3}(\mathbf{x})$ its gradient and higher order gradients.

Concerning the macro-displacement, a third-order Taylor polynomial expansion is chosen

$$U_i(\mathbf{x}) = \bar{U}_i + \bar{H}_{ip_1} x_{p_1} + \frac{1}{2} \bar{\kappa}_{ip_1p_2} x_{p_1} x_{p_2} + \frac{1}{6} \bar{\kappa}_{ip_1p_2p_3} x_{p_1} x_{p_2} x_{p_3}, \quad (9)$$

where the coefficients \bar{U}_i , \bar{H}_{ip_1} , $\bar{\kappa}_{ip_1p_2}$ and $\bar{\kappa}_{ip_1p_2p_3}$ are the macroscopic fields evaluated at point $\mathbf{x} = \mathbf{0}$, respectively. In order to identifying a micropolar continuum, the 20 independent coefficients must be properly reduced to 6 as detailed in [7].

At this point, by replacing the equation (9), suitably manipulated, in (8), the polynomial approximation of the microscopic displacement field is

$$\begin{aligned} u_1(\mathbf{x}, \boldsymbol{\xi}) = & \mathcal{B}_1^1(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{11} + \mathcal{B}_1^2(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{22} + \mathcal{B}_1^3(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{12} + \\ & + \mathcal{B}_1^4(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{122} + \mathcal{B}_1^5(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{211} + \mathcal{B}_1^6(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{1222}, \\ u_2(\mathbf{x}, \boldsymbol{\xi}) = & \mathcal{B}_2^1(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{11} + \mathcal{B}_2^2(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{22} + \mathcal{B}_2^3(\mathbf{x}, \boldsymbol{\xi}) \bar{E}_{12} + \\ & + \mathcal{B}_2^4(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{122} + \mathcal{B}_2^5(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{211} + \mathcal{B}_2^6(\mathbf{x}, \boldsymbol{\xi}) \bar{\kappa}_{1222}, \end{aligned} \quad (10)$$

where $\bar{E}_{ip_1} = (\bar{H}_{ip_1} + \bar{H}_{p_1i})/2$ and the localization functions $\mathcal{B}_i^j(\mathbf{x}, \boldsymbol{\xi})$ depend on the overall first order elastic tensor components and on the perturbation functions. By plugging equations (10) in equations (7), the micropolar rotation field $\Phi(\mathbf{x})$ and, in turn, the macroscopic curvature tensor components $K_1 = \partial\Phi/\partial x_1$ and $K_2 = \partial\Phi/\partial x_2$ are obtained.

5 Generalized macro-homogeneity condition

The overall micropolar elastic properties are derived by exploiting a generalized macro-homogeneity condition, establishing an energy equivalence between the macroscopic and the microscopic scales. Accordingly with [5, 8], the *microscopic mean strain energy* is defined as

$$\bar{\mathcal{E}}_m \doteq \frac{1}{2} \int_{\mathcal{A}} \int_{\mathcal{Q}} \underline{\boldsymbol{\varepsilon}}(\mathbf{x}, \boldsymbol{\xi})^T \underline{\underline{\mathbf{C}}}^m(\boldsymbol{\xi}) \underline{\boldsymbol{\varepsilon}}(\mathbf{x}, \boldsymbol{\xi}) d\boldsymbol{\xi} d\mathbf{x}, \quad (11)$$

where $\underline{\underline{\mathbf{C}}}^m$ is the elasticity matrix and $\underline{\boldsymbol{\varepsilon}}$ is the microscopic strain vector in the standard matrix notation. Under the assumption of scale separation, the $\bar{\mathcal{E}}_m$ related

to the strain field $\underline{\varepsilon}_0 = \underline{\varepsilon}(\mathbf{x} = \mathbf{0}, \xi)$ can be introduced as

$$\bar{\varepsilon}_m^0 \doteq \frac{1}{2} \int_{\mathcal{A}} \int_Q \underline{\varepsilon}(\mathbf{x} = \mathbf{0}, \xi)^T \underline{\underline{\mathbf{C}}}^m(\xi) \underline{\varepsilon}(\mathbf{x} = \mathbf{0}, \xi) d\xi d\mathbf{x} = \frac{|\mathcal{A}|}{2} \int_Q \underline{\varepsilon}_0^T \underline{\underline{\mathbf{C}}}^m \underline{\varepsilon}_0 d\xi, \quad (12)$$

being $|\mathcal{A}|$ the area of the periodic cell. More specifically, this strain vector is determined from the microscopic displacement components in equation (10), taking the form

$$\underline{\varepsilon}_0 = \underline{\underline{\mathbf{B}}}^\Xi \underline{\Xi} + \underline{\underline{\mathbf{B}}}^\Upsilon \underline{\Upsilon}, \quad (13)$$

being $\underline{\Xi} = \{ \bar{E}_{11} \ \bar{E}_{22} \ \bar{E}_{12} \ \bar{\kappa}_{1222} \}^T$, $\underline{\Upsilon} = \{ \bar{\kappa}_{122} \ \bar{\kappa}_{211} \}^T$ and $\underline{\underline{\mathbf{B}}}^\Xi, \underline{\underline{\mathbf{B}}}^\Upsilon$ properly defined strain localization matrices. The related *microscopic mean strain energy density* is consequently derived

$$\begin{aligned} \bar{\phi}_m^0 = \frac{\bar{\varepsilon}_m^0}{|\mathcal{A}|} = \frac{1}{2} & \left(\underline{\Xi}^T \int_Q \underline{\underline{\mathbf{B}}}^{\Xi T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Xi d\xi \underline{\Xi} + \underline{\Upsilon}^T \int_Q \underline{\underline{\mathbf{B}}}^{\Upsilon T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Upsilon d\xi \underline{\Upsilon} + \right. \\ & \left. + \underline{\Xi}^T \int_Q \underline{\underline{\mathbf{B}}}^{\Xi T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Upsilon d\xi \underline{\Upsilon} + \underline{\Upsilon}^T \int_Q \underline{\underline{\mathbf{B}}}^{\Upsilon T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Xi d\xi \underline{\Xi} \right). \end{aligned} \quad (14)$$

Furthermore, the macroscopic strain energy density evaluated in $\mathbf{x} = \mathbf{0}$ is introduced

$$\phi_M^0 = \frac{1}{2} \left(\underline{\Gamma}_0^T \underline{\underline{\mathbf{G}}}^M \underline{\Gamma}_0 + \underline{\mathbf{K}}_0^T \underline{\underline{\mathbf{S}}}^M \underline{\mathbf{K}}_0 + \underline{\Gamma}_0^T \underline{\underline{\mathbf{Y}}}^M \underline{\mathbf{K}}_0 + \underline{\mathbf{K}}_0^T \underline{\underline{\mathbf{Y}}}^{M T} \underline{\Gamma}_0 \right), \quad (15)$$

where the asymmetric micropolar strain vector and the curvature vector, evaluated in $\mathbf{x} = \mathbf{0}$ are defined as

$$\underline{\Gamma}_0 = \underline{\underline{\mathbf{A}}}^\Xi \underline{\Xi} + \underline{\underline{\mathbf{A}}}^\Upsilon \underline{\Upsilon}, \quad \underline{\mathbf{K}}_0 = \underline{\underline{\mathbf{A}}}^\Xi \underline{\Xi} + \underline{\underline{\mathbf{A}}}^\Upsilon \underline{\Upsilon}, \quad (16)$$

being $\underline{\underline{\mathbf{A}}}^\Xi, \underline{\underline{\mathbf{A}}}^\Upsilon, \underline{\underline{\mathbf{A}}}^\Upsilon, \underline{\underline{\mathbf{A}}}^\Xi$ transformation matrices.

By exploiting the generalized macro-homogeneity condition, establishing the equivalence between the microscopic and macroscopic strain energy density $\bar{\phi}_m^0 \doteq \phi_M^0(\mathbf{x} = \mathbf{0})$, after some manipulations, the overall elastic micropolar matrices are determined.

In the case the periodic cell is characterized by centrosymmetric topology, it results

$$\begin{aligned} \underline{\underline{\mathbf{G}}}^M &= \int_Q \underline{\underline{\mathbf{A}}}^{\Xi - T} \underline{\underline{\mathbf{B}}}^{\Xi T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Xi \underline{\underline{\mathbf{A}}}^{\Xi - 1} d\xi, \\ \underline{\underline{\mathbf{S}}}^M &= \int_Q \underline{\underline{\mathbf{A}}}^{\Upsilon - T} \underline{\underline{\mathbf{B}}}^{\Upsilon T} \underline{\underline{\mathbf{C}}}^m \underline{\underline{\mathbf{B}}}^\Upsilon \underline{\underline{\mathbf{A}}}^{\Upsilon - 1} d\xi, \end{aligned} \quad (17)$$

and the coupling matrix is $\underline{\underline{\mathbf{Y}}}^M = \mathbf{0}$.

6 Benchmark test

As an example, a strip of two-phase periodic medium, realized by assembling, along horizontal and vertical directions, periodic cells with a stiff matrix (phase 1) embedding soft square inclusions (phase 2), see Figure 2, is considered. The size of the inclusion is $\varepsilon/2$ and the material is characterized by $\eta_E = E_2/E_1 = 3/50$ and $\eta_\nu = \nu_1/\nu_2 = 1$ (with $E_1 = 500$ GPa, $\nu_1 = 0.1$). The specimen undergoes a system of discontinuous periodic forces, with period $L_1 = (4\alpha + \beta)\varepsilon$, located on both top and bottom sides of the strip characterized by width equal to $\beta\varepsilon$, with $\alpha = 4$, $\beta = 10$, and ε being the size of the periodic cell. Plane strain conditions are assumed.

The numerical results of the micro-mechanical model, in terms of displacement

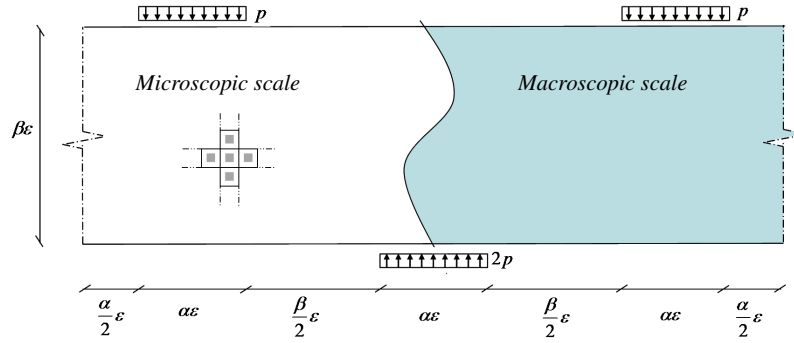


Fig. 2 Strip undergoing discontinuous periodic forces: schematic of the heterogeneous medium versus the homogenized one.

components, along a horizontal line located at a distance $9/2\varepsilon$ from the top side of the strip, are compared with the respective ones obtained considering the micropolar homogenized model.

In Figure 3(a) the dimensionless micro-mechanical displacement component u_1/L_1 (blue dotted line), and the respective macro-mechanical one U_1/L_1 (red solid line) are plotted versus the dimensionless coordinate x_1/L_1 . Analogously, in Figure 3(b) the dimensionless components u_2/L_1 and U_2/L_1 are reported with the same line styles. For both microscopic and macroscopic displacement components a very good agreement is shown.

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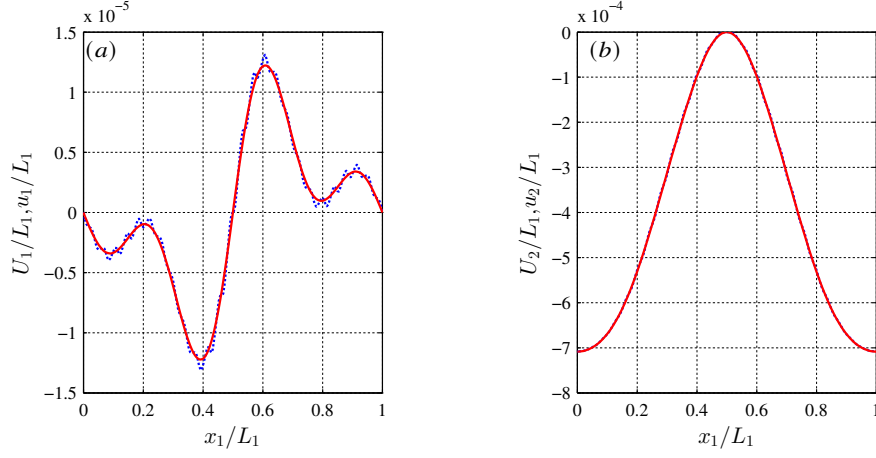


Fig. 3 Case with softer inclusion. Comparison between dimensionless micro-mechanical displacement components, in blue dotted lines, and the respective macro-mechanical ones versus x_1/L_1 . (a) Components u_1/L_1 , U_1/L_1 ; (b) components u_2/L_1 , U_2/L_1 .

References

1. E. Sanchez-Palencia. Comportements local et macroscopique d'un type de milieux physiques heterogenes. *International Journal of Engineering Science*, 12(4):331–351, 1974.
2. N. Bakhvalov and G. Panasenko. *Homogenization: Averaging Processes in Periodic Media*. Kluwer Academic Publishers, Dordrecht-Boston-London, 1984.
3. T.I. Zohdi and P. Wriggers. *An introduction to computational micromechanics*. Springer Science Business Media, 2008.
4. R. D. Mindlin. Micro-structure in linear elasticity. *Archive for Rational Mechanics and Analysis*, 16(1):51–78, 1964.
5. A. Bacigalupo. Second-order homogenization of periodic materials based on asymptotic approximation of the strain energy: formulation and validity limits. *Meccanica*, 49(6):1407–1425, 2014.
6. M.L. De Bellis and A. Bacigalupo and G. Zavarise. Characterization of hybrid piezoelectric nanogenerators through asymptotic homogenization. *Computer Methods in Applied Mechanics and Engineering*, 355:1148–1186, 2019.
7. A. Bacigalupo and M.L. De Bellis and G. Zavarise. Asymptotic homogenization approach for the micropolar modelling of periodic materials *Submitted 2021*
8. V. Smyshlyaev and K. Cherednichenko. On rigorous derivation of strain gradient effects in the overall behaviour of periodic heterogeneous media. *Journal of the Mechanics and Physics of Solids*, 48(6):1325–1357, 2000.