Solutions for periodically distributed materials with localised imperfections

M. Patrício¹, R. Mattheij² and G. de With³

Abstract: The behaviour of composite materials with periodically distributed constituents is considered. Mathematically, this can be described by a boundary value problem with highly oscillatory coefficient functions. An algorithm is proposed to handle the case when the underlying periodicity is locally disturbed. This procedure is constructed using fundamental concepts from homogenisation theory and domain decomposition techniques. Applications to layered materials are considered.

Keywords: Homogenisation, composites, domain decomposition.

1 Introduction

The increasing usage of high performance materials such as composites justifies that a lot of effort be put into the modelling of these materials, cf. for example [Aymerich and Serra (2006); Guz, J.Rushchitsky, and A.Guz (2008)]. Different approaches are possible, as the relevant phenomena occurring on these materials may be regarded on different lengthscales, see [Fitzgerald, Goldbeck-Wood, Kung, Petersen, Subramanian, and J.Wescott (2008)].

From the point of view of continuum mechanics, the coefficients of PDEs related to very heterogeneous materials vary so rapidly that applying classical techniques such as finite elements or boundary elements methods, see [Babuska and Strouboulis (2001); Becker (1992)] - becomes prohibitively expensive. One possible strategy to tackle this problem consists of employing domain decomposition. This allows the division of the computational domain into smaller subdomains where the original equation is to be solved. In this way, instead of solving one very complicated problem, one will solve several not-so-complicated problems.

¹ Technical University of Eindhoven, Department of Mathematics and Computer Science.

² Technical University of Eindhoven, Department of Mathematics and Computer Science.

³ Technical University of Eindhoven, Department of Chemical Engineering and Chemistry.

Domain decomposition methods are based on the alternative methods which were introduced in the second half of the XIX century. In order to prove the existence and uniqueness of the solution of Laplace's equation on a domain Ω which is the union of simple geometries, Schwarz decomposed Ω into overlapping subdomains, cf. [Schwarz (1870)]. He went on to propose an iterative procedure for which Dirichlet boundary conditions are imposed at the boundaries that arise at the subdomains. The applicability of this idea as a numerical solver for PDEs was later studied and since then, much has been published in this area, see for example [Allaire (2002); Bensoussan, Lions, and Papanicolaou (1978); Cioranescu and Donato (1999); Dubois (2003); Pavliotis and Stuart (2008); Quarteroni and Valli (1999)].

A distinct approach may be adopted when it is further assumed that the material is distributed in a periodic manner, with a small period ε . In spite of this simplification, the usage of classical techniques is still not advisable. Indeed, to obtain accurate results using finite element methods, one would have to ensure that the element size of the mesh is taken very small, definitely smaller than ε , cf. [Hou, Wu, and Cai (1999)]. On the bright side, several techniques have been devised which solve this class of problems, amongst which those suggested by the homogenisation theory, see [Cioranescu and Donato (1999); Pavliotis and Stuart (2008)], the multiscale finite element methods, cf. [Hou and H.Wu (1997); Hou, Wu, and Cai (1999)] or the heterogeneous multiscale method, [E, Engquist, Li, Ren, and Vanden-Eijnden (2005)].

In this paper, we study boundary value problems related to periodic materials with localised imperfections or which are such that there is a high activity region to which it may be assumed the relevant phenomenon is confined, cf. [Kakuba, Mattheij, and Anthonissen (2006)]. Mathematically, these are such that the coefficients of the PDEs have a highly oscillatory behaviour which is periodic with period ε everywhere except for a small subdomain. In order to solve this problem we propose an algorithm that borrows concepts from the techniques of domain decomposition and of homogenisation. The idea is to make use of the periodic structure of the material as much of possible. An accurate solution to the problem should then be found with reasonably small computational effort.

We start by analysing a one-dimensional problem in section 2. In 2.1 we consider the case in which the coefficient of the differential equation is a periodic function of a small period ε over the entire domain Ω , with $\varepsilon \ll 1$. A homogenised problem is deduced whose solution is an approximation to the exact solution of the original problem. Corrector functions that improve the accuracy of this approximation are sought. After this the more complex problem when the coefficients vary rapidly in a non-periodic manner is analysed in 2.2. Finally, in 2.3, we combine the two previous approaches for the case in which the coefficient is periodic on most of the domain. For that, an appropriate strategy is indicated and analysed.

In section 3 the results from section 2 are adapted for the problem of linear elasticity. Special emphasis is given to a hybrid algorithm that is inspired in both homogenisation and domain decomposition techniques.

Finally, in section 4, several numerical results are presented for the two problems considered. These examples show the effectiveness of the proposed hybrid approach.

2 One-dimensional problem

In this section we analyse two boundary value problems. The first is such that the coefficients of the differential equation are periodic functions with a small period ε . As for the second problem, it differs from the previous one in the sense that there exists a small region over which these coefficients are no longer of the same form as in the rest of the domain.

2.1 Periodic structure

As is well known, the theory of homogenisation allows for the approximation of the solution of boundary value problems with PDEs that have periodic and highly oscillatory coefficients

$$a^{\varepsilon}(x) = \widetilde{a}(x/\varepsilon).$$

Here a^{ε} is a smooth ε -periodic function with $\varepsilon \ll 1$. We consider the following boundary value problem

$$\begin{cases}
-\frac{\mathrm{d}}{\mathrm{d}x} \left[a^{\varepsilon}(x) \frac{\mathrm{d}}{\mathrm{d}x} u^{\varepsilon}(x) \right] &= f(x), \ x \in (0,1), \\
u^{\varepsilon}(0) = 0, \\
u^{\varepsilon}(1) = 0,
\end{cases}$$
(1)

where $f \in L^2(0,1)$ and there exist real constants α and β such that

$$0 < \alpha < a^{\varepsilon}(x) < \beta, \ x \in [0, \ 1].$$

In order to look for an approximation of the solution of (1), we use the multiple scale method. For that consider the ansatz

$$u^{\varepsilon}(x,y) = u_0(x,y) + \varepsilon u_1(x,y) + \varepsilon^2 u_2(x,y) + \dots,$$
(2)

where we assume the functions u_i , i = 0, 1, 2, ..., to be 1-periodic in y and to depend explicitly on x and $y := x/\varepsilon$. This is a mathematical translation of the idea that u^{ε} depends on two separate lengthscales, macroscopic and microscopic.

Now using the first three terms in the previous asymptotic expansion, we can show that the function u_0 actually depends only on x, cf. [Cioranescu and Donato (1999); Pavliotis and Stuart (2008)]. We denote it by $\overline{u} := u_0(x)$ and refer to it as the homogenised solution. It satisfies the boundary value problem

$$\begin{cases}
-\overline{a}\frac{d}{dx}\left(\frac{d\overline{u}}{dx}\right) &= f(x), x \in (0,1), \\
\overline{u}(0) &= 0, \\
\overline{u}(1) &= 0,
\end{cases}$$
(3)

where the homogenised coefficient \overline{a} is given by

$$\overline{a} = \int_0^1 \widetilde{a}(y) dy - \int_0^1 \widetilde{a}(y) \frac{d\chi}{dy}(y) dy$$
(4)

and χ is the solution of the so-called cell problem

$$\begin{cases}
-\frac{d}{dx}(\tilde{a}(y)\frac{d\chi}{dy}) = -\frac{d\tilde{a}}{dy}, & y \in [0, 1], \\
\chi \text{ is periodic,} \\
\int_{0}^{1} \chi(y)dy = 0.
\end{cases}$$
(5)

The function \overline{u} provides a cheap numerical approximation to u^{ε} . To obtain more accuracy, we look at the function u_1 appearing in the second term of the expansion, the first order corrector. This reads

$$u_1(x,y) = -\chi(y)\frac{d\overline{u}}{dx}(x).$$
(6)

The homogenised solution \overline{u} verifies the same boundary conditions as the heterogeneous solution u^{ε} . We note, however, that the same cannot be said about $\overline{u} + \varepsilon u_1$. A boundary corrector *C* should then be introduced so that $(\overline{u} + \varepsilon u_1 + C)|_{\{0,1\}} = 0$. Thus *C* is determined at the boundaries. Since it should also be defined at the remaining points of the domain, it is natural to let it satisfy the original heterogeneous equation with source term equal to zero

$$\begin{cases} -\frac{\mathrm{d}}{\mathrm{d}x} \left[a^{\varepsilon}(x) \frac{\mathrm{d}}{\mathrm{d}x} C(x) \right] &= 0, \ x \in (0,1), \\ C(0) &= -\varepsilon u_1(0), \\ C(1) &= -\varepsilon u_1(1). \end{cases}$$
(7)

In practice C may be approximated by a function which satisfies (7) with a^{ε} replaced by \overline{a} . It can be shown that there exists a constant d such that we have, cf. [Versieux and Sarkis (2006)],

$$\|u^{\varepsilon} - (\overline{u} + \varepsilon u_1 + \varepsilon C)\|_0 \le d\varepsilon^2 \|\overline{u}\|_3.$$
(8)

$$\|u^{\varepsilon} - (\overline{u} + \varepsilon u_1 + \varepsilon C)\|_1 \le d\varepsilon \|\overline{u}\|_2.$$
⁽⁹⁾

2.2 Complex structure

We will now look at the previous problem in a broader setting, for which the technique described earlier is no longer directly applicable. We drop the requirement that the coefficients of the differential equation in (1) are periodic and consider instead

$$\begin{cases}
-\frac{d}{dx} \left[a(x) \frac{d}{dx} u(x) \right] = f(x), x \in \Omega = (0, 1), \\
u(0) = 0, \\
u(1) = 0.
\end{cases}$$
(10)

This problem can be easily reformulated in the equivalent multi-domain form

$$\begin{cases}
-\frac{d}{dx} \left[a(x) \frac{d}{dx} v(x) \right] = f(x), x \in \Omega_1 = (0, \gamma), \\
v(0) = 0, \\
v(\gamma) = w(\gamma), \\
\frac{dv}{dx}(\gamma) = \frac{dw}{dx}(\gamma), \\
-\frac{d}{dx} \left[a(x) \frac{d}{dx} w(x) \right] = f(x), x \in \Omega_2 = (\gamma, 1), \\
w(1) = 0,
\end{cases}$$
(11)

where $v := u|_{\Omega_1}$, $w := u|_{\Omega_2}$ and $\gamma \in (0, 1)$. This formulation suggests that we can split (10) into separate problems that allow the determination of the functions *v* and *w*. Since the values of *u* and of its derivative are not known at $x = \gamma$, one must recur to iterative methods to implement this domain decomposition. We keep in mind that the transmission conditions expressed in the third and fourth lines of (11) must be satisfied at the boundary $\Gamma = {\gamma}$. Several iterative methods have been proposed and analysed in the literature, cf. [Smith, Bjørstad, and Gropp (1996); Quarteroni and Valli (1999); Toselli and Widlund (2004)]. They generate sequences of boundary value problems set on subdomains of Ω such that on each subdomain the solution of the boundary value problem converges to *u*. As an example, consider the following Dirichlet-Neumann method

$$\begin{cases}
-\frac{\mathrm{d}}{\mathrm{d}x}\left[a(x)\frac{\mathrm{d}}{\mathrm{d}x}v^{k+1}(x)\right] = f(x), x \in \Omega_1, \\
v^{k+1}(0) = 0, \\
\frac{\mathrm{d}v^{k+1}}{\mathrm{d}x}(\gamma) = \frac{\mathrm{d}w^{k+1}}{\mathrm{d}x}(\gamma),
\end{cases}$$
(12)

$$\begin{cases} -\frac{\mathrm{d}}{\mathrm{d}x} \left[a(x) \frac{\mathrm{d}}{\mathrm{d}x} w^{k+1}(x) \right] &= f(x), \ x \in \Omega_2, \\ w^{k+1}(\gamma) = \lambda^k, \\ w^{k+1}(1) = 0, \end{cases}$$
(13)

$$\lambda^{k+1} = \theta w^{k+1}|_{\Gamma} + (1-\theta)\lambda^k, \ k \ge 0.$$
(14)

Here, λ^0 is the initial guess for the value of *u* at Γ and θ is a positive acceleration parameter. It can be shown, as in [Quarteroni and Valli (1999)], that this method converges as long as θ is within a certain range.

This procedure may be generalised so that the computational domain is partitioned into any given number of subdomains. A parallel implementation allows for the numerical solution of rather complicated problems, cf. [Quarteroni and Valli (1999); Smith, Bjørstad, and Gropp (1996)].

Up to now, two distinct techniques were mentioned. These share the feature of reducing the computational complexity of the boundary value problem at hands. Homogenisation was presented for periodic structures, whilst domain decomposition is more general but requires the resolution of the heterogeneous scale. In what

follows we combine the previous approaches. This results in a hybrid approach algorithm suited for periodically distributed materials with localised imperfections or with a localised portion of the domain where a different analysis is required. Consider a problem of the general form (10) with coefficients given by

$$a(x) = \begin{cases} a_1(x), \ x \in [0, \ \gamma_1], \\ a_2^{\varepsilon}(x), \ x \in (\gamma_1, \ 1], \end{cases}$$
(15)

where a_2^{ε} is an ε -periodic function. Assume that $\gamma_1 < 1/2$ and

$$0 < a_1(x), x \in \Omega_1 \text{ and } 0 < \alpha < a_2^{\mathcal{E}}(x) < \beta, x \in \Omega_2.$$
(16)

The algorithm we will set up will iterate over an overlapping region $[\gamma_1, \gamma_2]$, for a convenient choice of γ_2 such that $\gamma_1 < \gamma_2 < 1$. Sequences of functions \hat{v}^{k+1} and \hat{w}^{k+1} will be generated, providing approximations for $u|_{[0,\gamma_2]}$ and $u|_{[\gamma_1,1]}$, respectively. The hybrid approach algorithm then reads

- Initialise choose an initial approximation $\widehat{\lambda}^0$ for $u(\gamma_2)$.
- For $k = 0, 1, 2, \ldots$

Solve

$$\begin{cases} -\frac{\mathrm{d}}{\mathrm{d}x} \left[a(x) \frac{\mathrm{d}}{\mathrm{d}x} \hat{v}^{k+1}(x) \right] &= f(x), \ x \in (0, \gamma_2), \\ \hat{v}^{k+1}(0) = 0, \\ \hat{v}^{k+1}(\gamma_2) = \hat{\lambda}^k. \end{cases}$$

$$(17)$$

Find an approximation \widehat{w}^{k+1} related to the solution of the problem

$$\begin{cases} -\frac{d}{dx} \left[a_2^{\varepsilon}(x) \frac{d}{dx} w^{k+1}(x) \right] &= f(x), \ x \in (\gamma_1, 1), \\ w^{k+1}(\gamma_1) = v^{k+1}(\gamma_1), \\ w^{k+1}(1) = 0. \end{cases}$$
(18)

• Update
$$\widehat{\lambda}^k$$
:
 $\widehat{\lambda}^{k+1} = \widehat{w}^{k+1}(\gamma_2).$ (19)

The function \widehat{w}^{k+1} used to approximate the solution of (18) needs to be worked out. Start by finding the homogenised function \overline{w}^{k+1} that satisfies (18) with a_2^{ε} replaced by the corresponding homogenised coefficient \overline{a} , as was done in section 2.1. Next, compute the first order corrector w_1^{k+1} and the boundary corrector C^{k+1} for the problem (18). Set $\widehat{w}^{k+1} := \overline{w}^{k+1} + \varepsilon w_1^{k+1} + C^{k+1}$. Alternatively, the previous step may be skipped by instead defining $\widehat{w}^{k+1} := \overline{w}^{k+1}$. This approach will then become less complex, but also less accurate.

We observe that this algorithm is a modification of the iterative overlapping scheme proposed by Schwarz, which has been shown to converge, see [Schwarz (1870)]. A major twist is being added to this scheme though, as a homogenisation error appears at each iteration step. Let us denote the error of the approximations \hat{v}^{k+1} and \hat{w}^{k+1} coming from the previous iterative scheme by $\hat{E}_1^{k+1} := \hat{v}^{k+1} - u|_{[0,\gamma_2]}$ and $\hat{E}_2^{k+1} := \hat{w}^{k+1} - u|_{[\gamma_1,1]}$, respectively. We will determine a stopping condition for the hybrid approach algorithm as well as the error of the approximation that we obtain. The error function \hat{E}_1^{k+1} satisfies

$$\begin{cases}
-\frac{d}{dx} \left[a(x) \frac{d}{dx} \widehat{E}_{1}^{k+1}(x) \right] = 0, x \in (0, \gamma_{2}), \\
\widehat{E}_{1}^{k+1}(0) = 0, \\
\widehat{E}_{1}^{k+1}(\gamma_{2}) = \widehat{E}_{2}^{k}(\gamma_{2}),
\end{cases}$$
(20)

while $\widehat{E}_{2}^{k+1}(x) = E_{2}^{k+1}(x) + \delta^{k+1}(x)$, where

$$\begin{cases}
-\frac{d}{dx} \left[a_{2}^{\varepsilon}(x) \frac{d}{dx} E_{2}^{k+1}(x) \right] = 0, \quad x \in (\gamma_{1}, 1), \\
E_{2}^{k+1}(\gamma_{1}) = \widehat{E}_{1}^{k+1}(\gamma_{1}), \\
E_{2}^{k+1}(1) = 0,
\end{cases}$$
(21)

and $\delta^{k+1}(x)$ is the homogenisation error at step k. Assume, without loss of generality, that $\widehat{E}_2^k(\gamma_2)$, the error coming from the previous iteration, is positive. From the differential equations in (20) and (21), it can be seen that both \widehat{E}_1^{k+1} and E_2^{k+1} are strictly monotonous functions. They are illustrated in Figure 1.



Figure 1: Error reduction scheme: as long as $\widehat{E}_2^{k+1}(\gamma_2) < \widehat{E}_1^{k+1}(\gamma_2)$, then $\widehat{E}_1^{k+2}(x) < \widehat{E}_1^{k+1}(x)$ and the error is reduced.

Then clearly

$$E_2^{k+1}(\gamma_2) < E_2^{k+1}(\gamma_1) = \widehat{E}_1^{k+1}(\gamma_1) < \widehat{E}_1^{k+1}(\gamma_2)$$

and as long as $\widehat{E}_1^{k+1}(\gamma_2) - E_2^{k+1}(\gamma_2) > |\delta^{k+1}(\gamma_2)|$, then also

$$\widehat{E}_2^{k+1}(\gamma_2) < \widehat{E}_1^{k+1}(\gamma_2) = \widehat{E}_2^k(\gamma_2).$$

In other words, at the end of the iteration step, the maximum of the approximation error coming from the previous iteration, $\hat{E}_1^{k+1}(\gamma_2) = \hat{E}_2^k(\gamma_2)$, will be reduced to $\hat{E}_1^{k+1}(\gamma_2) = \hat{E}_2^{k+1}(\gamma_2)$.

A natural stopping criterion for the hybrid approach algorithm would then be given by

$$|\widehat{E}_{1}^{k+1}(\gamma_{2}) - E_{2}^{k+1}(\gamma_{2})| \le \delta,$$
(22)

where δ is the maximum absolute error predicted for the homogenisation procedure. However, since $\hat{E}_1^{k+1}(\gamma_2)$ and $E_2^{k+1}(\gamma_2)$ are not known, we will adopt the following stopping criterion

$$|\widehat{E}_{1}^{k+1}(\gamma_{2}) - \widehat{E}_{2}^{k+1}(\gamma_{2})| \le \delta/2,$$
(23)

which can also be written as

$$|\hat{u}_1^{k+1}(\gamma_2) - \hat{u}_2^{k+1}(\gamma_2)| \le \delta/2.$$
(24)

This implies an inequality like (22) with the right hand side replaced by $3\delta/2$. We can now establish the following theorem which gives the error of the approximation obtained when the quantity $\hat{E}_1^{k+1}(\gamma_2) - \hat{E}_2^{k+1}(\gamma_2)$ decreases until (24) holds.

Theorem 2.1 Let k be the smallest natural number such that (24) holds. Then the approximation

$$\widehat{u}^{k+1}(x) = \begin{cases} \widehat{v}^{k+1}(x), \ x \in [0, \ \gamma_1], \\ \widehat{w}^{k+1}(x), \ x \in (\gamma_1, \ 1], \end{cases}$$
(25)

for the exact solution u of (10) with (15) is such that

$$\|\widehat{u}^{k+1} - u\|_{\infty} \le \left(\frac{3}{2} \frac{\int_{0}^{\gamma_{1}} 1/a(u)du}{\int_{\gamma_{1}}^{\gamma_{2}} 1/a(u)du} + 1\right)\delta.$$
(26)

Sketch of Proof: For each iteration, the maximum of the function

$$E^{k+1}(x) = \begin{cases} \widehat{E}_1^{k+1}(x), \ x \in [0, \ \gamma_1], \\ E_2^{k+1}(x), \ x \in (\gamma_1, \ 1], \end{cases}$$
(27)

is attained for $x = \gamma_1$. Now, since

$$\widehat{E}_2^{k+1}(x) = E_2^{k+1}(x) + \delta^{k+1}(x) \le E_2^{k+1}(x) + \delta,$$

the maximum of E^{k+1} added to δ gives an upper bound for the error function

$$\widehat{E}^{k+1}(x) = \begin{cases} \widehat{E}_1^{k+1}(x), \ x \in [0, \ \gamma_1], \\ \widehat{E}_2^{k+1}(x), \ x \in (\gamma_1, \ 1]. \end{cases}$$
(28)

Consequently,

$$\|\hat{u}^{k+1} - u\|_{\infty} \le E_2^{k+1}(\gamma_1) + \delta.$$
⁽²⁹⁾

Now, in order to estimate the value of $E_2^{k+1}(\gamma_1)$, we note that from (20) and (21) it can be easily seen that there exist constants c_i and d_i , i = 1, 2, such that

$$\widehat{E}_1^{k+1} = c_1 \int_0^x \frac{1}{a(u)} du + d_1 \text{ and } E_2^{k+1} = c_2 \int_{\gamma_1}^x \frac{1}{a(u)} du + d_2.$$

These constants can be determined in terms of integrals of the coefficient function *a* given by (15). For that we use the boundary conditions for \widehat{E}_1^{k+1} and E_2^{k+1} on x = 0 and x = 1 respectively, and also the conditions

$$\widehat{E}_{1}^{k+1}(\gamma_{1}) = E_{2}^{k+1}(\gamma_{1}) \text{ and } \widehat{E}_{1}^{k+1}(\gamma_{2}) = E_{2}^{k+1}(\gamma_{2}) + \frac{3}{2}\delta.$$

Given (16) we can rewrite the inequality (26) from the previous theorem as

$$\|\widehat{u}^{k+1}-u\|_{\infty} \leq (\frac{3}{2}\frac{\beta\int_{0}^{\gamma_{1}}1/a(u)du}{\gamma_{2}-\gamma_{1}}+1)\delta.$$

From this inequality, we infer that γ_2 should be chosen as large as possible in order to minimize the error at the end of the iterative process. The drawback is that choosing a larger value for γ_2 implies a bigger computational effort, which implies that it may not be chosen too large.

3 The elasticity problem

In this section we extend the theory of Section 2 to the problem of linear elasticity. We follow the logical structure of the previous section and reformulate the results of homogenisation and domain decomposition. We conclude this section by presenting the corresponding hybrid approach.

3.1 Periodic structure

Let Ω be a connected bounded open set in \mathscr{R}^2 and $\partial \Omega = \Gamma_N \cup \Gamma_D$ be Lipschitz continuous such that Γ_D is of measure greater than zero. Let us consider a composite material with constituents periodically distributed over Ω , such that Ω is covered by a mosaic of cells of the form $\varepsilon Y =]0, \varepsilon l_1[\times]0, \varepsilon l_2[$ over which the material is distributed as in the reference cell $Y =]0, l_1[\times]0, l_2[$ - Figure 2.



Figure 2: Representative cell.

We state the linear elasticity problem for the composite material as follows

$$\begin{cases}
-\nabla \cdot (\mathbf{A}^{\varepsilon}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{u}^{\varepsilon})) = \mathbf{f} & \text{in } \Omega, \\
\mathbf{u}^{\varepsilon} = \mathbf{0} & \text{on } \Gamma_{D}, \\
\boldsymbol{\sigma}(\mathbf{u}^{\varepsilon}) \cdot \mathbf{n} = \boldsymbol{\varphi}_{N} & \text{on } \Gamma_{N},
\end{cases}$$
(30)

cf. [Cioranescu and Donato (1999); Patrício, Mattheij, and de With (2007); Pavliotis and Stuart (2008)]. Here the vector functions $\boldsymbol{\varphi}_N$ and \mathbf{f} are given and $\boldsymbol{\varepsilon}, \boldsymbol{\sigma}$ and \mathbf{u} denote the strain tensor, the stress tensor and the displacement vector respectively. These are such that for a vector function \mathbf{w} defined over Ω ,

$$\boldsymbol{\varepsilon}(\mathbf{w}) = (\nabla \mathbf{w} + (\nabla \mathbf{w})^T), \ \boldsymbol{\sigma}(\mathbf{w}) = \mathbf{A}^{\varepsilon} \boldsymbol{\varepsilon}(\mathbf{w}).$$
(31)

The tensor \mathbf{A}^{ε} , which characterises the behaviour of the material, can be defined by extending the components of a fourth-order tensor $\widetilde{\mathbf{A}} = \widetilde{\mathbf{A}}(\mathbf{y}) = (\widetilde{a}_{ijkh})_{1 \le i,j,k,h \le 2}$ defined over the reference cell *Y* periodically to \mathscr{R}^2 . We define $\mathbf{A}^{\varepsilon} = \mathbf{A}^{\varepsilon}(\mathbf{x}) = (a_{ijkh}^{\varepsilon})_{1 \le i,j,k,h \le N}$ such that for $\mathbf{x} = (x_1, x_2) \in \mathscr{R}^2$,

$$a_{ijkh}^{\varepsilon}(\mathbf{x}) := \widetilde{a}_{ijkh}(\mathbf{y}) = \widetilde{a}_{ijkh}(\frac{\mathbf{x}}{\varepsilon}), \tag{32}$$

where we denote $\mathbf{y} := \frac{\mathbf{x}}{\varepsilon}$, for $\mathbf{y} = (y_1, y_2) \in \mathscr{R}^2$. In order to proceed some notation must be introduced. For any fourth-order tensor $\mathbf{A} = (a_{ijkh})_{1 \le i,j,k,h \le 2}$ and for any matrices $\mathbf{M} = (m_{ij})_{1 \le i,j \le 2}$ and $\mathbf{N} = (n_{ij})_{1 \le i,j \le 2}$, we denote

$$\|\mathbf{M}\| = (\sum_{i,j=1}^{2} m_{ij}^{2})^{1/2},$$

$$\mathbf{AM} = ((\sum_{k,h=1,2} a_{ijkh} m_{kh})_{ij})_{1 \le i,j \le 2},$$

$$\mathbf{AMN} = \sum_{i,j,k,h=1,2} a_{ijkh} m_{ij} n_{kh}.$$

Assume that there exist α , $\beta \in \mathscr{R}$ such that $\widetilde{\mathbf{A}} \in M_e(\alpha, \beta, Y)$, ie

• $\widetilde{a}_{ijkh} \in L^{\infty}(Y)$, for any $i, j, k, h \in \{1, 2\}$;

•
$$\widetilde{a}_{ijkh} = \widetilde{a}_{jikh} = \widetilde{a}_{khij}$$
, for any $i, j, k, h \in \{1, 2\}$;

- $\alpha \|\mathbf{M}\|^2 \leq \widetilde{\mathbf{A}}\mathbf{M}\mathbf{M}$, for any symmetric 2 × 2 matrix **M**;
- $\|\widetilde{\mathbf{A}}(\mathbf{y})\mathbf{M}\| \le \beta \|\mathbf{M}\|$, for any 2 × 2 matrix **M**, almost anywhere on *Y*.

We will now look at how to approximate the heterogeneous solution \mathbf{u}^{ε} of (30). Consider the following ansatz

$$\mathbf{u}^{\varepsilon}(\mathbf{x},\mathbf{y}) = \mathbf{u}_0(\mathbf{x},\mathbf{y}) + \varepsilon \mathbf{u}_1(\mathbf{x},\mathbf{y}) + \varepsilon^2 \mathbf{u}_2(\mathbf{x},\mathbf{y}) + \dots$$
(33)

Here, \mathbf{u}_i , i = 0, 1, 2, ... are periodic functions in $\mathbf{y} = \mathbf{x}/\varepsilon$. Following [Allaire (2002)] it can be shown that when we take the first three terms of this expansion into account and insert them in the differential equation in (30) we conclude that \mathbf{u}_0 depends only on \mathbf{x} , ie. $\mathbf{u}_0 = \overline{\mathbf{u}}(\mathbf{x}) = (\overline{u}_1(\mathbf{x}), \overline{u}_2(\mathbf{x}))$. Moreover, it is the solution of

$$\begin{cases} -\nabla \cdot (\overline{\mathbf{A}}\boldsymbol{\varepsilon}(\overline{\mathbf{u}})) = \mathbf{f} & \text{in } \Omega, \\ \overline{\mathbf{u}} = \mathbf{0} & \text{on } \Gamma_D, \\ \overline{\mathbf{u}} \cdot \mathbf{n} = \boldsymbol{\varphi}_N & \text{on } \Gamma_N. \end{cases}$$
(34)

The homogenised tensor $\overline{\mathbf{A}} = (\overline{a}_{ijkh})$ is symmetric and given by

$$\overline{a}_{ijkh} = \frac{1}{|Y|} \int_{Y} \widetilde{a}_{ijkh}(\mathbf{y}) d\mathbf{y} -$$

$$= \frac{1}{|Y|} \int_{Y} \sum_{l,m=1,2} \widetilde{a}_{ijlm}(\mathbf{y}) \frac{\partial \chi_{l}^{kh}}{\partial y_{m}}(\mathbf{y}) d\mathbf{y}.$$
(35)

As for the cell function $\boldsymbol{\chi}^{lm}(\mathbf{y}) = (\boldsymbol{\chi}_k^{lm})(\mathbf{y})$, it is the solution of the cell problem

$$\begin{cases} -\nabla \cdot (\widetilde{\mathbf{A}}(\mathbf{y})\nabla(\mathbf{\chi}^{lm} - \mathbf{P}^{lm})) = \mathbf{0} \text{ for } \mathbf{y} \in Y, \\ \mathbf{\chi}^{lm} \text{ is Y-periodic }, \\ \frac{1}{|Y|} \int_{Y} \mathbf{\chi}_{k}^{lm}(\mathbf{y}) d\mathbf{y} = 0. \end{cases}$$
(36)

Here we have used the vector valued functions $\mathbf{P}^{lm}(\mathbf{y}) = (P_k^{lm}(\mathbf{y}))$, defined as

$$P_k^{lm}(\mathbf{y}) := y_m \delta_{kl}, \text{ for } l, m, k \in \{1, 2\},$$
(37)

where δ_{kl} is the Kronecker symbol. It can be shown that $\boldsymbol{\chi}^{lm}$ is the unique solution of (36) in the set $W_{per}(Y)$ defined by

$$W_{per}(Y) := \{ \mathbf{v} \in H^1_{per}(Y) \mid \frac{1}{|Y|} \int_Y \mathbf{v}(\mathbf{y}) d\mathbf{y} = 0 \}$$
(38)

where $H_{per}^1(Y)$ is the closure for the H^1 -norm of $C_{per}^{\infty}(Y)$, the subset of $C^{\infty}(\mathscr{R}^2)$ of periodic functions over *Y*, cf Cioranescu and Donato (1999).

Finally, \mathbf{u}_1 takes the form

$$\mathbf{u}_{1}(\mathbf{x},\mathbf{y}) = \frac{1}{2} \sum_{i,j=1,2} \left(\frac{\partial \overline{u}_{i}}{\partial x_{j}} + \frac{\partial \overline{u}_{j}}{\partial x_{i}} \right) \boldsymbol{\chi}^{ij}(\frac{\mathbf{x}}{\varepsilon}).$$
(39)

We call $\overline{\mathbf{u}}$ and $\varepsilon \mathbf{u}_1$ the homogenised solution and the first corrector for the problem (30), respectively. We note that $\overline{\mathbf{u}}$ satisfies the same boundaries condition prescribed for the heterogeneous solution. This does not necessarily hold true for the approximation $\overline{\mathbf{u}} + \varepsilon \mathbf{u}_1$, which means that somehow we should force the right boundary

conditions to be respected. Like we did in the previous section, a boundary corrector **C** can be introduced. This verifies

$$\begin{cases}
-\nabla \cdot (\mathbf{A}^{\varepsilon}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{C})) = \mathbf{0} & \text{in } \Omega, \\
\mathbf{C} = -\varepsilon \mathbf{u}_{1} & \text{on } \Gamma_{D}, \\
\boldsymbol{\sigma}(\mathbf{C}) \cdot \mathbf{n} = \mathbf{0} & \text{on } \Gamma_{N}.
\end{cases}$$
(40)

Finally, we can approximate the solution of (30) by $\overline{\mathbf{u}} + \varepsilon \mathbf{u}_1 + \mathbf{C}$, once the homogenised coefficients (35) have been determined. This is computationally much cheaper than solving the full heterogeneous problem, but it still allows for the resolution of the heterogeneities.

3.2 Complex structure

Let us again consider the linear elasticity problem for a composite. Unlike what we did previously, we now assume that this is not necessarily periodically distributed. Then, instead of (30), we write

$$\begin{cases} -\nabla \cdot (\mathbf{A}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{u})) = \mathbf{f} & \text{in } \Omega, \\ \mathbf{u} = \mathbf{0} & \text{on } \Gamma_D, \\ \boldsymbol{\sigma}(\mathbf{u}) \cdot \mathbf{n} = \boldsymbol{\varphi}_N & \text{on } \Gamma_N, \end{cases}$$
(41)

where the parameter ε was suppressed. When the constituents of the composite in question are finely mixed, this is a rather complex problem, which requires the adoption of appropriate numerical techniques. In particular, as we have already stated in the previous section, one may recur to domain decomposition methods as described in [Quarteroni and Valli (1999); Toselli and Widlund (2004)]. These cut up the original problem into smaller more manageable problems.

In what follows, we will consider the problem of linear elasticity (41) where now the tensor **A** reads

$$\mathbf{A}(\mathbf{x}) = \begin{cases} \mathbf{A}_1(\mathbf{x}), \ \mathbf{x} \in \Omega_1, \\ \mathbf{A}_2^{\varepsilon}(\mathbf{x}), \ \mathbf{x} \in \Omega_2. \end{cases}$$
(42)

Here $\mathbf{A}_2^{\varepsilon}$ is an ε -periodic tensor and it is assumed that $|\Omega_1| < |\Omega_2|$. Note that the homogenisation method described earlier may not be employed to solve (41) with (42) as \mathbf{A} is not periodic everywhere. One possible alternative is the usage of domain decomposition techniques. The drawback is that these do not make use of the periodicity of the elasticity tensor over Ω_2 . We then proceed as in Section 2 and establish a hybrid approach for this problem where again we combine homogenisation and domain decomposition techniques.

We will introduce a sequence of problems set on the two overlapping subdomains $\widehat{\Omega}_1$ and Ω_2 , where $\Omega_1 \subset \widehat{\Omega}_1 \subset \Omega$. Let $\Gamma_1 = \partial \Omega_1 \cap \partial \Omega_2$ and $\Gamma_2 = \partial \widehat{\Omega}_1 - \partial \Omega$, as illustrated in Figure 3.



Figure 3: The computational domain Ω is the union of the overlapping subdomains $\widehat{\Omega}_1$ and Ω_2 .

The hybrid approach for elasticity reads

- Initialise choose $\widehat{\pmb{\lambda}}^0$ as an initial approximation for $\pmb{u}|_{\Gamma_2}.$
- For k = 0, 1, 2, ...

solve

$$\begin{cases}
-\nabla \cdot (\mathbf{A}\boldsymbol{\varepsilon}(\widehat{\mathbf{v}}^{k+1})) = \mathbf{f} & \text{in } \widehat{\Omega}_{1}, \\
\widehat{\mathbf{v}}^{k+1} = \mathbf{0} & \text{on } \Gamma_{D} \cap \partial \widehat{\Omega}_{1}, \\
\boldsymbol{\sigma}(\widehat{\mathbf{v}})^{k+1}) \cdot \mathbf{n} = \boldsymbol{\varphi}_{N} & \text{on } \Gamma_{N} \cap \partial \widehat{\Omega}_{1}, \\
\widehat{\mathbf{v}}^{k+1} = \widehat{\boldsymbol{\lambda}}^{k} & \text{on } \Gamma_{2}.
\end{cases}$$
(43)

Find an approximation $\widehat{\mathbf{w}}^{k+1}$ for the solution of the problem

$$\begin{cases}
-\nabla \cdot (\mathbf{A}_{2}^{\varepsilon} \boldsymbol{\varepsilon}(\mathbf{w}^{k+1})) = \mathbf{f} & \text{in } \Omega_{2}, \\
\mathbf{w}^{k+1} = \mathbf{0} & \text{on } \Gamma_{D} \cap \partial \widehat{\Omega}_{2}, \\
\boldsymbol{\sigma}(\mathbf{w}^{k+1}) \cdot \mathbf{n} = \boldsymbol{\varphi}_{N} & \text{on } \Gamma_{N} \cap \partial \widehat{\Omega}_{2}, \\
\mathbf{w}^{k+1} = \widehat{\mathbf{v}}^{k+1} & \text{on } \Gamma_{1}.
\end{cases}$$
(44)

Update
$$\widehat{\boldsymbol{\lambda}}^{k+1}$$

 $\widehat{\boldsymbol{\lambda}}^{k+1} = \widehat{w}^{k+1}|_{\Gamma_2}.$ (45)

As before, in order to determine $\widehat{\mathbf{w}}^{k+1}$, one must first compute the homogenised solution $\overline{\mathbf{w}}^{k+1}$ that satisfies (44) with $\mathbf{A}_2^{\varepsilon}$ replaced by the corresponding homogenised tensor $\overline{\mathbf{A}}$. At this point one may already define $\widehat{\mathbf{w}}^{k+1} := \overline{\mathbf{w}}^{k+1}$. If more accuracy is sought, one should compute the first order corrector \mathbf{w}_1^{k+1} and the boundary corrector \mathbf{C}^{k+1} for the problem (44). Set $\widehat{\mathbf{w}}^{k+1} := \overline{\mathbf{w}}^{k+1} + \mathbf{C}^{k+1}$.

As a stopping condition for this algorithm, we may generalise (24) and require

$$\max_{\mathbf{x}\in\Gamma_2} |\widehat{w}_1^{k+1}(\mathbf{x}) - \widehat{v}_1^{k+1}(\mathbf{x})| \leq \frac{1}{2}\delta_1,$$

$$\max_{\mathbf{x}\in\Gamma_2} |\widehat{w}_2^{k+1}(\mathbf{x}) - \widehat{v}_2^{k+1}(\mathbf{x})| \le \frac{1}{2}\delta_2,\tag{46}$$

where δ_1 and δ_2 are the estimated maximum homogenisation errors for the horizontal and vertical components of the displacement, respectively. We thus obtain an approximation to the solution of (41) with (42).

4 Numerical results

Our goal in this section is to apply the methods analysed earlier to boundary value problems with highly oscillatory coefficients. The following two subsections are related to sections 2 and 3, respectively.

4.1 One-dimensional examples

In what follows we start by examining a one-dimensional boundary value problem with ε -periodic coefficients. We use homogenisation techniques to approximate the solution of this problem. Next we look at a modification of this same problem; the ε -periodicity no longer holds on a small subdomain. Domain decomposition methods and the hybrid approach are then applied.

Example 4.1 - Periodic structure

Let us consider the boundary value problem (1) with

$$a^{\varepsilon}(x) := \frac{1}{2 + \sin(\frac{2\pi x}{\varepsilon})}, \ \varepsilon = 0.1, \ f(x) = 1.$$

$$(47)$$

The analytical solution u^{ε} of this problem, as well as of the corresponding solution \overline{u} of the homogenised problem (3), can be easily calculated. This allows for the determination of the error $\overline{E} = u^{\varepsilon} - \overline{u}$, which is displayed in the second line of the Table 1, in the norms $\|\cdot\|_{\infty}$ and $\|\cdot\|_{L^2(0,1)}$.

As we have seen, better approximations for u^{ε} can be achieved using the first order corrector u_1 given by (6) and the boundary corrector *C* which solves (7). The latter can be approximated by the solution of the homogenised problem

$$\begin{cases}
-\overline{a}\frac{d}{dx}\left[\frac{d}{dx}C(x)\right] &= 0, x \in (0,1), \\
C(0) &= -\varepsilon u_1(0), \\
C(1) &= -\varepsilon u_1(1),
\end{cases}$$
(48)

where \overline{a} is given by (4). We display the norms of the error $E_C = u^{\varepsilon} - (\overline{u} + \varepsilon u_1 + C)$ in the last line of Table 1. Note that in this case it is possible to determine both u_1 and *C* analytically.

As expected, the corrected homogenised solution is a better approximation to u^{ε} than \overline{u} . This is illustrated in Figure 4. The exact solution u^{ε} is depicted as a dotted line. The homogenised solution \overline{u} and its corrected counterpart $\overline{u} + \varepsilon u_1 + C$ are represented as the darker and lighter solid lines, respectively.

In conclusion, the homogenised solution \overline{u} captures the essential behaviour of the heterogeneous solution u^{ε} but disregards the oscillations. These can be recovered by the corrected homogenised solution in a very satisfactory manner. This is an

	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$
\overline{E}	1.5E - 2	5.6E - 3
E_C	4.1E - 4	2.4E - 4

 Table 1: Error of the homogenisation procedure.



Figure 4: Exact and approximated solutions.

advantageous process in the sense that it allows for a cheap solution to be obtained for a problem that would otherwise require a big computational effort.

Example 4.2 - Periodic structure with localised imperfections

Consider the problem (10) where the coefficients are of the form (15) and

$$a(x) = \begin{cases} 2+1.9\cos(2\pi x/0.03), \ x \in \Omega_1 = (0, \ 0.1) \\ \left[2+\sin(\frac{2\pi x}{\varepsilon})\right]^{-1}, \ x \in \Omega_2 = (0.1, \ 1) \end{cases},$$

$$f(x) = 1. \tag{49}$$

Note that the function a is ε -periodic throughout Ω except for a small subdo-

main Ω_1 . We start by computing a reference solution for (10) with (49) by using quadratic finite elements on a very fine mesh. As was seen in section 2.2, the solution of this problem can be found using domain decomposition. We will apply the scheme (12)-(13)-(14), where we again employ quadratic finite elements, now with element size h = 1E - 4.

A choice has to be made for the initial guess at $\gamma = 0.1$. Note that the problem at hand is very similar to the problem considered in Example 1. Indeed, the solutions of both problems satisfy the same boundary conditions at x = 0 and x = 1as well as the same differential equation everywhere except in Ω_1 . In this way the homogenised solution \overline{u} from Example 1 is a natural choice for an initial guess, and so we set $\lambda^0 = \overline{u}(0.1)$. The acceleration parameter θ is simply chosen as 0.5. More details in how to optimize this parameter are given in [Quarteroni and Valli (1999)].

With these choices for the initial guess and acceleration parameter, the errors of the successive approximations

$$u^{k}(x) = \begin{cases} v^{k}(x), \ x \in \Omega_{1}, \\ w^{k}(x), \ x \in \Omega_{2}, \end{cases}$$
(50)

coming from the iterative procedure are displayed in Table 2, for a few values of k.

k	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$
0	9.6 <i>E</i> – 3	
2	3.4E - 3	2.1E - 3
4	6.9E - 4	3.7E - 4
6	1.2E - 4	6.4E - 5

Table 2: Error of the domain decomposition procedure.

Note that the solution of this problem can also be determined using the hybrid approach algorithm (17)-(18)-(19), which makes use of the periodic behaviour of a_{2}^{e} . This will generate the sequence of approximations $\{\hat{u}^{k}\}, k = 1, 2, ...$ defined

in (25), as we iterate over the overlapping region $[0.1, \gamma_2]$. We choose $\lambda^0 = \overline{u}(\gamma_2)$ as an initial guess for the value of the solution *u* at $x = \gamma_2$, where, again, \overline{u} refers to the homogenised solution discussed in the previous example. In order to solve (17) and to find the homogenised corrected approximation of the solution of (18), we use quadratic finite elements with a different element size for each subdomain. A finer grid is required to solve the problem on [0, 0.1], so the grid size is taken 1E - 4 and 1E - 1, respectively.

	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	k	Upper bound
\overline{E}	1.5E - 2	5.7E - 3	2	5.0E - 2
E_C	7.9E - 4	3.9E - 4	6	1.4E - 3

Table 3: Error of the hybrid procedure for $\gamma_2 = 0.15$.

Table 4: Error of the hybrid procedure for $\gamma_2 = 0.25$.

	• ∞	$\ \cdot\ _{L^2(0,1)}$	k	Upper bound
\overline{E}	1.4E - 2	5.2E - 3	2	2.9E - 2
E_C	5.6E - 4	2.8E - 4	4	9.7 <i>E</i> – 4

Table 5: Error of the hybrid procedure for $\gamma_2 = 0.35$.

	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	k	Upper bound
\overline{E}	1.4E - 2	4.7 <i>E</i> −3	2	2.2E - 2
E_C	4.8E - 4	2.5E - 4	4	8.0E - 4

Tables 3-5 display the errors obtained by employing the procedure above for different sizes of the overlapping region. The parameter γ_2 which regulates this size is

taken 0.15, 0.25 and 0.35, respectively. As before, on the second lines of the tables, \overline{E} gives the error when simple homogenisation is applied on the domain Ω_2 . As for E_C , it corresponds to the error obtained by improving the homogenised solution with the first order corrector and the boundary corrector. The fourth column of the tables gives the number of iterations k required to satisfy the stopping condition (24), and the last column the theoretical upper bound given by (26). A prediction for the maximum error δ of the homogenisation procedure was taken from the second column of Table 1. Finally, in Figure 5 we show the exact solution of (10) with (49) as a dotted line, the hybrid homogenised solution as a light full line.



Figure 5: Exact and approximated solutions.

As one can see, the hybrid approach combines the economy of the homogenisation technique with the versatility allowed by the domain decomposition method. The accuracy of the results depends on that of the homogenisation procedure. A good approximation for the heterogeneous periodic solution is thus required.

4.2 Layered elastic materials

Here we present two examples related to the elasticity problems introduced in section 3. The first example illustrates the application of the homogenisation technique to a problem with periodically oscillating coefficients. The second demonstrates the capability of the hybrid approach to deal with materials with localised imperfections.

Example 4.3 - Periodic structure

Let us consider the problem (30) with $\Omega = [0,1]^2$ and assume that the underlying material is isotropic. This means that the components of the elasticity tensor $\widetilde{\mathbf{A}}$ can be written as

$$\widetilde{a}_{2222}(\mathbf{y}) = \widetilde{a}_{1111}(\mathbf{y}) = \frac{E(\mathbf{y})}{1 - v^2(\mathbf{y})};$$
(51)

$$\widetilde{a}_{2121}(\mathbf{y}) = \frac{E(\mathbf{y})}{2(1+\mathbf{v}(\mathbf{y}))};$$
(52)
$$E(\mathbf{y})\mathbf{v}(\mathbf{y})$$

$$\widetilde{a}_{2211}(\mathbf{y}) = \frac{E(\mathbf{y})\mathbf{v}(\mathbf{y})}{1 - \mathbf{v}^2(\mathbf{y})};$$
(53)

$$\widetilde{a}_{2111}(\mathbf{y}) = \widetilde{a}_{2221}(\mathbf{y}) = 0, \tag{54}$$

where *E* is the Young's modulus and *v* is the Poisson's ratio. We further assume that the material is also layered and that its reference cell $Y = [0, 1] \times [0, 1]$ can be decomposed into two subdomains $Y_1 = [0, \frac{1}{2}] \times [0, 1]$, $Y_2 = [\frac{1}{2}, 1] \times [0, 1]$, see Figure 6. These are such that for $i = 1, 2, Y_i$ is occupied by a linear elastic material with Young's modulus $E_i = E_i(y_1)$ and Poisson's ratio $v_i = v_i(y_1)$, where $\mathbf{y} = (y_1, y_2)$. We can then write

$$E(\mathbf{y}) = E_1 \chi_1(y_1) + E_2 \chi_2(y_1), \tag{55}$$

$$\mathbf{v}(\mathbf{y}) = \mathbf{v}_1 \chi_1(y_1) + \mathbf{v}_2 \chi_2(y_1), \tag{56}$$

where χ_1 and χ_2 are the characteristic functions of the sets Y_1 and Y_2 . These are given by

$$\chi_i(\mathbf{y}) = \begin{cases} 1, \text{ for } \mathbf{y} \in Y_i, \\ 0, \text{ for } \mathbf{y} \in Y - Y_i, \end{cases}$$
(57)

and can be extended periodically over Y.

Finally let

$$v_1 = v_2 = 0.3, E_1 = 1, E_2 = 3, \varepsilon = 2E - 2$$
 (58)



Figure 6: The reference cell *Y* is composed of two different materials.

and the boundary conditions be such that

$$\boldsymbol{\Gamma}_{D} = \{0\} \times [0,1], \ \boldsymbol{\varphi}_{N}(\mathbf{x}) = \begin{cases} (0,1) & \text{for } x_{2} = 1, \\ (0,0) & \text{for } x_{2} = 0, \\ (1,0) & \text{for } x_{1} = 1. \end{cases}$$
(59)

A reference solution for (30) with (51)-(59) can be determined using finite elements with a very fine mesh. What we want to do now is to approximate the solution to this problem using homogenisation. It can be shown, as in [Patrício, Mattheij, and de With (2007)], that the homogenised medium corresponding to the isotropic layered material we have mentioned is orthotropic with material constants given by

$$E_x = \frac{\overline{E}}{\overline{\nu}^2 + A\overline{E}}, \ E_y = \overline{E}, \tag{60}$$

$$\mathbf{v}_{xy} = \frac{\overline{\mathbf{v}}}{\overline{\mathbf{v}}^2 + A\overline{E}}, \ \mathbf{v}_{yx} = \overline{\mathbf{v}},\tag{61}$$

$$G = \frac{1}{\frac{2(1+\nu_1)}{E_1} + \frac{2(1+\nu_2)}{E_2}},\tag{62}$$

where

$$\overline{E} = \frac{1}{2}(E_1 + E_2), \ \overline{\nu} = \frac{1}{2}(\nu_1 + \nu_2), \ A = \frac{1}{2}(\frac{\nu_1^2}{E_1} + \frac{\nu_2^2}{E_2}).$$
(63)

We use quadratic finite elements to compute the homogenised solution $\overline{\mathbf{u}}$. A square grid with 50 × 50 elements is employed. The horizontal and vertical components of

	Horizonta	l component	Vertical component		
	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	
Ē	1.2E - 1	2.2E - 2	1.9 <i>E</i> – 1	6.2E - 2	
E _C	3.3E - 2	3.5E - 3	3.0E - 2	3.6 <i>E</i> – 3	

Table 6: Error of the homogenisation procedure.

the error $\overline{\mathbf{E}} = \overline{\mathbf{u}} - \mathbf{u}^{\varepsilon}$ of this approximation are displayed in the third line of Table 6.

In order to obtain a better approximation for \mathbf{u}^{ε} , we will make use of the first order corrector \mathbf{u}_1 given by (39) and the boundary corrector \mathbf{C} given by (40). The latter can be approximated by the solution of the following problem

$$\begin{cases}
-\nabla \cdot (\overline{\mathbf{A}}\boldsymbol{\varepsilon}(\mathbf{C})) = \mathbf{0} & \text{in } \Omega, \\
\mathbf{C} = -\boldsymbol{\varepsilon} \mathbf{u}_{1} & \text{on } \Gamma_{D}, \\
\boldsymbol{\sigma}(\mathbf{C}) \cdot \mathbf{n} = \mathbf{0} & \text{on } \Gamma_{N},
\end{cases}$$
(64)

where $\overline{\mathbf{A}}$ is the homogenised elasticity tensor. In order to compute \mathbf{u}_1 , we first have to first solve the cell problem (36). We do so by approximating the piecewise constant functions *E* and *v* by continuous smooth functions as in [Patrício, Mattheij, and de With (2007)]. As before, we employ square quadratic finite elements. The function \mathbf{u}_1 depends both on components of the cell function and on derivatives of components of the homogenised function $\overline{\mathbf{u}}$. These derivatives can be determined by numerical differentiation. As for the boundary corrector \mathbf{C} , it can be computed from (64) by again using finite elements.

The norms of the horizontal and vertical components of the error function $\mathbf{E}_C = (\overline{\mathbf{u}} + \varepsilon \mathbf{u}_1 + \mathbf{C}) - \mathbf{u}^{\varepsilon}$ are displayed in the last line of Table 6. As expected, this gives better results than using the homogenised solution $\overline{\mathbf{u}}$ as an approximation. In Figure 7 we plot the horizontal components of the exact solution of the problem \mathbf{u}^{ε} , the homogenised function $\overline{\mathbf{u}}$ and the homogenised corrected approximation $\overline{\mathbf{u}} + \varepsilon \mathbf{u}_1 + \mathbf{C}$ along y = 0.7.



Figure 7: Exact and approximated solutions for the horizontal component of the displacement along y = 0.7.

Example 4.4 - Periodic structure with localised imperfections

Consider (41) with (42) and (59), where the computational domain $\Omega = [0,1]^2$ is split into the non-overlapping subdomains $\Omega_1 = [0,0.1] \times [0,0.1]$ and $\Omega_2 = \Omega - \Omega_1$. The components of the elasticity tensor are assumed to satisfy (51)-(56) with (58) throughout Ω except for some circular inclusions on Ω_1 , see Figure 8.



Figure 8: Inclusions present on the subdomain Ω_1 .

The inclusions consist of a linear elastic material characterized by Young's modulus $E_3 = 4$ and Poisson's ratio $v_3 = 0.1$. The radius of each inclusion is r = 0.01. They are centered at the points

$$P_1 = (0.02, 0.02), P_2 = (0.05, 0.03),$$

$$P_3 = (0.08, 0.015), P_4 = (0.015, 0.05),$$

$$P_5 = (0.04, 0.07), P_6 = (0.08, 0.055),$$

$$P_7 = (0.015, 0.08), P_8 = (0.07, 0.085).$$

The problem we have described concerns a periodic structure with localised imperfections. We may handle this by employing the hybrid approach for elasticity algorithm (43)-(45) with the stopping condition (46), where we define $\hat{\Omega}_1 = [0, 0.15] \times [0, 0.15]$. This algorithm iterates over the overlapping region $\hat{\Omega}_1 - \Omega$, cf. Figure 3, generating a sequence of approximations

$$\widehat{\mathbf{u}}^{k}(\mathbf{x}) = \begin{cases} \widehat{\mathbf{v}}^{k}(\mathbf{x}), \ \mathbf{x} \in \Omega_{1}, \\ \widehat{\mathbf{w}}^{k}(\mathbf{x}), \ \mathbf{x} \in \Omega_{2}. \end{cases}$$
(65)

An initial guess $\widehat{\boldsymbol{\lambda}}^0$ for $\mathbf{u}|_{\Gamma_2}$ must be given. Here we take $\widehat{\boldsymbol{\lambda}}^0 = \overline{\mathbf{u}}|_{\Gamma_2}$, where $\overline{\mathbf{u}}$ is the homogenised solution calculated on previous example. A reference solution \mathbf{u} for the problem at hand can be determined using finite elements with a very fine mesh. The same method is employed to solve (43) for each iteration step. As for (44) we approximate its solution by applying homogenisation methods like before.

	Horizontal		Vertical		It.
	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	$\ \cdot\ _{\infty}$	$\ \cdot\ _{L^2(0,1)}$	k
E ⁰	1.7 <i>E</i> – 1	2.8E - 2	2.3E - 1	7.5E - 2	_
Ē	8.2E - 2	8.5E - 3	1.0E - 1	2.7E - 2	5
E _C	3.8E - 2	5.4E - 3	3.9E - 2	5.8E - 3	7

Table 7: Error of the hybrid procedure.

The third line of Table 7 displays the norms of the horizontal and vertical components of the error $\mathbf{E}^0 = \mathbf{u} - \overline{\mathbf{u}}$ of the initial approximation which we give as an initial guess. On the fourth and last lines of the table we show the norms of the approximations obtained by using the hybrid approach as described. We use the homogenised solution $\overline{\mathbf{w}}$ and the respective homogenised corrected solution to approximate the solution of (44), respectively.

5 Conclusions

In this paper we have described an approach to obtain solutions for problems involving materials which are periodically distributed but have localised imperfections. This combines homogenisation and domain decomposition techniques. It may be applied to a wide range of problems where local phenomena is taking an important role. It allows for the computation of a solution taking the heterogeneities into account.

References

Allaire, G. (2002): *Shape Optimization by the Homogenization Method.* Springer, New York.

Aymerich, F.; Serra, M. (2006): An ant colony optimization algorithm for stacking sequence design of composite laminates. *CMES: Computer Modeling in Engineering & Sciences*, vol. 13, no. 1, pp. 49–65.

Babuska, I.; Strouboulis, T. (2001): *The finite element method and its reliability.* Clarendon Press, Oxford.

Becker, A. (1992): *The Boundary Element Method in Engineering*. McGraw-Hill, Maidenhead.

Bensoussan, A.; Lions, J. L.; Papanicolaou, G. (1978): *Asymptotic Analysis of Periodic Structures*. North-Holland, Amesterdam.

Cioranescu, D.; Donato, P. (1999): *An introduction to homogenization*. Oxford University Press.

Dubois, O. (2003): *Optimized Schwarz Methods for the Advection-Diffusion Equation.* PhD thesis, McGill University, Montréal, 2003.

E, W.; Engquist, B.; Li, L.; Ren, W.; Vanden-Eijnden, E. (2005): The heterogeneous multiscale method: a review. http://www.math.princeton.edu/multiscale, 2005. **Fitzgerald, G.; Goldbeck-Wood, G.; Kung, P.; Petersen, M.; Subramanian, L.; J.Wescott** (2008): Materials modeling from quantum mechanics to the mesoscale. *CMES: Computer Modeling in Engineering & Sciences*, vol. 24, no. 3, pp. 169–183.

Guz, A. N.; J.Rushchitsky, J.; A.Guz, I. (2008): Comparative computer modeling of carbon-polymer composites with carbon or graphite microfibers or carbon nanotubes. *CMES: Computer Modeling in Engineering & Sciences*, vol. 26, no. 3, pp. 139–156.

Hou, T.; Wu, X.; Cai, Z. (1999): Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients. *Math. Comp*, vol. 227, no. 68, pp. 913–943.

Hou, T. Y.; H.Wu, X. (1997): A multiscale finite element method for elliptic problems in composite materials and porous media. *J. Comput. Phys.*, vol. 134, pp. 169–189.

Kakuba, G.; Mattheij, R.; Anthonissen, M. (2006): Local defect correction for the boundary element method. *CMES: Computer Modeling in Engineering & Sciences*, vol. 15, no. 3, pp. 127–135.

Patrício, M.; Mattheij, R.; de With, G. (2007): Homogenisation with application to layered materials. *submited to Mathematics and Computers in Simulation*.

Pavliotis, G.; Stuart, A. M. (2008): Multiscale methods: averaging and homogenization. http://www.warwick.ac.uk/~masor/hultiscale.pdf, 2008.

Quarteroni, A.; Valli, A. (1999): Domain Decomposition Methods for Partial Differential Equations. Clarendon Press, Oxford.

Schwarz, H. (1870): Über einen grenzübergang durch alternierendes verfahren. *Vierteljahrsschrift der Naturforschenden Gesellschaft in Zürich*, , no. 15, pp. 272–286.

Smith, B.; Bjørstad, P.; Gropp, W. (1996): Domain decomposition : parallel multilevel methods for elliptic partial differential equations. Cambridge University Press.

Toselli, A.; Widlund, O. (2004): *Domain Decomposition Methods - Algorithms and Theory*, volume 34. Springer Series in Computational Mathematics.

Versieux, H. M.; Sarkis, M. (2006): Numerical boundary corrector for elliptic equations with rapidly oscillating periodic coefficients. *Commun. Numer. Meth. Engng*, vol. 22, pp. 577–589.