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ON COMPUTATION OF MACRO-HETEROGENEOUS COMPOSITES

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A simplified computational model for solving the static problems of linear-elastic macro-heterogeneous composites is proposed. The approach is based on that discussed by Konieczny et al. (1994). The final result is presented in the form of algebraic linear equation system of the finite element method.

Key words: macro-heterogeneous composites

1. Introduction

It is known that composites are aggregates comprising two or more distinctly different materials which, on the macroscopic scale, form together a new medium with *apparent* properties different from those of the individual constituents, cf Thompson (1987). Hence, every composite represents, by definition, a certain micro-heterogeneous continuous medium. If the apparent properties of this medium do not change throughout a whole structural element then the composite is said to be *macro-homogeneous*. Such situations take place, e.g., for periodic composite materials having apparent *macro* properties determined by one representative volume element (cf Jones, 1980; Bensoussan et al., 1980). However, some engineering structures involve composite elements with apparent properties depending on their position in the body. These structural composite elements are not made of one standardized composite material but reveal different macro-properties in different parts of the body and will be referred to as the *macro-heterogeneous* composites.

So far, theoretical studies of the micro-modelling of composites have been restricted mainly to the *macro-homogeneous* structures (esp. micro-periodic bodies) leading to various homogenization theories; an extensive list of the related papers can be found in Jones (1980), Bensoussan et al. (1980). The approach to modelling of the macro-heterogeneus composite materials proposed by Jikov (1994) and based on the concept of G-convergence is to be applied to when solving the engineering problems. That is why the main aim of this contribution is to propose a simplified computational approach to mechanics of the *macro-heterogeneous* composites. The theoretical background of this approach is strictly related to that explored by Konieczny et al. (1994) but the main attention is focused here on formulation of the FEM approach which can be applied to calculations of stresses and displacements in the macro-heterogeneous composites. The considerations are confined to the linear-elastic composite materials on the assumption of perfect bonding between material constituents and for the deterministic description of these constituents distribution.

Notations. Subscripts i, j, k, l run over $1, 2, 3$ and are related to the Cartesian orthogonal coordinate system in the physical space. Indices a, b run over $1, 2, ..., n$. Summation convention holds for both i, j, k, l and a, b. For the spatial derivatives we use the notation $f_{,i} \equiv \partial f / \partial x_i$, where $f = f(\boldsymbol{x})$ is a differentiable function and $\boldsymbol{x} = (x_1, x_2, x_3)$ is a point in the physical space.

2. Basic notions

Let Ω be a region in the physical space occupied by the undeformed and unstressed composite body made of the perfectly bonded homogeneous constituents. Material properties of this body are assumed to be known being determined by the components of elasticity tensor field $a_{ijkl}(\cdot)$, which are piecewise constant functions, suffering jump discontinuities only across the interfaces between material constituents. We restrict ourselves to the composites for which there exist a decomposition of Ω into a very large number of small mutually disjointed cells (volume elements) V^A, $A = 1, 2, ..., S$ such that:

(i) Every volume element V^A is a small piece of the body but large enough to detect all material heterogeneities responsible for the macro-properties (apparent properties) of the composite in the vicinity of V^A

(ii) Every two adjacent volume elements have similar distributions of material constituents (and hence similar apparent properties) but the remote volume elements can be distinctly different.

The above conditions will be detailed at the end of this Section.

Volume elements V^A, $A = 1, 2, .., S$, are referred to as the macro-volume elements. In a special case of a micro-periodic body material the structures of all macro-volume elements coincide and hence can be determined by one representative volume element (cf Thompson, 1987). For every V^A we shall introduce the averaging operator

$$\langle f \rangle \equiv \frac{1}{\text{vol}(V^A)} \int\limits_{V^A} f(\boldsymbol{x})\, dv \qquad A = 1, 2, ..., S \quad dv \equiv dx_1 dx_2 dx_3$$

where $f(\cdot)$ is an arbitrary integrable function defined (almost everywhere) on Ω.

In order to formulate a computational model of the composite under consideration we shall introduce, following Konieczny et al. (1994), two fundamental concepts. The first of them is a concept of a *macro-function* by means of which we shall describe, roughly speaking, the macroscopic behaviour of the composite. To this end we define the microstructure parameter δ, setting $\delta = \max \delta_A$, $A = 1, 2, ..., S$, where δ_A is the maximum characteristic length dimension of V^A. Let $G(\cdot)$ be an arbitrary real-valued function defined on Ω. By λ_G we denote a *numerical tolerance parameter*, defined as the maximum admissible tolerance related to the computations of the values of function $G(\cdot)$. In the sequel both parameters δ, λ_G are assumed to be known. The triple $\big(G(\cdot), \lambda_G, \delta\big)$ is said to be the macro-function if for every $\boldsymbol{x}, \boldsymbol{y} \in \Omega$ and $\|\boldsymbol{x} - \boldsymbol{y}\| < \delta$ the condition $|G(\boldsymbol{x}) - G(\boldsymbol{y})| < \lambda_G$ holds. Hence for any intergrable function $f(\cdot)$ defined almost everywhere on Ω we obtain

$$\begin{aligned} \int\limits_{\Omega} f(\boldsymbol{x}G(\boldsymbol{x})\, dv &= \sum_{A=1}^{S} \langle f \rangle_A G(\boldsymbol{x}_A) \text{vol}(V^A) + 0(\lambda_G) = \\ &= \int\limits_{\Omega} F(\boldsymbol{x}G(\boldsymbol{x})\, dv + 0(\lambda_G) + 0(\lambda_F) \end{aligned} \tag{2.1}$$

provided that $\big(G(\cdot), \lambda_G, \delta\big)$ is the macro-function, $\boldsymbol{x}_A$ is the center of V^A and $\big(F(\cdot), \lambda_F, \delta\big)$ is a macro-function satisfying conditions $F(\boldsymbol{x}_A) = \langle f \rangle_A$, $A = 1, ..., S$.

Returning to the conditions (i), (ii) given at the begining of this Section, we shall assume that there exist the continuous macro-functions $A_{ijkl}(\cdot)$, $A_{aijk}(\cdot)$, $A_{abij}(\cdot)$, defined on Ω, satisfying conditions

$$\begin{aligned} A_{ijkl}(\boldsymbol{x}^A) &= \langle a_{ijkl}\rangle_A \\ A_{aijk}(\boldsymbol{x}^A) &= \langle a_{ijkl}h_{a,l}\rangle_A \\ A_{abij}(\boldsymbol{x}^A) &= \langle a_{ikjl}h_{a,k}h_{b,l}\rangle_A \end{aligned} \tag{2.2}$$

for some $\boldsymbol{x}^A \in V^A$ and $A = 1, 2, ..., S$.

The above conditions, at the proper choice of micro-shape functions $h_a(\cdot)$, determine the class of macro-heterogeneous composites under consideration.

3. Macro-modelling assumptions

The modelling procedure leading from equations of the linear elasticity theory for a composite material structure with the highly-oscillating properties to a certain macro-model of this composite will be based on two assumptions. The first of them is called the *micro-macro kinematic hypothesis* and states that the displacement field $u_i(\cdot)$ can be assumed in the form (cf Konieczny et al., 1994)

$$u_i(\boldsymbol{x}) = U_i(\boldsymbol{x}) + h_a(\boldsymbol{x})Q_i^a(\boldsymbol{x}) \qquad \boldsymbol{x} \in \Omega \tag{3.1}$$

where $h_a(\cdot)$, $a = 1, ..., n$, is a known system of the so called micro-shape functions (postulated a priori in every problem under consideration) which satisfy the conditions $\langle h_a\rangle_A = 0$ and $|h_a(\boldsymbol{x})| \leq \delta$, $\delta h_{a,i}(\boldsymbol{x}) \in 0(\delta)$, for every $A = 1, ..., S$ and every $\boldsymbol{x} \in \Omega$. Moreover, $U_i(\cdot)$, $Q_i^a(\cdot)$ are arbitrary independent regular macro-functions (together with their first and second derivatives) constituting basic kinematic unknowns. Fields $U_i(\cdot)$ will be called the *macro-displacements* and satisfy conditions $U_i(\boldsymbol{x}) = \langle u_i\rangle_A + O(\delta)$ for every $\boldsymbol{x} \in V^A$ and $A = 1, ..., S$. Functions $Q_i^a(\cdot)$ will be referred to as the *correctors*. It will be shown in Section 4 that the correctors describe, from the quantitative wievpoint, the disturbances of displacements caused by the micro-heterogeneous structure of the composite.

Let λ stand for the numerical tolerance parameter related to the functions $U_i(\cdot)$, $Q_i^a(\cdot)$ and their derivatives. The second macro-modelling assumption will be called the *asymptotic approximation hypothesis* and states that terms $O(\delta)$ and $O(\lambda)$ in all equations obtained in the course the modelling procedure can be neglected (cf Konieczny et al., 1994). Hence, the linearized strain components ε_{ij}, obtained from Eq (3.1) will be assumed in the form

$$\varepsilon_{ij}(\boldsymbol{x}) = U_{(i,j)}(\boldsymbol{x}) + h_{a,(i}(\boldsymbol{x})Q_{j)}^a(\boldsymbol{x}) \tag{3.2}$$

Similarly, terms $O(\lambda_F)$, $O(\lambda_G)$ in Eq (2.1) will be neglected.

4. Analysis

For the sake of simplicity let us restrict the considerations to the plane static problems. Setting

$$\boldsymbol{U} = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \qquad \boldsymbol{Q}^a = \begin{bmatrix} Q_1^a \\ Q_2^a \end{bmatrix} \qquad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \end{bmatrix}$$
$$\mathbf{C}_a = \begin{bmatrix} h_{a,1} & 0 \\ 0 & h_{a,2} \\ h_{a,2} & h_{a,1} \end{bmatrix} \qquad \boldsymbol{\partial} = \begin{bmatrix} \frac{\partial}{\partial x_1} & 0 \\ 0 & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} \end{bmatrix} \tag{4.1}$$

we shall rewrite Eq (3.2) to the form

$$\boldsymbol{\varepsilon} = \boldsymbol{\partial} \boldsymbol{U} + \mathbf{C}_a \boldsymbol{Q}^a \tag{4.2}$$

Representing the elasticity tensor field $a_{ijkl}(\cdot)$ for the plane strain problem under consideration by the 3×3 matrix $\mathbf{a}$ and denoting by $\boldsymbol{\sigma}$ the column of the stress components, we obtain the matrix form of the stress-strain relations

$$\boldsymbol{\sigma} = \mathbf{a}\boldsymbol{\varepsilon} \tag{4.3}$$

Let us denote by $\boldsymbol{p}$ and $\boldsymbol{f}$ the columns of surface tractions and volume body forces, respectively. The priciple of virtual work will be postulated in the well known form

$$\int\limits_{\Omega} \{\delta\boldsymbol{\varepsilon}\}^\top \boldsymbol{\sigma}\, d\Omega = \oint\limits_{\partial\Omega} \{\delta\boldsymbol{U}\}^\top \boldsymbol{p}\, dS + \int\limits_{\Omega} \{\delta\boldsymbol{U}\}^\top \boldsymbol{f}\, d\Omega \tag{4.4}$$

Macro-functions $A_{ijkl}(\cdot)$, $A_{aijk}(\cdot)$, $A_{abij}(\cdot)$ satisfying Eq (2.2) can be determined by means of the interpolation formulas (cf Konieczny et al., 1994)

$$\begin{aligned} A_{ijkl}(\boldsymbol{x}) &= \sum_K \langle a_{ijkl} \rangle_K \eta^K(\boldsymbol{x}) \\ A_{aijk}(\boldsymbol{x}) &= \sum_K \langle a_{ijkl} h_{a,l} \rangle_K \eta^K(\boldsymbol{x}) \\ A_{abij}(\boldsymbol{x}) &= \sum_K \langle a_{ijkl} h_{a,k} h_{b,l} \rangle_K \eta^K(\boldsymbol{x}) \end{aligned} \tag{4.5}$$

where $\eta^K(\boldsymbol{x})$ are suitable interpolation functions and index K runs over a certain subsequence of the sequence $1, 2, ..., S$.

Combining Eqs (4.2) ÷ (4.4), using (2.1) and *asymptotic approximation hypothesis*, after representing the macro-functions (4.5) in the form of 3×3 matrix functions $\mathbf{A}(\cdot)$, $\mathbf{A}_a(\cdot)$, $\mathbf{A}_{ab}(\cdot)$, respectively, we obtain

$$\begin{aligned}
&\int\limits_{\Omega} \{\delta \boldsymbol{U}\}^\top \boldsymbol{\partial}^\top \mathsf{A}(\boldsymbol{x}) \boldsymbol{\partial U}\; d\Omega + \int\limits_{\Omega} \{\delta \boldsymbol{Q}^a\} \mathsf{A}_a(\boldsymbol{x}) \boldsymbol{\partial U}\; d\Omega + \\
&+ \int\limits_{\Omega} \{\delta \boldsymbol{U}\}^\top \boldsymbol{\partial}^\top [\mathsf{A}_a(\boldsymbol{x})]^\top \boldsymbol{Q}^a\; d\Omega + \int\limits_{\Omega} \{\delta \boldsymbol{Q}^a\} \mathsf{A}_{ab}(\boldsymbol{x}) \boldsymbol{Q}^a\; d\Omega = \\
&= \oint\limits_{\delta\Omega} \{\delta \boldsymbol{U}\}^\top \boldsymbol{p}\; dS + \int\limits_{\Omega} \{\delta \boldsymbol{U}\}^\top \boldsymbol{f}\; d\Omega
\end{aligned} \tag{4.6}$$

On condition that $\boldsymbol{U}, \boldsymbol{Q}^a$ are arbitrary linear-independent basic unknowns, the variational conditions (4.6) lead to the system of partial differential equations in $\boldsymbol{U}$ coupled with the linear algebraic equations in $\boldsymbol{Q}^a$. Discretizing the region Ω, we assume that

$$\boldsymbol{U} = \mathbf{N}\boldsymbol{q} \tag{4.7}$$

where $\boldsymbol{q}$ is the generalized nodal displacement vector. Moreover, we assume that in every finite element the vectors $\boldsymbol{Q}^a$ are constant

$$\boldsymbol{Q}^a = \mathbf{M}\boldsymbol{q}^a \tag{4.8}$$

where $\boldsymbol{q}^a$ is the vector of constant values of $\boldsymbol{Q}^a$ in all finite elements. In this case

$$\begin{aligned}
&\{\delta \boldsymbol{U}\} = \mathbf{N}\{\delta \boldsymbol{q}\} \qquad\qquad \{\delta \boldsymbol{Q}^a\} = \mathbf{M}\{\delta \boldsymbol{q}^a\} \\
&\boldsymbol{\partial U} = \boldsymbol{\partial}\mathbf{N}\boldsymbol{q} = \mathbf{B}\boldsymbol{q}
\end{aligned} \tag{4.9}$$

where $\mathbf{B} = \boldsymbol{\partial}\mathbf{N}$. Substituting Eqs (4.7) ÷ (4.9) into Eq (4.6) and denoting

$$\begin{aligned}
\mathbf{K} &= \int\limits_{\Omega} \mathbf{B}^\top \mathsf{A}(\boldsymbol{x}) \mathbf{B}\; d\Omega \\
\mathbf{K}_a &= \int\limits_{\Omega} \mathbf{B}^\top \mathsf{A}_a(\boldsymbol{x}) \mathbf{M}\; d\Omega \\
\mathbf{K}_{ab} &= \int\limits_{\Omega} \mathbf{M}^\top \mathbf{A}_{ab}(\boldsymbol{x}) \mathbf{M}\; d\Omega \\
\boldsymbol{F} &= -\oint\limits_{\partial\Omega} \mathbf{N}^\top \boldsymbol{p}\; dS - \int\limits_{\Omega} \mathbf{N}^\top \boldsymbol{f}\; d\Omega
\end{aligned} \tag{4.10}$$

we arrive finally at the following system of equations in $\boldsymbol{q}$ and $\boldsymbol{q}^a$, $a = 1, ..., n$

$$
\begin{aligned}
&\mathsf{K}\boldsymbol{q} + \mathsf{K}_a\boldsymbol{q}^a + \boldsymbol{F} = \mathbf{0} \\
&\mathsf{K}_a^{\top}\boldsymbol{q} + \mathsf{K}_{ab}\boldsymbol{q}^b = \mathbf{0}
\end{aligned}
\tag{4.11}
$$

After obtaining solutions $\boldsymbol{q}$, $\boldsymbol{q}^a$, $a = 1, ..., n$, to Eqs (4.11), we calculate the macro-displacements $\boldsymbol{U}$ and correctors $\boldsymbol{Q}^a$ using Eqs (4.7), (4.8), respectively.

Let us observe that for homogeneous bodies $\mathsf{A}_a(\boldsymbol{x}) = \mathbf{0}$ and hence $\mathsf{K}_a = \mathbf{0}$. Since K_{ab} represents the invertible linear transformation then Eqs (4.11) yield $\boldsymbol{q}^b = \mathbf{0}$. Thus from Eq (4.8) it follows that also $\boldsymbol{Q}^a = \mathbf{0}$. Hence the correctors Q_i^a in Eq (3.1) describe the effect of micro-heterogeneity of a composite on its behaviour.

Examples of applications of Eqs (4.11) will be presented in the subsequent paper.

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O obliczaniu makro-niejednorodnych kompozytów

Streszczenie

W pracy zaproponowano uproszczony model obliczeniowy dla statyki makro-niejednorodnych liniowo-sprężystych kompozytów. Wykorzystano podejście przedstawione w pracy Konieczny i inni (1994). Zagadnienie doprowadzono do układu algebraicznych równań liniowych.

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