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Asymptotic homogenisation in linear elasticity. Part I: Mathematical formulation and finite element modelling

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A B S T R A C T

The asymptotic expansion homogenisation method is an excellent methodology to model physical phenomena on media with periodic microstructure and a useful technique to study the mechanical behaviour of structural components built with composite materials. In the first part of this work the authors present a detailed form of the mathematical formulation of the asymptotic expansion homogenisation for linear elasticity problems, as well the explicit mathematical equations that characterise the microstructural stress and strain fields associated with a given macrostructural equilibrium state – the localisation procedure. From this mathematical basis, the authors also present the numerical equations resulting from the finite element modelling of the asymptotic expansion homogenisation method in linear elasticity.

1. Introduction

The numerical simulation of the mechanical behaviour of complex microstructure composite materials often leads to the need for significant resources in terms of memory and CPU time. In this context, numerical models used to predict the behaviour of these materials are developed. One of these methods is the asymptotic expansion homogenisation (AEH). Applying the AEH, overall material properties can be derived from the mechanical behaviour of selected microscale representative volumes (also known as representative unit-cells, RUC) with specific periodic boundary conditions.

The homogenisation method equations for cellular media have been previously presented, in a weak form derivation, by Guedes and Kikuchi [1]. Although this derivation is suitable for the finite element method formulation, the use of the strong form allows a better understanding of the mathematical and physical multiscale relations of the method. With this in mind, the authors present a detailed strong form derivation of the asymptotic expansion homogenisation for linear elasticity problems. In addition, some of the main aspects of the higher-order displacement correctors and localisation procedure, as well as the numerical equations resulting from the finite element modelling of the method, are also discussed.

2. Asymptotic expansion homogenisation in linear elasticity

The detailed numerical modelling of the mechanical behaviour of composite material structures often involves high computational costs. In this scope, the use of homogenisation methodologies can lead to significant benefits. These techniques allow the substitution of a heterogeneous medium for an equivalent homogenous medium, therefore allowing the use of macrostructural behaviour laws obtained from microstructural information.

On the other hand, composite materials typically have heterogeneities with characteristic dimensions much smaller than the dimensions of the structural component itself. If the distribution of the heterogeneities is roughly periodical, it can usually be approximated by the periodical repetition of a unit-cell, representative of the microstructural details of the composite material.

With this in mind, the asymptotic expansion homogenisation method is an excellent methodology to model physical phenomena

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on media with periodic microstructure, as well as a useful technique to study the mechanical behaviour of structural components built with composite materials. The main numerical advantages of this method are (i) the fact that it allows a significant reduction of the number of degrees of freedom and (ii) the capability to find the stress and strain microstructural fields associated with a given macrostructural equilibrium state. In fact, unlike other common homogenisation methods, the AEH leads to explicit mathematical equations to characterise those fields. This process is often called localisation.

The concept of homogenisation applied to physical properties goes back to the nineteenth century [2–4]. However, the first published work on mathematical homogenisation theory dates to the end of the 1960s [5–7]. Since then, several homogenisation methods have been proposed, from which the AEH stands out as one of the most important [8,9]. This method allows the calculation of average (homogenised) values for the mechanical properties of a given composite material. However, the AEH cannot be used with non-periodical microstructures. In this case, other homogenisation methodologies are better suited, such as the G-convergence [5] – for symmetric non-periodic problems –, H-convergence [10] – for non-symmetric non-periodic problems – and Γ-convergence [11] – for problems that allow a variational formulation. Even so, these methodologies do not lead to the homogenised properties the composite material, but only to estimates for its upper and lower bounds.

In this section the authors present the main features associated to the application of the AEH methodology to the linear elasticity problem. Some notions about higher-order terms of the asymptotic expansion of the displacement field are also presented and the formulation for the localisation problem is shown.

2.1. Differential formulation of the elasticity problem

Consider a heterogeneous linear elastic material associated to a material body Ω. The microstructure of Ω is made of a spatially periodic distribution of a representative unit-cell associated to a region Y, as illustrated in Fig. 1. Most heterogeneous materials with periodic microstructures have a very small relation ϵ ($\epsilon \ll 1$) between the micro- and macroscale characteristic dimensions. The mechanical loading of such materials creates periodic oscillations on the resulting displacement, stress or strain fields. These oscillations are a consequence of the periodicity of the microstructural heterogeneities and are evident in a neighbouring region of dimension ϵ of any point of Ω. In this context, the existence of two different scales $\mathbf{x}$ and $\mathbf{y}$, each associated respectively to the material behaviour phenomena on the macroscale Ω and microscale Y levels (see Fig. 1), is often assumed. Thus, the variables associated to the referred fields become functionally dependent on both $\mathbf{x}$ and $\mathbf{y}$ systems, where

$$\mathbf{y} = \mathbf{x}/\epsilon. \tag{1}$$

The functional dependence on $\mathbf{y}$ is periodical in Y. This property is usually called Y-periodicity. In terms of elastic properties, the Y-periodicity of the microstructural heterogeneities reflects itself on the fact that the elasticity tensor $\mathbf{D}$ is Y-periodic in $\mathbf{y}$. In contrast, the material homogeneity at the macroscale level results from the fact that the elasticity tensor components do not depend on the macroscale system of coordinates, $\mathbf{x}$. Therefore, the components of the elasticity tensor are

$$D_{ijkl} = D_{ijkl}(\mathbf{y}). \tag{2}$$

However, on the macroscale system of coordinates, $\mathbf{x}$, the microstructural heterogeneity appears over periods ϵ^{-1} times smaller than the characteristic dimension of the domain Y. According to Eq. 1, this is denoted by

$$D^{\epsilon}_{ijkl}(\mathbf{x}) = D_{ijkl}(\mathbf{x}/\epsilon), \tag{3}$$

where the superindex ϵ stands for the ϵ Y-periodicity of $\mathbf{D}$ in the system of coordinates $\mathbf{x}$, thus depending indirectly on $\mathbf{x}$. Assuming infinitesimal strains associated to a static equilibrium state and considering Einstein's convention for tensor notation, the linear-elasticity problem can be described using equilibrium equations, linearised strain–displacement relations and constitutive laws that may be written as [12]

$$\frac{\partial \sigma^{\epsilon}_{ij}}{\partial x^{\epsilon}_{j}} + f_i = 0 \qquad \text{in } \Omega, \tag{4}$$

$$\varepsilon^{\epsilon}_{ij} = \frac{1}{2}\left(\frac{\partial u^{\epsilon}_{i}}{\partial x^{\epsilon}_{j}} + \frac{\partial u^{\epsilon}_{j}}{\partial x^{\epsilon}_{i}}\right) \qquad \text{in } \Omega \text{ and} \tag{5}$$

$$\sigma^{\epsilon}_{ij} = D^{\epsilon}_{ijkl}\varepsilon^{\epsilon}_{kl} \quad \text{in } \Omega, \tag{6}$$

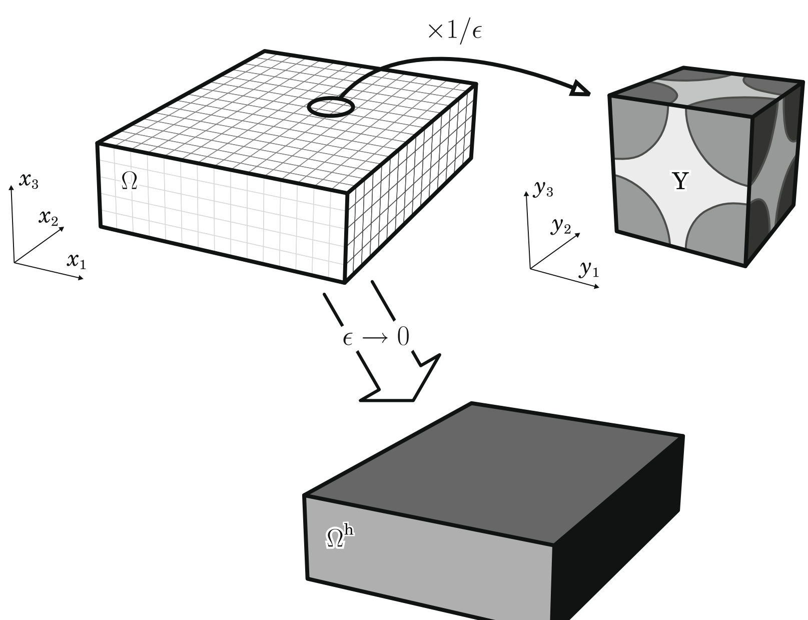

Fig. 1. Schematic representation of the heterogeneous elastic material Ω and the unit-cell Y, representative of the microscale, used in the asymptotic expansion homogenisation method, which results, with $\epsilon \to 0$, in the homogenous material Ω^{h}.

respectively, for $i,j,k,l \in \{1,2,3\}$. σ_{ij} and ε_{ij} are the components of the Cauchy stress and strain tensors, respectively. f_i and u_i represent the vector components of volume loads and displacements, respectively. The index ϵ stands for the ϵY-periodicity of a given variable on the macroscale coordinate system, $\mathbf{x}$. The boundary of Ω is disjointly defined by the surfaces Γ_u and Γ_t, which are related to Dirichlet's and Neumann's boundary conditions, defined as

$$u_i^\epsilon = \bar{u}_i \quad \text{in } \Gamma_u \quad \text{and} \tag{7}$$

$$\sigma_{ij}^\epsilon n_j = \bar{t}_i \quad \text{in } \Gamma_t, \tag{8}$$

respectively, with $\Gamma_u \cup \Gamma_t = \Gamma$ and $\Gamma_u \cap \Gamma_t = \emptyset$. $\bar{u}_i$ and $\bar{t}_i$ are prescribed displacement and surface load values, respectively. n_j are the components of an outward versor normal to the surface Γ_t.

In this context, the resolution of the elasticity problem consists on the determination of the displacement field corresponding to the solution $\mathbf{u}^\epsilon \in V_\Omega^0$ of the variational problem

$$\int_\Omega D_{ijkl}^\epsilon \frac{\partial u_k^\epsilon}{\partial x_l^\epsilon} \frac{\partial v_i}{\partial x_j^\epsilon} \mathrm{d}\Omega = \int_\Omega f_i v_i \mathrm{d}\Omega + \int_{\Gamma_{N_u}} \bar{t}_i v_i \mathrm{d}\Gamma, \qquad \forall v \in V_\Omega^0, \tag{9}$$

where V_Ω^0 is the set of continuous and sufficiently regular functions, zero-valued in Γ_u.

As heterogeneous materials are made of $n > 1$ homogenous materials, the linear elasticity problem consists of n equations, analogous to Eq. (4), associated to continuity conditions for displacements and surface loads in each of the interfaces between subdomains.

2.2. Asymptotic expansion of the displacement field

Assuming the existence of two distinct scales associated to the material behaviour phenomena at the macroscale Ω and microscale Y levels, the displacement field is approximated using the following asymptotic expansion in ϵ:

$$u_i^\epsilon(\mathbf{x}) = u_i^{(0)}(\mathbf{x},\mathbf{y}) + \epsilon u_i^{(1)}(\mathbf{x},\mathbf{y}) + \epsilon^2 u_i^{(2)}(\mathbf{x},\mathbf{y}) + \cdots, \tag{10}$$

where the terms $u_i^{(r)}(\mathbf{x},\mathbf{y})$, with $r \in \mathbb{N}_0$, are Y-periodic functions called correctors of order r of the displacement field. With $\mathbf{y} = \mathbf{x}/\epsilon$, according to the chain rule of function differentiation,

$$\frac{\partial \cdot}{\partial x_i^\epsilon} = \frac{\partial \cdot}{\partial x_i} + \frac{1}{\epsilon}\frac{\partial \cdot}{\partial y_i}. \tag{11}$$

In this context, replacing the asymptotic expansion of the displacements (expression (10)) in the strain–displacement relations (Eq. (5)), using relation (11) and correctly manipulating the indexes and regrouping the powers of ϵ,

$$\varepsilon_{ij}^\epsilon = \epsilon^{-1}\varepsilon_{ij}^{(0)} + \epsilon^0 \varepsilon_{ij}^{(1)} + \epsilon^1 \varepsilon_{ij}^{(2)} + \cdots, \tag{12}$$

where

$$\varepsilon_{ij}^{(0)} = \frac{1}{2}\left(\frac{\partial u_i^{(0)}}{\partial y_j} + \frac{\partial u_j^{(0)}}{\partial y_i}\right) \quad \text{and} \tag{13}$$

$$\varepsilon_{ij}^{(r)} = \frac{1}{2}\left(\frac{\partial u_i^{(r-1)}}{\partial x_j} + \frac{\partial u_j^{(r-1)}}{\partial x_i} + \frac{\partial u_i^{(r)}}{\partial y_j} + \frac{\partial u_j^{(r)}}{\partial y_i}\right), \qquad r \in \mathbb{N}. \tag{14}$$

Replacing relations (12) in the constitutive equations (Eq. (6)) and considering Eqs. (1) and (3) leads to

$$\sigma_{ij}^\epsilon = \epsilon^{-1}\sigma_{ij}^{(0)} + \epsilon^0 \sigma_{ij}^{(1)} + \epsilon^1 \sigma_{ij}^{(2)} + \cdots, \tag{15}$$

where according to expressions (13) and (14),

$$\sigma_{ij}^{(0)} = \frac{1}{2} D_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(0)}}{\partial y_l} + \frac{\partial u_l^{(0)}}{\partial y_k}\right) \quad \text{and} \tag{16}$$

$$\sigma_{ij}^{(r)} = \frac{1}{2} D_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(r-1)}}{\partial x_l} + \frac{\partial u_l^{(r-1)}}{\partial x_k} + \frac{\partial u_k^{(r)}}{\partial y_l} + \frac{\partial u_l^{(r)}}{\partial y_k}\right), \qquad r \in \mathbb{N}. \tag{17}$$

Replacing expression (15) in the equilibrium Eq. (4), using the relations (11) and regrouping the powers of ϵ,

$$\epsilon^{-2}\frac{\partial \sigma_{ij}^{(0)}}{\partial y_j} + \epsilon^{-1}\left(\frac{\partial \sigma_{ij}^{(0)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(1)}}{\partial y_j}\right) + \epsilon^0\left(\frac{\partial \sigma_{ij}^{(1)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(2)}}{\partial y_j} + f_i\right) + \cdots = 0. \tag{18}$$

Since the previous equations must be valid for any given $\epsilon \to 0$, it is necessary that any coefficient of the powers of ϵ is zero. Thus, for the various power orders of ϵ (*i.e.* for the several orders of correction) it is possible to obtain the following (infinite) enumerable set of differential equations:

$$\epsilon^{-2} \to \frac{\partial \sigma_{ij}^{(0)}}{\partial y_j} = 0, \tag{19}$$

$$\epsilon^{-1} \to \frac{\partial \sigma_{ij}^{(0)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(1)}}{\partial y_j} = 0, \tag{20}$$

$$\epsilon^{0} \to \frac{\partial \sigma_{ij}^{(1)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(2)}}{\partial y_j} + f_i = 0 \quad \text{and} \tag{21}$$

$$\epsilon^{r} \to \frac{\partial \sigma_{ij}^{(r+1)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(r+2)}}{\partial y_j} = 0, \qquad r \in \mathbb{N}. \tag{22}$$

Considering the asymptotic expansions (10) and (15), Dirichlet's (expression (7)) and Neumann's (expression (8)) boundary conditions of the original problem become

$$\epsilon^0 u_i^{(0)} + \epsilon^1 u_i^{(1)} + \epsilon^2 u_i^{(2)} + \cdots = \bar{u}_i \quad \text{in } \Gamma_u \quad \text{and} \tag{23}$$

$$\left(\epsilon^{-1}\sigma_{ij}^{(0)} + \epsilon^0 \sigma_{ij}^{(1)} + \epsilon^1 \sigma_{ij}^{(2)} + \cdots\right) n_j = \bar{t}_i \quad \text{in } \Gamma_t, \tag{24}$$

respectively. Therefore, Dirichlet's and Neumann's boundary conditions linked to each order of correction are

$$\epsilon^0 \to u_i^{(0)} = \bar{u}_i \quad \text{and} \tag{25}$$

$$\epsilon^r \to u_i^{(r)} = 0 \quad \text{in } \Gamma_u,\ r \in \mathbb{N}, \ \text{and} \tag{26}$$

$$\epsilon^{-1} \to \sigma_{ij}^{(0)} n_j = 0, \tag{27}$$

$$\epsilon^{0} \to \sigma_{ij}^{(1)} n_j = \bar{t}_i \quad \text{and} \tag{28}$$

$$\epsilon^{r} \to \sigma_{ij}^{(r+1)} n_j = 0 \quad \text{in } \Gamma_t,\ r \in \mathbb{N}. \tag{29}$$

The solutions of the differential equations defined in relations (19)–(22), associated to the boundary conditions (25)–(29), can be calculated recursively. It is possible to determine the solutions $\sigma_{ij}^{(1)}$ in terms of $\sigma_{ij}^{(0)}$ having the solutions $\sigma_{ij}^{(0)}$ of Eq. (19), by substitution on Eq. (20). The solutions for the equations of a given order of correction can be calculated from the solutions of the equations of higher orders.

2.3. Microscale differential equations

From the differential equations of the correction order −2 of the stress field (expression (19)), it results that

$$\sigma_{ij}^{(0)} = \sigma_{ij}^{(0)}(\mathbf{x}). \tag{30}$$

Nonetheless, considering expression (16) and the symmetry of the elasticity tensor,

$$\sigma_{ij}^{(0)} = D_{ijkl}(\mathbf{y})\frac{\partial u_k^{(0)}}{\partial y_l}. \tag{31}$$

This way, conditions (30) and (31) become [13]

$$\sigma_{ij}^{(0)} = 0 \quad \text{and} \tag{32}$$

$$u_i^{(0)} = u_i^{(0)}(\mathbf{x}). \tag{33}$$

Thus, displacement $u_i^{(0)}$ is independent of the microscale coordinates $\mathbf{y}$, corresponding therefore to the global displacement field of the macroscale homogenised material. Hence, replacing Eq. (32) in the differential equations associated to the stress field correction order -1 (expression (20)) leads to

$$\frac{\partial \sigma_{ij}^{(1)}}{\partial y_j} = 0. \tag{34}$$

Considering expression (17) with $r = 1$ as well as the symmetry of the elasticity tensor,

$$\sigma_{ij}^{(1)} = D_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right), \tag{35}$$

from where Eq. (34) lead to

$$\frac{\partial}{\partial y_j}\left[D_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right)\right] = 0. \tag{36}$$

The fact that the term $\partial u_k^{(0)}/\partial x_l$ on expression (36) is constant relative to the operators $\partial \cdot /\partial y_j$ (see Eq. (33)) leads, according to the principle of superposition, to the following solutions of Eq. (36):

$$u_i^{(1)}(\mathbf{x},\mathbf{y}) = -\chi_i^{kl}(\mathbf{y})\frac{\partial u_k^{(0)}}{\partial x_l}(\mathbf{x}) + \bar{u}_i^{(1)}(\mathbf{x}). \tag{37}$$

$\bar{u}_i^{(1)}(\mathbf{x})$ are integration constants in $\mathbf{y}$ and χ_i^{kl} are the Y-periodic components of the characteristic displacement field tensor, $\boldsymbol{\chi}$. Replacing Eq. (37) in the expression (35), leads to

$$\sigma_{ij}^{(1)} = \hat{\sigma}_{ij}^{mn}\frac{\partial u_m^{(0)}}{\partial x_n}, \tag{38}$$

where

$$\hat{\sigma}_{ij}^{mn} = D_{ijkl}(\mathbf{y})\left(I_{kl}^{mn} - \frac{\partial \chi_k^{mn}}{\partial y_l}\right) \tag{39}$$

are Y-periodic functions, in which

$$I_{kl}^{mn} = \delta_{km}\delta_{ln}. \tag{40}$$

δ_{ij} is the Kronecker delta. Considering Eq. (33) and replacing Eq. (38) in expression (34) results in

$$\frac{\partial \hat{\sigma}_{ij}^{mn}}{\partial y_j}\frac{\partial u_m^{(0)}}{\partial x_n} = 0. \tag{41}$$

On the previous equations, since the second factor of the first member is arbitrary, the first factor has to be zero. Therefore, the differential microscale equilibrium equations can be written as

$$\frac{\partial \hat{\sigma}_{ij}^{mn}}{\partial y_j} = 0 \tag{42}$$

or, according to expression (39), as

$$\frac{\partial}{\partial y_j}\left[D_{ijkl}\left(I_{kl}^{mn} - \frac{\partial \chi_k^{mn}}{\partial y_l}\right)\right] = 0. \tag{43}$$

The characteristic displacement field tensor components are the solutions $\chi_i^{kl} \in \widetilde{V}_Y$ of the auxiliary variational problem

$$\int_Y D_{ijkl}\frac{\partial \chi_k^{mn}}{\partial y_l}\frac{\partial v_i}{\partial y_j}\mathrm{d}Y = \int_Y D_{ijmn}\frac{\partial v_i}{\partial y_j}\mathrm{d}Y, \qquad \forall v_i \in \widetilde{V}_Y, \tag{44}$$

where $\widetilde{V}_Y$ is the set of Y-periodic continuous and sufficiently regular functions with zero average value in Y. The average value of a Y-periodic in Y function $\Phi(\mathbf{x},\mathbf{y})$ is defined as

$$\langle\Phi\rangle_Y = \frac{1}{|Y|}\int_Y \Phi(\mathbf{x},\mathbf{y})\mathrm{d}Y. \tag{45}$$

The need for null average values in Y for the solutions of Eq. (44) is a unicity condition for the characteristic displacement tensor $\boldsymbol{\chi}$ [13].

2.4. Macroscale differential equations

Applying the operator $\langle\cdot\rangle_Y$ – average value in Y – to both terms of the equilibrium differential equations associated to the stress field correction of order 0 (expression (21)) leads to

$$\left\langle\frac{\partial \sigma_{ij}^{(1)}}{\partial x_j}\right\rangle_Y + \left\langle\frac{\partial \sigma_{ij}^{(2)}}{\partial y_j}\right\rangle_Y + \langle f_i\rangle_Y = 0. \tag{46}$$

According to the definition of average value of a Y-periodic function in Y and the divergence theorem,

$$\left\langle\frac{\partial \sigma_{ij}^{(2)}}{\partial y_j}\right\rangle_Y = \frac{1}{|Y|}\int_Y \frac{\partial \sigma_{ij}^{(2)}}{\partial y_j}\mathrm{d}Y = \frac{1}{|Y|}\int_{\Gamma_Y}\sigma_{ij}^{(2)}n_j\mathrm{d}\Gamma = 0, \tag{47}$$

taking into account the anti-symmetry of the versors n_j in Γ_Y. Thus, due to the fact that the operator $\langle\cdot\rangle_Y$ commutes with operators $\partial\cdot/\partial x_j$ and the volume load vector, f_i, does not depend on $\mathbf{y}$, expression (46) becomes

$$\frac{\partial\left\langle\sigma_{ij}^{(1)}\right\rangle_Y}{\partial x_j} + f_i = 0. \tag{48}$$

The previous relation represents the homogenised macroscale equilibrium differential equations. Replacing expression (39) in (38) and applying the average operator, the homogenised constitutive relations become

$$\left\langle\sigma_{ij}^{(1)}\right\rangle_Y = D_{ijmn}^{h}\frac{\partial u_m^{(0)}}{\partial x_n}, \tag{49}$$

where

$$D_{ijmn}^{h} = \frac{1}{|Y|}\int_Y D_{ijkl}(\mathbf{y})\left[I_{kl}^{mn} - \frac{\partial \chi_k^{mn}}{\partial y_l}\right]\mathrm{d}Y \tag{50}$$

are the homogenised elasticity tensor components, $\mathbf{D}^{h}$. The integration of Eq. (28) on surface Γ_t, according to the divergence theorem, results in

$$\int_\Omega \frac{\partial \sigma_{ij}^{(1)}}{\partial x_j}\mathrm{d}\Omega = \int_{\Gamma_t}\bar{t}_i\mathrm{d}\Gamma. \tag{51}$$

Applying the average operator to both members of Eq. (51) and considering the divergence theorem, equations

$$\left\langle\sigma_{ij}^{(1)}\right\rangle_Y n_j = \bar{t}_i \qquad \text{in} \quad \Gamma_t \tag{52}$$

are obtained. These are Neumann's boundary conditions associated to the variables of the problem defined in Eq. (48). In this context, considering

$$\Sigma_{ij} = \left\langle\sigma_{ij}^{(1)}\right\rangle_Y \tag{53}$$

and Eqs. (48), (25), (52) and (49), the displacement field $u_i^{(0)}$ is the solution of the homogenised elasticity problem, defined as

$$\frac{\partial \Sigma_{ij}}{\partial x_j} + f_i = 0 \qquad \text{in } \Omega, \tag{54}$$

$$u_i^{(0)} = \bar{u}_i \qquad \text{in } \Gamma_u, \tag{55}$$

$$\Sigma_{ij} n_j = \bar{t}_i \qquad \text{in } \Gamma_t, \text{ with} \tag{56}$$

$$\Sigma_{ij} = D^h_{ijkl} \frac{\partial u_k^{(0)}}{\partial x_l} \qquad \text{in } \Omega, \tag{57}$$

where the components D^h_{ijkl} of the homogenised elasticity tensor are determined solving the microscale equilibrium differential equations (expression (43)) and, adequately manipulating the tensor indexes, from Eq. (50). Σ_{ij} represents the macrostructural homogenised stress field.

In this context, the resolution of the homogenised elasticity problem consists on the determination of the macrostructural displacement field corresponding to the solution $\mathbf{u}^{(0)} \in V^0_\Omega$ of the variational problem

$$\int_\Omega D^h_{ijkl} \frac{\partial u_k^{(0)}}{\partial x_l} \frac{\partial v_i}{\partial x_j} d\Omega = \int_\Omega f_i v_i d\Omega + \int_{\Gamma_{N_u}} \bar{t}_i v_i d\Gamma \qquad \forall v \in V^0_\Omega, \tag{58}$$

where V^0_Ω is the set of continuous and sufficiently regular functions, zero-valued in Γ_u.

Once the displacement field $u_i^{(0)}$ is obtained, Eq. (37) lead to the determination of the displacement field $u_i^{(1)}$. Nevertheless, the consideration of both $\mathbf{x}$ and $\mathbf{y}$ scales – associated to material behaviour phenomena at the macroscale Ω and microscale Y levels, respectively – is based, as referred in Section 2.1, on the hypothesis of the existence of periodical oscillations of the resulting displacement fields, due to the periodicity of the microstructural heterogeneities. These oscillations overlie on the macroscopic fields where the influence of microstructural heterogeneities are not considered. These oscillations may be seen as fluctuations around the macroscopic average value (see Fig. 2). In this sense, the integration constants $\bar{u}_i^{(1)}(\mathbf{x})$ in $\mathbf{y}$ of the term $u_i^{(1)}$ associated to the displacement field asymptotic expansion (10) can, without loss of generality, be considered equal to zero, *i.e.* $\bar{u}_i^{(1)}(\mathbf{x}) = 0$. Thus, the presented methodology leads to the definition of a first-order approximation $\tilde{u}_i^\epsilon(\mathbf{x})$, linear in relation to ϵ, for the asymptotic expansion of the displacement field $u_i^\epsilon(\mathbf{x})$ (see Fig. 2). This approximation, according to expressions (10) and (33), can be written as

$$u_i^\epsilon(\mathbf{x}) \approx \tilde{u}_i^\epsilon(\mathbf{x}) = u_i^{(0)}(\mathbf{x}) + \epsilon u_i^{(1)}(\mathbf{x}, \mathbf{y}). \tag{59}$$

Replacing expression (37) in Eq. (59) and relying on $\bar{u}_i^{(1)}(\mathbf{x}) = 0$, the following equations are obtained as a function of the characteristic displacement tensor components:

$$u_i^\epsilon(\mathbf{x}) \approx \tilde{u}_i^\epsilon(\mathbf{x}) = u_i^{(0)}(\mathbf{x}) - \epsilon \chi_i^{kl}(\mathbf{y}) \frac{\partial u_k^{(0)}}{\partial x_l}(\mathbf{x}). \tag{60}$$

Due to the linear character, in ϵ, of the previous approximation, $\boldsymbol{\chi}$ is often designated the first-order characteristic displacement field tensor.

2.5. Higher-order displacement correctors

Higher-order correctors, part of the asymptotic expansion of the displacement field (10), can be calculated by the recursive use of the differential equations associated to higher orders of correction (see Section 2.2). As an example, consider the second-order corrector $u_i^{(2)}$ for the asymptotic expansion of the displacement field (expression (10)). In this case, Eq. (21) must be solved based on the solutions $u_i^{(0)}$ and $u_i^{(1)}$ of Eqs. (19) and (20), respectively. This way, considering $r = 2$ in Eq. (17), with the symmetry of the elasticity tensor, and replacing it, along with expression (35), in the equilibrium differential equations of the stress field corrector of order 0 (expression (21)),

$$D_{ijkl}(\mathbf{y}) \left[\frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l} + \frac{\partial^2 u_k^{(1)}}{\partial x_j \partial y_l} \right] + \frac{\partial}{\partial y_j} \left[D_{ijkl}(\mathbf{y}) \left(\frac{\partial u_k^{(1)}}{\partial x_l} + \frac{\partial u_k^{(2)}}{\partial y_l} \right) \right] + f_i = 0. \tag{61}$$

On the other hand, replacing the expression (57) in Eq. (54) and recalling that the homogenised elasticity tensor $\mathbf{D}^h$ is constant,

$$f_i = -D^h_{ijkl} \frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l}. \tag{62}$$

Replacing Eqs. (37) (with $\bar{u}_i^{(1)}(\mathbf{x}) = 0$) and (62) in Eq. (61), manipulating the indexes and regrouping the terms leads to

$$\frac{\partial}{\partial y_j} \left[D_{ijkl}(\mathbf{y}) \frac{\partial u_k^{(2)}}{\partial y_l} \right] = \overline{D}_{ijkl} \frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l}, \tag{63}$$

where

$$\overline{D}_{ijkl} = D^h_{ijkl} - D_{ijkl}(\mathbf{y}) + D_{ijmn}(\mathbf{y}) \frac{\partial \chi_m^{kl}}{\partial y_n} + \frac{\partial}{\partial y_n} \left[D_{inmj}(\mathbf{y}) \chi_m^{kl} \right]. \tag{64}$$

The fact that the term $\partial^2 u_k^{(0)} / \partial x_j \partial x_l$ of expression (63) is constant in relation to the operators $\partial \cdot / \partial y_j$ (see Eq. (33)) allows, according to the superimposition principle, to assume the following solutions to Eq. (63):

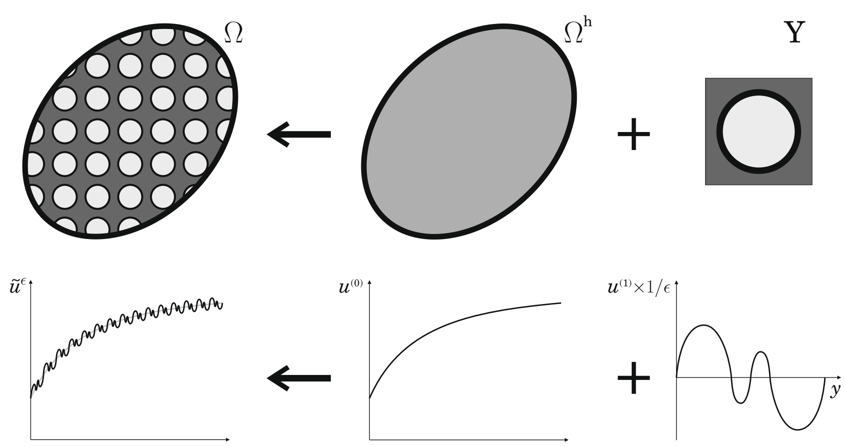

Fig. 2. Illustration of the first-order approximation of the asymptotic expansion of the displacement field, for a one-dimensional case: the displacement field, in Ω, is approximated by the overlapping of the macroscale homogenised field, in Ω^h, with the oscillations that result from the Y-periodicity of the microscale field, in Y.

$$u_i^{(2)}(\mathbf{x},\mathbf{y}) = -\Theta_i^{kjl}\frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l} + \bar{u}_i^{(2)}(\mathbf{x}). \tag{65}$$

$\bar{u}_i^{(2)}(\mathbf{x})$ are integration constants in $\mathbf{y}$ and Θ_i^{kjl} are the Y-periodic components of the second-order characteristic displacement field tensor.

According to expressions (63) and (64), the second-order characteristic displacement field tensor components are the solutions $\Theta_k^{mnp} \in \widetilde{\mathrm{V}}_{\mathrm{Y}}$ of the auxiliary variational problem

$$\int_{\mathrm{Y}} D_{ijkl}\frac{\partial \Theta_k^{mnp}}{\partial y_l}\frac{\partial v_i}{\partial y_j}\mathrm{d}Y = \int_{\mathrm{Y}}\left(D^{\mathrm{h}}_{inmp} - D_{inmp} + D_{inkj}\frac{\partial \chi_k^{mp}}{\partial y_j}\right)v_i \mathrm{d}Y - \int_{\mathrm{Y}} D_{ijkn}\chi_k^{mp}\frac{\partial v_i}{\partial y_j}\mathrm{d}Y, \qquad \forall v_i \in \widetilde{\mathrm{V}}_{\mathrm{Y}}, \tag{66}$$

in which $\widetilde{\mathrm{V}}_{\mathrm{Y}}$ is the set of Y-periodic continuous and sufficiently regular functions with zero average value in Y.

It is possible to obtain the remaining higher-order correctors of the asymptotic expansion of the displacement field (10). The correctors of order $k \in \mathrm{N}_0$ are proportional to a partial derivative of order k of the global displacements of the homogenised material associated to the macroscale, $u_i^{(0)}$. The relation factors are the components of the characteristic displacement fields of order k. In this context, further assuming integration constants in $\mathbf{y}$ as equal to zero for higher orders, expression (10) becomes

$$u_i^{\epsilon}(\mathbf{x}) = u_i^{(0)}(\mathbf{x}) - \epsilon\chi_i^{kl}(\mathbf{y})\frac{\partial u_k^{(0)}}{\partial x_l}(\mathbf{x}) - \epsilon^2\Theta_i^{kjl}(\mathbf{y})\frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l}(\mathbf{x}) - \cdots \tag{67}$$

Though the displacement field u_i^{ϵ} is defined as a set of (infinite) enumerable terms (see expression (67)), it can be shown that, for a small relation between characteristic dimensions of the micro- and macroscale domains ($\epsilon \ll 1$), the higher-order terms are not numerically significant when compared to the first order approximation (60) [14].

2.6. Conventional homogenisation methodology

In practice, a significant part of structural engineering applications based on heterogeneous materials with periodic microstructures is associated to values of $\epsilon \ll 1$. In this case, according to Section 2.5, a first-order approximation for the displacement field is often adequate to represent the displacement field u_i^{ϵ}. Ignoring the higher-order terms simplifies the asymptotic expansion homogenisation methodology, giving way to the conventional homogenisation methodology [14].

According to the previous sections, the conventional homogenisation methodology applied to the elasticity problem is an exact mathematical technique. It is possible to solve a problem associated to a partial differential operator with constant coefficients (see Eqs. (54)–(57) instead of a problem associated to a partial differential operator with coefficients of high-frequency periodic spatial variations (see Eqs. (4)–(8)). This is called homogenised elasticity problem. In turn, the coefficients of the homogenised problem are determined from the solution of a problem defined on a microscale unit-cell, with boundaries restrained by periodicity boundary constraints (see Eqs. (44) and (50)).

In this context, in numerical terms, one of the main advantages of this methodology is the significant reduction of the number of degrees of freedom involved in the resolution of the elasticity problem. This technique allows the modelling of the microstructural details based on a single representative unit-cell. The macroscale is modelled as a homogenous material body.

2.7. Conventional localisation methodology

An advantage of the asymptotic homogenisation expansion method is that it allows the detailing of the microstructural stress and strain fields. In fact, unlike other common homogenisation methods, this method explicitly defines equations for the determination of the microscale stress and strain levels. This process is called localisation and can be seen as the inverse of the homogenisation procedure (see Fig. 3).

With Eqs. (13), (16) and (32) was shown that $\sigma_{ij}^{(0)} = 0$ and $\varepsilon_{ij}^{(0)} = 0$. According to expressions (15) and (12), the stress and strain fields are defined by

$$\sigma_{ij}^{\epsilon} = \epsilon^0\sigma_{ij}^{(1)} + \epsilon^1\sigma_{ij}^{(2)} + \cdots \qquad \text{and} \tag{68}$$

$$\varepsilon_{ij}^{\epsilon} = \epsilon^0\varepsilon_{ij}^{(1)} + \epsilon^1\varepsilon_{ij}^{(2)} + \cdots, \tag{69}$$

respectively. Expressions (68) and (69) are serial expansions of the stress and strain fields that result from the Y-periodicity of the microstructural heterogeneities. However, a first order approximation (in ϵ) of the displacement field is considered in the conventional homogenisation methodology. Thus, according to the relations (14) and (17) for $r = 1$, approximations $\widetilde{\sigma}_{ij}^{\epsilon}$ and $\widetilde{\varepsilon}_{ij}^{\epsilon}$ of order zero in ϵ are defined for the microstructural stress and strain fields. These approximations are

$$\sigma_{ij}^{\epsilon}(\mathbf{x}) \approx \widetilde{\sigma}_{ij}^{\epsilon}(\mathbf{x}) = \epsilon^0\sigma_{ij}^{(1)}(\mathbf{x},\mathbf{y}) \qquad \text{and} \tag{70}$$

$$\varepsilon_{ij}^{\epsilon}(\mathbf{x}) \approx \widetilde{\varepsilon}_{ij}^{\epsilon}(\mathbf{x}) = \epsilon^0\varepsilon_{ij}^{(1)}(\mathbf{x},\mathbf{y}). \tag{71}$$

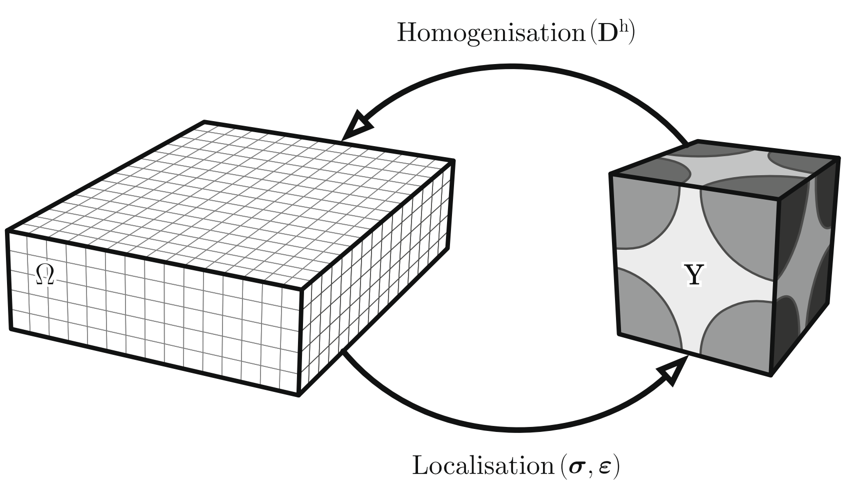

Fig. 3. Schematic illustration of the information flow in homogenisation and localisation procedures, between the macroscale Ω and the microscale Y.

According to expressions (38) and (39), the microstructural stress field associated to the conventional localisation methodology (expression (70)) is defined by

$$\sigma_{ij}^{(1)}(\mathbf{x},\mathbf{y}) = D_{ijkl}(\mathbf{y})\left(I_{kl}^{mn} - \frac{\partial \chi_k^{mn}}{\partial y_l}\right)\frac{\partial u_m^{(0)}}{\partial x_n}. \tag{72}$$

Replacing expression (37) in Eq. (14) for $r = 1$ and adjusting indexes, the microstructural strain field associated to the conventional localisation methodology (expression (71)) becomes

$$\varepsilon_{ij}^{(1)}(\mathbf{x},\mathbf{y}) = T_{ij}^{kl}\left(I_{kl}^{mn} - \frac{\partial \chi_k^{mn}}{\partial y_l}\right)\frac{\partial u_m^{(0)}}{\partial x_n}, \tag{73}$$

where

$$T_{ij}^{kl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right). \tag{74}$$

Eqs. (72) and (73) allow, for a given point of the macroscale $\mathbf{x}$, the computation of approximate values for the stress and strain fields within the heterogeneous microstructure. However, the macrostructural homogenised stress field Σ_{ij}, as it is an average of the microstructural stress field $\sigma_{ij}^{(1)}$ in Y (see Eq. 53)), is unable to represent any microstructural stress fluctuations.

2.8. Additional remarks

In previous sections the authors presented the asymptotic expansion homogenisation method applied to the linear elasticity problem. Proposed functions are considered sufficiently regular. In general this is not entirely verified. The components of the elasticity tensor D_{ijkl} are most often discontinuous at the matrix–reinforcement interface of a composite material. Thus, although the asymptotic expansion of the displacement field is useful to solve the linear elasticity problem, questions arise as the exact proof of the method requires overly regular functions. The exact (non-formal) mathematical study of the method with non-regular functions involves the use of concepts such as weak convergence. In this context, the exact development of the homogenisation theory is based on methods such as the one proposed by Tartar [15] or the two-scale convergence method [16].

3. Finite element modelling equations

The numerical implementation of the finite element equations is described along the next paragraphs.

3.1. Corrector of the displacement field

The solution of Eq. (44) is called the corrector (χ) and contains the eigendeformations of the representative periodic geometry [17]. The element strain and stress matrices are respectively $\boldsymbol{\varepsilon} = \mathbf{Bu}$ and $\boldsymbol{\sigma} = \mathbf{DBu}$, where all the variables belong to the microscale problem, that is, are related to the geometry and material of the representative unit-cell. $\mathbf{D}$ and $\mathbf{B}$ are the matrices of elasticity and partial derivatives of the interpolation functions, respectively. $\mathbf{u}$ is the vector of the element's nodal displacements. Therefore, the finite element approximation to Eq. (44) results as

$$\int_{Y^e} \mathbf{B}^{\mathrm{T}}\mathbf{DB}\,\mathrm{d}Y\boldsymbol{\chi} = \int_{Y^e} \mathbf{B}^{\mathrm{T}}\mathbf{D}\,\mathrm{d}Y = \mathbf{F}^{\mathrm{D}}, \tag{75}$$

where the index e denotes element quantities from the meshed unit-cell domain (body Y) [18]. The corrector $\boldsymbol{\chi}$ is a matrix, not a vector. The second term of Eq. (75) is made of the columns of a matrix $\mathbf{F}^{\mathrm{D}}$ [18]. These columns are six load vectors, leading to the same number of systems of equations that need to be solved. Accordingly, the results are different solutions that make up the corrector columns. Each one defines an eigendeformation mode. The definition of matrix $\mathbf{F}^{\mathrm{D}}$ shows that the force vectors are built from the integration of the gradient of elastic properties between the material components that form the composite material.

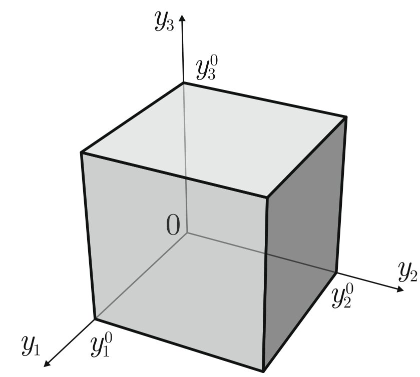

Fig. 4. Coordinate system and boundaries for a hexahedral representative unit-cell.

3.2. Periodicity boundary conditions

The periodicity boundary conditions are imposed over the representative unit-cell external surface boundaries. For a hexahedral unit-cell in $y_1 \in [0, y_1^0]$, $y_2 \in [0, y_2^0]$ and $y_3 \in [0, y_3^0]$ (see Fig. 4), the boundary conditions are as follows:

$$\begin{aligned} &\chi_i^{jk}(0, y_2, y_3) = \chi_i^{jk}(y_1^0, y_2, y_3),\\ &\chi_i^{jk}(y_1, 0, y_3) = \chi_i^{jk}(y_1, y_2^0, y_3) \quad \text{and}\\ &\chi_i^{jk}(y_1, y_2, 0) = \chi_i^{jk}(y_1, y_2, y_3^0). \end{aligned} \tag{76}$$

In order to avoid rigid body motion, displacements and rotations of an arbitrary point of the unit-cell must be fixed. This restriction is created acting only upon the translation degrees of freedom of one of the corners. Rigid body motion is therefore avoided through the periodicity constraints which, as shown in relations (76), force the restriction to act accordingly over all the remaining cell corners.

3.3. Homogenised elasticity matrix

The homogenised elasticity matrix, $\mathbf{D}^{\mathrm{h}}$, is obtained by adapting Eq. (50), leading to

$$\mathbf{D}^{\mathrm{h}} = \sum_{k=1}^{n_e} \frac{Y^k}{Y}\mathbf{D}^k(\mathbf{I} - \mathbf{B}^k\boldsymbol{\chi}^k), \tag{77}$$

where Y^k is the volume of element k, Y the total geometry volume and $\mathbf{I}$ the identity matrix. n_e is the number of elements of Y. If $\boldsymbol{\chi} = \mathbf{0}$, Eq. (77) becomes the volume average of the elastic properties of the microscale elements.

3.4. Localisation procedure

For a given integration (Gauss) point of a finite element of the macroscale mesh, the microscale strain is (see Eq. (73))

$$\boldsymbol{\varepsilon}^{(1)}(\mathbf{x},\mathbf{y}) = (\mathbf{I} - \mathbf{B}^e\boldsymbol{\chi}^e)\boldsymbol{\varepsilon}^{(0)}(\mathbf{x},\mathbf{y}). \tag{78}$$

The microstructural stress may be calculated for each microscale element multiplying the matching strain field by the corresponding elasticity matrix:

$$\boldsymbol{\sigma}^{(1)}(\mathbf{x},\mathbf{y}) = \mathbf{D}^e(\mathbf{I} - \mathbf{B}^e\boldsymbol{\chi}^e)\boldsymbol{\varepsilon}^{(0)}(\mathbf{x},\mathbf{y}). \tag{79}$$

4. Final remarks

The formal mathematical formulation of the asymptotic expansion homogenisation for linear elasticity problems was shown in a detailed form. The numerical equations resulting from the finite element modelling of the asymptotic expansion homogenisation method where also presented, as the starting point for the second part of this work.

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