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Solutions for Periodically Distributed Materials with Localised Imperfections

M. Patrício[1], R. Mattheij[1] and G. de With [2]

Summary

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 linearly elastic materials are considered.

Introduction

When dealing with materials with complex microstructures such as composites, the coefficients of the related PDEs vary so rapidly that applying classical techniques such as finite elements or boundary elements methods becomes prohibitively expensive. One may think for example of a material which consists of two phases bonded together along the interface, the matrix and the inclusions. The number of the latter is then typically very large. This makes for a very complex problem to deal with from the numerical point of view.

One possible strategy to tackle this problem consists of employing domain decomposition techniques. This allows the division of the computational domain into smaller subdomains where the original equation is to be solved - see for example [7].

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 - [5]. On the bright side, several techniques have been devised which solve this class of problems, amongst which those suggested by the homogenisation theory [2], the multiscale finite element methods [4] or the heterogeneous multiscale method [3].

The goal of this work is to analyse boundary value problems related to periodic materials with localised imperfections. 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. This is done for a one dimensional problem -

[1]Department of Mathematics and Computer Science, Technische Universiteit Eindhoven
[2]Department of Chemical Engineering and Chemistry, Technische Universiteit Eindhoven

which we omit here for the sake of brevity - and also for the two dimensional elasticity problem. An accurate solution to the problem is then found with reasonably small computational effort.

Periodic structure

Let us consider a composite material with constituents periodically distributed over Ω. Assume 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 1.

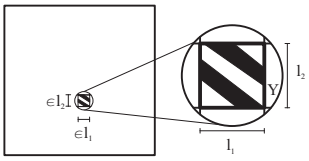

Figure 1: Representative cell.

We state the well-known linear elasticity problem for the composite material as follows - cf. [2] -

$$\begin{cases} -\nabla\cdot\ (\mathbf{A}^{\varepsilon}(\mathbf{x})\mathbf{e}(\mathbf{u}^{\varepsilon})) = \mathbf{f} & \mathbf{x}\ \in\ \Omega, \\ \mathbf{u}^{\varepsilon} = \mathbf{0} & \text{on } \Gamma_D, \\ \sigma(\mathbf{u}^{\varepsilon})\cdot\mathbf{n} = \mathbf{g}_N & \text{on } \Gamma_N. \end{cases} \tag{1}$$

where $\mathbf{g}_N$ is a vector function and $\mathbf{e}$ and σ are the strain and stress tensors, respectively. The tensor $\mathbf{A}^{\varepsilon}$, which characterizes 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 IR^2. We define $\mathbf{A}^{\varepsilon} = \mathbf{A}^{\varepsilon}(\mathbf{x}) = (a^{\varepsilon}_{ijkh})_{1\le i,j,k,h\le N}$ such that for $\mathbf{x} = (x_1,\ x_2) \in IR^2$, one has $a^{\varepsilon}_{ijkh}(\mathbf{x}) := \widetilde{a}_{ijkh}(\mathbf{y}) = \widetilde{a}_{ijkh}(\mathbf{x}/\varepsilon)$, where we denote $\mathbf{y} := \mathbf{x}/\varepsilon$, for $\mathbf{y} = (y_1,\ y_2) \in IR^2$. We will now look at how to approximate the heterogeneous solution $\mathbf{u}^{\varepsilon}$ of (1). Consider the following ansatz

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

Here, $\mathbf{u}_i,\ i = 1,\ 2,\ \dots$ are periodic functions in $\mathbf{y} = \mathbf{x}/\varepsilon$. Following [1] 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 (1) 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, $\overline{\mathbf{u}}$ is the solution of

$$\begin{cases} -\nabla\cdot\ (\overline{\mathbf{A}}\mathbf{e}(\overline{\mathbf{u}})) = \mathbf{f} & \mathbf{x}\ \in\ \Omega, \\ \\ \overline{\mathbf{u}} = \mathbf{0} & \text{on } \Gamma_D, \\ \overline{\mathbf{u}}\cdot\mathbf{n} = \mathbf{g}_N & \text{on } \Gamma_N. \end{cases} \tag{3}$$

The homogenised tensor $\overline{\mathbf{A}} = (\overline{a}_{ijkh})$ is symmetric and does not depend on $\mathbf{x}$. In order to compute it, one must first solve a cell problem in order to determine the cell function $\chi^{lm}(\mathbf{y}) = (\chi^{lm}_k)(\mathbf{y})$. More terms of the asymptotic expansion may be calculated. In particular, $\mathbf{u}_1$ takes the form

$$\mathbf{u}_1(\mathbf{x},\mathbf{y}) = \frac{1}{2}\sum_{i,j=1,2}\left(\frac{\partial\overline{u}_i}{\partial x_j} + \frac{\partial\overline{u}_j}{\partial x_i}\right)\chi^{ij}(\frac{\mathbf{x}}{\varepsilon}). \tag{4}$$

We call $\overline{\mathbf{u}}$ the homogenised solution for the problem (1). It captures the macroscopic behaviour of $\mathbf{u}^\varepsilon$. To recover the effect of the heterogeneities, we consider the approximation $\overline{\mathbf{u}} + \varepsilon\mathbf{u}_1$. It does not necessarily satisfy the same boundaries condition prescribed for the heterogeneous solution. This may be remedied by introducing a boundary corrector $\mathbf{C}$ which is given by $-\varepsilon\mathbf{u}_1$ at the boundaries, in similarity to [8]. We call $\overline{\mathbf{u}} + \varepsilon\mathbf{u}_1 + \mathbf{C}$ the homogenised corrected solution.

This approximation is computationally much cheaper to obtain than solving the full heterogeneous problem, and it still allows for the resolution of the heterogeneities.

Complex structure

Let us again consider the linear elasticity problem for a composite. Unlike what we did previously, we now assume that the material is not necessarily periodically distributed. Then, instead of (1), we consider

$$\begin{cases} -\nabla\cdot\ (\mathbf{A}(\mathbf{x})\mathbf{e}(\mathbf{u})) = \mathbf{f} & \mathbf{x}\ \in\ \Omega, \\ \\ \mathbf{u} = \mathbf{0} & \text{on } \Gamma_D, \\ \sigma(\mathbf{u})\cdot\mathbf{n} = \mathbf{g}_N & \text{on } \Gamma_N, \end{cases} \tag{5}$$

where the parameter ε was suppressed and the tensor $\mathbf{A}$ reads

$$\mathbf{A}(\mathbf{x}) = \begin{cases} \mathbf{A}_1(\mathbf{x}),\ \mathbf{x}\in\Omega_1, \\ \mathbf{A}_2^\varepsilon(\mathbf{x}),\ \mathbf{x}\in\Omega_2. \end{cases} \tag{6}$$

Here $\mathbf{A}_2^\varepsilon$ is an ε-periodic tensor and it is assumed that $|\Omega_1| < |\Omega_2|$, where Ω_1 and Ω_2 are two non-overlapping subsets of Ω such that $\Omega = \Omega_1 \cup \Omega_2$. The homogenisation method described earlier may not be employed to solve (5) with (6)

as **A** is not periodic everywhere. One possible alternative, with the drawback of not making use of the periodicity of the elasticity tensor over Ω_2, is the usage of domain decomposition techniques. In what follows, we will establish a hybrid approach for this problem where 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 $\Gamma_2 = \partial\widehat{\Omega}_1 \cap \partial\Omega_2$, as illustrated in Figure 2.

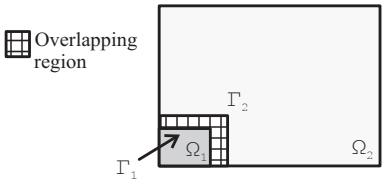

Figure 2: The computational domain Ω .

The hybrid approach algorithm reads

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

  solve

$$\begin{cases} -\nabla\cdot\ (\mathbf{A}\mathbf{e}(\widehat{\mathbf{v}}^{k+1})) = \mathbf{f} & \mathbf{x} \in\ \widehat{\Omega}_1, \\ \widehat{\mathbf{v}}^{k+1} = \mathbf{0} & \text{on } \Gamma_D \bigcap \Omega_1, \\ \sigma(\widehat{\mathbf{v}}^{k+1})\cdot\mathbf{n} = \mathbf{g}_N & \text{on } \Gamma_N \bigcap \Omega_1, \\ \widehat{\mathbf{v}}^{k+1} = \widehat{\mathbf{h}}^k & \text{on } \Gamma_2. \end{cases} \tag{7}$$

  Use homogenisation techniques to find the homogenised corrected solution $\widehat{\mathbf{w}}^{k+1} := \overline{\mathbf{w}}^{k+1} + \varepsilon\mathbf{w}_1^{k+1} + \mathbf{C}^{k+1}$ which approximates the solution of the problem

$$\begin{cases} -\nabla\cdot\ (\mathbf{A}_2^{\varepsilon}\mathbf{e}(\mathbf{w}^{k+1})) = \mathbf{f} & \mathbf{x}\ \in\ \Omega_2, \\ \mathbf{w}^{k+1} = \mathbf{0} & \text{on } \Gamma_D \bigcap \Omega_2, \\ \sigma(\mathbf{w}^{k+1})\cdot\mathbf{n} = \mathbf{g}_N & \text{on } \Gamma_N \bigcap \Omega_2, \\ \mathbf{w}^{k+1} = \mathbf{v}^{k+1} & \text{on } \Gamma_1. \end{cases} \tag{8}$$

  Update $\widehat{\mathbf{h}}^{k+1}$

$$\widehat{\mathbf{h}}^{k+1} = \widehat{\mathbf{w}}^{k+1}|_{\Gamma_1}. \tag{9}$$

This procedure generates a sequence of approximations $\widehat{\mathbf{u}}^k$ to (5) with (6) defined by $\widehat{\mathbf{v}}^k$ over Ω_1 and by $\widehat{\mathbf{w}}^k$ over Ω_2. A stopping condition for this algorithm is defined in terms of the norms of the components of $(\widehat{\mathbf{w}}^k - \widehat{\mathbf{v}}^k)|_{\Gamma_2}$.

Example

Consider (5) with (6), where the computational domain $\Omega = [0,1] \times [0,1]$ 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 described a layered material throughout Ω except for some circular inclusions on Ω_1, see Figure 3. The plate is kept fixed along $x = 0$, and along its upper, lower and right boundaries $\sigma \cdot \mathbf{n}$ is given by $(0,1)$, $(0,0)$ and $(1,0)$, respectively.

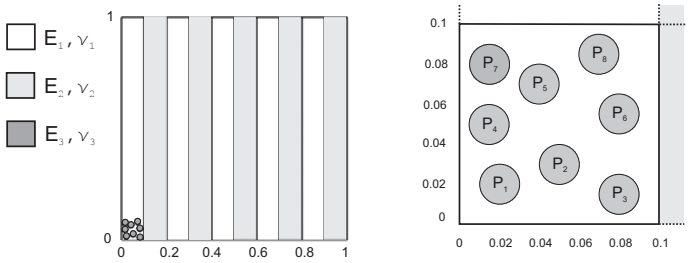

Figure 3: Left: plate with layered material and inclusions. Right: zoom up of the subdomain Ω_1.

The constituents of the layered material have Young's Modulus and Poisson's ratio $E_1 = 1,\ \nu_1 = 0.3$ and $E_2 = 3,\ \nu_2 = 0.3$. We like to think of the inclusions as being randomly distributed. They consist of a linear elastic material characterized by Young's modulus $E_3 = 4$ and Poisson's ratio $\nu_3 = 0.1$. The radius of each inclusion is $r = 0.01$. They are centered at the points $P_1 = (0.02,\ 0.02)$, $P_2 = (0.05,\ 0.03)$, $P_3 = (0.08,\ 0.015)$, $P_4 = (0.015,\ 0.05)$, $P_5 = (0.04,\ 0.07)$, $P_6 = (0.08,\ 0.055)$, $P_7 = (0.015,\ 0.08)$, $P_8 = (0.07,\ 0.085)$.

This problem concerns a periodic structure with localised imperfections. We may handle this by employing the hybrid approach for elasticity algorithm (7)-(9) with the prescribed stopping condition, where we define $\widehat{\Omega}_1 = [0,\ 0.15] \times [0,\ 0.15]$.

A reference solution $\mathbf{u}$ for this problem can be determined using finite elements with a very fine mesh. For the algorithm, an initial guess $\widehat{\mathbf{h}}^0$ for $\mathbf{u}|_{\Gamma_2}$ must be given. Here we take $\widehat{\mathbf{h}}^0 = \overline{\mathbf{u}}|_{\Gamma_2}$, where $\overline{\mathbf{u}}$ is the homogenised solution corresponding to a modification of the current problem at hand - instead of considering inclusions, we assume that the material is periodic and layered over Ω. Finite elements are also employed to solve (7) for each iteration step. As for (8) we approximate its solution by applying homogenisation methods like before.

Table 1: Error of the hybrid procedure.

	Horizontal component		Vertical component		Iterations
	Maximum norm	L^2 norm	Maximum norm	L^2 norm	k
$\mathbf{E}^0$	$1.7E-1$	$2.8E-2$	$2.3E-1$	$7.5E-2$	–
$\mathbf{E}_C$	$3.8E-2$	$5.4E-3$	$3.9E-2$	$5.8E-3$	7

The third line of Table 1 displays the norms of the error $\mathbf{E}^0 = \mathbf{u} - \overline{\mathbf{u}}$. On the last line of the table we show the norm of the error of the approximation obtained by using the hybrid approach as described.

Conclusion

In this work we describe an approach to obtain solutions for problems involving materials which are periodically distributed but have localised imperfections. This approach combines homogenisation and domain decomposition techniques. It may be applied to a wide range of problems where local phenomena is taking an important role, and for which local resolution of the microscale is required.

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