A SEMI-ANALITYCAL APPROACH FOR THE CALCULATION OF EFFECTIVE PROPERTIES OF ELASTIC COMPOSITE MATERIALS WITH IMPERFECT INTERFACES

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Abstract. *The present work provides details on the application of three well-known methods for the computation of the effective anisotropic elastic tensor of fibrous composite materials provided with a periodic microstructure. We assume imperfect interfaces of linear spring type between the constituents. The methods are the asymptotic homogenization method (AHM), the domain decomposition method (DDM) and the finite element method (FEM). Examples of the application of the approach for fibrous composites with several phases, using the free code FreeFEM++, are presented. Comparisons with other works are reported.*

Keywords: *effective elastic properties, asymptotic homogenization, finite elements, domain decomposition*

1 INTRODUCTION

The design and production of composites materials with mechanical, thermal and electromagnetic properties that surpass the ones of their constituent is an area of intensive development. Savings in this effort are achieved if the macro-behavior of the composite can be accurately predicted given the physical properties of the constituent phases and the geometrical description of its arrangement. In linear elasticity the micro-heterogeneity of fiber-reinforced composites produces a rapid oscillation of the coefficients involved in the partial differential equations model. The analytic solution of this system of equations for general anisotropic constituents is impossible. Numerical methods, on the other hand, require a very fine discretization, of the domain depicted by the composite, that considerably increases the computational cost and compromises the convergence of the methods. An alternative to this problem is the use of some homogenization theory. Mathematical homogenization allows obtaining approximations to the so-called effective or homogenized properties of heterogeneous media taking into account the physical and geometric characteristics of their constituents, see for instance Allaire (2002); Bravo-Castillero et al. (2013). Effective properties characterize a homogeneous medium ”equivalent” to the heterogeneous one under study.

Among the mathematical homogenization methods, the asymptotic homogenization method (AHM) is a rigorous one, relevant when the structure of the media is periodic. A detailed explanation of this method can be found in Auriault et al. (2009); Bakhvalov and Panasenko (1989); Bensoussan et al. (1978); Oleĭnik et al. (1992). The AHM presents a mathematical framework for the calculation of effective coefficients that rely on the solution of so-called *local problems* posed on the periodic cell. These local problems are analytically solved only in exceptional cases. For example, in Rodríguez-Ramos et al. (2001) and Guinovart-Díaz et al. (2001), analytical expressions are obtained for the effective elastic properties of biphasic composites with square and hexagonal geometry of the periodic cell and fibers of circular cross-section respectively. They consider both phases transversely isotropic and perfectly glued. In López-Realpozo et al. (2014) analytical expressions are obtained for a composite with transversely isotropic phases, reinforced by long fibers of circular cross-section, with rhombic periodic cell and imperfect contact.

When analytic solutions to the local problems are not available, an alternative is to apply some numerical method. The most used is the finite element method (FEM), Otero et al. (2013), Würkner et al. (2014). However, most works are restricted to periodic cells with square or parallelogram shape and circular, elliptical or square fiber cross-section. It is our assumption that study of more complicated geometries have been limited by the meshing capabilities of the software being used. In the context of FEM, problems such as the local problems are known as elliptic interface problems, see Babuška (1970).

In this work the effective elastic properties of composite materials with micro-periodic distribution of parallel unidirectional fibers are studied. The study of such materials can be done in the plane (2D) and they are characterized by a periodic repetition of a basic cell, called the unit cell or periodicity cell. We allow arbitrary shapes for the periodic cell and the cross-sections of the fibers. The constituent materials, matrix and fibers, may be anisotropic and the linear-spring interface model, Duan et al. (2007), is assumed. The numerical solution of the local problems is obtained iteratively from the decomposition in sub-problems, on the domain of the fibers and on the matrix domain, which are coupled by the imperfect contact conditions. This type of approach is characteristic of the domain decomposition methods (DDM) Dolean et al. (2015); Mathew (2008). In this work, we use the free software FreeFEM ++ Hecht (2012), for the solution of the subproblems via FEM. FreeFEM ++ is based on directly discretizing the variational formulation of the problem, which makes it very close to the mathematical formulation of FEM. The benefits of the methodology have been already shown in the computation of the thermal effective conductivity tensor of composite materials in León-Mecías et al. (2017).

2 THEORETICAL FRAMEWORK

To determine elastic effective properties of fiber-reinforced composites some method of homogenization has to be used. Among the eligible methods, we use the AHM. In the AHM the problem over the composite medium is embedded in a family of problems parametrized by the period size ε. This family of problems weakly converges to the solution of a problem with constant coefficients, the effective elastic coefficients. The AHM is mathematically rigorous and provides an analytic formulation for the effective coefficients. However, the basis for the analytic formulae of the effective coefficients are the solutions of the local problems over the periodic cell and these, seldom have closed form expressions. In most cases, the use of numerical methods is unavoidable. Therefore, we call such an approach semi analytic.

In the following we describe the AHM approach. We will consider arbitrary shapes for the cross-sections of the fibers. The periodic cells can have arbitrary polygonal boundary but they must provide a translations only tiling of the plane. To simplify the exposition we study materials with a periodic arrangement of two different fibers. The two fibers can be distinguish by cross-section shape or elastic properties and all fibers are aligned with the x_3-axis of a three dimensional Cartesian coordinate system.

2.1 Governing elastic equations

For two no colinear vectors $\mathbf{v} = (v_1, v_2) \in \mathbb{R}^2$, $\mathbf{w} = (w_1, w_2) \in \mathbb{R}^2$, a point $\mathbf{z} = (z_1, z_2) \in \mathbb{Z}^2$ and any set $S \subset \mathbb{R}^2$ define

$$\mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}}(S) = \left\{\mathbf{y} \in \mathbb{R}^2 : \mathbf{y} = \mathbf{x} + z_1\mathbf{v} + z_2\mathbf{w},\ \mathbf{x} \in S\right\},$$

and

$$\dim(S) = \max_{\mathbf{y}_1,\mathbf{y}_2 \in S} \|\mathbf{y}_1 - \mathbf{y}_2\|.$$

Let's denote with $\Omega_\#$ the Lipschitz domain with polygonal boundary $\Gamma_\# = \partial\Omega_\#$ that defines the periodic cell. Then $\Omega_\#$ is a periodic cell if an only if there exist two vectors $\mathbf{v} \in \mathbb{R}^2$ and $\mathbf{w} \in \mathbb{R}^2$ such that:

- $\mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}_1}(\Omega_\#) \cap \mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}_2}(\Omega_\#) = \emptyset$ if $\mathbf{z}_1 \neq \mathbf{z}_2$,
- $\cup_{\mathbf{z}\in\mathbb{Z}^2}\mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}}\left(\overline{\Omega}_\#\right) = \mathbb{R}^2$.

The cross-section of the two fibers are represented by the Lipschitz domains $F_1 \subset \Omega_\#$ and $F_2 \subset \Omega_\#$ such that $F_1 \cap F_2 = \partial F_1 \cap \partial F_2 = \emptyset$. Allowing an arbitrary shape for $\Gamma_\#$ we can always achieve $\partial F_1 \cap \Gamma_\# = \partial F_2 \cap \Gamma_\# = \emptyset$. We denote $\Omega_\#^{(M)} = \Omega_\# \setminus \left\{\overline{F}_1 \cup \overline{F}_2\right\}$.

Suppose the cross-section of a 3D sample of the composite material is given by the Lipschitz domain $\Omega \subset \mathbb{R}^2$ with $\Omega_\# \subset \Omega$ and $\dim(\Omega) \gg \dim(\Omega_\#)$. Then we have that $\varepsilon = \dim(\Omega_\#) / \dim(\Omega) \ll 1$ and to represent the fact that a network of periodic repetitions of $\Omega_\#$ is embedded in Ω we denote the cross-section of the composite with Ω^ε. Note that we can let $\varepsilon \to 0$ by increasing the size of the composite material sample and this have no effect on the effective properties of the fibrous material.

Hereinafter Einstein summation convention holds and Latin alphabet indices take on values $1, 2$, or 3 while Greek alphabet indices take on values 1 or 2. The constitutive equations of linear elasticity for $\mathbf{x} = (x_1, x_2) \in \Omega^\varepsilon$ are given by

$$\sigma_{ij} = C_{ijkl}(\mathbf{x})\,\epsilon_{kl},$$
$$\epsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k^\varepsilon}{\partial x_l} + \frac{\partial u_l^\varepsilon}{\partial x_k}\right),$$

where C_{ijkl} are the elastic coefficients satisfying the usual symmetries and u_i^ε are components of the displacement vector function $\mathbf{u}^\varepsilon : \Omega^\varepsilon \to \mathbb{R}^3$. Let be

$$\Omega_\alpha^\varepsilon = \cup_{\mathbf{z}\in\mathbb{Z}^2}\left\{\mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}}(F_\alpha) \cap \Omega^\varepsilon\right\}$$

and define $\Omega_M^\varepsilon = \Omega^\varepsilon \setminus \left\{\overline{\Omega}_1^\varepsilon \cup \overline{\Omega}_2^\varepsilon\right\}$. Observe that Ω_1^ε and Ω_2^ε are not connected sets with boundaries defined by

$$\partial\Omega_\alpha^\varepsilon = \cup_{\mathbf{z}\in\mathbb{Z}^2}\left\{\mathcal{T}_{\mathbf{v},\mathbf{w},\mathbf{z}}(\partial F_\alpha) \cap \Omega^\varepsilon\right\},$$

while Ω_M^ε is a multiply connected set. Assuming that each component of the composite is homogeneous we have

$$C_{ijkl}(\mathbf{x}) = \begin{cases} C_{ijkl}^{(M)}, & \mathbf{x} \in \Omega_M^\varepsilon, \\ C_{ijkl}^{(1)}, & \mathbf{x} \in \Omega_1^\varepsilon, \\ C_{ijkl}^{(2)}, & \mathbf{x} \in \Omega_2^\varepsilon. \end{cases}, \tag{1}$$

and C_{ijkl} is $\Omega_\#$ periodic in Ω^ε.

A boundary value problem for static elasticity problem over Ω^ε can be stated as follows

$$\frac{\partial \sigma_{i\alpha}^\varepsilon}{\partial x_\alpha} = 0, \text{ in } \Omega_M^\varepsilon \setminus \{\partial\Omega_1^\varepsilon \cup \partial\Omega_2^\varepsilon\}, \tag{2}$$
$$\mathbf{u}^\varepsilon = 0, \text{ on } \partial_D\Omega^\varepsilon, \tag{3}$$
$$\sigma_{i\alpha}^\varepsilon n_\alpha = 0, \text{ on } \partial_N\Omega^\varepsilon, \tag{4}$$

where n_α are the components of the outward normal unitary vector $\mathbf{n}(\mathbf{x}) = (n_1(\mathbf{x}), n_2(\mathbf{x}))^T \in \mathbb{R}^2$ for $\mathbf{x} \in \partial\Omega^\varepsilon$. We remark that boundary conditions (3) and (4) on Ω^ε does not hat effect in the value of the effective elastic properties of the composite. However, contact conditions at the interface between matrix and fibers, that means in the sets $\partial\Omega_1^\varepsilon$ and $\partial\Omega_2^\varepsilon$, are of great importance. In this work we consider *imperfect contact of linear spring type* between matrix and fibers.

To state the linear spring type contact conditions in a form more amenable to FEM we define the matrices

$$\mathcal{K}_{ij} = (C_{i\alpha j\beta}) \in \mathbb{R}^{2\times 2}.$$

Given the symmetries of C_{ijkl} we have $\mathcal{K}_{21} = \mathcal{K}_{12}^\top$, $\mathcal{K}_{31} = \mathcal{K}_{13}^\top$, $\mathcal{K}_{32} = \mathcal{K}_{23}^\top$ and $\mathcal{K}_{ii}$ symmetric. Denoting

$$\sigma_i^\varepsilon = \mathcal{K}_{i1}\nabla u_1^\varepsilon + \mathcal{K}_{i2}\nabla u_2^\varepsilon + \mathcal{K}_{i3}\nabla u_3^\varepsilon,$$

then the system of partial differential equations defined in (2) is equivalent to

$$\nabla \cdot \sigma_1^\varepsilon = 0, \text{ in } \Omega_M^\varepsilon \setminus \{\partial\Omega_1^\varepsilon \cup \partial\Omega_2^\varepsilon\}, \tag{5}$$
$$\nabla \cdot \sigma_2^\varepsilon = 0, \text{ in } \Omega_M^\varepsilon \setminus \{\partial\Omega_1^\varepsilon \cup \partial\Omega_2^\varepsilon\}, \tag{6}$$
$$\nabla \cdot \sigma_3^\varepsilon = 0, \text{ in } \Omega_M^\varepsilon \setminus \{\partial\Omega_1^\varepsilon \cup \partial\Omega_2^\varepsilon\}. \tag{7}$$

Let $\mathbf{n}_M(\mathbf{x}) = \left(n_1^{(M)}(\mathbf{x}), n_2^{(M)}(\mathbf{x})\right)^T$ be the outward normal unitary vector for $\mathbf{x} \in \partial\Omega_M^\varepsilon$ and analogously define $\mathbf{n}_\alpha(\mathbf{x})$ for $\mathbf{x} \in \partial\Omega_\alpha^\varepsilon$. The vector of tractions in direction of $\mathbf{n}_{(h)}(\mathbf{x})$, $h = M, 1, 2$, is defined as

$$\mathbf{T}^{(h)} = \begin{pmatrix} T_1^{(h)} & T_2^{(h)} & T_3^{(h)} \end{pmatrix}^\top = \begin{pmatrix} \sigma_1^\varepsilon|_{\Omega_h^\varepsilon} \cdot \mathbf{n}_{(h)} & \sigma_2^\varepsilon|_{\Omega_h^\varepsilon} \cdot \mathbf{n}_{(h)} & \sigma_3^\varepsilon|_{\Omega_h^\varepsilon} \cdot \mathbf{n}_{(h)} \end{pmatrix}^\top,$$

where, for a function f defined in Ω_h^ε and a point $\mathbf{x} \in \partial\Omega_h^\varepsilon$

$$f|_{\Omega_h^\varepsilon}(\mathbf{x}) = \lim_{\mathbf{y}\in\Omega_h^\varepsilon \to \mathbf{x}} f(\mathbf{y}).$$

The traction vector $\mathbf{T}^{(h)}(\mathbf{x})$ is given by Cartesian components and on each $\mathbf{x} \in \{\partial\Omega_M^\varepsilon \cup \partial\Omega_1^\varepsilon \cup \partial\Omega_2^\varepsilon\}$ it can be decomposed into its normal, tangential and axial components by

$$\mathbf{T}_{\{n,t,a\}}^{(h)}(\mathbf{x}) = \begin{pmatrix} T_n^{(h)} & T_t^{(h)} & T_a^{(h)} \end{pmatrix}^\top = \mathcal{N}^{(h)}\mathbf{T}^{(h)} \tag{8}$$

where

$$\mathcal{N}^{(h)} = \begin{pmatrix} n_1^{(h)} & n_2^{(h)} & 0 \\ -n_2^{(h)} & n_1^{(h)} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Analogously we obtain

$$\mathbf{u}_{\{n,t,a\}}^\varepsilon = \begin{pmatrix} u_n^{(\varepsilon)} & u_t^{(\varepsilon)} & u_a^{(\varepsilon)} \end{pmatrix}^\top = \mathcal{N}^{(h)}\mathbf{u}^\varepsilon. \tag{9}$$

The linear spring type interface conditions in $\mathbf{x} \in \partial\Omega_\alpha^\varepsilon$ are then given by

$$\mathbf{T}_{\{n,t,a\}}^{(M)}(\mathbf{x}) = -\mathcal{K}^{(\alpha)}[\![\mathbf{u}_{\{n,t,a\}}^\varepsilon]\!]_{\partial\Omega_\alpha^\varepsilon}(\mathbf{x}) \tag{10}$$

where

$$\mathcal{K}^{(\alpha)} = \begin{pmatrix} k_n^{(\alpha)} & 0 & 0 \\ 0 & k_t^{(\alpha)} & 0 \\ 0 & 0 & k_a^{(\alpha)} \end{pmatrix}$$

and, for $\mathbf{x} \in \partial\Omega_{\alpha}^{\varepsilon}$,

$$[\![(\cdot)]\!]_{\partial\Omega_{\alpha}^{\varepsilon}}(\mathbf{x}) = (\cdot)|_{\Omega_{M}^{\varepsilon}}(\mathbf{x}) - (\cdot)|_{\Omega_{\alpha}^{\varepsilon}}(\mathbf{x}),\ h = n, t, a,$$

is the jump of a quantity across the interface $\partial\Omega_{\alpha}^{\varepsilon}$.

Note that, for $h = n, t, a$, $k_h^{(\alpha)} \geq 0$ and when $k_h^{(\alpha)} \rightarrow \infty$ we have perfect contact of displacements and tractions across the interface, whereas for $k_h^{(\alpha)} = 0$ we obtain what is called total debonding.

Summarizing we have the following displacements problem over the composite medium.

Problem 1 *In the domain Ω^{ε} find $\mathbf{u}^{\varepsilon}$ that satisfy the system of partial differential equations (5)-(7), boundary conditions (3) and (4) and the interface contact conditions (10) on $\partial\Omega_1^{\varepsilon}$ and $\partial\Omega_2^{\varepsilon}$.*

Problem 1 is not solvable analytically. For any numerical solution the meshes must be extremely dense. Therefore, the computational cost of solving problem 1 can be very high. One way to deal with such a situation is to find approximate solutions for $\varepsilon \longrightarrow 0$. In this regard the asymptotic homogenization method is an efficient choice. In the following section a brief description of this method is given.

3 SEMIANALYTICAL APPROACH OF THE EFFECTIVE ELASTIC PROPERTIES

The AHM provides a rigorous approach to obtain approximate solutions of problem 1 for any $\varepsilon > 0$. Moreover, as $\varepsilon \rightarrow 0$ this approximate solutions weakly converge to the solution of problem 1. In the AHM the solution $\mathbf{u}^{\varepsilon}$ is stated in the two scale formal asymptotic ansatz

$$\mathbf{u}^{\varepsilon}(\mathbf{x}) = \mathbf{u}_0(\mathbf{x}) + \sum_{i=1}^{\infty} \varepsilon^i \mathbf{u}_i(\mathbf{x}, \mathbf{y}). \tag{11}$$

In (11) $\mathbf{y} = \mathbf{x}/\varepsilon$ is called local or rapid variable and $\mathbf{x}$ is the global or slow variable. Substituting the asymptotic expansion (11) in (5)-(7), applying the chain rule to each component of $\mathbf{u}_i$ and equating the terms in power of ε to zero, an infinite system of equations is obtained, to determine the functions $\mathbf{u}_i$ in (11). From the equations for ε^{-1} we can find $\mathbf{u}_1(\mathbf{x}, \mathbf{y}) = (u_{11}(\mathbf{x}, \mathbf{y}), u_{21}(\mathbf{x}, \mathbf{y}), u_{31}(\mathbf{x}, \mathbf{y}))$ and also establish the so called local problems on the periodic cell $\Omega_{\#}$ that only involves the fast variable $\mathbf{y}$. The computation of effective coefficients depends on the solution of these problems. For details see Penta and Gerisch (2015). The local problems are six and they are identified with indices 11, 22, 33, 23, 13 and 12. For $pq \in \{11, 22, 33, 23, 13, 12\}$ they are stated as following.

Problem 2 (Local Problem pq) *Find $\mathbf{N}^{pq} : \Omega_{\#} \rightarrow \mathbb{R}^3$, $\mathbf{y} \mapsto \mathbf{N}^{pq}(\mathbf{y})$, $\mathbf{N}^{pq} = (N_1^{pq}, N_2^{pq}, N_3^{pq})$,*

$\mathbf{y} = (y_1, y_2)$, *such that* N_i^{pq} $\Omega_\#$*-periodic and*

$$\nabla \cdot \sigma_i^{(\#)} = 0, \text{ in } \Omega_\# \setminus \{\partial F_1 \cup \partial F_2\}, \tag{12}$$

$$\sigma_i^{(\#)}\Big|_{\Omega_\#^{(M)}} \cdot \mathbf{n}_M + \sigma_i^{(\#)}\Big|_{F_\alpha} \cdot \mathbf{n}_\alpha = 0, \text{ on } \partial F_\alpha, \tag{13}$$

$$T_n^{(M)} = -k_n^{(\alpha)} [\![N_n^{pq}]\!]_{\partial F_\alpha}, \tag{14}$$

$$T_t^{(M)} = -k_t^{(\alpha)} [\![N_t^{pq}]\!]_{\partial F_\alpha}, \tag{15}$$

$$T_a^{(M)} = -k_a^{(\alpha)} [\![N_a^{pq}]\!]_{\partial F_\alpha}, \tag{16}$$

where

$$\sigma_i^{(\#)} = \mathcal{K}_{i1} \nabla N_1^{pq} + \mathcal{K}_{i2} \nabla N_2^{pq} + \mathcal{K}_{i3} \nabla N_3^{pq} + \mathbf{k}_i^{pq},$$
$$\mathbf{k}_i^{pq} = (C_{i1qp}, C_{i2qp})^\top \in \mathbb{R}^2,$$

and $T_n^{(M)}$, $T_t^{(M)}$ *and* $T_n^{(M)}$ *are respectively the normal, tangential and axial components of the tractions vector*

$$\left(T_1^{(M)}, T_2^{(M)}, T_3^{(M)}\right) = \left(\sigma_1^{(\#)} \cdot \mathbf{n}_M, \sigma_2^{(\#)} \cdot \mathbf{n}_M, \sigma_2^{(\#)} \cdot \mathbf{n}_M\right)$$

on $\mathbf{y} \in \partial F_\alpha$.

The effective coefficients are computed as

$$\hat{C}_{ijkl} = \left\langle C_{ijkl} + C_{ijpq} \frac{\partial N_i^{pq}}{\partial y_j} \right\rangle_{\Omega_\#} \tag{17}$$

where

$$\langle (\cdot) \rangle_{\Omega_\#} = \frac{1}{|\Omega_\#|} \int_{\Omega_\#} (\cdot)\, d\mathbf{y}.$$

From (17) is easy to note that $\mathbf{N}^{pq}$ allows the calculation of the six different effective coefficients $\hat{C}_{ijpq}$.

3.1 Solving the local problems. FEM combined with a DDM

The local problems (12)-(16) over the periodic cell $\Omega_\#$, have analytic solutions only in exceptional cases. The solution of such problems are usually sought by numerical methods. One of the most used is the FEM, Babuška (1970). However, the linear spring type interface conditions (13)-(16) can not be easily imposed in standard finite element analysis software implementations because these lacks appropriate jump operators on interfaces.

Interface conditions (14)-(16) are not stated in the directions useful for the variational formulation of the problem needed by FEM. We will analyze how to state these in convenient form only on ∂F_1 since on ∂F_2 the procedure is the same changing only the spring type constants.

Let us denote

$$\mathbf{T}_{\{n,t,a\}}^{(M)} = \left(T_n^{(M)}, T_t^{(M)}, T_a^{(M)}\right)^\top,$$
$$\mathbf{N}_{\{n,t,a\}}^{pq} = (N_n^{pq}, N_t^{pq}, N_a^{pq})^\top.$$

Written in matrix form, conditions (14)-(16) on ∂F_1 are

$$\mathbf{T}^{(M)}_{\{n,t,a\}} = -\mathcal{K}[\![\mathbf{N}^{pq}_{\{n,t,a\}}]\!]_{\partial F_1}$$

but

$$\mathbf{T}^{(M)}_{\{n,t,a\}} = \mathcal{N}\mathbf{T}^{(M)},\ \mathbf{N}^{pq}_{\{n,t,a\}} = \mathcal{N}^{(1)}[\![\mathbf{N}^{pq}]\!]_{\partial F_1},$$

where

$$\mathcal{K}^{(1)} = \left(\begin{array}{ccc} k_n^{(1)} & 0 & 0 \\ 0 & k_t^{(1)} & 0 \\ 0 & 0 & k_a^{(1)} \end{array}\right),\ \mathcal{N}^{(1)} = \left(\begin{array}{ccc} n_1^{(1)} & n_2^{(1)} & 0 \\ -n_2^{(1)} & n_1^{(1)} & 0 \\ 0 & 0 & 1 \end{array}\right).$$

Then

$$\mathbf{T}^{(M)} = \left(\mathcal{N}^{(1)}\right)^{-1}\mathcal{K}^{(1)}\mathcal{N}^{(1)}[\![\mathbf{N}^{pq}]\!]_{\partial F_1}$$

or

$$T_1^{(M)} = -\left(k_{11}^{(1)}[\![N_1^{pq}]\!]_{\partial F_1} + k_{12}^{(1)}[\![N_2^{pq}]\!]_{\partial F_1}\right), \tag{18}$$

$$T_2^{(M)} = -\left(k_{12}^{(1)}[\![N_1^{pq}]\!]_{\partial F_1} + k_{22}^{(1)}[\![N_2^{pq}]\!]_{\partial F_1}\right), \tag{19}$$

$$T_3^{(M)} = -k_a^{(1)}[\![N_3^{pq}]\!]_{\partial F_1}, \tag{20}$$

where

$$k_{11}^{(1)} = k_n\left(n_1^{(1)}\right)^2 + k_t\left(n_2^{(1)}\right)^2,$$

$$k_{12}^{(1)} = n_1^{(1)}n_2^{(1)}\left(k_n - k_t\right),$$

$$k_{22}^{(1)} = k_t\left(n_1^{(1)}\right)^2 + k_n\left(n_2^{(1)}\right)^2.$$

In (18)-(19) we see that $T_1^{(M)}$ and $T_2^{(M)}$ linearly depend on $[\![N_1^{pq}]\!]$ and $[\![N_2^{pq}]\!]$. Taking into account equations (13) and (18)-(20) we can replace the interface conditions (13) of the local problems on ∂F_1 with

$$T_1^{(1)} = -\left(k_{11}^{(1)}[\![N_1^{pq}]\!]_{\partial F_1} + k_{12}^{(1)}[\![N_2^{pq}]\!]_{\partial F_1}\right), \tag{21}$$

$$T_2^{(1)} = -\left(k_{12}^{(1)}[\![N_1^{pq}]\!]_{\partial F_1} + k_{22}^{(1)}[\![N_2^{pq}]\!]_{\partial F_1}\right), \tag{22}$$

$$T_3^{(1)} = -k_a^{(1)}[\![N_3^{pq}]\!]_{\partial F_1}. \tag{23}$$

Having the interface conditions in a form more straightforward for FEM we consider the use of domain decomposition methods to solve the local problems with interface conditions (18)-(23). The idea for DDM arises from the fact that $\sigma_i^{(\#)}$ in (12) can be decompose in

$$\sigma_i^{(\#)} = \begin{cases} \mathcal{K}_{i1}^{(M)}\nabla N_1^{pq} + \mathcal{K}_{i2}^{(M)}\nabla N_2^{pq} + \mathcal{K}_{i3}^{(M)}\nabla N_3^{pq} + \mathbf{k}_i^{(M)pq}, & \mathbf{y} \in \Omega_M \\ \mathcal{K}_{i1}^{(1)}\nabla N_1^{pq} + \mathcal{K}_{i2}^{(1)}\nabla N_2^{pq} + \mathcal{K}_{i3}^{(1)}\nabla N_3^{pq} + \mathbf{k}_i^{(1)pq}, & \mathbf{y} \in F_1 \\ \mathcal{K}_{i1}^{(2)}\nabla N_1^{pq} + \mathcal{K}_{i2}^{(2)}\nabla N_2^{pq} + \mathcal{K}_{i3}^{(2)}\nabla N_3^{pq} + \mathbf{k}_i^{(2)pq}, & \mathbf{y} \in F_2 \end{cases}. \tag{24}$$

with, considering (1), constant matrices $\mathcal{K}_{ij}^{(h)}$, $h = M, 1, 2$. This means that we can separate the equations (12) in equations with constant coefficients over the matrix and fiber domains.

3.2 *Domain decomposition method for the local problems*

To address the imperfect contact condition at the interface, in this work, a variant of a domain decomposition method, Dolean et al. (2015), Mathew (2008), is applied. The basic idea of this method consists in decompose a region in subdomains, which allow to approximate the solution independently in each subdomain. This way, the solution over the whole region can be calculated by iterative substructuring as in Jelassi et al. (2013), or as in our work, linking the subdomains by means of interface conditions Lions (1990).

Considering (24) we decompose

$$\mathbf{N}^{pq}(\mathbf{y}) = \begin{cases} \mathbf{N}^{pq}_{(M)}(\mathbf{y}), & \mathbf{y} \in \Omega_M \\ \mathbf{N}^{pq}_{(1)}(\mathbf{y}), & \mathbf{y} \in F_1 \\ \mathbf{N}^{pq}_{(2)}(\mathbf{y}), & \mathbf{y} \in F_2 \end{cases}$$

and, for $h = M, 1, 2$, denote

$$\sigma_i^{(h)} = \mathcal{K}_{i1}^{(h)} \nabla N_{1(h)}^{pq} + \mathcal{K}_{i2}^{(h)} \nabla N_{2(h)}^{pq} + \mathcal{K}_{i3}^{(h)} \nabla N_{3(h)}^{pq} + \mathbf{k}_i^{(h)pq}.$$

We can then rewrite the local problems as

Problem 3 *Find $\mathbf{N}^{pq}_{(M)}(\mathbf{y})$, $\mathbf{N}^{pq}_{(1)}(\mathbf{y})$ and $\mathbf{N}^{pq}_{(2)}(\mathbf{y})$ such that $\mathbf{N}^{pq}_{(M)}(\mathbf{y})$ Ω_M-periodic,*

$$\begin{aligned} \nabla \cdot \sigma_i^{(M)} &= 0, \ \textit{in}\ \Omega_M, \\ \nabla \cdot \sigma_i^{(1)} &= 0, \ \textit{in}\ F_1, \\ \nabla \cdot \sigma_i^{(2)} &= 0, \ \textit{in}\ F_2, \end{aligned}$$

interface conditions (18)-(23) are enforced in ∂F_1, ∂F_2 and uniqueness conditions

$$\left\langle \mathbf{N}^{pq}_{(M)}(\mathbf{y}) \right\rangle_{\Omega_M} = \left\langle \mathbf{N}^{pq}_{(1)}(\mathbf{y}) \right\rangle_{F_1} = \left\langle \mathbf{N}^{pq}_{(2)}(\mathbf{y}) \right\rangle_{F_2} = 0 \tag{25}$$

hold.

Observe that in problem 3 the system of partial differential equations are separated in domains but coupled through the interface conditions. If the solution in Ω_M is known we can compute with FEM the solutions in F_1 and F_2. Conversely, knowing the solutions in F_1 and F_2 allows the computation of the solution in Ω_M. This provides the idea for the following simple DDM iterative scheme. Given guessed initial values $\mathbf{N}^{pq}_{0(1)}$ of the solution in F_1, $\mathbf{N}^{pq}_{0(2)}$ of the solution in F_2 and an error tolerance $\epsilon \ll 1$ then, for $n \geq 0$

1. With $\mathbf{N}^{pq}_{n(1)}$ and $\mathbf{N}^{pq}_{n(2)}$ compute the solution $\mathbf{N}^{pq}_{n(M)}$ in Ω_M,
2. With $\mathbf{N}^{pq}_{n(M)}$ compute solutions $\mathbf{N}^{pq}_{n+1(1)}$ and $\mathbf{N}^{pq}_{n+1(2)}$,
3. If $\max\left\{ \left\| \mathbf{N}^{pq}_{n+1(1)} - \mathbf{N}^{pq}_{n(1)} \right\|, \left\| \mathbf{N}^{pq}_{n+1(2)} - \mathbf{N}^{pq}_{n(2)} \right\| \right\} < \epsilon$ stop with the solution

$$\left\{ \mathbf{N}^{pq}_{n(M)}, \mathbf{N}^{pq}_{n+1(1)}, \mathbf{N}^{pq}_{n+1(2)} \right\}$$

, else set $n = n + 1$ and go back to step 1.

Table 1: Comparison of the results of Otero et al. (2013) (O2013) with our approach (A-D-F) for a porous material formed by circular holes in a isotropic matrix. The periodic cell is unit a square and the area fractions of the circular holes are $0.05, 0.2, 0.35, 0.55, 0.75$.

	$\widehat{c}_{11}$ (O2013)	$\widehat{c}_{11}$ A-D-F	$\widehat{c}_{12}$ (O2013)	$\widehat{c}_{12}$ A-D-F
0.05	8.052537E+01	8.057222E+01	3.314981E+01	3.315992E+01
0.2	5.339001E+01	5.341426E+01	1.836599E+01	1.837110E+01
0.35	3.653604E+01	3.654994E+01	9.781059E+00	9.783213E+00
0.55	2.049858E+01	2.050756E+01	3.378678E+00	3.378741E+00
0.75	5.849942E+00	5.859657E+00	2.891222E-01	2.881649E-01
	$\widehat{c}_{13}$ (O2013)	$\widehat{c}_{13}$ A-D-F	$\widehat{c}_{33}$ (O2013)	$\widehat{c}_{33}$ A-D-F
0.05	3.410255E+01	3.411964E+01	8.696153E+01	8.697176E+01
0.2	2.152680E+01	2.153561E+01	6.891608E+01	6.892136E+01
0.35	1.389513E+01	1.389994E+01	5.383708E+01	5.383998E+01
0.55	7.163179E+00	7.165901E+00	3.579791E+01	3.579955E+01
0.75	1.841719E+00	1.844342E+00	1.860503E+01	1.860658E+01
	$\widehat{c}_{44}$ (O2013)	$\widehat{c}_{44}$ A-D-F	$\widehat{c}_{66}$ (O2013)	$\widehat{c}_{66}$ A-D-F
0.05	2.435897E+01	2.436334E+01	2.320944E+01	2.323223E+01
0.2	1.794506E+01	1.794812E+01	1.342208E+01	1.344047E+01
0.35	1.291530E+01	1.291738E+01	6.616327E+00	6.629126E+00
0.55	7.459089E+00	7.460579E+00	1.808771E+00	1.816486E+00
0.75	2.111431E+00	2.113931E+00	7.890091E-02	8.675641E-02

The iterative schema given above is trouble-free to realize with FEM software with the capabilities of FreeFEM++. The variational formulation of the problems to solve in steps one and two is easy to obtain. Details about the norms used in step three depends of the FEM spaces used in the numerical implementation. In the next section we present some numerical results obtained with our approach.

4 NUMERICAL RESULTS AND DISCUSSION

The strength of the combination of methods exposed above will be illustrated with some examples. To prove the accuracy we first compare with the also semi-analytical approach, presented in Otero et al. (2013), where a unit square periodic cell with a circular hole is considered. The constitutive material of the matrix is isotropic and given by a Young's modulus of 70GPa and a Poisson's ratio of 0.3. In Otero et al. (2013) (see table 2 in it) results for porous material are given and compared with analytical results. In Table 1 we compare our results with the, semi-analytical solutions calculated in Otero et al. (2013), for several area fractions

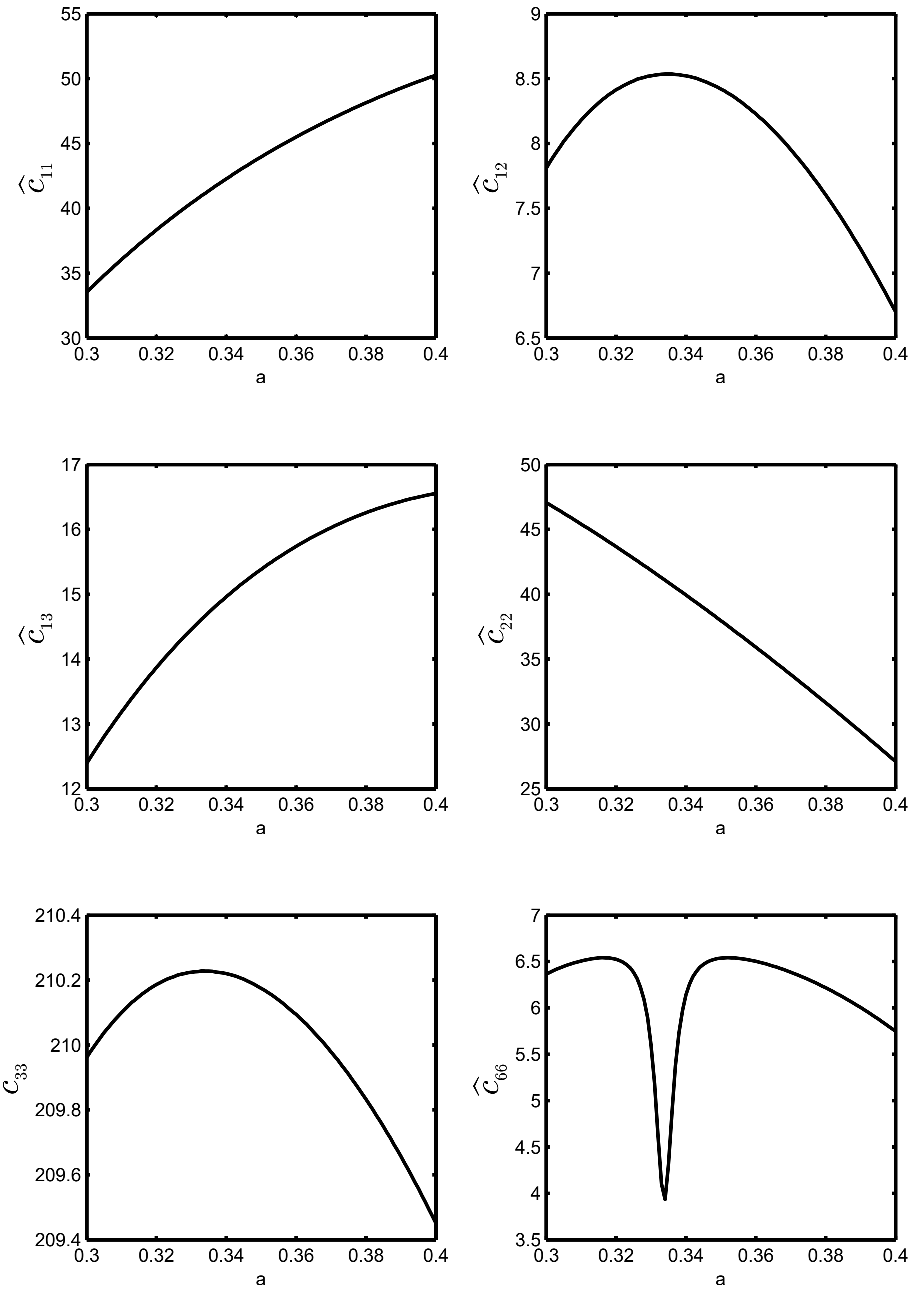

Figure 1: Effect of the aspect ratio of an elliptical fiber in a square periodic cell. The area fraction of the ellipse remains 0.35 and the semimajor axis a varies 0.3 and 0.4.

of the circular hole. In the table the results of Otero et al. (2013) are identified with O2013 and ours with A-D-F to save space. In this case the linear spring type interface constants are

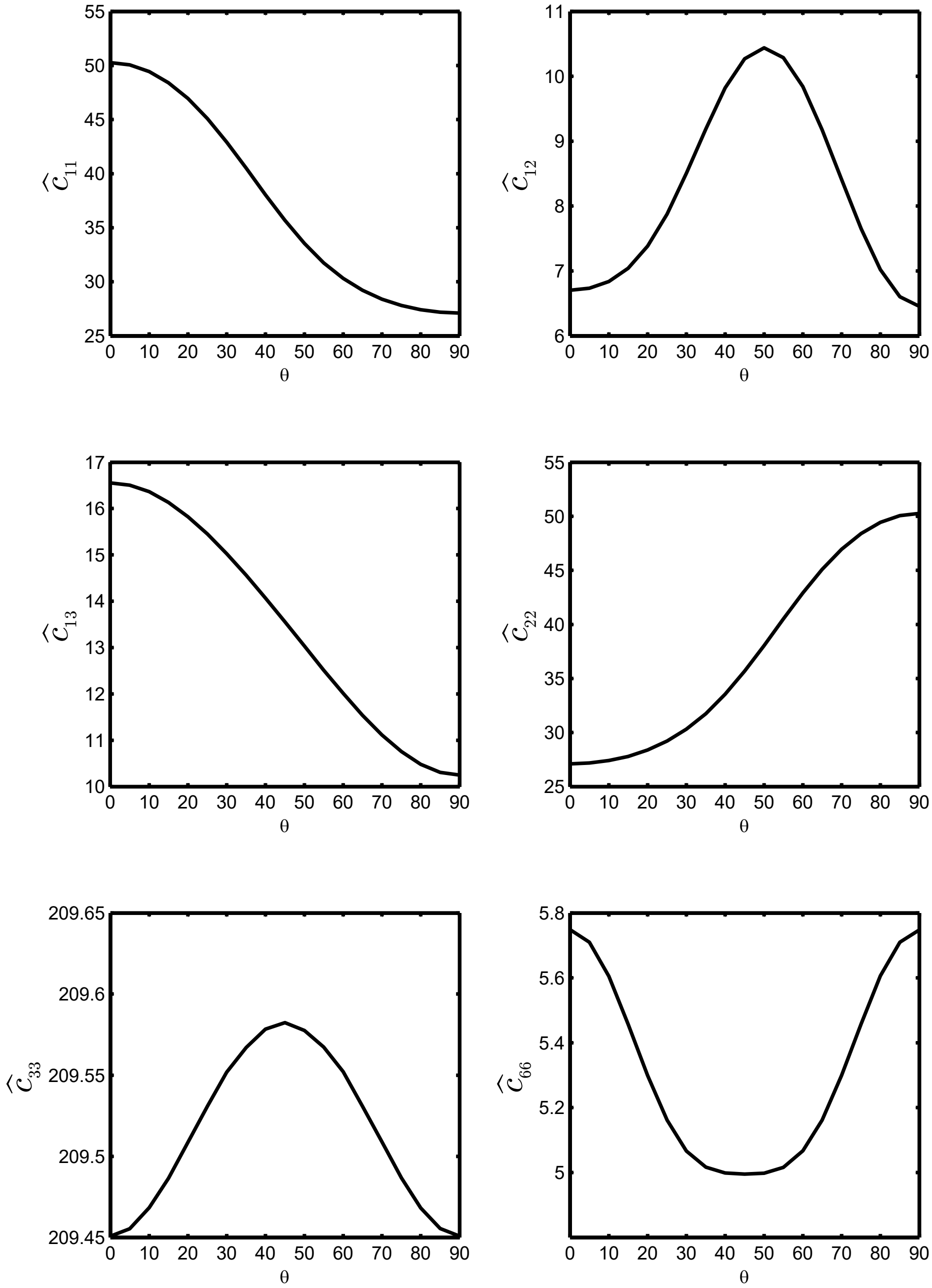

Figure 2: Influence of the angle of rotation of an elliptical fiber in unit square for the effective behavior of the composite. The elliptical fiber has a semimajor axis $a = 0.4$, an area fraction of 0.35 and a rotation angle θ varying from 0° to 90° degrees.

$k_n = k_t = k_a = 0$. The effective coefficients are presented in Voigt notation. The chosen error tolerance in step three of the iterative scheme is $\epsilon = 1 \times 10^{-10}$ and the norm used is $\left\| \mathbf{N}^{pq}_{n+1(1)} - \mathbf{N}^{pq}_{n(1)} \right\|_{L_2(F_1)}$. We observe a good agreement of our AHM-DDM-FEM (denoted by DDFEM) approach with the one in Otero et al. (2013).

To show the capabilities of our method we developed the a numerical experiment consisting in study the effect of the aspect ratio of an elliptical fiber in a square periodic cell. The matrix elastic properties as the same as before, the isotropic fiber has a Young's modulus of 450GPa and a Poisson's ratio of 0.17. We took the area fraction of the ellipse to be constantly 0.35 and change the aspect ratio by varying the semimajor axis a between 0.3 and 0.4. For this experiment we take the linear spring type interface constants $k_n = 10$, $k_t = k_a = 0.01$. The effective properties obtained by AHM-DDM-FEM are shown in Fig. 1 for efective coefficients $\hat{c}_{11}$, $\hat{c}_{12}$, $\hat{c}_{13}$, $\hat{c}_{33}$, $\hat{c}_{44}$ and $\hat{c}_{66}$.

Another experiment carried out, again for an elliptical inclusion in a square unit cell, consists of the study of the influence of the angle of rotation of the ellipse in the effective behavior of the composite. The matrix and fiber have same elastic properties as before. The elliptical fiber has a semimajor axis $a = 0.4$ and an area fraction of 0.35. We let the ellipse rotate from $0°$ to $90°$ and impose imperfect interface contact conditions with $k_n = k_t = k_a = 0.001$. The results are shown in Fig. 2 for the same efective coefficients and same tolerance as in Fig. 1.

To demonstrate the efficacy of the proposed procedure we show a last computational experiment with a composite whose cross-section is illustrated in Fig. 3.

Among the different possibilities for the choice of the periodic cell, the one illustrated with continuous line there, allows to have the fibers completely contained within the matrix. This reduce the number of domains used in the DDM scheme and therefore the computational complexity. Note that the other two periodic cells marked with discontinuous lines have at least seven different domains. The choosen one, with the form of a plus sign, only consists of three domains. In FreeFEM++ is easy to implement and meshing complex shapes and also to impose appropriate periodicity conditions.

For this two-fibers computational experiment we take the elastic tensor $C^{(M)}$ (in Voigt notation) of the matrix to be formed by $c_{11}^{(M)} = 8.65$, $c_{12}^{(M)} = 4.75$ and $c_{44}^{(M)} = 1.95$ corresponding to isotropic epoxy resin LY558. The elasticity tensors $C^{(1)}$ and $C^{(2)}$ for the fibers are formed by $c_{11}^{(1)} = 12.10$, $c_{12}^{(1)} = 6.49$, $c_{13}^{(1)} = 6.50$, $c_{33}^{(1)} = 410.00$, $c_{44}^{(1)} = 13.70$, $c_{66}^{(1)} = 2.80$ and $c_{11}^{(1)} = 20.40$, $c_{12}^{(1)} = 9.40$, $c_{13}^{(1)} = 10.50$, $c_{33}^{(1)} = 240.00$, $c_{44}^{(1)} = 24.00$, $c_{66}^{(1)} = 5.50$ corresponding to transversely isotropic Morganite "Modmor" type I and type II fibers respectively. The effective elastic tensor, obtained through our AHM-DDM-FEM schema for $k_n^{(1)} = k_t^{(1)} = k_s^{(1)} = 1.0 \times 10^0$,

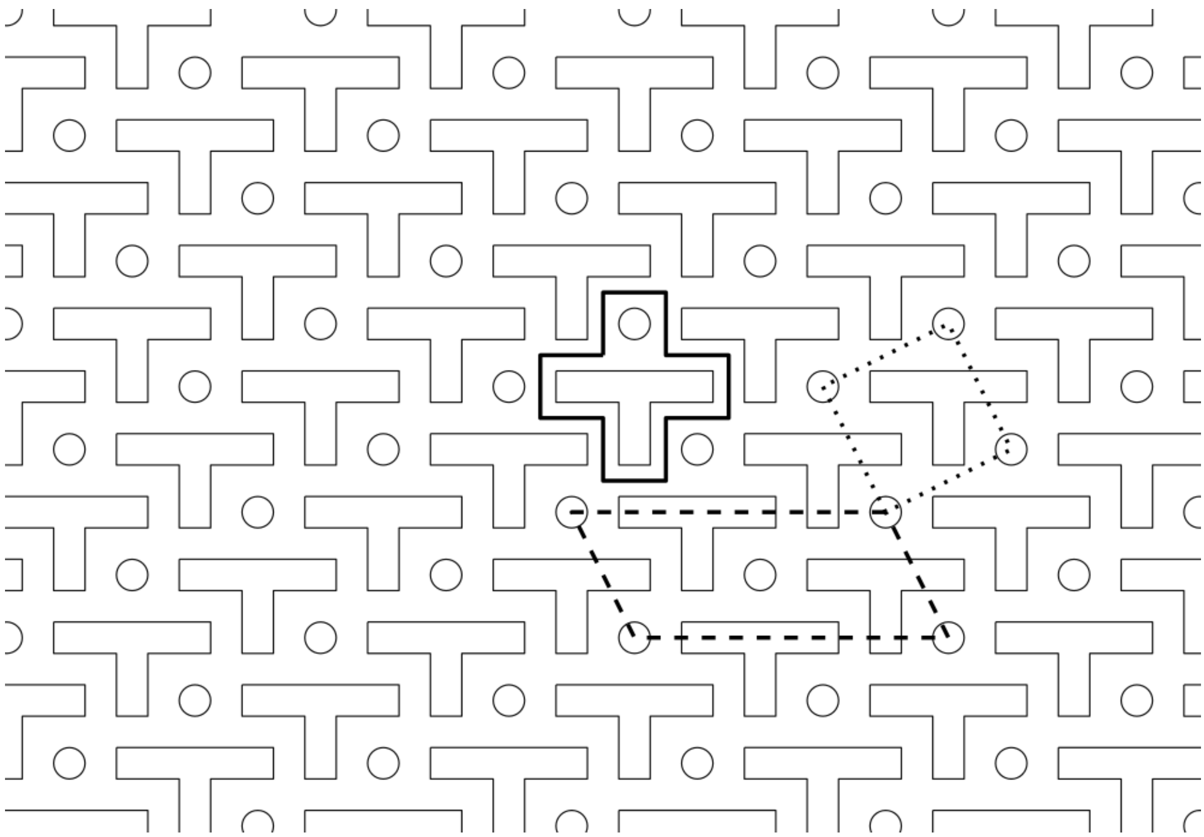

Figure 3: Periodic arrangement of two fibers in a imaginary composite. Different possible periodic cells are marked with different line types. The cell marked with continuous line is the one with the smaller number of subdomains for a DDM schema.

$k_n^{(2)} = k_t^{(2)} = k_s^{(2)} = 1.0 \times 10^{-3}$, is

$$\hat{C} = \begin{pmatrix} 6.34 & 2.98 & 3.29 & 0 & 0 & 0 \\ 2.98 & 5.90 & 3.14 & 0 & 0 & 0.02 \\ 3.29 & 3.14 & 102.83 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.73 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.88 & 0 \\ 0 & 0.02 & 0 & 0 & 0 & 1.61 \end{pmatrix}.$$

Figure 4 shows the solutions of the cell problems corresponding to the composite described above for $pq \in \{11, 22, 33, 23, 13, 12\}$. In each row we show N_1^{pq}, N_2^{pq} and N_3^{pq}. We can observe the rigth periodic behavior on the boundary of the plus sign shaped cell and the effect of the imperfec contact in the two fibers. For this experiment $\epsilon = 1 \times 10^{-10}$ and we iterate in each problem until $\max\left\{\left\|\mathbf{N}^{pq}_{n+1(1)} - \mathbf{N}^{pq}_{n(1)}\right\|_{L_2(F_1)}, \left\|\mathbf{N}^{pq}_{n+1(2)} - \mathbf{N}^{pq}_{n(2)}\right\|_{L_2(F_1)}\right\} \leq \epsilon$.

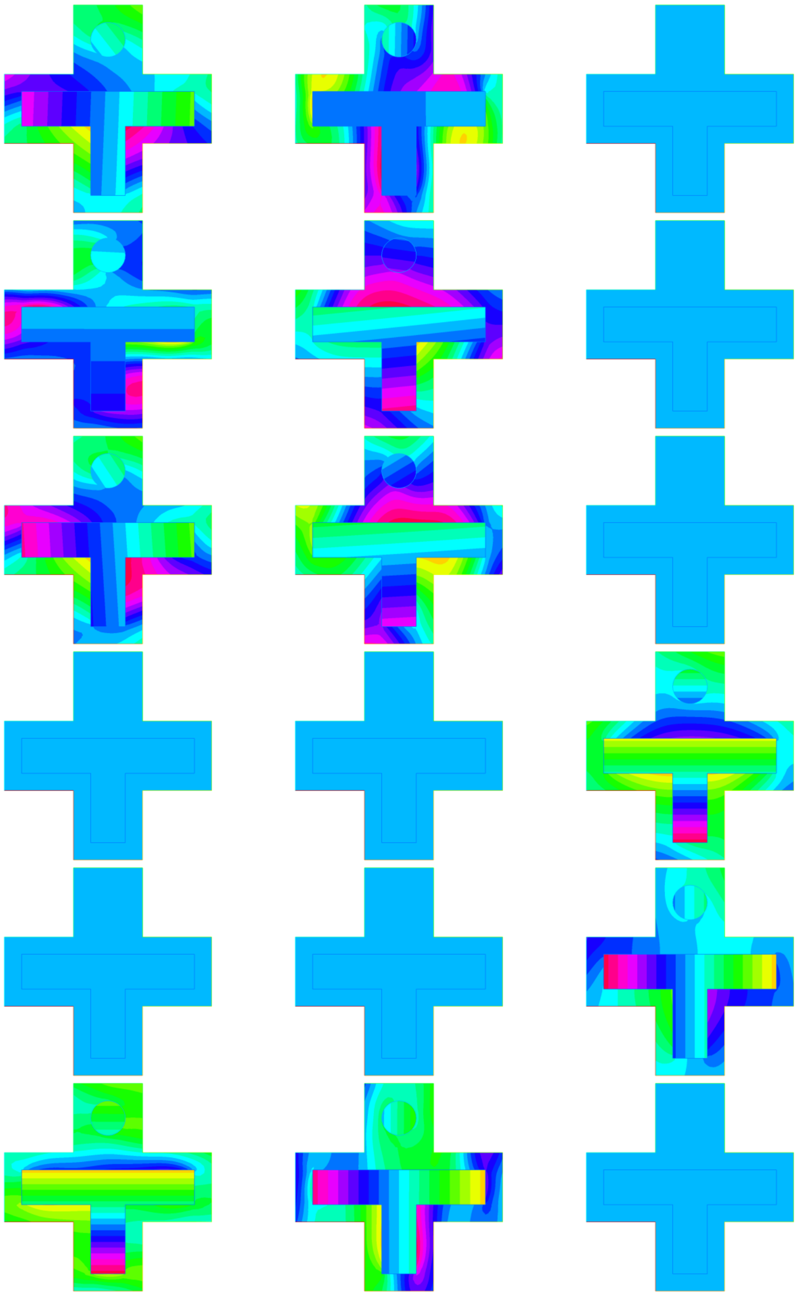

Figure 4: Solutions of the cell problems N_1^{pq}, N_2^{pq} and N_3^{pq} for the composite with periodic cell shown in Figure 3. From top to bottom $pq \in \{11, 22, 33, 23, 13, 12\}$.

5 CONCLUSIONS

The present work presents a method for the calculation of effective properties of composite materials with periodic structure in the presence of imperfect interfaces. The difference with other similar works as Otero et al. (2013) is that our method allows arbitrary shaped periodic cells as well as completely anisotropic constituent materials. These capabilities are achieved using the DDM technique in a novel way that allows the use of FEM software implementations without complications. We chose FreeFEM ++ because of its good 2D meshing capabilities and the way of assemble stiffness matrices directly from the variational formulation of the problem.

The results presented in the previous section validate the quality of the proposed method. They were achieved on a Notebook Dell Vostro 3560 (Intel Core i7-3632QM @ 2.20GHz, 6 GB RAM, 64-bits OS). The number of iterations of the DDM iterative scheme for the examples presented varied between 4 and 56 for all the pq problems. For $k_n, k_t, k_a \ll 1$ the number of iterations were always less than 10. We used moderate mesh sizes in all the experiments. For the last example the mesh size was 0.02 resulting in a mesh with 3998 triangles and 2302 vertices.

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