

A straightforward methodology to predict composite mechanical properties using asymptotic homogenization technique combined to a simple method to determine fiber distribution arrangement

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Abstract. The present work aims to present a methodology that applies the asymptotic homogenization technique, which lies on a rigorous mathematical foundation, combined to a simple method of real fiber arrangement identification in order to predict the elastic mechanical properties of unidirectional carbon fiber reinforced composites. The asymptotic homogenization, is implemented with support of the commercial finite element software ABAQUS[®]. The fiber arrangement is obtained directly from micrographs of a polished cross-section sample. A simple algorithm to identify fibers and matrix from micrographs is implemented using commercial software MATLAB[™]. The numerical prediction is then compared to the experimental results providing good agreements.

Keywords: homogenization techniques, fiber distribution, finite element modeling, composite materials

INTRODUCTION

Lightweight structures are largely applied in several areas and its use is growing every day. In this context conventional materials have been replaced by composite materials increasing the performance of the final structure. In the composite materials area there exist many fields of study among which the multi-scale modeling are very suitable to understand the material behavior, mostly when it is very difficult to be obtained experimentally. This modeling is generally applied considering a sub-volume of a whole reducing the simulation time with good results. The multi-scale modeling can be implemented using different types of domain discretization. The homogenization technique based on Representative Volume Elements (RVE) is often used viewing that it can be easily implemented in a commercial software of finite element analysis which contributes to model complex micro-structures.

The use of RVE techniques to predict the mechanical properties of composite materials have been proposed over the years. Recent works (Zeman and Šejnoha, 2007; Yang et al., 2013; Catalanotti, 2016; Wu et al., 2018) have presented methodologies to create random fiber distributions that can statistically represent the real fiber arrangement. Yang et al. (2013) compared the predicted mechanical properties with experimental results which showed reasonable agreement. These approaches are very interesting from the point of view of more realistic representations. However, they assume that the micro-structure of a composite material is completely random regardless other factors, e.g. the manufacturing process which can affect the fiber spatial distribution (Vaughan and McCarthy, 2010).

Vaughan and McCarthy (2010) applied statistical tools over cross-section images of high volume fraction composite samples to generate an equivalent fiber distribution which takes into account the manufacturing process effects over the micro-structure. Qi et al. (2018) investigated the effects of irregular pores on transverse mechanical properties of composite materials combining cross-section images and RVE techniques. Both works compared the predicted mechanical properties with experimental results which showed good agreement.

The previous mentioned works provided proper methodologies to predict the mechanical properties of composite materials. However they are based on the RVE techniques which does not lie on rigorous mathematical theory since it depends on the average stress. Moreover the techniques applied to generate the fiber distribution for both complete randomly arrangement and cross-section sample images can be sometimes complicated to be implemented.

Motivation and Objectives

In view of the mathematical assumptions of RVE techniques and the recent methods proposed to generate fiber distributions in a unit cell, the present work aims to present a straightforward methodology to predict the mechanical properties

of composite materials using a more robust homogenization technique, namely asymptotic homogenization, combined to a simple method to generate fiber distribution based on cross-section images. The asymptotic homogenization presents rigorous mathematical theory but its implementation can be arduous when complex micro-structures are considered. In this context, a different strategy of implementation is applied in order to simplify it. Moreover, a simple algorithm to determine the fiber distribution based on color threshold of cross-section sample micrographs is proposed. In order to confirm its robustness, the algorithm is applied to determine the fiber positioning of a carbon fiber reinforced epoxy composite material.

ASYMPTOTIC HOMOGENIZATION TECHNIQUE

The asymptotic homogenization technique can be applied to predict the elastic mechanical properties of a composite material which unit cell arrangement is assumed to be periodic. The detailed mathematical formulation can be found in the works of Guedes and Kikuchi (1990) and Hassani and Hinton (1998). According to Guedes and Kikuchi (1990), the homogenized properties E_{ijkl}^H are given by:

$$E_{ijkl}^H = \frac{1}{|Y|} \int_Y \left(E_{ijkl} - E_{ijmn} \frac{\partial \chi_m^{kl}(y)}{\partial y_n} \right) dY, \quad (1)$$

where Y corresponds to the unit cell volume, y_n denotes the set of coordinates used to define the problem at the micro-scale level, E_{ijkl} is the material constitutive tensor and $\chi_m^{kl}(y)$ are the auxiliary displacement fields defined at the domain of the unit cell.

The auxiliary displacement fields $\chi_m^{kl}(y)$ can be obtained solving the micro level problem:

$$\int_Y E_{ijmn} \frac{\partial \chi_m^{kl}}{\partial y_n} \frac{\partial \delta u_i}{\partial y_i} dY = \int_Y E_{ijkl} \frac{\partial \delta u_i}{\partial y_i} dY. \quad (2)$$

The solution of the problem in the micro-level for the $\chi_m^{kl}(y)$ can be obtained by the finite element method, discretizing the domain of the unit cell. Nevertheless, if the unit cell presents a complicated micro-structure, more work can be demanded on its implementation. In this context Cheng, Cai and Xu (2013) presented a simple implementation using a finite element commercial software to discretize the unit cell. At first, the Eq. (1) is rewritten in the bi-linear form and assuming unitary pre-strains, it can be defined in function of strains as (Sigmund, 1994):

$$E_{ijkl}^H = \frac{1}{|Y|} \int_Y E_{pqrs} \left(\epsilon_{pq}^{0(kl)} - \epsilon_{pq}^{*(kl)} \right) \left(\epsilon_{rs}^{0(ij)} - \epsilon_{rs}^{*(ij)} \right) dY, \quad (3)$$

which rewritten in the matrix form gives:

$$[E^H] = \frac{1}{|Y|} \int_Y \left(\{\epsilon^0\} - \{\epsilon^*\} \right)^T [E] \left(\{\epsilon^0\} - \{\epsilon^*\} \right) dY. \quad (4)$$

Equation (4) can still be described in terms of characteristic displacements, where $\{\epsilon\} = [B]\{\chi\}$, as:

$$[E^H] = \frac{1}{|Y|} \int_Y \left(\{\chi^0\} - \{\chi^*\} \right)^T [B]^T [E] [B] \left(\{\chi^0\} - \{\chi^*\} \right) dY. \quad (5)$$

It is known from the finite element formulation that the stiffness matrix is defined by:

$$[K] = \frac{1}{|Y|} \int_Y [B]^T [E] [B] dY, \quad (6)$$

and the reaction force vector is:

$$\{f\} = [K] \{\chi\}. \quad (7)$$

The homogenized mechanical properties in Eq. (1) are then written in terms of nodal displacements and nodal forces as:

$$E_{ijkl}^H = \frac{1}{|Y|} \left(\chi^{0(ij)} - \chi^{*(ij)} \right)^T \left(f^{0(kl)} - f^{*(kl)} \right) dY, \quad (8)$$

where $\chi^{0(ij)}$ are the prescribed nodal displacements which results in unit strains, $f^{0(kl)}$ are the nodal forces obtained after prescribing $\chi^{0(ij)}$, $\chi^{*(ij)}$ are the nodal displacements obtained after prescribing $f^{0(kl)}$ and $f^{*(kl)}$ are the nodal forces after prescribing $\chi^{*(ij)}$. More details of the development of this novel implementation can be found in Cheng, Cai and Xu (2013). In the present work this technique is implemented on ABAQUS® software using Python subroutines according to the workflow presented in Fig. 1. Among the advantages of implementing the asymptotic homogenization technique in a commercial finite element software, it can be mentioned:

- Rigorous mathematical theory is preserved;
- Different types of elements are available to discretize the periodic unit cell;
- Flexibility to model unit cells with specific fiber arrangement.

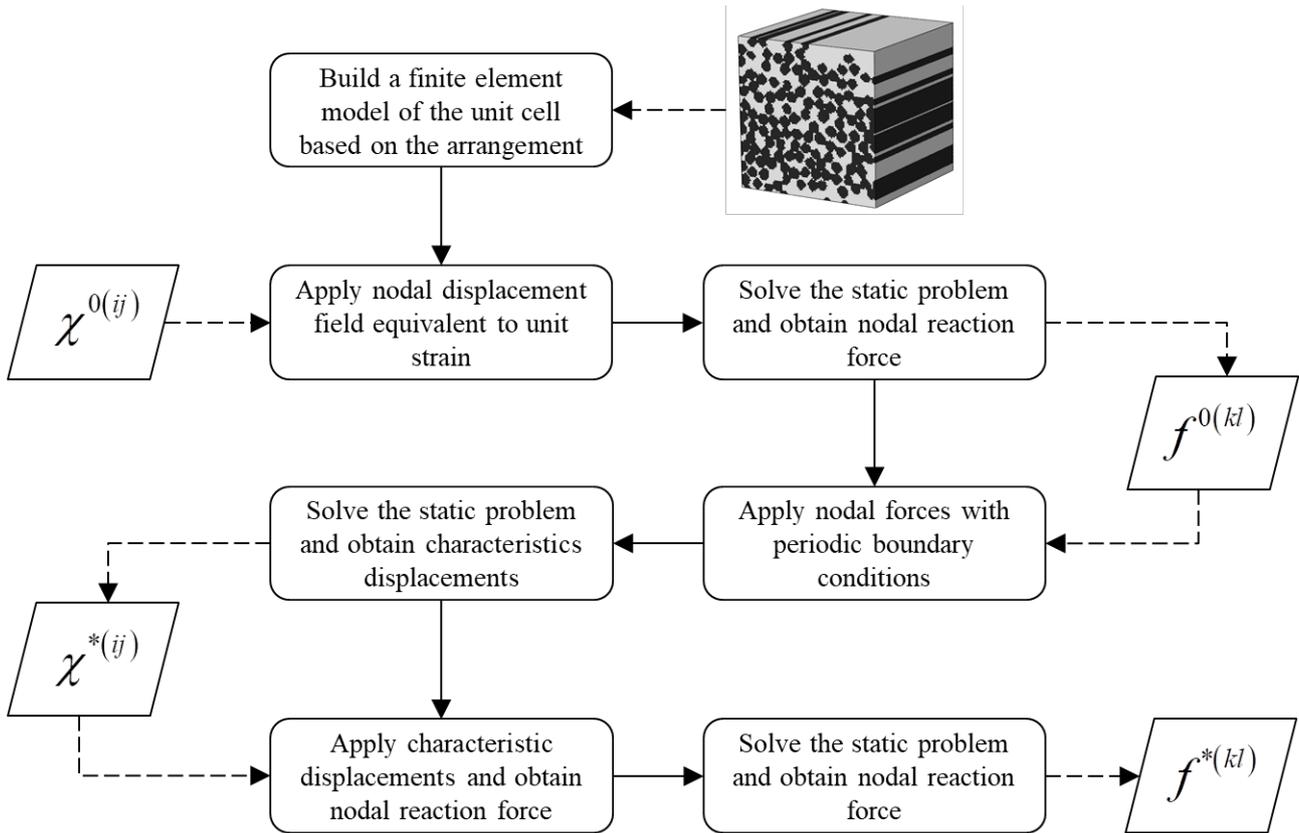


Figure 1 – Workflow of asymptotic homogenization implementation in a commercial finite element software.

The asymptotically homogenized properties of a 3D unit cell are obtained by applying the steps on the workflow presented in Fig. 1 at six different load cases (each one for solving one column of matrix $[E^H]$). The boundary conditions of the steps where the static problem is solved to obtain the nodal reaction forces, are already given by the applied nodal displacements.

Regarding to the step where the static problem is solved to obtain the characteristic displacements, i.e. nodal forces are applied to the nodes, it is worth noting that the required periodic boundary conditions are not straightly available on

ABAQUS[®] as can be seen in ABAQUS (2014). Nevertheless, it is possible to apply periodic boundary conditions through linear constraints on ABAQUS[®] using equations to define the relative motion between the degrees of freedom of two or more nodes. Thus, a general linear homogeneous equation is defined on ABAQUS[®] as:

$$\sum_{i=1}^n A_i^k u_i^k = 0, \quad (9)$$

where i is the degree of freedom, k refers to the node and A is a constant coefficient which defines the relative motion of nodes.

In an attempt to clarify the implementation of periodic boundary conditions on ABAQUS[®], it is considered the Fig. 2 which illustrates an example of a 3D unit cell with periodic faces where nodes A and B have the same coordinate in the plane 2 – 3.

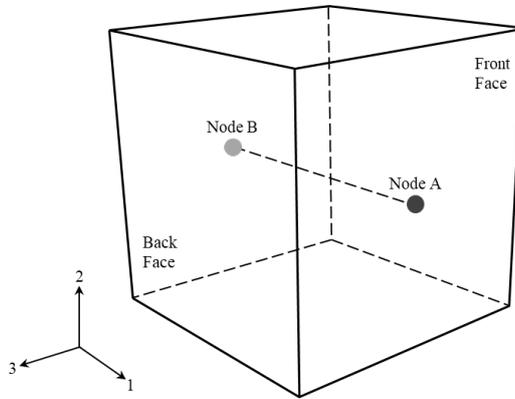


Figure 2 – Example of an unit cell with periodic boundary conditions applied to the face nodes.

Viewing that nodes A and B shall have the same displacements in all directions, the equations defining the relative motion between their degrees of freedom can be written as:

$$\begin{aligned} u_1^A - u_1^B &= 0, \\ u_2^A - u_2^B &= 0, \\ u_3^A - u_3^B &= 0. \end{aligned} \quad (10)$$

Therefore, all the external paired nodes of the unit cell, i.e. all the nodes that are under periodic boundary conditions, need to be identified and their respective constraint equations created. It may perhaps be observed that, in a discretized unit cell with a large number of nodes, it is highly recommended to write a Python script in order to create these equations on ABAQUS[®].

FIBER ARRANGEMENT ALGORITHM

The present work proposes a simple algorithm to identify the material constituents, i.e. matrix and fiber, from micrographs of composite materials cross-section. It is important to remark that the performance of the algorithm is directly linked to the image quality. If the image presents marks or blurred portions, the identification of fibers can be compromised. Besides, if the constituents have pixels with close values in a gray scale, the threshold shall be finely adjusted.

Thus, in the first step the cross-section micrograph is read and a selected region is cropped. Then, a threshold value in gray scale, which is applied to identify the fibers in the image, and the fiber diameter in pixels are also computed. For each computed fiber, it is also necessary to determine the pixels in the neighborhood which have the geometrical position inside the pre-defined fiber diameter. In this case, a simple distance in the midst of two points is calculated in order to determine the neighboring pixels. Lastly, an output file is written containing the geometrical position and the pixels assigned values which corresponds to the material constituents, e.g. 0 for the matrix and 1 for the fibers. This file is used as an input data to

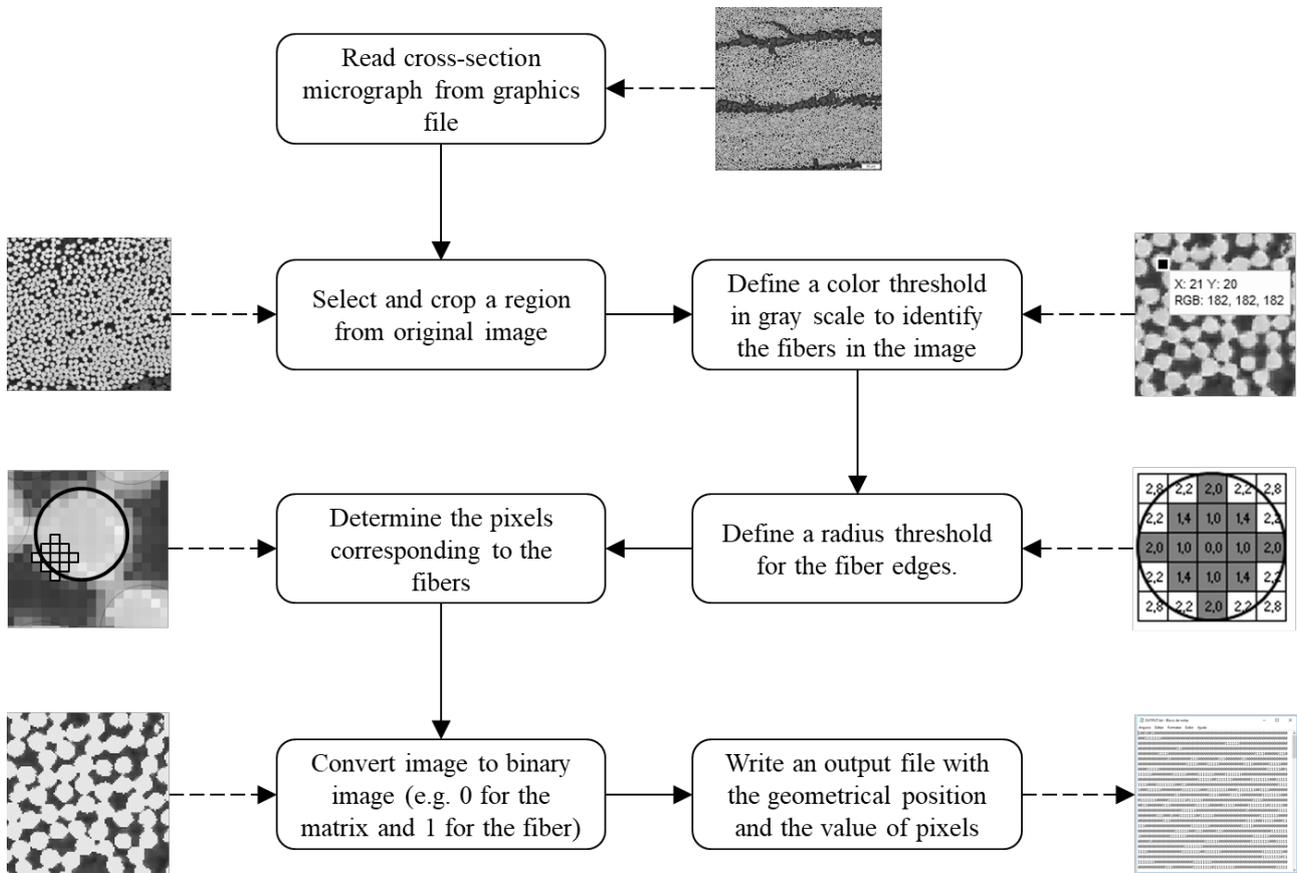


Figure 3 – Proposed algorithm to identify the fiber and matrix from cross-section micrographs.

asymptotic homogenization analysis. The proposed algorithm was implemented using commercial software MATLAB™ and follows the procedure presented in Fig. 3.

It is worth to say that the proposed algorithm does not take into account voids or pores. However, it could be easily implemented defining another color threshold related to the voids/pores. These pixels would have another value assigned corresponding to another constituent. Depending on the region where the micrograph is taken, the fiber volume fraction may change. In cases of very random fiber arrangement, a very large representative region may be necessary requiring a significant computational time. Alternatively, micrographs can be taken from different regions and an statistical study can be performed in order to determine the equivalent fiber arrangement. This alternative proposition is not in the scope of this work but to be explored in future works by the authors.

RESULTS AND DISCUSSION

In order to demonstrate the proposed methodology application, a micrograph of a unidirectional carbon fiber reinforced epoxy was chosen. Figure 4 presents the original micrograph of the sample cross-section. It can be seen in Fig. 4 that there is a good contrast between fiber/matrix besides no void or pores were identified. Figures 5 and 6 present, respectively, the cropped region of the original micrograph cross-section and the computed micro-structure generated by the proposed algorithm. In Fig. 6 the light color regions represent the fibers and dark color represent the matrix. The computed fiber volume fraction, by performing a pixels counting, is $V_f = 0.60$. Figure 7 presents the unit cell with discretized domain of the computed micro-structure. The finite element model was discretized using the eight nodes, reduced integration, C3D8R solid elements available in ABAQUS®. More details about the element formulation can be found in ABAQUS (2014).

Table 1 presents the mechanical properties of the carbon fiber and epoxy matrix used in the finite element model employed in asymptotic homogenization method. The constituents mechanical properties were obtained directly from the manufacturer data sheet.

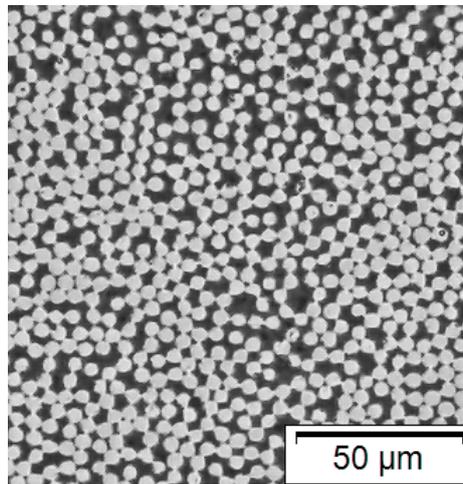


Figure 4 – Original micrograph of the sample cross-section.

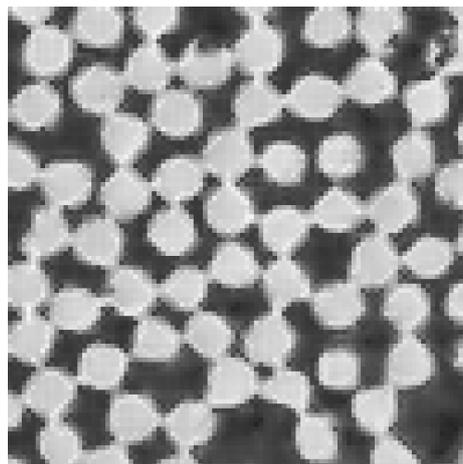


Figure 5 – Cropped region from original micrograph used for computing the micro-structure.

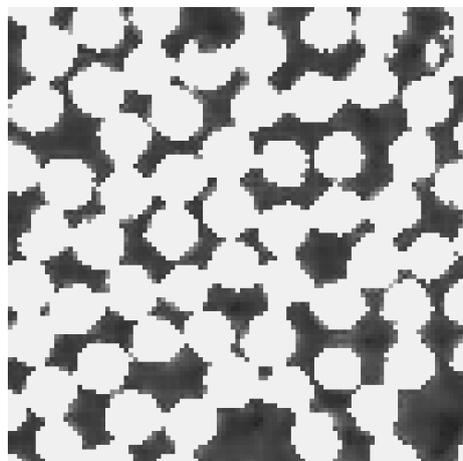


Figure 6 – Computed micro-structure using the proposed algorithm.

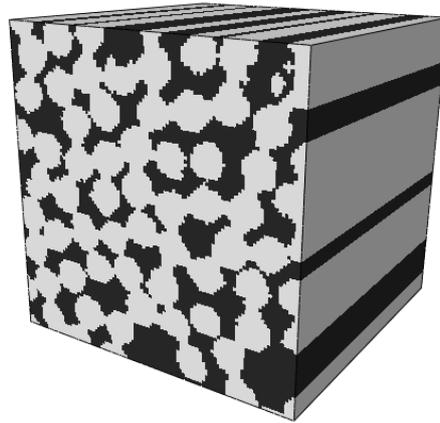


Figure 7 – Unit cell discretized according to computed micro-structure.

Table 1 – Mechanical properties of carbon fiber and epoxy matrix.

Mechanical Properties	Carbon Fiber	Epoxy Matrix
Longitudinal Modulus [GPa]	294	3.5
Transverse Modulus [GPa]	19	3.5
Density [g/cm ³]	1.79	1.28

Table 2 presents a comparison between the predicted mechanical properties and the experimental results range which were obtained from specimens tested in tensile (longitudinal and transverse) and in-plane shear. It must be highlighted that the fiber volume fraction of the specimens and the fiber volume fraction computed in cross-section micrograph are not exactly the same. Taking into account the reinforcement fiber areal weight and the fiber density, as well as the measured cured ply thickness, it was possible to estimate the fiber volume fraction of the tested specimens. In this case, a fiber volume fraction $V_f = 0.584$ was estimated for the tested specimens which differed slightly from that obtained for the computed micro-structure. Despite of the small difference, the predicted longitudinal properties were normalized to a unique fiber volume fraction.

The normalization of mechanical test results to a specified fiber volume fraction is often performed for direct comparison of values. Although the longitudinal properties can be normalized to a specified fiber volume fraction, the same cannot be done for the other properties viewing that it intends to reduce variability in fiber-dominated properties. In this case, it is justified on the basis that most of the load is carried by the fibers.

Table 2 – Comparison of predicted mechanical properties with experimental results.

Mechanical Properties	Prediction	Experimental
Longitudinal Modulus E_1 [GPa]	174.8 ¹	164.7 – 173.4
Transverse Modulus E_2 [GPa]	9.8	6.8 – 9.2
In-plane Shear Modulus G_{12} [GPa]	4.5	3.4 – 5.3

¹ Normalized to 58.4% fiber volume.

The results in Tab. 2 demonstrate that good agreement with the experimental results was achieved using the proposed methodology to predict composite mechanical properties. As already expected, the predicted results are within the superior limit of the properties range which could be plausibly attributed to the imperfections in the tested specimens.

CONCLUSION

A novel methodology applying a robust homogenization technique, i.e. asymptotic homogenization, combined to a simple method to determine the fiber distribution arrangement was presented. The proposed methodology showed to be very interesting from the consistency, implementation and performance points of view. The methodology was applied to predict the mechanical properties of a carbon fiber reinforced epoxy composite which values were compared with experimental results. In this context, the methodology demonstrated to have a great potential of application since it lies on

simple methods combined to mathematical consistency. The application of the proposed methodology for other materials plays an important role on authors' ongoing work.

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