Homogenisation with application to layered materials

Patricio Dias, M.J.; Mattheij, R.M.M.; de With, G.

Published: 01/01/2007

Document Version
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
• A submitted manuscript is the author’s version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

Citation for published version (APA):
Homogenisation with application to layered materials.

M. Patrício* R. Mattheij* G. With**

*Adress: Department of Mathematics and Computer Science
Technische Universiteit Eindhoven
**Adress: Department of Chemical Engineering and Chemistry
Technische Universiteit Eindhoven

Abstract

In this paper we are concerned with the elliptic PDEs with highly oscillating coefficients which model the behaviour of composite linear elastic materials. Analytical expressions for the effective coefficients are obtained for the case of layered materials using the theory of homogenisation. Some properties of the homogenised materials are analysed. An efficient algorithm for the numerical determination of the effective coefficients is proposed.

Keywords: Homogenisation, layered materials, composites, finite elements, effective coefficients.

1 Introduction

Linear elastic materials can be modelled by second order elliptic PDEs. The equations are obtained in terms of the displacements [11, 16] and there are many situations in which their solutions are either known [15] or can be easily computed using classical numerical techniques such as finite elements or boundary elements methods, cf. [3, 7].

Particularly, when dealing with composite materials, the coefficients of the PDEs that arise are material dependent. It is often the case that the constituents of the composite are finely mixed and the coefficients jump between different values along the spatial coordinates very rapidly. We are then left with PDEs with highly oscillatory coefficients. These are usually very hard to solve not only analytically but also from the point of view of numerical computing.
Many different strategies that extend and adapt the method of finite elements for this particular class of problems have been developed. For example, some authors [1, 2] proposed that the choice of the space of admissible functions and test functions should depend on the problem that one is trying to solve. The multiscale finite element methods is a technique in which the base functions are taken to solve the problem locally. These are then used to generate a space of finite elements. The idea is to be able to automatically take information from the small scale to the macro scale, see [12, 13]. An alternative is given by the heterogeneous multiscale method which follows a top-down strategy; the starting point is an incomplete macroscale model and the missing numerical data from the microscale model is estimated and used as a complement [10].

In this paper, we focus on the theory of homogenisation, an asymptotic method for PDEs with rapidly oscillating coefficients, which henceforth we assume to be periodic with period $\epsilon$, $\epsilon \ll 1$. This is a popular technique that is used in many applications such as fibre optics, composite materials and flow in porous media. It allows for the approximation of the solution of the original equations in terms of simpler PDEs, the homogenised or effective equations. This way we establish the macroscopic behaviour of a system which has heterogeneities on the microscopic level.

For periodic materials, this homogenisation or upscaling procedure we have described has allowed for significant progress. On the other hand, for natural phenomena which are better described by nonlinear differential equations in a random nonhomogeneous medium, many problems still remain open. Also, the usage of phenomenological parameters such as the coefficient of elasticity that appears in the context of linear elasticity has in itself limitations. In recent years, detailed microscopic studies have been revealing interesting aspects on the microscopic realm, some of which in contrast to common expectations. For instance, the hardness of a material does not grow monotonously with a reduction of the crystal size [4, 5].

The concept of homogenisation has been associated to other techniques and looked at from different points of view, giving rise to very efficient algorithms. Much has been written on this subject - [14, 18]. We like to cite [9] in particular, which updates the earlier writings of [6, 8, 20].

Our starting point is the relation between the effective coefficients and the coefficients of the original PDE. This involves the corrector functions, which in turn are the solutions of the cell problem. For layered materials, it is sometimes possible to find closed form expressions for the effective coefficients, see [9, 18]. We adapt and extend these results for the more complicated problem of linear elasticity. We will obtain useful analytical expressions enabling us to characterize the nature of the homogenised materials. More precisely, we show that the homogenised material corresponding to a composite with linear elastic components is orthotropic. Its material constants will be related to those of the components of the original material.
We start by presenting a one dimensional example of an elliptic PDE with oscillating coefficients in section 2. Applying classical finite elements would require a prohibitive computational cost when the parameter $\epsilon$ is very small. The effective solution for this problem is obtained and compared to the solution of the original heterogeneous problem.

Next, in section 3 the elasticity problem for composite materials is formulated. We follow [9] to analyse the asymptotic behaviour of the underlying equations. The necessary fundamental concepts of homogenisation theory are introduced and the homogenised equations are presented, as well as the main convergence result.

Section 4 is devoted to layered composite materials. We use the theory of the previous section to deduce the effective coefficients. It is shown that the homogenised material which corresponds to an isotropic elastic layered material is orthotropic. The engineering constants are determined. We conclude this section with an example which illustrates the application of the theory.

Finally, in section 5 we propose an algorithm to determine the effective solution numerically for the more general case. We discuss its application to several examples, with particular attention being given to layered materials.

## 2 One-dimensional model

In order to illustrate many of the relevant issues present in more sophisticated problems, we will look for the solution of a one-dimensional Dirichlet boundary value problem with periodically oscillating coefficients

$$a(\epsilon x) := a(\frac{x}{\epsilon}). \quad (2.1)$$

Here, $a(\epsilon x)$ is an $\epsilon$-periodic function and $\epsilon \ll 1$. This is a simple example to justify why the usage of classical finite elements is not a good choice for problems with rapidly oscillating coefficients and to show how the homogenisation theory provides a good solution without having to resolve the microscale. Let, more particularly,

$$a^\epsilon(x) := \frac{1}{2 + \sin(\frac{2\pi x}{\epsilon})}. \quad (2.2)$$

and consider the problem

$$\left\{ \begin{array}{ll}
- \frac{d}{dx} \left[ a^\epsilon(x) \frac{d}{dx} u^\epsilon(x) \right] &= f(x), \ x \in (0,1), \\
\epsilon u^\epsilon(0) &= 0, \\
\epsilon u^\epsilon(1) &= 0, 
\end{array} \right. \quad (2.3)$$

If $\epsilon$ tends to zero, $a^\epsilon$ becomes an increasingly oscillating function, see Figure 1.
Let us now take $f(x) = 1$. The solution $u^\epsilon$ of problem (2.3), represented in Figure 2 a), is given by

$$u^\epsilon(x) = \int_0^x \left( \frac{-y + c_0}{a(y/\epsilon)} \right) dy, \quad c_0 = \frac{\int_0^1 [a(y/\epsilon)]^{-1} y dy}{\int_0^1 [a(y/\epsilon)]^{-1} dy}. \quad (2.4)$$

In general, it is hard or even not possible to find the analytical solution for problems like (2.3). We must then recur to numerical methods. The classical finite elements are not very appropriate unless the mesh size $h$ is taken sufficiently smaller than $\epsilon$ - [13]. This is computationally very expensive when as in many real world problems $\epsilon$ is very small. In that case, even with heavy computer efforts it is impossible to take $h < \epsilon$. Let $f \in L^2(0,1)$ and suppose that there exist two real constants $\alpha$ and $\beta$ such that

$$0 < \alpha \leq a(x) \leq \beta.$$ 

Let $\{x_i\}_{i=1,...,N+1}$, with $x_i = i/(N + 1)$ be a discretization of the interval $[0,1]$ into disjoint subintervals of length $h$. Denote by $V^h_0$ the subspace of $H^1(0,1)$ given by the functions that are linear in every interval $[x_{i-1}, x_i]$, for $i = 1, \ldots, N + 1$. Then the error of the finite element approximation $u_h \in V^1(0,1)$ to $u^\epsilon \in H^1_0(0,1)$ which satisfies

$$\int_0^1 a(x/\epsilon) \frac{d u_h}{d x}(x) \frac{d v_h}{d x}(x) dx = \int_0^1 f(x)v_h(x)dx, \forall v_h \in V^h_0 \quad (2.5)$$

is estimated by

$$\|u^\epsilon - u_h\|_{H^1(0,1)} \leq c \frac{\beta^2 h}{\alpha^3 \epsilon} \|f\|_{L^2(0,1)}, \quad (2.6)$$

with $c \in \mathbb{R}$, cf. [17]. Though it is clear that for a fixed value of $\epsilon$, $u_h$ converges to $u^\epsilon$, the convergence of this method is not uniform in $\epsilon$ - [19]. This implies that when finite elements are used the grid size $h$ must be taken much smaller than $\epsilon$. 

Figure 1: Oscillating behaviour of $a^\epsilon$, $\epsilon = 0.1$. 

Let $\{x_i\}_{i=1,...,N+1}$ be a discretization of the interval $[0,1]$ into disjoint subintervals of length $h$. Denote by $V^h_0$ the subspace of $H^1(0,1)$ given by the functions that are linear in every interval $[x_{i-1}, x_i]$, for $i = 1, \ldots, N + 1$. Then the error of the finite element approximation $u_h \in V^1(0,1)$ to $u^\epsilon \in H^1_0(0,1)$ which satisfies

$$\int_0^1 a(x/\epsilon) \frac{d u_h}{d x}(x) \frac{d v_h}{d x}(x) dx = \int_0^1 f(x)v_h(x)dx, \forall v_h \in V^h_0 \quad (2.5)$$

is estimated by

$$\|u^\epsilon - u_h\|_{H^1(0,1)} \leq c \frac{\beta^2 h}{\alpha^3 \epsilon} \|f\|_{L^2(0,1)}, \quad (2.6)$$

with $c \in \mathbb{R}$, cf. [17]. Though it is clear that for a fixed value of $\epsilon$, $u_h$ converges to $u^\epsilon$, the convergence of this method is not uniform in $\epsilon$ - [19]. This implies that when finite elements are used the grid size $h$ must be taken much smaller than $\epsilon$. 

4
One alternative approach which allows for a good numerical approximation using a mesh size $h > \epsilon$ is given by the homogenisation theory. It allows for the formulation of a second problem, still of the form of (2.3) but with constant coefficients - called effective coefficients - so we are rid of the oscillations. The effective solution $\bar{u}$ of the new problem should capture the macroscopic behaviour of $u^\epsilon$, but not the oscillations on the microscopic scale.

It can be shown that the homogenised problem related to (2.2) - (2.3), and again with $f(x) = 1$, reads

$$
\begin{align*}
- \int_0^1 1/a(y)dy \frac{d^2}{dx^2} \bar{u}(x) &= 1, \ x \in (0,1), \\
\bar{u}(0) &= 0, \\
\bar{u}(1) &= 0.
\end{align*}
$$

(2.7)

Its solution, plotted in Figure 2b), is given by

$$
\bar{u}(x) = - \int_0^1 \frac{1}{a(y)}dy \left[ \frac{1}{2} (x^2 - x) \right].
$$

(2.8)

We now follow [9, 21] to relate $u^\epsilon$ and $\bar{u}$. Let $a(x)$ be a positive function in $L^\infty(0, l_1)$, which we extend to $\mathbb{R}$ such that it is $l_1$-periodic. In these conditions, the following theorem justifies the validity of the approximation provided by the homogenisation theory.

**Theorem 2.1.** Given $f \in L^2(d_1, d_2)$, let $u^\epsilon \in H^1_0(d_1, d_2)$ be the unique solution of the problem
\[
\begin{aligned}
\begin{cases}
-\frac{d}{dx} [a'(x) \frac{d}{dx} u'(x)] &= f(x), \ x \in (d_1, d_2), \\
u'(d_1) &= 0, \\
u'(d_2) &= 0,
\end{cases}
\end{aligned}
\]  
(2.9)

and \( \Sigma \in H^1_0(0,1) \) be the unique solution of the problem

\[
\begin{aligned}
\begin{cases}
-\Sigma \frac{d^2}{dx^2} \Sigma(x) &= f(x), \ x \in (d_1, d_2), \\
\Sigma(d_1) &= 0, \\
\Sigma(d_2) &= 0,
\end{cases}
\end{aligned}
\]  
(2.10)

where the effective coefficient \( \Sigma \) is given by

\[
\Sigma = \frac{1}{\int_{0}^{1} [a(y)]^{-1} dy}.
\]  
(2.11)

Then the solution of problem (2.9) converges to the solution of problem (2.10) in \( H^1_0(0,1) \), i.e

\[
u' \rightharpoonup \Sigma \text{ weakly in } H^1_0(0,1).
\]  
(2.12)

In other words, this allows us to find an approximation for the solution of (2.9) without having to solve the microscale. Instead, we are left to deal with the simpler homogenised problem (2.10), once the effective coefficient \( \Sigma \) has been determined.

Finally, let \( a \in W^{1,p}(\mathbb{R}) \), for some \( p > 2 \). Under the conditions of the previous theorem it can be shown, as in [17], that there exists a constant \( C \in \mathbb{R} \) such that

\[
\|u' - \Sigma\|_{H^1(d_1,d_2)} \leq C \epsilon \|\Sigma\|_{H^2(d_1,d_2)}.
\]  
(2.13)

3 Homogenisation for elasticity

In what follows, we briefly analyse the asymptotic behaviour of the solution of elasticity problems associated to periodic composite materials using the theory of homogenisation - [9, 18]. We present these results for a 2D plane stress situation, though they can be extended to higher dimensions in a straightforward way.

Consider a composite material with constituents periodically distributed over \( \Omega \subseteq \mathbb{R}^2 \). We can then define a reference cell \( Y = [0,l_1] \times [0,l_2] \) such that \( \Omega \) is covered by a mosaic of cells of the form \( \epsilon Y = [0,\epsilon l_1] \times [0,\epsilon l_2] \) - Figure 3.
Figure 3: Domain $\Omega$ and reference cell $Y$.

Now consider the fourth-order tensor $A = A(y) = (a_{i,j,k,h})_{1 \leq i,j,k,h \leq 2}$ defined over the reference cell $Y$. For any $2 \times 2$ matrices $M = (m_{ij})_{1 \leq i,j \leq 2}$ and $N = (n_{ij})_{1 \leq i,j \leq 2}$, we denote

\[
\|M\| = \left( \sum_{i,j=1}^{2} m_{ij}^2 \right)^{1/2},
\]

\[
AM = \left( \sum_{k,h=1}^{2} a_{i,j,k,h}m_{k,h} \right)_{1 \leq i,j \leq 2},
\]

\[
AMN = \sum_{i,j,k,h=1}^{2} a_{i,j,k,h}m_{ij}n_{kh}.
\]

Now, assume that there exist $\alpha, \beta \in \mathbb{R}$ and with $A \in M_e(\alpha, \beta, Y)$, ie

- $a_{i,j,k,h} \in L^\infty(Y)$, for any $i,j,k,h \in \{1,2\}$;
- $a_{i,j,k,h} = a_{j,i,k,h} = a_{k,h,i,j}$, for any $i,j,k,h \in \{1,2\}$;
- $\alpha\|M\|^2 \leq AMM$, for any symmetric $2 \times 2$ matrix $M$;
- $\|A(y)M\| \leq \beta\|M\|$, for any $2 \times 2$ matrix $M$, almost anywhere on $Y$.

We extend the functions $a_{i,j,k,h}$ to $\mathbb{R}^2$ periodically, which allows us to define a second tensor $A^\epsilon = A^\epsilon(x) = (a_{i,j,k,h}^\epsilon)_{1 \leq i,j,k,h \leq N}$ such that for $x = (x_1, x_2) \in \mathbb{R}^2$,

\[
a_{i,j,k,h}^\epsilon(x) := a_{i,j,k,h}(y) = a_{i,j,k,h}(\frac{x}{\epsilon}),
\]

where we denote $y := \frac{x}{\epsilon}$, for $y = (y_1, y_2) \in \mathbb{R}^2$. It can be shown that $A \in M_e(\alpha, \beta, Y)$ implies that $A^\epsilon \in M_e(\alpha, \beta, Y)$.

We now formulate the linear elasticity problem for the composite material. Let $\Omega$ be a connected bounded open set in $\mathbb{R}^n$. Moreover, let $\partial \Omega = \Gamma_N \cup \Gamma_D$ be Lipschitz continuous such that $\Gamma_D$ is of measure greater than zero. Then the problem is stated as
\[
\begin{cases}
- \nabla \cdot (A\epsilon(x)\epsilon(u)) = f & \text{in } \Omega, \\
u^\epsilon = 0 & \text{on } \Gamma_D, \\
\sigma(u^\epsilon) \cdot n = \varphi_N & \text{on } \Gamma_N,
\end{cases}
\] (3.2)

where the functions \( \varphi_N \) and \( f \) are given and \( \epsilon, \sigma \) and \( u \) denote the strain tensor, the stress tensor and the displacement vector respectively. These are such that for every function \( w \),

\[
\epsilon(w) = (\nabla w + (\nabla w)^T), \quad \sigma(w) = A\epsilon(w).
\] (3.3)

We look for weak solutions of (3.2) in the space \( V \) defined by

\[
V = \{ v \mid v \in H^1(\Omega), \quad \gamma(v) = 0 \text{ on } \Gamma_1 \},
\] (3.4)

cf. [9]. Note that \( \gamma(v) = v|_{\partial \Omega} \) is the trace of \( v \) on \( \partial \Omega \), the unique linear continuous map \( \gamma : H^1(\Omega) \to L^2(\partial \Omega) \). We then look for the unique \( u^\epsilon \in V = V^2 \) and define the following norm

\[
\|v\|_V = \left( \sum_{i=1}^2 \|\nabla v_i\|_{L^2(\Omega)}^2 \right)^{1/2},
\] (3.5)

for \( v = (v_1, v_2) \in V \).

In order to find the homogenised version for the problem (3.2) it is useful to introduce some auxiliary functions. Consider the family of vector valued functions \( P^{lm}(y) = (P^{lm}_k(y)) \) defined by

\[
P^{lm}_k(y) := y_m \delta_{kl}, \quad k = 1, 2,
\] (3.6)

where \( \delta_{kl} \) is the Kronecker symbol and \( l, m \in \{1, 2\} \). Let \( \chi^{lm}(y) = (\chi^{lm}_k(y)) \in (W_{per}(Y))^2 \) be the unique solution of the cell problem

\[
\begin{cases}
- \nabla \cdot (A(y)\nabla(\chi^{lm} - P^{lm})) = 0 \text{ for } y \in Y, \\
\chi^{lm} \text{ is } Y\text{-periodic}, \\
M_Y(\chi^{lm}_k) = 0,
\end{cases}
\] (3.7)

where the notation

\[
M_Y(f) := \frac{1}{|Y|} \int_Y f(y)dy
\] (3.8)

was used,

\[
W_{per}(Y) := \{ v \in H^1_{per}(Y) | M_Y(v) = 0 \}.
\] (3.9)

and \( H^1_{per}(Y) \) is the closure for the \( H^1 \)-norm of \( C^\infty_{per}(Y) \), the subset of \( C^\infty_{per}(\mathbb{R}) \) of periodic functions over \( Y \). For \( l, m \in \{1, 2\} \), it can be shown that the solution of (3.7) is unique.
We now aim at characterizing the homogeneous solution of the elasticity problem. The following theorem, given as in [9], is the equivalent of the theorem presented earlier on section 2 but now in the context of elasticity.

**Theorem 3.1.** Let us consider the heterogeneous elasticity problem for a composite

\[
\begin{align*}
-\nabla \cdot (A(\varepsilon(x))\varepsilon(u)) &= f & \text{in } \Omega, \\
\varepsilon(u) &= 0 & \text{on } \Gamma_D, \\
\sigma(\varepsilon(u)) \cdot n &= \varphi_N & \text{on } \Gamma_N,
\end{align*}
\]

(3.10)

where \( f \in V' \), \( \varphi_N \in (H^{-1/2}(\Gamma_2))^2 \) and \( u' \in V \) is its unique solution.

Then

\[
\begin{align*}
\varepsilon(u') &\to \varepsilon(\bar{u}) \text{ weakly in } V, \\
A'\varepsilon(u') &\to A\varepsilon(\bar{u}) \text{ weakly in } (L^2(\Omega))^2, \\
\end{align*}
\]

(3.11)

where \( \bar{u} \in V \) is the unique solution of the homogenised problem

\[
\begin{align*}
-\nabla \cdot (A\varepsilon(\bar{u})) &= f & \text{in } \Omega, \\
\bar{u} &= 0 & \text{on } \Gamma_D, \\
\bar{u} \cdot n &= \varphi_N & \text{on } \Gamma_N.
\end{align*}
\]

(3.13)

The homogenised tensor \( A = (\bar{a}_{ijkh}) \) is symmetric and

\[
\bar{a}_{ijkh} = \frac{1}{|Y|} \int_Y a_{ijkh}(y) dy - \frac{1}{|Y|} \int_Y \sum_{l,m=1,2} a_{ijlm}(y) \frac{\partial \lambda_{kh}}{\partial y_m}(y) dy.
\]

(3.14)

This theorem is the fundamental result which allows us to undergo the analysis of layered materials in the next section. In practical terms, one may avoid computing the solution of (3.10) directly. This implies solving the cell problem (3.7) to find the effective coefficients \( \bar{a}_{ijkh} \) and finally computing the approximation \( \bar{u} \) for \( u' \).

## 4 Effective solution for layered composites

In this section we will consider layered periodic composite materials, such that their properties vary only along one spatial coordinate. We show how the effective coefficients can be determined analytically and use this result to characterize the homogenised material.

Let us consider the elasticity problem
\[
\begin{aligned}
\begin{cases}
-\nabla \cdot (A'(x)\epsilon(u')) = f & \text{in } \Omega, \\
u' = 0 & \text{on } \Gamma_D, \\
\sigma(u') \cdot n = \varphi_N & \text{on } \Gamma_N,
\end{cases}
\end{aligned}
\] (4.1)

where

\[
a_{ijkh}'(x) = a_{ijkh}(\frac{x}{\epsilon}) = a_{ijkh}(\frac{x_1}{\epsilon}) = a_{ijkh}'(x_1).
\] (4.2)

We further assume that the reference cell is such that \(|Y| = 1\), for the sake of simplicity and without loss of generality. Then under the conditions of theorem 3.1, we make use of (4.2) to solve the cell problem analytically and find explicit expressions for the effective coefficients.

**Theorem 4.1.** Consider the problem (4.1), where the components of the tensor \(A'\) satisfy

\[
det(y_1) := a_{1111}(y_1)a_{2121}(y_1) - a_{2111}^2(y_1) \neq 0 \quad \forall y_1 \in [0, l_1].
\] (4.3)

Furthermore, we denote

\[
\begin{align*}
\text{Det} & := \left[ M_Y \left( \frac{a_{2111}}{\det} \right)^2 - M_Y \left( \frac{a_{1111}}{\det} \right) M_Y \left( \frac{a_{2121}}{\det} \right) \right], \\
A_{ij} & := -M_Y \left( \frac{a_{ij11}a_{2121}}{\det} \right) + M_Y \left( \frac{a_{ij21}a_{1111}}{\det} \right), \\
B_{ij} & := M_Y \left( \frac{a_{ij11}a_{1121}}{\det} \right) - M_Y \left( \frac{a_{ij21}a_{1111}}{\det} \right).
\end{align*}
\] (4.4) (4.5) (4.6)

Then the effective solution \(\overline{u}\) for this problem satisfies

\[
\begin{aligned}
\begin{cases}
-\nabla \cdot (\overline{A}(\overline{u})) = f & \text{in } \Omega, \\
\overline{u} = 0 & \text{on } \Gamma_D, \\
\sigma(\overline{u}) \cdot n = \varphi_N & \text{on } \Gamma_N,
\end{cases}
\end{aligned}
\] (4.7)

where the components of \(\overline{A}\) are symmetric and given by

\[
\overline{\pi}_{ijlm}(x) = \frac{A_{ij}}{\text{Det}} M_Y(\frac{a_{111m}}{\det}) + \frac{B_{ij}}{\text{Det}} M_Y(\frac{a_{211m}}{\det}),
\] (4.8)

for all \(i, j, l, m \in \{1, 2\}\) with \(i + j \geq l + m\), except for \(i = j = l = m = 2\). In the later case,
\[ \sigma_{2222}(x) = M_Y(a_{2222}) + M_Y\left( \frac{2a_{2211}a_{2221}a_{2111} - a_{2111}^2a_{2121} - a_{2221}^2a_{2111}}{\det} \right) \]

\[ -\frac{A_{22}}{\text{Det}} M_Y\left( \frac{a_{1111}}{\det} \right) + \frac{B_{22}}{\text{Det}} M_Y\left( \frac{a_{1111}}{\det} \right) A_{22} \]

\[ -\frac{B_{22}}{\text{Det}} M_Y\left( \frac{a_{2121}}{\det} \right) + \frac{A_{22}}{\text{Det}} M_Y\left( \frac{a_{2111}}{\det} \right) B_{22}. \tag{4.9} \]

**Sketch of a proof:**
Since \( a_{ijkh}(y) = a_{ijkh}(y_1) \), the homogenised coefficients given in (3.14) read

\[ \pi_{ijkh} = \frac{1}{|Y|} \int_Y a_{ijkh}(y_1) dy_1 - \frac{1}{|Y|} \int_Y a_{ijlm}(y_1) \frac{\partial \chi_{kh}}{\partial y_m}(y_1) dy_1. \tag{4.10} \]

The family of functions \( \frac{\partial \chi_{lm}^{i}}{\partial x_s} \) are determined by integrating the first equation in (3.7), which yields

\[ a_{1111} \frac{\partial \chi_{lm}^{i}}{\partial y_1} + a_{1121} \frac{\partial \chi_{lm}^{i}}{\partial y_1} = -a_{11lm} + c_{1}^{lm}, \tag{4.11} \]

\[ a_{2111} \frac{\partial \chi_{lm}^{i}}{\partial y_1} + a_{2121} \frac{\partial \chi_{lm}^{i}}{\partial y_1} = -a_{21lm} + c_{2}^{lm}. \tag{4.12} \]

The integration constants \( c_{k}^{lm} \) can be determined using the fact that the functions \( \chi_{k}^{lm} \) are \( Y \)-periodic. The result then follows from (4.10).

This is the fundamental step which allows for the formulation of the homogenised problem (3.13)-(3.14). The solution of this problem approximates the solution of (3.2), and we can now relate these two.

In particular, we can apply the previous result to a linear elastic isotropic non-homogeneous material with Poisson’s ratio \( \nu = \nu(y_1) \) and with Young’s modulus \( E = E(y_1), y \in Y \). The heterogeneous elasticity problem for this material is given by (4.1), where the symmetrical coefficients \( a_{ijkh} \) of the tensor \( A \) are now

\[ a_{2222} = a_{1111} = \frac{E}{1 - \nu^2}; \quad a_{2211} = \frac{E\nu}{1 - \nu^2}; \tag{4.13} \]

\[ a_{2121} = \frac{E}{2(1 + \nu)}; \quad a_{2111} = a_{2221} = 0. \tag{4.14} \]

In these conditions, we may compute the elasticity tensor \( \bar{A} \) explicitly.
Property 4.2. The homogeneous problem related to (4.1)-(4.13)-(4.14) is

\[
-\nabla \cdot (\mathcal{A}e(\mathbf{u})) = f \quad \text{in } \Omega, \\
\mathbf{u} = 0 \quad \text{on } \Gamma_D, \\
\sigma(\mathbf{u}) \cdot \mathbf{n} = \varphi_N \quad \text{on } \Gamma_N.
\]

The effective coefficients \(a_{ijlm}\) are symmetric and given by

\[
a_{1111} = \frac{1}{MY(1/a_{1111})}, \quad a_{2111} = a_{2221} = 0; \quad (4.16)
\]

\[
a_{2211} = \frac{MY(a_{2211}/a_{1111})}{MY(1/a_{1111})}, \quad a_{2121} = \frac{1}{MY(1/a_{2121})}; \quad (4.17)
\]

\[
a_{2222} = MY(a_{2222}) - MY\left(\frac{a_{2211}^2}{a_{1111}}\right) + MY\left(\frac{a_{2211}/a_{1111}}{a_{2222}}\right)^2. \quad (4.18)
\]

Proof: It is a consequence of Theorem 4.1.

Next, we consider the following

Lemma 4.3. In the conditions of Theorem (4.1) assume that there exist constants \(c_{ijlm}\) and a function \(E = E(y_1)\) such that the coefficients \(a_{ijlm}\) read

\[
a_{ijlm} = E(y_1)c_{ijlm}. \quad (4.19)
\]

Then the effective coefficients \(\overline{a}_{ijlm}\) are

\[
\overline{a}_{ijlm}(y_1) = \frac{1}{[c_{2111} - c_{1111}c_{2121}]/MY(1/E)\left(c_{1111}(-c_{ij11}c_{2121} + c_{ij21}c_{2111})
\right. + c_{2111}(c_{ij11}c_{2111} - c_{ij21}c_{2111})} \quad (4.20)
\]

for all indices \(i, j, l, m \in \{1, 2\}\) not simultaneously 2 and \(i + j \geq l + m\). In the later case,
\[ \pi_{2222}(y_1) = M_Y(E) \left[ c_{2222} + \right. \\
\left. \frac{2c_{2211}c_{2221}c_{2111} - c_{2111}^2c_{2211} - c_{2221}^2c_{1111}}{c_{2111}^2 - c_{1111}c_{2121}} \right] - \]
\[ \frac{2c_{2211}c_{2111}^2(-c_{2211}c_{2121} + c_{2221}c_{1111})}{(c_{2111}^2 - c_{1111}c_{2121})^2} + \]
\[ \frac{c_{2221}c_{1111}c_{2111}c_{2211}c_{2121} - c_{2221}c_{1111}^2}{(c_{2111}^2 - c_{1111}c_{2121})^2} + \]
\[ \frac{c_{1111}(-c_{2211}c_{2121} + c_{2221}c_{1111})^2}{(c_{2111}^2 - c_{1111}c_{2121})^2} + \]
\[ \frac{c_{2121}(c_{2211}c_{2111} - c_{2221}c_{1111})^2}{(c_{2111}^2 - c_{1111}c_{2121})^2} \right] \left[ \frac{1}{M_Y(1/E)} \right]. \quad (4.21) \]

**Proof:** It is a consequence of Theorem 4.1.

It is well known that the homogenised problem for an isotropic elastic material is not necessarily isotropic, cf. [18]. We will show that it is also not fully anisotropic if the Poisson’s ratio is constant - in fact, it is orthotropic, which means that the coefficients of the elasticity tensor \( A \) are given by

\[ a_{1111} = \frac{E_x}{1 - \nu_{xy}\nu_{yx}}; \quad a_{2211} = \frac{E_x\nu_{yx}}{1 - \nu_{xy}\nu_{yx}}; \quad (4.22) \]
\[ a_{2222} = \frac{E_y}{1 - \nu_{xy}\nu_{yx}}; \quad a_{2121} = G_{xy}; \quad (4.23) \]
\[ a_{2111} = a_{2221} = 0; \quad (4.24) \]

where \( \nu_{xy}E_y = \nu_{yx}E_x \).

**Property 4.4.** Let us consider the problem \((4.1)-(4.13)-(4.14)\), where \( \nu \) is a constant function and \( E = E(y_1) \).

Then the effective coefficients are such that the homogenised material is orthotropic. The corresponding material constants read

\[ E_x = \frac{AB}{A + \nu^2(B - A)}; \quad E_y = A, \quad (4.25) \]
\[ \nu_{xy} = \frac{B\nu}{A + \nu^2(B - A)}; \quad \nu_{yx} = \nu, \quad (4.26) \]
\[ G_{xy} = \frac{B}{2(1 + \nu)}; \quad (4.27) \]
where

\[ A = M_Y(E), \quad B = \frac{1}{M_Y(1/E)}. \]

**Proof:** It is a consequence of the previous lemma.

Upper and lower bounds for the material constants given in (4.25)-(4.27) can be determined in terms of the Young’s modulus and Poisson’s ratio of the original heterogeneous material.

**Property 4.5.** The material constants of the homogenised material satisfy

\[ \frac{1}{M_Y(1/E)} \leq E_x \leq M_Y(1/E), \]

\[ \frac{1}{M_Y(1/E)M_Y(1/E)} \nu \leq \nu_{xy} \leq \nu. \]

**Proof:** It is a consequence of the Cauchy-Schwarz inequality.

Finally, we construct a mixture of two isotropic homogeneous materials. Consider a composite layered material on \( \Omega \), which is such that its reference cell \( Y = [0,1] \times [0,1] \) can be decomposed into two subdomains \( Y_1 = [0, \frac{1}{2}] \times [0,1] \), \( Y_2 = [\frac{1}{2}, 1] \times [0,1] \). Suppose that for \( i = 1, 2 \), \( Y_i \) is occupied by a linear elastic material with Young’s modulus \( E_i \) and Poisson’s ratio \( \nu_i \).

Then, for a given value of \( \epsilon > 0 \) the domain \( \Omega \) can be decomposed into two subdomains

\[ \Omega_1^\epsilon = \{ x \in \Omega \mid \chi_1(\frac{x}{\epsilon}) = 1 \}, \]

\[ \Omega_2^\epsilon = \{ x \in \Omega \mid \chi_2(\frac{x}{\epsilon}) = 1 \}. \]

Here, \( \chi_1 \) and \( \chi_2 \) are the characteristic functions of the sets \( Y_1 \) and \( Y_2 \) given respectively by

\[ \chi_i(x) = \begin{cases} 1, & \text{for } x \in Y_i, \\ 0, & \text{for } x \in Y - Y_i, \end{cases} \]

that are extended by periodicity over \( Y \). In this conditions, we state the following
Property 4.6. Let us consider the problem (4.1) - (4.13) - (4.14), where

\[ E(x) = E_1 \chi_1(x_1) + E_2 \chi_2(x_1), \quad (4.31) \]
\[ \nu(x) = \nu_1 \chi_1(x_1) + \nu_2 \chi_2(x_1). \quad (4.32) \]

Then the corresponding homogenised material is orthotropic with engineering constants given by

\[ E_x = \frac{E}{\nu^2 + AE}, \quad E_y = E, \quad (4.33) \]
\[ \nu_{xy} = \frac{\nu}{\nu^2 + AE}, \quad \nu_{yx} = \nu, \quad (4.34) \]
\[ G = \frac{1}{\frac{2(1+\nu_1)}{E_1} + \frac{2(1+\nu_2)}{E_2}}, \quad (4.35) \]

where

\[ \overline{E} = \frac{1}{2}(E_1 + E_2), \quad \overline{\nu} = \frac{1}{2}(\nu_1 + \nu_2), \quad A = \frac{1}{2}(\frac{\nu_1^2}{E_1} + \frac{\nu_2^2}{E_2}). \quad (4.36) \]

Proof: It is a consequence of Property 4.2.

We conclude this section with an example to illustrate the previous property. Let \( \nu_1 = 0.1, \nu_2 = 0.3, E_1 = 1, E_2 = 10 \) and the boundary conditions be such that:

\[ \Gamma_D = \{0\} \times [0,1], \quad \varphi_N(x) = \begin{cases} 0 & \text{for } x_2 = 1, \\ 0 & \text{for } x_2 = 0, \\ (1,0) & \text{for } x_1 = 1. \end{cases} \quad (4.37) \]

We use a triangular grid with quadratic finite elements to solve the problem for \( \epsilon = 0.1 \). The vertical component of the displacements is plotted in Figures 4 a). We also plot the value of the horizontal displacement along the vertical line \( y = 0.5 \) in Figure 4 b).
Finally we represent the solution of the homogenised version of the problem in Figures 6 a) and b), obtained by applying Property 4.6. Again we used finite elements in the same manner as before.

As expected, the effective solution captures the essence of the behaviour of the original heterogeneous solution, disregarding only the oscillations.

5 Numerical examples

In this section we include examples of boundary value problems with coefficients which are material dependent, for different material properties. We consider two examples of layered materials. In the first, the coefficients of the underlying PDE are continuous functions of space. In the second example they are only piecewise continuous, as one would expect when dealing with composite materials.
Let us again consider the elasticity problem (4.1)-(4.13)-(4.14). In order to determine the effective solution of this problem, it is necessary to first solve the cell problem and determine the effective coefficients. We then consider the following algorithm:

Step 1 - solve the cell problem (3.7);

Step 2 - compute the coefficients $a_{ijkh}$ by means of (3.14);

Step 3 - determine the solution of the homogenised problem (4.15).

We note that numerical techniques may have to be used. In that case, it is important to estimate the error committed on each step, as the precision of the estimate $\bar{u}$ allowed by Theorem 3.1 depends also on these errors.

**Example 5.1 Continuous coefficients**

Consider the previous problem (4.1)-(4.13)-(4.14), where the reference cell is now given by $Y = [-0.5, 0.5] \times [-0.5, 0.5]$ and the material properties characterized by

$$E(y) = E(y_1) = 1 + y_1^2, \quad \nu = 0.3.$$  \hspace{1cm} (5.1)

The non-trivial effective coefficients for this problem are easily determined using Property 4.2. The exact values of the coefficients are displayed in the second column of Table 1 with 6 significant digits.

We now follow steps 1 and 2 of the previous algorithm, where we have applied numerical techniques to determine an approximation for the coefficients.

We use finite element analysis on a rectangular mesh with quadratic elements and step size $h = 0.01$ in order to solve the cell problem. The solution functions $\chi_{lm}^k$ are either the constant zero function or have similar shapes. We represent $\chi_{11}^k$ over the reference cell in figure 7.

For the second step, two distinct strategies were followed in order to determine an approximation for the effective coefficients. Both aim at solving (3.14), but they differ in how the integrals are dealt with.

The first approach employs the expression of the heterogeneous coefficients $a_{ijkh}$. In this case it is possible to compute the exact value of the integrals in (5.2) when we use a least square polynomial approximation for $\chi_{i1}^{kh}$. In the third and fourth columns of Table 1 we display the approximations $A_{p3}$ and $A_{p9}$ for the relevant effective coefficients, obtained by using the mentioned polynomials with degree 3 and 9, respectively.
Figure 7: The periodic cell function $\chi_{11}^{11}$ of Example 5.1.

Table 1: Effective coefficients.

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Exact</th>
<th>$A_{p_4}$</th>
<th>$A_{p_9}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi_{111}$</td>
<td>1.18506</td>
<td>1.18350</td>
<td>1.18506</td>
</tr>
<tr>
<td>$\pi_{212}$</td>
<td>0.41477</td>
<td>0.41423</td>
<td>0.41477</td>
</tr>
<tr>
<td>$\pi_{221}$</td>
<td>0.35552</td>
<td>0.35505</td>
<td>0.35552</td>
</tr>
<tr>
<td>$\pi_{222}$</td>
<td>1.18999</td>
<td>1.18985</td>
<td>1.18999</td>
</tr>
</tbody>
</table>

The values of the residuals of the approximations of the relevant non-zero functions $\chi_{kh}^{kh}$, denoted by $Res_3$ and $Res_9$, are given in Table 2.

Table 2: Residual of the approximation of $\chi_{kh}^{kh}$.

<table>
<thead>
<tr>
<th>Function</th>
<th>$Res_3$</th>
<th>$Res_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_{11}^{11}$</td>
<td>$2.1E - 3$</td>
<td>$1.7E - 7$</td>
</tr>
<tr>
<td>$\chi_{21}^{21}$</td>
<td>$2.1E - 3$</td>
<td>$1.7E - 7$</td>
</tr>
<tr>
<td>$\chi_{12}^{22}$</td>
<td>$6.2E - 4$</td>
<td>$5.1E - 8$</td>
</tr>
</tbody>
</table>

The second strategy that we adopt consists of computing the right hand side of (3.14) thus avoiding fitting. Instead, numerical differentiation and integration
techniques are used. Firstly, for the approximation of \( \frac{\partial \chi_k}{\partial y_l} \), central differences are employed for all points except for the boundaries, where forward and backward differences are used on \( x = -0.5 \) and \( x = 0.5 \), respectively. For the integration of the integrals, the classical composite Trapezoidal and composite Simpson rules with 101 and 25 equidistant points are used. The values of the estimates for the coefficients are given in Table 3.

Table 3: Effective coefficients.

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Trapezoidal</th>
<th>Simpson</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \pi_{111} )</td>
<td>1.18539</td>
<td>1.18508</td>
</tr>
<tr>
<td>( \pi_{2121} )</td>
<td>0.41489</td>
<td>0.41478</td>
</tr>
<tr>
<td>( \pi_{2211} )</td>
<td>0.35562</td>
<td>0.35552</td>
</tr>
<tr>
<td>( \pi_{2222} )</td>
<td>1.19029</td>
<td>1.19001</td>
</tr>
</tbody>
</table>

We conclude that by using finite differences followed by the Simpson rule with 101 points one obtains results which are quite accurate. These are indeed nearly as accurate as the ones obtained by employing fitting with a polynomial of degree 9.

**Example 5.2** Piecewise coefficients

Let us consider the previous problem, where now instead of (5.1) we have

\[
E(y) = E(y_1) = \chi_1(y_1) + 3\chi_2(y_1); \quad \nu = 0.3,
\]

whereas \( \chi_1 \) and \( \chi_2 \) are the characteristic functions of the sets \( Y_1 = [-0.5, 0] \times [-0.5, 0.5] \) and \( Y_2 = [0, 0.5] \times [-0.5, 0.5] \), respectively, as defined in (4.30). We start by approximating \( E(y) \) by the continuous function

\[
E_\lambda(y_1) = 2 + \frac{\pi}{2} \arctan(\lambda y_1).
\]

We note that the approximation is more accurate as the value of \( \lambda \) grows - Figure 8.

We now use the second strategy described earlier. Table 4 contains the values of the approximations obtained for the non-zero coefficients of the underlying PDE. These can be compared to the exact solution given by Property 4.2, displayed in the second row of table 4, with 6 significant digits.
Figure 8: The functions $E_\lambda$. Better approximations for $E = E(y_1)$ are obtained for bigger values of $\lambda$.

Table 4: Effective coefficients.

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Exact</th>
<th>Approximation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\overline{\sigma}_{1111}$</td>
<td>$1.64835$</td>
<td>$1.64835$</td>
</tr>
<tr>
<td>$\overline{\sigma}_{2121}$</td>
<td>$0.57692$</td>
<td>$0.57692$</td>
</tr>
<tr>
<td>$\overline{\sigma}_{2211}$</td>
<td>$0.49451$</td>
<td>$0.49451$</td>
</tr>
<tr>
<td>$\overline{\sigma}_{2222}$</td>
<td>$2.14835$</td>
<td>$2.14835$</td>
</tr>
</tbody>
</table>

As one would expect, the results are more accurate for larger values of $\lambda$. This parameter may be taken arbitrarily large, but at the cost of having to work with a fine mesh, locally around $y_1 = 0$, the material interface.

**Example 5.3** A complicated structure

Let us again consider the elasticity problem (4.1)-(4.13)-(4.14) where over the reference cell $Y = [0,1] \times [0,1]$ the material properties now vary along both spatial coordinates. They are characterized by

$$E(y) = 1.1 + \cos(2\pi y_1) \sin(2\pi y_2), \quad \nu = 0.3. \quad (5.5)$$

The boundary conditions are such that:
\[ \Gamma_D = \{0\} \times [0,1], \varphi_N(x) = \begin{cases} (0,1), & x_2 = 1, \\ 0, & x_2 = 0, \\ (1,0), & x_1 = 1. \end{cases} \] (5.6)

As before, we compute the solution functions \( \chi_k^{\text{fin}} \) of the cell problem using finite elements and a fine triangular grid with 42778 quadratic elements. For illustration, \( \chi_1^{12} \) and \( \chi_2^{12} \) are plotted in Figure 9.

![Figure 9](image)

**Fig 9 a)** The periodic cell function \( \chi_1^{12} \) of Example 5.3. **b)** The periodic cell function \( \chi_2^{12} \) of Example 5.3.

We follow the algorithm described earlier to approximate the value of the effective coefficients of the homogenised PDE. In Figure 10 a) we compare the horizontal components of the effective and the heterogeneous solutions along the line \( y = 0.5 \) and in Figure 10 b) the respective vertical components along \( x = 0.5 \) and with \( \epsilon = 1/4 \). The homogeneous solution is represented by the dashed lines.

![Figure 10](image)

**Fig 10 a)** Horizontal components of \( \mathbf{u} \) and the approximation \( \mathbf{u}^\epsilon \) along \( y = 0.5 \). **b)** Vertical components of \( \mathbf{u} \) and the approximation \( \mathbf{u}^\epsilon \) along \( x = 0.5 \).

Finally, we compute the norms of the differences between the components of \( \mathbf{u}^\epsilon \) and \( \mathbf{u} \), for different values of \( \epsilon \) - Table 5.
Table 5: Error in $\| \cdot \|_{L^2(\Omega)}$.

<table>
<thead>
<tr>
<th></th>
<th>$\epsilon = 1/4$</th>
<th>$\epsilon = 1/8$</th>
<th>$\epsilon = 1/12$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|u_1' - \pi_1|_{L^2(\Omega)}$</td>
<td>$1.4E - 2$</td>
<td>$7.0E - 3$</td>
<td>$4.6E - 3$</td>
</tr>
<tr>
<td>$|u_2' - \pi_2|_{L^2(\Omega)}$</td>
<td>$9.5E - 3$</td>
<td>$4.4E - 3$</td>
<td>$3.0E - 3$</td>
</tr>
</tbody>
</table>

As one would expect, for smaller values of $\epsilon$, the heterogeneous solution is closer to the homogenised solution.

**Conclusion**

For layered composites we look for approximations of the solution of (3.2). One such approximation, with low computational cost, is the solution of a homogenised problem (3.13). In order to find this, one needs first to determine the coefficients of the latter problem. We do so for layered materials, analytically. For the more general case of periodically distributed composites, we propose a numerical algorithm to determine the effective coefficients.

This procedure is restricted to periodically distributed materials, hence excluding random nonhomogeneous media. It requires the numerical solution of a cell problem, which can still require much computer power. However, it can be adapted to more phenomena other than linear elasticity, such as heat propagation, fluid flow, radiation and in general for both linear and non-linear models, as well as to higher dimensions.

**References**


