MULTISCALE HOMOGENIZATION OF MULTILAYERED STRUCTURES

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Abstract: In this paper, the analytical solution of the multiple-step homogenization problem for multi-rank composites with generalized periodicity made of elastic materials is presented. The proposed homogenization scheme is combined with computational homogenization for solving more complex microstructures. Two numerical examples are presented, concerning a “chevron” composite and a wavy fiber reinforced composite.

1 INTRODUCTION

Materials may exhibit complex structures with more than one length scale, in a manner that a “hierarchical” structure could be defined. This “hierarchy” plays a major role in determining the bulk material properties ([3]) with great technological importance ([7]). Microstructures with periodicity are often characterized by the repetition of the same material element with respect to one or two or three-dimensional coordinate axis. However, there are structures that can not be obtained by the repetition of the same micro-volume. Following [4], one of the simplest composite, that called rank-one, is a stratified material where the material properties vary only in one direction, called the direction of lamination. In multiple-rank laminates, there is a large difference in the scales of the successive laminations, which are in different directions. The existence of a sequence of scales of decreasing order allows for performing a succession of homogenization steps, in which the “homogenized” material from every step acts as initial (“heterogeneous”) material for the next step. In every step, the homogenization scheme requires the solution of a cell problem with data corresponding to the material “homogenized” properties obtained from the previous step and to the volume fractions corresponding to the actual size.

In Section 2 we define the problem that this paper treats while in Section 3 we present the analytical solution of the microequation during a homogenization step, which is necessary in order to compute the effective elastic matrix. In Section 4 we present two numerical examples.

2 FORMULATION OF THE PROBLEM

In mathematical homogenization at least two scales are introduced. The first one is the macroscale denoted by $x \in \Omega'$, where $\Omega'$ is the volume occupied by the heterogeneous body, at which the heterogeneities, characterized by $\varepsilon$, are very small compared to the whole structure. The second one is the microscale denoted by $x', \varepsilon$, which is the actual scale for the heterogeneities. At every step of homogenization, the scale is much bigger than the scale of the previous step.

The choice of the repeated unit cell (RUC) is made with respect to the generalized periodicity function $\varrho(x')$ (for
more details see [5]) and $Y = [0, y_1] \times [0, y_2] \times [0, y_3]$ is chosen to be the basic cell, where

$$y = \frac{\varrho(x)}{\epsilon}.$$  \hfill (1)

The dependence of functions on the microcoordinate is performed (generally in a non-periodic way) via

$$\bar{y} = \frac{x}{\epsilon}.$$  \hfill (2)

We denote field variables $\sigma^0$, $\varepsilon^0$ and $u^1$ as microscopic variables and $\Sigma$, $E$ and $u^0$ as the macroscopic variables where the macroscopic quantities depend only on the macrocoordinate $x$. Both classes of deformation fields are related to the RUC located at $x$. Away from the boundaries $\partial\Omega$, stress and strain fields conform at the microlevel to the generalized periodicity conditions:

$$\sigma^0, \varepsilon^0 \text{ are } Y - \text{periodic functions of } y.$$  \hfill (3)

The actual displacement $u^0$ within $Y$ located at $x$ has two properties: it is oscillating and it has a generalized periodicity. We assume that $u^0$ can be expressed as a sum of a linear and a periodic part ([1],[2],[5])

$$u^0_i(x, \bar{y}, y) = E_{ij} \bar{y}_j + u^1_i,$$  \hfill (4)

where

$$u^1_i = u^1_i(x, y),$$  \hfill (5)

is periodic with respect to $y$. We remind that the difference with [2] is that, there, the function $u^1_i$ is periodic with respect to the microvariable $\bar{y}$, while here it is periodic only with respect to the generalized periodicity ([5]).

Microstrain is defined from (4) with respect to the microcoordinate,

$$\varepsilon^0_{ij} = \text{sym} \left( \frac{\partial u_i}{\partial \bar{y}_j} \right) = \frac{1}{2} \left( \frac{\partial u_i}{\partial \bar{y}_j} + \frac{\partial u_j}{\partial \bar{y}_i} \right),$$  \hfill (6)

while the macrostrain is defined with respect to the macrocoordinate,

$$E_{ij} = \text{sym} \left( \frac{\partial u^0_i}{\partial x_j} \right) = \frac{1}{2} \left( \frac{\partial u^0_i}{\partial x_j} + \frac{\partial u^0_j}{\partial x_i} \right).$$  \hfill (7)

It was proved ([6]) that

$$\langle \varepsilon^0_{ij} \rangle = E_{ij}.$$  \hfill (8)

Two main hypotheses hold. The first is the perfect bonding among layers of the constituents (see in [8] the effect of debonded fibers of a composite under traction). The second one is that there is no cracking in the structure. The elastic coefficients are assumed of the form,

$$C_{ijkh}(y) = C_{ijkh} \left( \frac{\varrho(x)}{\epsilon} \right), \quad C_{ijkh}(y) \text{ } Y - \text{periodic, } C_{ijkh} \in L^\infty(\mathbb{R}^m),$$  \hfill (9)

$$\varrho \in C^2(\mathbb{R}^m), \quad m \leq 3,$$  \hfill (10)

$$C_{ijkh} \xi_{ij} \xi_{kh} \geq \lambda \xi_{ij} \xi_{ij}, \quad \forall \xi \text{ symmetric, } C_{ijkh} = C_{jikh} = C_{ijkh} = C_{khij},$$  \hfill (11)

$$\sum_{i=1}^{n} \sum_{k=1}^{m} \left( \frac{\partial \varrho_k(x)}{\partial x_i} \right)^2 \eta_k^2 \geq \beta \sum_{k=1}^{n} \eta_k^2, \quad \forall \eta.$$  \hfill (12)
We note that, at every scale $\epsilon$, the generalized periodicity is related only to the actual scale. The sequentially formed composite allows for a succession of homogenization steps based on one-dimensional cell problems.

We study the elasticity problem

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i(x) = 0 \quad \text{in} \quad \Omega^\epsilon,$$

(13)

$$u_i^\epsilon = 0 \quad \text{on} \quad S_d,$$

(14)

$$\sigma_{ij}^\epsilon n_j = t_i(x) \quad \text{on} \quad S_t,$$

(15)

$$\sigma_{ij}^\epsilon(x) = C_{ijkh}(x)\varepsilon_{kh}(u^\epsilon),$$

(16)

where $\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ is the infinitesimal strain tensor.

By putting

$$V = \{v \in (H^1(\Omega))^3|v|_{S_d} = 0\},$$

(17)

where $v|_{S_d}$ is the value of $v$ on the boundary $S_d$, the equations of equilibrium (13), in weak formulation, are written

$$\int_{\Omega} \nabla_j \sigma_{ij} \omega_i d\Omega + \int_{\Omega} f_i \omega_i d\Omega = 0, \quad \forall \omega_i \in V.$$

(18)

We apply the asymptotic expansion homogenization technique and we conclude (15) that the microstress satisfies the equation of equilibrium,

$$\frac{\partial \sigma_{ij}^0}{\partial y_j} = 0,$$

(19)

or

$$\frac{\partial \sigma_{ij}^0}{\partial y_m} \frac{\partial \varrho_m}{\partial x_j} = 0.$$

(20)

The microequation or cell equation (19) or (20) is written as

$$\frac{\partial}{\partial y_l} \left( \frac{\partial g_l}{\partial x_j} C_{ijkz} \frac{\partial \varrho_m}{\partial x_z} \frac{\partial w_{kh}^0}{\partial y_m} + \frac{\partial g_l}{\partial x_j} C_{ij\phi\theta} \right) = 0$$

(21)

with respect to the unknowns $w_{ij}^{kh}$ (where the indices $l, m$ take the value 1, the indices $i, k$ take the values 1,2,3 and the indices $j, z$ take the values 1,2) under appropriate periodicity and continuity conditions.

3 THE SOLUTION OF THE MICROEQUATION

By expanding (13) for $l, m, j, z,$ and $k,$ and after intergration [10] we conclude to the following equation in matrix form

\[
\begin{pmatrix}
\text{mat} \frac{\partial w_1^{0\alpha}}{\partial y_1} \\
\text{mat} \frac{\partial w_1^{0\alpha}}{\partial y_2} \\
\text{mat} \frac{\partial w_1^{0\alpha}}{\partial y_3}
\end{pmatrix}
\begin{pmatrix}
\text{mat} C_{1\alpha}^{\alpha} \\
\text{mat} C_{2\alpha}^{\alpha} \\
\text{mat} C_{3\alpha}^{\alpha}
\end{pmatrix}
= \begin{pmatrix}
\text{mat} C_{1\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_1} (\text{mat}) C_{1\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_2} (\text{mat}) C_{1\alpha}^{\alpha} \\
\text{mat} C_{2\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_1} (\text{mat}) C_{2\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_2} (\text{mat}) C_{2\alpha}^{\alpha} \\
\text{mat} C_{3\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_1} (\text{mat}) C_{3\alpha}^{\alpha} - \frac{\partial \varrho}{\partial x_2} (\text{mat}) C_{3\alpha}^{\alpha}
\end{pmatrix},
\]


NUMERICAL EXAMPLES.

4.1 “Chevron” structure

The first example is the two-dimensional, two-phase, second-rank laminate shown in Fig. 1. The widths \( \theta_{II} \) of the slabs should be much larger than the thicknesses of the layers within each slab. The layers within each slab form angles \( \theta_1 \) and \( \theta_2 \), not necessarily equal. One case is considered: \( \theta_1 = 30^\circ \), \( \theta_2 = 60^\circ \). The constituents are assumed isotropic with mechanical properties shown in Tables 1 and 2.

We follow a two-step homogenization procedure. According to this procedure, the problem will be solved first to the direction normal to the layers of the initial composite and as a result we will obtain a “new intermediate”
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Next we will apply the same procedure along \( x_1 \) axis for the constituents of the “new intermediate” composite, resulting from the first step. It is obvious that two generalized functions are required. The generalized periodicity function for the first step of the homogenization is \( \varrho^I = x_2 - x_1 \tan \theta \) with gradients
\[
\frac{\partial \varrho^I}{\partial x_1} = -\tan \theta \quad \text{and} \quad \frac{\partial \varrho^I}{\partial x_2} = 1.
\]
The generalized periodicity function for the second step is \( \varrho^{II} = x_1 \) with gradients
\[
\frac{\partial \varrho^{II}}{\partial x_1} = 1 \quad \text{and} \quad \frac{\partial \varrho^{II}}{\partial x_2} = 0.
\]

Figure 1: “Chevron” structure. Two microscale composite with laminate structure, forming angles \( \theta_1 \) and \( \theta_2 \) with \( x_1 \) axis in the macrocoordinate system, the one - dimensional cell in the framework of generalized periodicity in microcoordinate system of the first step and the corresponding of the second step. The material to be homogenized of the second step is a two - phase stratified material.

The RUC of the first step of homogenization (parameter of heterogeneity \( \epsilon^I \)) consists of 90% metal and 10% ceramic, while the volume fractions for the second step are 75% for the slab forming angle \( \theta_1 \) with the \( x_1 \) axis and 25% for the slab forming angle \( \theta_2 \) with the \( x_1 \) axis. We compute the effective elastic matrix from equation (26) using a MATLAB code that we have developed.

This is the simplest case since in both steps only two materials (the initial constituents in the first step and the results of the first step as constituents in the second step) are used.

Table 1: “Chevron” structure. Mechanical properties of constituents.

<table>
<thead>
<tr>
<th>Property</th>
<th>Metal</th>
<th>Ceramic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young Modulus (GPa)</td>
<td>72.4</td>
<td>420</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.33</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 2: “Chevron” structure. Elastic (symmetric) matrix coefficients of the two constituents (in GPa).

<table>
<thead>
<tr>
<th>Mechanical Properties</th>
<th>Metal</th>
<th>Ceramic</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{11}, C_{22}, C_{33} )</td>
<td>107.271</td>
<td>504</td>
</tr>
<tr>
<td>( C_{12}, C_{13}, C_{23} )</td>
<td>52.835</td>
<td>168</td>
</tr>
<tr>
<td>( C_{44}, C_{55}, C_{66} )</td>
<td>27.218</td>
<td>168</td>
</tr>
<tr>
<td>( C_{14}, C_{15}, C_{16} )</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( C_{24}, C_{25}, C_{26} )</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( C_{34}, C_{35}, C_{36} )</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

The results of the first step of homogenization are depicted in Tables 3 and 4, while the effective elastic matrix for the whole RUC is depicted in Table 5. Comparing Table 5 with Table 6, we conclude that the results of the present approach are in very good agreement with the results of the DIPH (see [9]).

4.2 Matrix reinforced by wavy fibers in two directions

Wavy fiber reinforced composite exhibit a nice mechanical behavior. In this example we consider a three - dimensional, two - phase composite consisting of a matrix reinforced by wavy fibers in two directions (see Fig. 2), parallel to \( x_2 \) – and \( x_1 \) – axis respectively, ordered vertically to \( x_3 \) – axis and forming two successive layers of
Table 3: “Chevron” structure. Effective elastic matrix for $\theta_1=30^\circ$ from the first step of homogenization (in GPa).

$$C^{\text{eff } I \theta_1} = \begin{pmatrix} 131.579 & 61.306 & 60.210 & 0 & 0 & 9.403 \\ 61.306 & 117.610 & 57.067 & 0 & 0 & 2.694 \\ 60.210 & 57.067 & 144.373 & 0 & 0 & 2.722 \\ 0 & 0 & 0 & 32.605 & 5.018 & 0 \\ 0 & 0 & 0 & 5.018 & 38.399 & 0 \\ 9.403 & 2.694 & 2.722 & 0 & 0 & 35.518 \end{pmatrix}$$

Table 4: “Chevron” structure. Effective elastic matrix for $\theta_2=60^\circ$ from the first step of homogenization (in GPa).

$$C^{\text{eff } I \theta_2} = \begin{pmatrix} 117.610 & 61.306 & 57.067 & 0 & 0 & -2.694 \\ 61.306 & 131.579 & 60.210 & 0 & 0 & -9.403 \\ 57.067 & 60.210 & 144.373 & 0 & 0 & -2.722 \\ 0 & 0 & 0 & 38.399 & -5.018 & 0 \\ 0 & 0 & 0 & -5.018 & 32.605 & 0 \\ -2.694 & -9.403 & -2.722 & 0 & 0 & 35.518 \end{pmatrix}$$

Table 5: “Chevron” structure, $\theta_1 = 30^\circ$, $\theta_2 = 60^\circ$. Effective elastic matrix from the second step of homogenization by the proposed method (in GPa).

$$C^{\text{eff } I} = \begin{pmatrix} 127.017 & 60.536 & 59.010 & 0 & 0 & 6.119 \\ 60.536 & 120.330 & 57.506 & 0 & 0 & -0.328 \\ 59.010 & 57.506 & 144.202 & 0 & 0 & 1.303 \\ 0 & 0 & 0 & 33.499 & 2.189 & 0 \\ 0 & 0 & 0 & 2.189 & 36.766 & 0 \\ 6.119 & -0.328 & 1.303 & 0 & 0 & 35.291 \end{pmatrix}$$

Table 6: “Chevron” structure, $\theta_1 = 30^\circ$, $\theta_2 = 60^\circ$. Effective elastic matrix by DIPH (in GPa) ([9]).

$$\tilde{C}^{\text{eff } I} = \begin{pmatrix} 128.087 & 61.306 & 59.424 & 0 & 0 & 6.379 \\ 61.306 & 121.102 & 57.853 & 0 & 0 & -0.330 \\ 59.424 & 57.853 & 144.373 & 0 & 0 & 1.361 \\ 0 & 0 & 0 & 35.053 & 2.509 & 0 \\ 0 & 0 & 0 & 2.509 & 36.950 & 0 \\ 6.379 & -0.330 & 1.361 & 0 & 0 & 35.518 \end{pmatrix}$$
thickness $\epsilon^{II}$ much larger than the distance $\epsilon^{I}$ between the wavy fibers. Then, the composite can be considered as a multilayered with two types of successive reinforced layers.

Each layer consists of a matrix reinforced by fibers of waviness 0.20. The volume fraction of fiber into each layer is 10%. The first layer is piled with angle 0° and the other with angle 90° and so on. The properties of both matrix and fiber are shown in Tables 7 and 8.

Table 7: Matrix reinforced by wavy fibers in two directions. Mechanical properties of the two constituents.

<table>
<thead>
<tr>
<th>Property</th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young Modulus (GPa)</td>
<td>276</td>
<td>3</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 8: Matrix reinforced by wavy fibers in two directions. Elastic (symmetric) matrix coefficients of the two constituents (in GPa).

<table>
<thead>
<tr>
<th>Mechanical Properties</th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$, $C_{22}$, $C_{33}$</td>
<td>371.538</td>
<td>4.038</td>
</tr>
<tr>
<td>$C_{12}$, $C_{13}$, $C_{23}$</td>
<td>159.231</td>
<td>1.731</td>
</tr>
<tr>
<td>$C_{44}$, $C_{55}$, $C_{66}$</td>
<td>106.154</td>
<td>1.154</td>
</tr>
<tr>
<td>$C_{14}$, $C_{15}$, $C_{16}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$C_{24}$, $C_{25}$, $C_{26}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$C_{34}$, $C_{35}$, $C_{36}$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

In order to solve this problem, we follow a two-step strategy. In the first step, we compute the effective elastic modulus in the RUC of each layer, that consists of a fiber reinforced matrix cube (see Fig. 3, 4, 5 and 6). This is a three-dimensional problem that has no analytical solution. In this case, we use the FEA commercial software DS Simulia Abaqus v.13 in order to solve the cell problem.

Figure 2: Matrix reinforced by wavy fibers in two directions. Laminate structure consists of fiber reinforced layers, piled with angles 0° (layer A) and 90° (layer B).

In the second step, where we will use the result of the first step as input data and we will apply the homogenization method as has been mentioned above (see “chevron” example). The volume fraction for the layer A is 70.0% and for the layer B is 30.0%. This is an one-dimensional problem with two equal volume phases. The generalized periodicity function for the second step is $\varphi^{II} = x_3$ with gradients $\frac{\partial \varphi^{II}}{\partial x_1} = 0$ and $\frac{\partial \varphi^{II}}{\partial x_3} = 1$. The results of the first step of homogenization are shown in Tables 9 and 10 while the results of the second step are shown in Table 11.

It should be remarked that, contrarily of the corresponding example in [10], the usage of not equal volume fractions for the layers in the second step, lead to a non symmetrical improvement of the effective elastic matrix (see $C_{11}^{eff}$ vs $C_{22}^{eff}$).

This example illustrates the advantages of the proposed method, namely the lower computational cost, the flexibility and the great adaptativity to many cases of “hierarchical” multi-scale composites, comparing to a full FE method.

5 CONCLUSIONS

In this paper, we presented a multi-step homogenization scheme for a sequentially laminated composite made of elastic isotropic materials. We formulated the microproblem and gave the analytical solution of it, as well as the effective coefficients at every step of the homogenization process. We confirm that homogenization causes
Figure 3: Matrix reinforced by wavy fibers in two directions. Meshing of the fiber for the first step of homogenization.

Figure 4: Matrix reinforced by wavy fibers in two directions. (a) Displacement loading of the fiber and (b) the corresponding shear stress field of the fiber for the first step of homogenization.

Table 9: Matrix reinforced by wavy fibers in two directions. Layer A (angle $0^\circ$). Effective elastic matrix from the first step of homogenization by DS Simulia Abaqus (in GPa).

$$C_{eff \, \text{A}} = \begin{pmatrix}
20.320 & 2.010 & 2.260 & 0 & 0 & 0 \\
2.010 & 4.810 & 2.000 & 0 & 0 & 0 \\
2.260 & 2.000 & 5.040 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.390 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.620 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.500
\end{pmatrix}$$

Table 10: Matrix reinforced by wavy fibers in two directions. Layer B (angle $90^\circ$). Effective elastic matrix from the first step of homogenization by DS Simulia Abaqus (in GPa).

$$C_{eff \, \text{B}} = \begin{pmatrix}
4.810 & 2.010 & 2.000 & 0 & 0 & 0 \\
2.010 & 20.320 & 2.260 & 0 & 0 & 0 \\
2.000 & 2.260 & 5.040 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.620 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.390 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.500
\end{pmatrix}$$

Table 11: Matrix reinforced by wavy fibers in two directions. Effective elastic matrix from the second step of homogenization (in GPa).

$$C_{eff \, \text{II}} = \begin{pmatrix}
15.667 & 2.010 & 2.182 & 0 & 0 & 0 \\
2.010 & 9.463 & 2.078 & 0 & 0 & 0 \\
2.182 & 2.078 & 5.040 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.459 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.551 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.500
\end{pmatrix}$$
Table 12: Matrix reinforced by wavy fibers in two directions. Percent improvement of the effective elastic matrix comparing to pure matrix.

\[
\begin{pmatrix}
+287.989\% & +16.118\% & +26.054\% & 0 & 0 & 0 \\
+16.118\% & +134.349\% & +20.046\% & 0 & 0 & 0 \\
+26.054\% & +20.046\% & +24.814\% & 0 & 0 & 0 \\
0 & 0 & 0 & +26.430\% & 0 & 0 \\
0 & 0 & 0 & 0 & +34.402\% & 0 \\
0 & 0 & 0 & 0 & 0 & +29.983\%
\end{pmatrix}
\]

Figure 5: Matrix reinforced by wavy fibers in two directions. Meshing of the RUC for the first step of homogenization.

Figure 6: Matrix reinforced by wavy fibers in two directions. (a) Displacement loading of the fiber and (b) the corresponding shear stress field of the RUC for the first step of homogenization.
anisotropy. We presented a combination of this method with computational homogenization techniques in order to reduce the computational cost of three-dimensional problems. The advantages of the proposed method are the lower computational cost, the flexibility and the great adaptativity to many cases of multiscale composites, comparing to a full FEA method. Finally, we presented two numerical examples, a “chevron” composite and a matrix reinforced with wavy fibers in two directions.

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