Variational methods for the homogenization of periodic heterogeneous media

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Abstract. – In this paper, several variational principles for the evaluation of the overall properties of composite materials with periodic microstructure are introduced. The two classical homogenization problems corresponding to assigned average strain or assigned average stress are considered. The periodicity of the variables governing the problem is enforced either by considering special representations (i.e. Fourier series) of the periodic part of the displacement and stress fields or by adopting appropriate boundary conditions on the unit cell. In particular, the boundary conditions ensuring the periodicity of the governing variable are introduced in the functionals by using Lagrangian multipliers. Once the variational principles are introduced, the Fourier series technique and the finite element method are adopted to obtain rational approximation procedures. Finally, numerical applications are carried out in order to assess the performances of the proposed methods in the computation of estimates or bounds on the overall elastic properties of a composite material, and in the determination of the displacement and stress distribution in the unit cell. © Elsevier, Paris.

1. Introduction

An evaluation of the overall mechanical properties of heterogeneous materials can be obtained using homogenization techniques. Many studies have been developed to determine analytical expressions and to obtain numerical models for the evaluation of the overall behavior of composite materials. Thus, several methods of homogenization are available in literature.

Many analytical homogenization procedures are based on the so-called equivalent eigenstrain method proposed by Eshelby (1957), who considered the problem of a single ellipsoidal inclusion embedded in an infinite elastic medium. Mori and Tanaka (1973) used the Eshelby solution and developed a method which approximately takes the interactions between the inclusions present in the matrix into account. A mathematical clarification of the approximations involved in the Mori-Tanaka method was presented by Benveniste (1987) and it has been observed, Weng (1992), that this method reduces to the Hashin and Shtrikman based formula of Willis (1977) in the case of a matrix containing a population of aligned ellipsoidal inclusions.

One of the most used homogenization technique is the self-consistent method proposed by Hill (1965) and Budiansky and O’Connell (1976). They considered a random distribution of the inclusions in an infinite medium characterized by the unknown effective properties of the composite which are to be determined. An iterative numerical procedure was used to obtain the overall moduli. The self-consistent method was developed and adopted by, for instance, Budiansky and O’Connell (1976) and Laws et al. (1983) for the analysis of cracked solids.

The effective mechanical behavior of weakly heterogeneous nonlinear materials was analyzed by Ponti Castañeda and Suquet (1995) for the case of random and periodic composites.

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Instead of estimates, bounds on the overall properties can be obtained. Several variational principles were developed by Hashin and Shtrikman (1963) in order to evaluate bounds on the homogenized elastic properties of macroscopically-isotropic heterogeneous materials (Willis, 1977 and Willis, 1983). Those bounds depend only on the volume fractions and the physical properties of the constituents. Hashin and Shtrikman type bounds on the effective elastic properties of composites were proposed by Willis (1991) in the case of nonlinear elastic constituents for a general distribution of inclusions.

For very regular composites, i.e. for composites with inclusions periodically distributed in the matrix, a periodic model has been proposed. A mathematical presentation of periodic composite materials and their homogenization can be found in Suquet (1987), Sanchez-Hubert and Sanchez-Palencia (1992). Many authors solved the homogenization problem for composite materials with periodic microstructure by using an extension of the Eshelby inclusion problem and the Fourier series technique, in this way they obtained estimates and bounds on the overall stiffness matrix (Suquet, 1990; Nemat-Nasser et al., 1993; Luciano and Barbero, 1994). These authors adopted variational principles defined on a homogeneous reference material subject to appropriate polarization fields simulating the different behaviors of the actual constituents of the original body. Further, Barbero and Luciano (1995) and Luciano and Barbero (1995) adopted the equivalent periodic eigenstrain method to determine the overall relaxation moduli of linear viscoelastic composite materials. The cell method for periodic media was proposed by Aboudi (1991), who considered a unit cell with a square inclusion. Finally, Moulinc and Suquet (1994) developed a new fast numerical method to compute the overall response of periodic composite materials with local linear and nonlinear behavior. Specifically, they formulated the homogenization problem in the form of a periodic Lippman-Schwinger equation (Suquet, 1990) and solved it iteratively.

In order to study the nonlinear behavior of the unit cell of a periodic composite, numerical methods, mainly the finite element method, are employed. In Antheine (1995) a displacement based linear finite element analysis for a masonry material modeled as a two- or three-dimensional elastic body was proposed. Nonlinear finite element analyses of a metal matrix composite was developed by Tvergaard (1993) for short whisker reinforced material, and by Hallen et al. (1994) for reinforcement in the form of long fibres. They studied the behavior of a unit cell subjected to an assigned loading history. Bounds on overall instantaneous elastoplastic properties of composites were derived by Teply and Dvorak (1988), by using the minimum principles, approximated by the finite element method. In a recent study, Luciano and Sacco (1997) recovered a macromechanical damage law for a masonry material using a numerical micromechanical analysis.

In this paper several new variational formulations of the homogenization problem for periodic media, characterized by any geometry of the inclusions, with or without orthogonal axes of symmetry, are proposed. Initially the homogenization problem of heterogeneous periodic media is formulated for the case of assigned average strain or assigned average stress. Then, the reduction of the elastostatic problem of an infinite periodic media to the corresponding single unit cell is presented. Two reduction strategies are discussed. The first one uses appropriate formulae for the representation of the strain or stress fields, while the second strategy considers average constraints on strain or stress fields and suitable boundary conditions on the unit cell, which guarantee the current enforcement of the periodicity of the strain and stress fields. The two methods are examined and new variational formulations, based on the Hu-Washizu functional in conjunction with the Lagrange multipliers technique, are proposed in order to develop rational numerical procedures to obtain approximate solutions of the problem. In particular, Fourier series and appropriate finite element methods are applied.

It is worth noting that, by adopting appropriate variational formulations, bounds on the overall elastic properties of a heterogeneous material can be computed. Finally, in order to evaluate the efficiency of the proposed methods, numerical analyses are developed and the obtained results are compared with results available in the literature.
2. Statement of the problem

A periodic composite body is obtained by assembling an infinite number of repetitive adjacent unit cells \( V \). In this paper, parallelepiped unit cells are considered with the total dimensions along the three coordinate axes \( x_1, x_2, x_3 \) denoted by \( 2a_1, 2a_2, \) and \( 2a_3 \).

An estimate of the overall stiffnesses of a periodic composite material is derived from the solution of the heterogeneous medium subject to load conditions, such that the stress and the strain fields are periodic. In particular, the elastostatic problems of a solid with periodic microstructure subject to a mean strain state \( \varepsilon_{ij}^{0} \) or to a mean stress state \( \sigma_{ij}^{0} \) are considered, with \( i, j = 1, 2, 3 \). They consist of the determination of the elastic state \( \{ u_i, \varepsilon_{ij}, \sigma_{ij} \} \), i.e. the displacement, strain and stress fields satisfying the classical equations for heterogeneous media in \( \mathbb{R}^3 \):

\[
\sigma_{ij,j}(x_1, x_2, x_3) = 0
\]

\[
2\varepsilon_{ij}(x_1, x_2, x_3) = u_{i,j}(x_1, x_2, x_3) + u_{j,i}(x_1, x_2, x_3)
\]

\[
C_{ijhk}(x_1, x_2, x_3) \varepsilon_{hk}(x_1, x_2, x_3) = \sigma_{ij}(x_1, x_2, x_3)
\]

In this framework, the strain and stress fields admit the representation formulae:

\[
\varepsilon_{ij}(x_1, x_2, x_3) = \varepsilon_{ij}^{0} + \varepsilon_{ij}^{p}(x_1, x_2, x_3)
\]

\[
\sigma_{ij}(x_1, x_2, x_3) = \sigma_{ij}^{0} + \sigma_{ij}^{p}(x_1, x_2, x_3)
\]

where the repeated indices imply summation, the comma subscript \((\bullet)_j\) indicates the partial derivative \( \partial / \partial x_j \), and \( C_{ijhk}(x_1, x_2, x_3) \) are the components of the fourth-order constitutive matrix which are \( V \)-periodic. Further, \( \varepsilon_{ij}^{0} \) and \( \sigma_{ij}^{0} \) are the averages of the strain and stress fields:

\[
\varepsilon_{ij}^{0} = \frac{1}{V} \int_{V} \varepsilon_{ij}(x_1, x_2, x_3) \, dV
\]

\[
\sigma_{ij}^{0} = \frac{1}{V} \int_{V} \sigma_{ij}(x_1, x_2, x_3) \, dV
\]

so that, \( \varepsilon_{ij}^{p} \) and \( \sigma_{ij}^{p} \) are \( V \)-periodic defined as the parts of the strain and stress fields with null average in \( V \):

\[
0 = \int_{V} \varepsilon_{ij}^{p}(x_1, x_2, x_3) \, dV
\]

\[
0 = \int_{V} \sigma_{ij}^{p}(x_1, x_2, x_3) \, dV
\]

In summary, the periodic elastostatic problem is governed by the field Eqs. (1)-(3) and by the additive Eq. (4) or (5). Note that when the mean strain \( \varepsilon_{ij}^{0} \) is assigned then the Eq. (4) must be considered to impose the given
average strain, and Eq. (7) is necessary for the post-computation of the mean stress \(\sigma_{ij}^0\); analogously, when the mean stress \(\sigma_{ij}^0\) is assigned then Eq. (5) must be considered, and Eq. (6) is necessary for the post-computation of the mean strain \(\varepsilon_{ij}^0\). In Suquet (1987) and Sanchez-Hubert and Sanchez-Palencia (1992), it has been emphasized that the periodic problem is well posed and admits a unique solution in terms of stresses.

The overall stiffness and compliance \(C_{ijk}\) and \(A_{ijk}\) are defined as:

\[
C_{ijk}\varepsilon_{hk}^0 = \sigma_{ij}^0, \quad A_{ijk}\sigma_{hk}^0 = \varepsilon_{ij}^0
\]

**Remark 1.** – The combination of (4) with the congruence Eq. (2) allows the displacement to be represented as (Suquet, 1987; Anthoine, 1995):

\[
u_i(x_1, x_2, x_3) = \varepsilon_{ij}^0 x_j + u_i^p(x_1, x_2, x_3)
\]

where \(u_i^p(x_1, x_2, x_3)\) is the periodic part of the displacement, such that \(u_{ij}^p(x_1, x_2, x_3) + u_{ij}^p(x_1, x_2, x_3) = 2\varepsilon_{ij}^p(x_1, x_2, x_3)\). The strain \(\varepsilon_{ij}^p(x_1, x_2, x_3)\) is \(V\)-periodic in \(R^3\) with null average in \(V\), i.e. it satisfies (8).

**Remark 2.** – Because of the periodicity and continuity of \(u_i^p(x_1, x_2, x_3)\), the following conditions are to be satisfied on the boundary \(\partial V\) of any unit cell:

\[
u_i^p(a_1, x_2, x_3) = \nu_i^p(-a_1, x_2, x_3) \quad \forall x_2 \in [-a_2, a_2] \forall x_3 \in [-a_3, a_3]
\]

\[
u_i^p(x_1, a_2, x_3) = \nu_i^p(x_1, -a_2, x_3) \quad \forall x_1 \in [-a_1, a_1] \forall x_3 \in [-a_3, a_3]
\]

\[
u_i^p(x_1, x_2, a_3) = \nu_i^p(x_1, x_2, -a_3) \quad \forall x_1 \in [-a_1, a_1] \forall x_2 \in [-a_2, a_2]
\]

**Remark 3.** – By taking (11) into account, the continuity conditions (12) become:

\[
u_i(a_1, x_2, x_3) - \nu_i(-a_1, x_2, x_3) - 2\varepsilon_{ij}^0 a_1 = 0 \quad \forall x_2 \in [-a_2, a_2] \forall x_3 \in [-a_3, a_3]
\]

\[
u_i(x_1, a_2, x_3) - \nu_i(x_1, -a_2, x_3) - 2\varepsilon_{ij}^0 a_2 = 0 \quad \forall x_1 \in [-a_1, a_1] \forall x_3 \in [-a_3, a_3]
\]

\[
u_i(x_1, x_2, a_3) - \nu_i(x_1, x_2, -a_3) - 2\varepsilon_{ij}^0 a_3 = 0 \quad \forall x_1 \in [-a_1, a_1] \forall x_2 \in [-a_2, a_2]
\]

**Remark 4.** – The equilibrium of the periodic part of the tractions between two adjacent cells requires:

\[
\sigma_{ij}^p(a_1, x_2, x_3) n_j(a_1, x_2, x_3) = -\sigma_{ij}^p(-a_1, x_2, x_3) n_j(-a_1, x_2, x_3) \quad \forall x_2 \in [-a_2, a_2] \forall x_3 \in [-a_3, a_3]
\]

\[
\sigma_{ij}^p(x_1, a_2, x_3) n_j(x_1, a_2, x_3) = -\sigma_{ij}^p(x_1, -a_2, x_3) n_j(x_1, -a_2, x_3) \quad \forall x_1 \in [-a_1, a_1] \forall x_3 \in [-a_3, a_3]
\]

\[
\sigma_{ij}^p(x_1, x_2, a_3) n_j(x_1, x_2, a_3) = -\sigma_{ij}^p(x_1, x_2, -a_3) n_j(x_1, x_2, -a_3) \quad \forall x_1 \in [-a_1, a_1] \forall x_2 \in [-a_2, a_2]
\]

where \(n_j\) is the outward normal to \(\partial V\).
By taking (14) into account, the classical theorem of mean stresses (e.g., see Aboudi, 1991) allows condition (9) to be rewritten as:

\[
0 = \int_{A_1} a_1 \left( \sigma_{ij}^p n_j n_k + n_i \sigma_{kij}^p n_j \right) dx_2 dx_3 \\
+ \int_{A_2} a_2 \left( \sigma_{ij}^p n_j n_k + n_i \sigma_{kij}^p n_j \right) dx_1 dx_3 \\
+ \int_{A_3} a_3 \left( \sigma_{ij}^p n_j n_k + n_i \sigma_{kij}^p n_j \right) dx_1 dx_2
\]

where \( A_i \) is the boundary of \( \partial V \) defined at \( x_i = a_i \).

Note that, while a strain \( \varepsilon_{ij}^p \) associated with a displacement field \( u_i^p \) satisfying conditions (12) has null average, a stress \( \sigma_{ij}^p \) satisfying boundary conditions (14) could have a non-zero average. Hence, in order to completely characterize the field \( \sigma_{ij}^p \), Eqs. (14) and (15) must be enforced.

By taking the above remarks into account, it can be noted that the elastostatic problem governed by (1)-(3) and (4), or by (1)-(3) and (5), can be rewritten in different equivalent forms.

**Problem 1**: given the mean strain \( \varepsilon_{ij}^0 \), find the elastic state \( \{ u_i^p, \varepsilon_{ij}, \sigma_{ij}^p \} \) satisfying the equations in \( R^3 \):

\[
\sigma_{ij,j}(x_1, x_2, x_3) = 0 \\
2\varepsilon_{ij} = 2\varepsilon_{ij}^0 + u_{ij}^p(x_1, x_2, x_3) + u_{j,i}(x_1, x_2, x_3) \\
C_{ijhk}(x_1, x_2, x_3) \varepsilon_{hk}(x_1, x_2, x_3) = \sigma_{ij}(x_1, x_2, x_3)
\]

then, compute the mean stress using (7) and finally the overall elastic tensor using (10);

**Problem 2**: given the mean stress \( \sigma_{ij}^0 \), find the elastic state \( \{ u_i, \varepsilon_{ij}, \sigma_{ij}^p \} \) satisfying the equations in \( R^3 \):

\[
\sigma_{ij,j}(x_1, x_2, x_3) = 0 \\
2\varepsilon_{ij} = u_{i,j}(x_1, x_2, x_3) + u_{j,i}(x_1, x_2, x_3) \\
C_{ijhk}(x_1, x_2, x_3) \varepsilon_{hk}(x_1, x_2, x_3) = \sigma_{ij}^0 + \sigma_{ij}^p(x_1, x_2, x_3)
\]

then, compute the mean strain using (6) and finally the overall elastic tensor using (10).

As the original periodic elastostatic problem, these two problems admit a unique solution apart from a rigid motion.

The elastostatic problem written in its original form (i.e., (1)-(3) and (4) or (1)-(3) and (5)) as well as in the equivalent form (16) and (17), is posed in the whole space \( R^3 \). By taking into account the periodicity of the involved functions, the problem can be recast only in \( V \). Then, the solution in \( R^3 \) can be recovered by periodically extending the solution obtained in \( V \). Two different ways can be adopted to enforce the \( V \)-periodicity of \( u_i^p, \varepsilon_{ij}^p \) and \( \sigma_{ij}^p \):

- by using opportune representation formulae;
- by considering the average constraints of (8) and (9) and suitable boundary conditions on the unit cell.

Next, new variational formulations for the periodic elastostatic problems (16) and (17) are exploited, by reducing the problem in \( V \). It can be emphasized that the variational principles are the bases for developing approximate methods, which allows the solution of problems (16) and (17) to be estimated. In particular, they can be used to get bounds on the overall composite properties.

It can be pointed out that the variational principles corresponding to the elastostatic problems (16) and (17) are defined on the heterogeneous body; hence they are different from the Hashin and Shtrikman type
variational principles (Nemat-Nasser et al., 1993), which introduce the periodic polarization fields simulating the heterogeneity as further unknowns of the problem.

3. Fourier series

In order to solve the periodic elastostatic problems (16) and (17), the Fourier representation of the governing variables appears to be convenient since it allows the constraints on the periodicity and on the average of the strain or stress to be automatically satisfied.

3.1. Fourier approach for problem 1

The following complex exponential form of the triple Fourier series representation for $u^p_k$ is considered:

$$(18) \quad u^p_k(x_1, x_2, x_3) = \sum_{n_1}^{\pm\infty} \sum_{n_2}^{\pm\infty} \sum_{n_3}^{\pm\infty} \tilde{u}^p_k(\xi_1, \xi_2, \xi_3)e^{i \xi_j x_j}$$

where $e$ is the base of the natural logarithm, $i = \sqrt{-1}$, $\xi_j = n_j \pi / a_j \ (n_j = 0, \pm 1, \pm 2, \ldots, \ j \ \text{not summed})$, and $\tilde{u}^p_k(\xi_1, \xi_2, \xi_3)$ are the unknown coefficients of the series.

The Hu-Washizu functional (Washizu, 1982) for problem (16), defined on the space of the restrictions in $V$ of the governing variables, takes finite values and hence can be introduced:

$$(19) \quad H^1(u^p_i, \varepsilon_{ij}, \sigma_{ij}) = \frac{1}{2} \int_V C_{ijk} \varepsilon_{hk} \varepsilon_{ij} \ dV - \int_V \sigma_{ij} \varepsilon_{ij} \ dV$$

$$\quad + \frac{1}{2} \int_V \sigma_{ij} (2\varepsilon^o_{ij} + u^p_{i,j} + u^p_{j,i}) \ dV$$

Note that in Eq. (19), as well as in the following equations, the dependence of the functions on $x_1, x_2, x_3$ in the integrals is implicitly understood.

The stationary conditions for the functional (19) with respect to $\sigma_{ij}$ and $\varepsilon_{ij}$ lead to Eqs. (16)$_2$ and (16)$_3$, respectively. The stationary condition with respect to $u^p_i$ yields:

$$(20) \quad 0 = \frac{1}{2} \int_V \sigma_{ij} (\delta u^p_{i,j} + \delta u^p_{j,i}) \ dV = - \int_V \sigma_{ij,j} \delta u^p_i \ dV + \int_{\partial V} \sigma_{ij} n_j \delta u^p_i \ ds$$

Because of the representation formula (18), Eq. (20) leads to the equilibrium Eq. (16)$_1$ and to conditions (14) written in terms of $\sigma_{ij}$ (Washizu, 1982). Furthermore, by satisfying implicitly Eqs. (16)$_2$ and (16)$_3$, the potential energy functional is obtained as:

$$(21) \quad \Phi(u^p_i) = \frac{1}{2} \int_V C_{ijk} \left[ \varepsilon^o_{hk} + \frac{1}{2} \left( u^p_{i,k} + u^p_{k,i} \right) \right] \left[ \varepsilon^o_{ij} + \frac{1}{2} \left( u^p_{i,j} + u^p_{j,i} \right) \right] \ dV$$

By substituting the representation formula (18) with $|n_j| \leq N \ (j = 1, 2, 3)$ into the functional $\Phi$, a consistent approximation of the potential energy is obtained and an approximated solution of the periodic elastostatic problem can be determined. In fact, by minimization of the approximated $\Phi$, it is possible to obtain an approximation of $3(2N + 1)^3$ coefficients of the series (18). In fact, for each of the 3 components of the
displacement vector, $n_1$, as well as $n_2$ and $n_3$, assumes $2N + 1$ values from $-N$ to $N$; as a consequence the triplet $(n_1, n_2, n_3)$ has $(2N + 1)^3$ different combinations.

It is a simple matter to verify that the approximate solution of the periodic problem leads to an estimate $\bar{C}_ijhk^{(N)}$ of the overall elastic tensor, corresponding to an upper bound on $\tilde{C}_ijhk$. In fact, let $u_i^{(\infty)}$ and $u_i^{(N)}$ denote the exact and the approximate stationary points for the functional given in (21), by taking into account Hill’s theorem (1965), we find:

$$\frac{1}{2}C_{ijk}^0e^{ij}_h e^{ij}_k = \Phi(u_i^{(N)}) = \frac{1}{2}C_{ijhk}^0 e^{ij}_h e^{ij}_k V$$

Inequality (22) leads to bounds on the diagonal coefficients: $\bar{C}_ijij \geq \bar{C}_ijij$.

3.2. Fourier approach for problem 2

Equations (17) can be equivalently written in $V$, when an explicit representation formula, which accounts for the $V$-periodicity of the stress $\sigma^p_{ij}$ is considered:

$$\sigma^p_{ij}(x_1, x_2, x_3) = \sum_{n_1}^{\pm\infty} \sum_{n_2}^{\pm\infty} \sum_{n_3}^{\pm\infty} \sigma^p_{ij}(\xi_1, \xi_2, \xi_3)e^{i\xi_h x_h} \quad \text{with } (\xi_1, \xi_2, \xi_3) \neq (0, 0, 0)$$

Note that the case $(\xi_1, \xi_2, \xi_3) = (0, 0, 0)$ is not considered in order to have a null average of $\sigma^p_{ij}$. Once the representation formula (23) is introduced, it is possible to define the Hu-Washizu functional (Washizu, 1982) corresponding to problem (17) posed in $V$ as:

$$H^2(u_i, \varepsilon_{ij}, \sigma^p_{ij}) = \frac{1}{2} \int_V C_{ijkl} e_{hk} e_{ij} dV - \int_V (\sigma^p_{ij} + \sigma^0_{ij}) \varepsilon_{ij} dV$$

$$+ \frac{1}{2} \int_V (\sigma^p_{ij} + \sigma^0_{ij})(u_{ij,i} + u_{ji,j}) dV - \int_{\partial V} (\sigma^p_{ij} + \sigma^0_{ij}) n_j u_i ds$$

The difference between the functionals (19) and (24) is apparent. The stationary conditions for functional (24) with respect to $\varepsilon_{ij}$ yields the Eq. (17)$_3$, and with respect to $\sigma^p$ leads to:

$$0 = \frac{1}{2} \int_V \delta \sigma^p_{ij}(u_{ij,i} + u_{ji,j} - 2\varepsilon_{ij}) dV - \int_{\partial V} \delta \sigma^p_{ij} n_j u_i ds$$

i.e. to Eqs. (17)$_2$ and, by using the null-average stress condition (15), to the expressions:

$$u_i(a_1, x_2, x_3) - u_i(-a_1, x_2, x_3) = 2\chi_{i1} a_1 \quad \forall x_2 \in [-a_2, a_2]$$

$$\forall x_3 \in [-a_3, a_3]$$

$$u_i(x_1, a_2, x_3) - u_i(x_1, -a_2, x_3) = 2\chi_{i2} a_2 \quad \forall x_1 \in [-a_1, a_1]$$

$$\forall x_3 \in [-a_3, a_3]$$

$$u_i(x_1, x_2, a_3) - u_i(x_1, x_2, -a_3) = 2\chi_{i3} a_3 \quad \forall x_1 \in [-a_1, a_1]$$

$$\forall x_2 \in [-a_2, a_2]$$

with $\chi_{ij} = \chi_{ji}$. Relations (26) are exactly the relations (13), with $\chi_{ij} = \varepsilon_{ij}^0$, i.e. $\chi_{ij}$ is the average of the strain compatible with $u_i$. The stationary condition for $H^2$ with respect to $u_i$ yields the equilibrium Eq. (17)$_1$.
Furthermore, by satisfying implicitly Eqs. \((16)_1\) and \((16)_3\), the complementary energy functional is obtained as:

\[
\Psi(\sigma_{ij}^p) = \frac{1}{2} \int_V A_{ijhkk}(\sigma_{hjk}^p + \sigma_{hkk}^p)(\sigma_{ij}^p + \sigma_{ij}^p) \, dV
\]

where \(A_{ijhkk}\) is the inverse of \(C_{ijhkk}\).

A consistent approximation of the complementary energy is obtained by substituting the representation formula (23) with \(|n_j| \leq M\) \((j = 1, 2, 3)\) into functional (27). The minimization of functional (27), under the equilibrium constraint, allows an approximation of \(6\left[(2M + 1)^3 - 1\right]\) coefficients of series (23) to be determined. In fact, for each of the 6 components of the symmetric stress tensor, \(n_1\), as well as \(n_2\) and \(n_3\), assumes \(2M + 1\) values from \(-M\) to \(M\); as a consequence the triplet \((n_1, n_2, n_3)\) has \((2M + 1)^3\) different combinations, but the triplet \((0, 0, 0)\) corresponding to the mean value of the functions has not to be considered, as previously emphasized.

This approximate solution of the periodic inclusion problem leads to an estimate \(\overline{A}^{(M)}_{ijhkk}\) of the overall elastic compliance tensor, corresponding to an upper bound on \(\overline{A}_{ijhkk}\). In fact, let \(\sigma_{ij}^{p(\infty)}\) and \(\sigma_{ij}^{p(M)}\) denote the exact and the approximate stationary points for the functional given in (27), by taking into account Hill’s theorem (1965), we find:

\[
\frac{1}{2} \overline{A}^{(M)}_{ijhkk} \sigma_{hjk}^0 \sigma_{ij}^p \, V = \Psi(\sigma_{ij}^{p(\infty)}) \geq \Psi(\sigma_{ij}^{p(M)}) = \frac{1}{2} \overline{A}_{ijhkk} \sigma_{hjk}^0 \sigma_{ij}^p \, V
\]

Of course, if \(\overline{c}_{ijhkk}\) is the inverse of \(\overline{A}^{(M)}_{ijhkk}\), then \(\overline{c}_{ijhkk} \leq \overline{c}_{ijhkk}\). Note that, by using both (22) and (28), it is possible to obtain bounds on the off-diagonal coefficients \(\overline{c}_{ijhkl}\) as proposed by Bisegna and Luciano (1996).

4. Average constraints and boundary conditions

In this section, an alternative approach to the Fourier series is presented. Specifically, the average constraints and suitable boundary conditions on \(\partial V\) are imposed to reduce the problem from \(\mathbb{R}^3\) to \(V\).

4.1. \(V\)-periodicity of \(u_i^p\) FOR PROBLEM 1

The \(V\)-periodicity and the continuity on \(\partial V\) of \(u_i^p\) allows the restriction of \(u_i^p\) in \(V\), satisfying the boundary conditions (12) to be considered. Thus, problem 1 governed by Eq. (16) can be recast only in \(V\) with constraint (12). These boundary conditions are imposed by using the Lagrange multipliers technique within the Hu-Washizu functional (19) as follows:

\[
W^1(u_i^p, \varepsilon_{ij}, \sigma_{ij}, \lambda_i^1, \lambda_i^2, \lambda_i^3) = \frac{1}{2} \int_V C_{ijhkk} \varepsilon_{hjk} \varepsilon_{ij} \, dV - \int_V \sigma_{ij} \varepsilon_{ij} \, dV + \frac{1}{2} \int_V \sigma_{ij}(2\varepsilon_{ij} + u_i^p + u_i^p) \, dV
\]

\[
- \int_{a_1}^{a_1} \int_{-a_2}^{a_2} \lambda_1^1 \left( u_i^p(a_1, x_2, x_3) - u_i^p(-a_1, x_2, x_3) \right) \, dx_2 dx_3
\]

\[
- \int_{a_1}^{a_1} \int_{-a_3}^{a_3} \lambda_2^2 \left( u_i^p(x_1, a_2, x_3) - u_i^p(x_1, -a_2, x_3) \right) \, dx_1 dx_3
\]

\[
- \int_{-a_1}^{-a_1} \int_{a_2}^{a_2} \lambda_3^3 \left( u_i^p(x_1, x_2, a_3) - u_i^p(x_1, x_2, -a_3) \right) \, dx_1 dx_2
\]
The stationary conditions for the functional (29) with respect to \( \sigma_{ij} \), \( \varepsilon_{ij} \) and \( \lambda_i^1, \lambda_i^2, \lambda_i^3 \) lead to Eqs. (16)_2, (16)_3 and the boundary conditions (12), respectively. The stationary condition with respect to \( u_i^p \) yields:

\[
0 = - \int_V \sigma_{ij,j} \delta u_i^p \, dV + \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} \left\{ \left[ \sigma_{ij,n_j} - \lambda_i^1 \right] \delta u_i^p \right\}_{x_1 = a_1} - \left\{ \left[ \sigma_{ij,n_j} + \lambda_i^1 \right] \delta u_i^p \right\}_{x_1 = -a_1} \, dx_2 \, dx_3 \\
+ \int_{-a_3}^{a_3} \int_{-a_3}^{a_3} \left\{ \left[ \sigma_{ij,n_j} - \lambda_i^2 \right] \delta u_i^p \right\}_{x_2 = a_2} - \left\{ \left[ \sigma_{ij,n_j} + \lambda_i^2 \right] \delta u_i^p \right\}_{x_2 = -a_2} \, dx_1 \, dx_3 \\
+ \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \left\{ \left[ \sigma_{ij,n_j} - \lambda_i^3 \right] \delta u_i^p \right\}_{x_3 = a_3} - \left\{ \left[ \sigma_{ij,n_j} + \lambda_i^3 \right] \delta u_i^p \right\}_{x_3 = -a_3} \, dx_1 \, dx_2
\]

which gives:

\[
\lambda_i^1 = \sigma_{ij,n_j} \big|_{x_1 = a_1} = -\sigma_{ij,n_j} \big|_{x_1 = -a_1} \quad \forall x_2 \in [-a_2, a_2] \quad \forall x_3 \in [-a_3, a_3] \\
\lambda_i^2 = \sigma_{ij,n_j} \big|_{x_2 = a_2} = -\sigma_{ij,n_j} \big|_{x_2 = -a_2} \quad \forall x_1 \in [-a_1, a_1] \quad \forall x_3 \in [-a_3, a_3] \\
\lambda_i^3 = \sigma_{ij,n_j} \big|_{x_3 = a_3} = -\sigma_{ij,n_j} \big|_{x_3 = -a_3} \quad \forall x_1 \in [-a_1, a_1] \quad \forall x_2 \in [-a_2, a_2]
\]

Hence, the Lagrange multipliers \( \lambda_i^1, \lambda_i^2, \lambda_i^3 \) represent the tractions between adjacent cells. Furthermore, it can be emphasized that when boundary conditions (12) are imposed, because of Eqs. (31), the requirements of (14) on the stress on \( \partial V \) are automatically guaranteed.

By satisfying implicitly Eqs. (16)_2 and (16)_3 the potential energy functional is obtained as:

\[
\phi(u_i^p, \lambda_i^1, \lambda_i^2, \lambda_i^3) = \Phi(u_i^p) \\
\quad - \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} \lambda_i^1 \left( u_i^p(a_1, x_2, x_3) - u_i^p(-a_1, x_2, x_3) \right) \, dx_2 \, dx_3 \\
\quad - \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \lambda_i^2 \left( u_i^p(x_1, a_2, x_3) - u_i^p(x_1, -a_2, x_3) \right) \, dx_1 \, dx_3 \\
\quad - \int_{-a_1}^{a_1} \int_{-a_2}^{a_2} \lambda_i^3 \left( u_i^p(x_1, x_2, a_3) - u_i^p(x_1, x_2, -a_3) \right) \, dx_1 \, dx_2
\]

where the functional \( \Phi \) is defined in (21).

By substituting relation (11) into the functional (32), a new potential energy is obtained in terms of total displacement \( u_i \) and Lagrange multipliers \( \lambda_i^1, \lambda_i^2, \lambda_i^3 \):

\[
\tilde{\phi}(u_i, \lambda_i^1, \lambda_i^2, \lambda_i^3) = \frac{1}{2} \int_V C_{ijh} \frac{1}{2}(u_{h,k} + u_{k,h}) \frac{1}{2}(u_{i,j} + u_{j,i}) \, dV \\
\quad - \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} \lambda_i^1 \left( u_i(a_1, x_2, x_3) - u_i(-a_1, x_2, x_3) - 2\varepsilon_{11}^0(a_1) \right) \, dx_2 \, dx_3 \\
\quad - \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \lambda_i^2 \left( u_i(x_1, a_2, x_3) - u_i(x_1, -a_2, x_3) - 2\varepsilon_{22}^0(a_2) \right) \, dx_1 \, dx_3 \\
\quad - \int_{-a_1}^{a_1} \int_{-a_2}^{a_2} \lambda_i^3 \left( u_i(x_1, x_2, a_3) - u_i(x_1, x_2, -a_3) - 2\varepsilon_{33}^0(a_3) \right) \, dx_1 \, dx_2
\]
which could be obtained directly by adding the Lagrangian term due to constraint (13) to the potential energy in terms of \( u_i \).

The discretization via the finite element method of the functionals (32) and (33) allows an approximate solution of problem 1 to be obtained. It is a simple matter to prove that, by means of this approximate solution, an upper bound for the diagonal coefficients of the overall elastic tensor is obtained.

4.2. \( V \)-PERIODICITY OF \( \sigma_{ij}^p \) FOR PROBLEM 2

The stress \( \sigma_{ij}^p \) must satisfies the constraint (15) and, for \( V \)-periodicity and continuity of the tractions on \( \partial V \), it can be considered as a function defined only in \( V \) which also satisfies the boundary conditions (14). Thus, problem 2 governed by Eq. (17) can be recast in \( V \) with the constraints (14) and (15), which are imposed by using the Lagrange multipliers technique within the Hu-Washizu functional (24):

\[
W^2(u_i, \varepsilon_{ij}, \sigma_{ij}^p, \mu_{ij}, \kappa_1, \kappa_2, \kappa_3) = \frac{1}{2} \int_V C_{ijkl} \varepsilon_{kl} \varepsilon_{ij} dV - \int_V (\sigma_{ij}^p + \sigma_{ij}^p) \varepsilon_{ij} dV + \int_V (\sigma_{ij}^p + \sigma_{ij}^p) \frac{1}{2} (u_{ij} + u_{ij,i}) dV - \int_{\partial V} (\sigma_{ij}^p + \sigma_{ij}^p) n_j u_i ds + \mu_{ij} \int_{\partial A_1} a_1 (\sigma_{ih} n_h n_j + n_i \sigma_{ijh} n_h) dx_2 dx_3 + \int_{\partial A_2} a_2 (\sigma_{ih} n_h n_j + n_i \sigma_{ijh} n_h) dx_1 dx_3 + \int_{\partial A_3} a_3 (\sigma_{ih} n_h n_j + n_i \sigma_{ijh} n_h) dx_1 dx_2  
\]

\[
- \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \kappa_1 \left( \sigma_{ij}^p (a_1, x_2, x_3) - \sigma_{ij}^p (-a_1, x_2, x_3) \right) n_j \bigg|_{x_1 = a_1} dx_2 dx_3  
\]

\[
- \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \kappa_2 \left( \sigma_{ij}^p (x_1, a_2, x_3) - \sigma_{ij}^p (x_1, -a_2, x_3) \right) n_j \bigg|_{x_2 = a_2} dx_1 dx_3  
\]

\[
- \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \kappa_3 \left( \sigma_{ij}^p (x_1, x_2, a_3) - \sigma_{ij}^p (x_1, x_2, -a_3) \right) n_j \bigg|_{x_3 = a_3} dx_1 dx_2  
\]

where the relations \( n_h \big|_{x_i = a_i} = -n_h \big|_{x_i = -a_i} \) with \( i = 1, 2, 3 \) are implicitly accounted for. The vectors \( \kappa_1(x_2, x_3) \), \( \kappa_2(x_1, x_3) \), \( \kappa_3(x_1, x_2) \) and the constant tensor \( \mu_{ij} \) are the Lagrange multipliers of the constraints (14) and (15), respectively. The stationary conditions for functional (34) with respect to \( u_i, \varepsilon_{ij} \) and to the Lagrange multipliers \( \kappa_1, \kappa_2, \kappa_3 \) and \( \mu_{ij} \) lead to Eqs. (17)1, (17)3 and to conditions (14) and (15), respectively. The stationary condition with respect to \( \sigma_{ij}^p \) yields:

\[
0 = -\int_V \varepsilon_{ij} \delta \sigma_{ij}^p dV + \int_V \frac{1}{2} (u_{ij} + u_{ij,i}) \delta \sigma_{ij}^p dV  
+ \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \left\{ (2a_1 \mu_{ij} n_j - u_i - \kappa_1) \delta \sigma_{ij}^p n_j \right\} \bigg|_{x_1 = a_1} dx_2 dx_3  
+ \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \left\{ (2a_2 \mu_{ij} n_j - u_i - \kappa_2) \delta \sigma_{ij}^p n_j \right\} \bigg|_{x_2 = a_2} dx_1 dx_3  
+ \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \left\{ (2a_3 \mu_{ij} n_j - u_i - \kappa_3) \delta \sigma_{ij}^p n_j \right\} \bigg|_{x_3 = a_3} dx_1 dx_2  
\]
which gives:

\begin{align}
  u_i(a_1, x_2, x_3) - u_i(-a_1, x_2, x_3) - 2\mu_1 a_1 &= 0 \quad \forall x_2 \in [-a_2, a_2] \\
  u_i(x_1, a_2, x_3) - u_i(x_1, -a_2, x_3) - 2\mu_2 a_2 &= 0 \quad \forall x_3 \in [-a_3, a_3] \\
  u_i(x_1, x_2, a_3) - u_i(x_1, x_2, -a_3) - 2\mu_3 a_3 &= 0 \quad \forall x_2 \in [-a_2, a_2]
\end{align}

(36)

\begin{align}
  u_i(-a_1, x_2, x_3) + \kappa_1^i(x_2, x_3) &= 0 \quad \forall x_2 \in [-a_2, a_2] \\
  u_i(x_1, -a_2, x_3) + \kappa_2^i(x_1, x_3) &= 0 \quad \forall x_3 \in [-a_3, a_3] \\
  u_i(x_1, x_2, -a_3) + \kappa_3^i(x_1, x_2) &= 0 \quad \forall x_2 \in [-a_2, a_2]
\end{align}

(37)

By a simple comparison of Eqs. (36) with the formulae given in (13), the mechanical meaning of the Lagrange multiplier \( \mu_{ij} \) clearly appears: it represents the average strain in the unit cell, i.e. \( \mu_{ij} = \varepsilon_{ij}^0 \). Note that when the boundary conditions (14) and (15) are imposed, because of Eqs. (36), the requirements on the displacement on \( \partial V \) given by (12) are automatically satisfied. Furthermore, Eqs. (37) shows that the negative of the Lagrange multipliers \( \kappa_1^i, \kappa_2^i \), and \( \kappa_3^i \) are the displacements of the boundary surfaces of the unit cell defined at \( x_1 = -a_1, x_2 = -a_2 \) and \( x_3 = -a_3 \), respectively.

By satisfying implicitly Eqs. (17)_1 and (17)_3 and by taking into account (15), the complementary energy can be written in terms of \( \sigma_{ij}^p \), and the Lagrangian multipliers \( \mu_{ij}, \kappa_1^i, \kappa_2^i, \kappa_3^i \) as:

\begin{align}
  \psi(\sigma_{ij}^p, \mu_{ij}, \kappa_1^i, \kappa_2^i, \kappa_3^i) &= \tilde{\psi}(\sigma_{ij}^p, \mu_{ij}) \\
  &= \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} \left[ \sigma_{ij}^p(a_1, x_2, x_3) - \sigma_{ij}^p(-a_1, x_2, x_3) \right] n_j \left|_{x_1=a_1} \right. dx_2 dx_3 \\
  &\quad - \int_{-a_1}^{a_1} \int_{-a_3}^{a_3} \left[ \sigma_{ij}^p(x_1, a_2, x_3) - \sigma_{ij}^p(x_1, -a_2, x_3) \right] n_j \left|_{x_2=a_2} \right. dx_1 dx_3 \\
  &\quad - \int_{-a_1}^{a_1} \int_{-a_2}^{a_2} \left[ \sigma_{ij}^p(x_1, x_2, a_3) - \sigma_{ij}^p(x_1, x_2, -a_3) \right] n_j \left|_{x_3=a_3} \right. dx_1 dx_2
\end{align}

(38)

where the functional \( \tilde{\psi} \) is:

\[
\tilde{\psi}(\sigma_{ij}^p, \mu_{ij}) = \frac{1}{2} \int_V A_{ij, hh} (\sigma_{hh}^0 + \sigma_{ij}^p + \sigma_{ij}^p) dV + \mu_{ij} \int_V \sigma_{ij}^p dV
\]

Furthermore, the equilibrium condition of (17)_1 can be simply enforced in the complementary energy \( \psi \), by using the penalty method (Brezzi and Fortin, 1991). Thus, a new penalized functional is obtained:

\[
\psi^p(\sigma_{ij}^p, \mu_{ij}, \kappa_1^i, \kappa_2^i, \kappa_3^i) = \psi(\sigma_{ij}^p, \mu_{ij}, \kappa_1^i, \kappa_2^i, \kappa_3^i) + \frac{1}{2\eta} \int_V \left\| \sigma_{ij}^p \right\|^2 dV
\]

(39)

where \( \eta \) is the penalty parameter. For this functional, it appears convenient to apply Uzawa’s method (Brezzi and Fortin, 1991) to treat the constraint on the average of the stress field. This method allows a sequence of
\((\sigma_{ij}^p, \mu_{ij}, \kappa_i^1, \kappa_i^2, \kappa_i^3)\), whose \(k\)-th term is indicated as \((\sigma_{ij}^{[k]}, \mu_{ij}^{[k]}, \kappa_i^{1[k]}, \kappa_i^{2[k]}, \kappa_i^{3[k]})\), to be defined using the following scheme:

1. choose an arbitrary \(\mu_{ij}^{[0]}\) as first approximation of the Lagrange multipliers
2. with \(\mu_{ij}^{[k]}\) assigned, find \(\sigma_{ij}^{[k]}, \kappa_i^{1[k]}, \kappa_i^{2[k]}, \kappa_i^{3[k]}\) such that \(\psi(\sigma_{ij}^{[k]}, \mu_{ij}^{[k]}, \kappa_i^{1[k]}, \kappa_i^{2[k]}, \kappa_i^{3[k]})\) is stationary
3. compute \(\mu_{ij}^{[k+1]} = \mu_{ij}^{[k]} + \rho \left( \frac{1}{V} \int_V \sigma_{ij}^{[k]} \, dV \right)\)
4. if the quantity \(|\mu_{ij}^{[k+1]} - \mu_{ij}^{[k]}|\) is greater than a fixed tolerance, go to step 2, otherwise stop the procedure.

Note that \(\rho\) is an appropriate numerical parameter. The use of the Uzawa procedure allows the solution of the constrained problem to be obtained in terms of \(\sigma_{ij}^p, \kappa_i^1, \kappa_i^2, \kappa_i^3\) and Lagrange multiplier \(\mu_{ij}\), representing the average strain, in fact \(\lim_{k \to \infty} \mu_{ij}^{[k]} = \varepsilon_{ij}^0\).

The discretization of functional (39) via the finite element method allows the determination of an approximate solution of problem 2. It is possible to prove that, by means of this approximate solution, a lower bound on the diagonal coefficients of the overall elastic tensor is obtained.

5. Numerical applications

In this section, numerical examples are carried out by adopting the approximate numerical methods previously proposed for the homogenization of solids with periodic microstructures. The applications are developed for two-dimensional plane strain problems.

Three unit cells are considered in the computations and their geometries are reported in Figures 1 and 2, and are denoted by cell 1, cell 2a and cell 2b. The numerical values adopted are \(h = 75\) mm, \(s = 225\) mm and \(t = 15\) mm. The matrix \((m)\) and the inclusions \((i)\) are isotropic with elastic moduli: \(E_i = 15000\) MPa, \(\nu_i = 0.25\), \(E_m = 1000\) MPa, and \(\nu_m = 0.3\). These values are equal to the ones adopted in Kralj et al. (1991) and Luciano and Sacco (1997).

Indeed, cells 1, 2a and 2b represent two classical repetitive cells of a masonry structure, as shown in Figures 1 and 2, since unit cells 2a and 2b characterize the same periodic microstructure. In particular, cell 2a has two perpendicular axes of symmetry, while cell 2b is not symmetric.

First, the Fourier method is adopted both for the displacement and the stress formulation. The minima of the functionals \(\Phi\) and \(\Psi\) are obtained numerically by considering only \(2(2N + 1)^2\) and \((2M + 1)^2 - 1\) terms of the Fourier series representations of \(u_1^p, u_2^p\) and of \(\sigma_{11}^p, \sigma_{22}^p, \sigma_{12}^p\), respectively. In particular, the minimization of the complementary energy \(\Psi\) is performed by using a Fourier representation of the stress components which automatically satisfy the equilibrium equation (1). By using both the formulations, lower and upper bounds on the effective properties of the material are obtained. In particular, the analyses are carried out by setting \(N = 12\) and \(M = 12\).

Next, the elastic moduli of the unit cells are derived by employing the finite element approximation of the variational principles previously presented and also by applying homogeneous boundary conditions on cells 1 and 2a. Initially, the formulation based on the functional \(\psi\) is considered. Successively, the stress formulation based on the functional \(\psi^S\) is used and the solution technique, based on the Uzawa method and presented in the previous section, is applied. This iterative procedure appears efficient and presents a fast convergence. When cell 1 is considered, a mesh of 768 isoparametric four node elements have been adopted for both the displacement and stress analyses. Cells 2a and 2b are discretized by a smaller number of elements, but of the
masonry type 1

cell 1

Fig. 1. – Periodic masonry: arrangement type 1.

same size as the ones adopted for cell 1. The penalty and the Uzawa parameters are taken as \(1/\eta = 20000\) mm²/MPa and \(\rho = 1\) (MPa)\(^{-1}\), respectively.

It is worth noting that, when the unit cell presents two perpendicular axes of symmetry and a very particular mean strain is considered (i.e., \(\{\varepsilon_{11}^0, \varepsilon_{22}^0, \varepsilon_{12}^0\} = \{1, 0, 0\}\) or \(\{\varepsilon_{11}^0, \varepsilon_{22}^0, \varepsilon_{12}^0\} = \{0, 1, 0\}\) or \(\{\varepsilon_{11}^0, \varepsilon_{22}^0, \varepsilon_{12}^0\} = \{0, 0, 1\}\)), the periodic boundary conditions can be transformed into homogeneous ones as discussed by Suquet (1987). For this reason, cell 1 and cell 2a can be also analyzed by using the displacement finite element method with appropriate homogeneous boundary conditions; on the contrary, cell 2b must be studied by employing the variational principles presented in this paper. Furthermore, even when a unit cell has two perpendicular axes of symmetry and a particular mean stress is considered (i.e., \(\{\sigma_{11}^0, \sigma_{22}^0, \sigma_{12}^0\} = \{1, 0, 0\}\) or \(\{\sigma_{11}^0, \sigma_{22}^0, \sigma_{12}^0\} = \{0, 1, 0\}\) or \(\{\sigma_{11}^0, \sigma_{22}^0, \sigma_{12}^0\} = \{0, 0, 1\}\)), a standard finite element stress approach involving appropriate homogeneous boundary conditions cannot be used since the null average constraint (15) must be enforced.

The elastic moduli obtained by using the four approaches proposed herein (Fourier stress, Fourier displacement, F.E.M. stress and F.E.M. displacement) for cell 1 are compared in Table I with the results obtained in Kralj et al. (1991) and Luciano and Sacco (1997) and the estimates carried out by using the Hashin and Shtrikman (H-S) principles with \(12 \times 12\) piecewise constant periodic polarization fields (Nemat-Nasser et al., 1993). Furthermore, the elastic moduli were also determined by a displacement finite element method with homogeneous boundary
masonry type 2

cell 2a  cell 2b

Fig. 2. – Periodic masonry: arrangement type 2.

<table>
<thead>
<tr>
<th>Moduli (MPa)</th>
<th>$\bar{c}_{1111}$</th>
<th>$\bar{c}_{2222}$</th>
<th>$\bar{c}_{1212}$</th>
<th>$\bar{c}_{1122}$</th>
<th>$\bar{c}_{1222}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>estimate in Luciano and Sacco (1997)</td>
<td>8942</td>
<td>5595</td>
<td>1562</td>
<td>1578</td>
<td></td>
</tr>
<tr>
<td>estimate in Kralj et al. (1991)</td>
<td>8242</td>
<td>5593</td>
<td>1521</td>
<td>1504</td>
<td></td>
</tr>
<tr>
<td>H-S (lower)</td>
<td>(bound)</td>
<td>(bound)</td>
<td>(bound)</td>
<td>(estimate)</td>
<td>(bound)</td>
</tr>
<tr>
<td>H-S (upper)</td>
<td>8213</td>
<td>5440</td>
<td>1521</td>
<td>1726</td>
<td>371</td>
</tr>
<tr>
<td>Fourier stress (lower)</td>
<td>10203</td>
<td>6678</td>
<td>1952</td>
<td>1941</td>
<td>3296</td>
</tr>
<tr>
<td>Fourier displacement (upper)</td>
<td>8595</td>
<td>5501</td>
<td>1556</td>
<td>1670</td>
<td>283</td>
</tr>
<tr>
<td>F.E.M. stress (lower)</td>
<td>11584</td>
<td>6474</td>
<td>1811</td>
<td>1988</td>
<td>3375</td>
</tr>
<tr>
<td>F.E.M. displacement (lower)</td>
<td>8452</td>
<td>5473</td>
<td>1554</td>
<td>1498</td>
<td>1292</td>
</tr>
<tr>
<td>F.E.M. displacement (upper)</td>
<td>8986</td>
<td>5615</td>
<td>1566</td>
<td>1567</td>
<td>1773</td>
</tr>
</tbody>
</table>

conditions, but they are not reported since they are exactly equal to the F.E.M. displacement results given in the last row of Table I.

The overall properties computed for cell 2a via the displacement and stress approaches are equal to the ones of cell 2b, and are reported in Table II. Analogous to cell 1, a displacement finite element analysis of cell 2a subject to ordinary boundary conditions provides results equal to the ones reported in the last row of Table II.

A comparison of the results given in Tables I and II shows the influence of the arrangement of the inclusions on the overall behavior of the composite material.
Table II. - Elastic moduli for the masonry material characterized by unit cell 2.

<table>
<thead>
<tr>
<th>Moduli (MPa)</th>
<th>$\bar{C}_{1111}$ (bound)</th>
<th>$\bar{C}_{2222}$ (bound)</th>
<th>$\bar{C}_{1212}$ (bound)</th>
<th>$\bar{C}_{1122}$ (estimate)</th>
<th>$\bar{C}_{1122}$ (bound)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-S (lower)</td>
<td>8499</td>
<td>5561</td>
<td>1450</td>
<td>1524</td>
<td>1021</td>
</tr>
<tr>
<td>H-S (upper)</td>
<td>9404</td>
<td>5965</td>
<td>1593</td>
<td>1626</td>
<td>2129</td>
</tr>
<tr>
<td>Fourier stress (lower)</td>
<td>8475</td>
<td>5539</td>
<td>1453</td>
<td>1541</td>
<td>731</td>
</tr>
<tr>
<td>Fourier displacement (upper)</td>
<td>10419</td>
<td>6152</td>
<td>1716</td>
<td>1823</td>
<td>2632</td>
</tr>
<tr>
<td>F.E.M. stress (lower)</td>
<td>8340</td>
<td>5551</td>
<td>1451</td>
<td>1541</td>
<td>1378</td>
</tr>
<tr>
<td>F.E.M. displacement (upper)</td>
<td>8690</td>
<td>5627</td>
<td>1461</td>
<td>1482</td>
<td>1645</td>
</tr>
</tbody>
</table>

Note that the diagonal coefficients $\bar{C}_{ijij}$ reported in Tables I and II represent bounds on the overall elastic properties. On the other hand, the values of the off-diagonal coefficient $\bar{C}_{1122}$ are not bounds, but they are used to compute the bounds on $\bar{C}_{1212}$ given in the last columns of Tables I and II, by applying the following formulas proposed by Bisegna and Luciano (1996):

$$\bar{C}_{1122}^{\text{upper}} = \min \left\{ \bar{C}_{1122}^{-}, \bar{C}_{1122}^{+} \right\} + \sqrt{\left( \bar{C}_{1111}^{\text{upper}} - \bar{C}_{1111}^{\text{lower}} \right) \left( \bar{C}_{2222}^{\text{upper}} - \bar{C}_{2222}^{\text{lower}} \right)}$$

$$\bar{C}_{1122}^{\text{lower}} = \max \left\{ \bar{C}_{1122}^{-}, \bar{C}_{1122}^{+} \right\} - \sqrt{\left( \bar{C}_{1111}^{\text{upper}} - \bar{C}_{1111}^{\text{lower}} \right) \left( \bar{C}_{2222}^{\text{upper}} - \bar{C}_{2222}^{\text{lower}} \right)}$$

where $\bar{C}_{1122}^{+}$ and $\bar{C}_{1122}^{-}$ are the estimates of $\bar{C}_{1122}$ associated with the upper and lower bounds of the diagonal coefficients, respectively.

In Figures 3 and 4 plots of the periodic stress components $\sigma_{11}^{\rho}$ and $\sigma_{22}^{\rho}$ in MPa of cells 1 and 2a, corresponding to an assigned average strain tensor $\bar{e}_{11}^{\rho} = 0$, $\bar{e}_{22}^{\rho} = 0$, and $\bar{e}_{12}^{\rho} = 1$, are presented. Analogously, in Figures 5 and 6 the same results are reported for the case of an assigned stress with components $\sigma_{11}^{\rho} = 0$, $\sigma_{22}^{\rho} = 0$, and $\sigma_{12}^{\rho} = 1$. It is important to note that the results obtained by imposing the average strain $\bar{e}^{\rho}$ or the average stress $\sigma^{\rho}$ cannot be directly compared, since the load conditions enforced on the cells are not equal. The distributions of the stresses for cell 2b are equal to those for cell 2a.

An analysis of the numerical results indicates that, although the overall behavior of the two masonry is not very different, the local distribution of the governing variables changes completely. In fact different stress distributions are obtained for the two cases considered. Figures 3-6 show that stress concentrations are present along the horizontal or vertical axes in the matrix of the composite for cell 1. On the contrary, in cell 2a or 2b stress concentrations are localized only at the corners of the inclusion.

Finally, in Figure 7, upper and lower bounds of the elastic coefficient $C_{1212}$, obtained by adopting the displacement and the stress finite element formulation, respectively, are plotted versus the mesh discretization parameter $\rho$. The number of elements is given by (16 $\rho$) x (6 $\rho$). Convergence of the overall elastic coefficient to a constant value can be observed when a finer mesh is used, and furthermore the numerical demonstration that the displacement and the stress approach provide upper and lower bounds, respectively.

It is worth noting that improvements of the results can be obtained by increasing the number of unknowns adopted (i.e. the number of Fourier coefficients or finite elements). In fact, both the Fourier and finite element methods are Galerkin's approximation procedures, and adopt subspaces of interpolation functions dense in the original spaces where the periodic elastostatic problems of (16) and (17) are posed. Hence, the convergence of the overall elastic coefficients obtained by using the Fourier series and the finite element methods to the exact values is warranted even when there are singularities of the stresses at sharp corners (Oden and Reddy, 1976).
Fig. 3. – Stress component $\sigma_{11}$ for $\varepsilon_{11}' = 0, \varepsilon_{22}'' = 0, \varepsilon_{12}'' = 1$.

Fig. 4. – Stress component $\sigma_{22}$ for $\varepsilon_{11}' = 0, \varepsilon_{22}'' = 0, \varepsilon_{12}'' = 1$.  

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Fig. 5. Stress component $\sigma_{11}$ for $\sigma_{11}^{(i)} = 0, \sigma_{22}^{(i)} = 0, \sigma_{ij}^{(i)} = 1$.

Fig. 6. Stress component $\sigma_{22}$ for $\sigma_{11}^{(i)} = 0, \sigma_{22}^{(i)} = 0, \sigma_{ij}^{(i)} = 1$. 
6. Conclusions

Several new variational formulations of the periodic elastostatic problem have been proposed in terms of displacements or stresses, in order to solve the homogenization problem for heterogeneous media with periodic microstructures. These formulations are the bases for numerical approximation techniques. Herein, the Fourier series and the finite element methods have been developed and appropriate computer codes have been implemented to obtain numerical estimates of the effective elastic properties of periodic composite materials.

Two interesting examples have been analyzed by using the numerical techniques presented and, the results have been compared with those available in the literature. In particular, the numerical results show that the methods herein proposed provide good estimates and bounds on the overall properties.

Further, it is worth noting that, by using the proposed formulations, it is possible to obtain the stress or the displacement distribution in the cell by fully accounting for the interactions between the inclusions, even when they present complex unsymmetric geometries.

Acknowledgments

Financial support of the Italian National Research Council (CNR) and Ministry of University and Research (MURST) are gratefully acknowledged.

REFERENCES

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(Manuscript received March 03, 1997; Revised August 18, 1997.)