On determination of periodic unit cell for plain weave fabric composites: Geometrical modeling of real world materials

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Abstract

In this contribution, we present the final outcome of the program, initiated in [23], aimed at the determination of a periodic unit cell for plain weave composites with reinforcement imperfections. The emphasis is put on a realistic geometrical description of these material systems utilizing the information provided by in-situ two-dimensional micrographs. Complex geometry of an analyzed composite is approximated using a two-layer periodic unit cell allowing for a mutual shift as well as nesting of individual layers. The parameters of the idealized unit cell are derived via matching appropriate statistical descriptors related to the real material and the idealized geometrical model. Once the optimal geometry of the unit cell is determined, it can be converted to a CAD model and used to generate the periodic finite element mesh applicable in the subsequent numerical treatment. The individual steps of this procedure are demonstrated in detail for a real world carbon-carbon composite system.

Keywords. balanced woven composites, image processing techniques, random microstructure, quantification of microstructure morphology, periodic unit cell, CAD modeling

1 Introduction

A rapid development in image analysis hardware in the last two decades opened a way for a substantial improvement of the modeling of mechanical response of complex material systems such as composites. Often used assumption about well-defined geometrical arrangement of reinforcements in the fiber/matrix composite aggregate fails when inspecting the high-resolution images of cross-sections of such systems on different length scales; see, e.g. [1, 16, 20, 21] and Fig. 1b). However, a natural choice of detailed numerical analysis of large material samples with the observed geometry has been found inadequate. First, a computer power is still lacking the efficiency required to solve such a complex task particularly when examining the response of materials beyond their elastic limits.

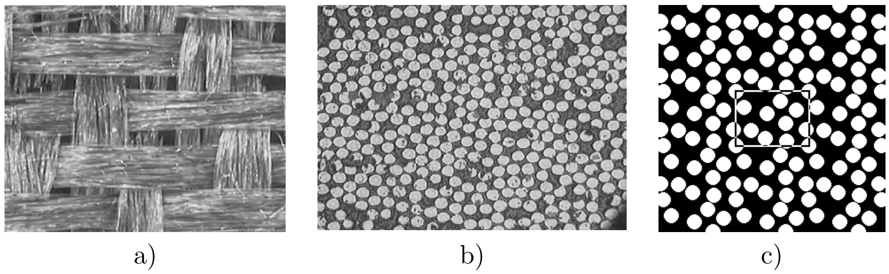


Figure 1: Multi-inclusion periodic unit cells. a) textile composite (mesoscale level) laminate, b) tow cross-section (microscale level), c) idealized unit cell

Second, even large samples of real world microstructures may not reveal all microstructural details of the entire composite. Accepting a random nature of such systems thus becomes a necessity when searching for tools that would allow a reliable description of actual materials with disordered microstructures from both geometrical and mechanical points of view.

Exploiting geometrical statistics of real material systems in the formulation of representative volume elements (RVEs) used for numerical estimates of the true material response has proved advantageous in number of applications [2, 18, 17, 13, 15, 22]. In particular, moving in the footsteps of [10], the authors demonstrated a possibility of specifying a suitable RVE of fibrous composites on the basis of a certain statistically optimal periodic unit cell (SOPUC) with geometrical parameters derived by matching the two-point probability function of real microstructure and the searched PUC. Here, the two-dimensional binary images of real microstructure disclosing a random distribution of reinforcements in the plane normal to the fibers direction served as a point of departure. A representative of such a micrograph is displayed in Fig. 1b) with an example of a corresponding unit cell shown in Fig. 1c).

Derivation of a suitable RVE on microscale, however, is only a first step in the successful analysis of more complex structures such as textiles. Although not evident from microstructural distribution of fibers, an example of the plane view of a C/P textile composite laminate plotted in Fig. 1a) clearly shows a periodic character of the geometrical arrangement of individual fiber tows. Apart from that the figure also suggests various geometrical imperfections attributed to the manufacturing processes. Assuming for example the plain weave C/C composite laminates the material properties are mainly influenced by two technologies: (i) textile (woven fabric preparation) and (ii) composite (impregnation of fabric reinforcement by matrix precursor, pressing and heat treatment). In particular, the woven technology leads to changes in carbon tow cross-section geometry and brings typical lenticular shape of a carbon tow. Pressing of woven laminate may cause tow deformation, which may have quasi-periodic or stochastic character. Heat treatment (curing, carbonization and graphitization) may further initialize pores and cracks development in the composite [16]. The systematic classification and discussion of sources of individual types of imperfections can be found in [9]. A comprehensive quantification of the actual yarn arrangement is provided in [16]. For further experimental evidence of woven path imperfections see also works [4, 9].

It thus becomes clear that such a complex three-dimensional structure of woven fabric composite impaired by various types of imperfections may cause the prediction of the overall properties to be prohibitively expensive if no action is taken. In particular, learning from the knowledge gained from the treatment of transverse plane cross-sections of random composites we advocate the use of a relatively simple SOPUC that incorporates, at least to some extent, the most severe types of imperfections identified from digitized micrographs of plain weave cross-sections of real material systems.

The theoretical grounds of the proposed approach were laid by Zeman and Šejnoha in [23] and further refined in [24]. Starting from the geometrical model of Kuhn and Charalambides [5] it has been concluded from a carefully selected set of numerical experiments, carried out for several artificial systems with predefined imperfections, that the resulting single ply SOPUC is too simple to satisfactorily address even the basic set of geometrical imperfections typical for laminates. This led to the definition of a new two-layer SOPUC that accounts for most of the geometrical imperfections that can be measured from binary images of real material systems. Formulation of a two-layer SOPUC suitable for the geometrical description of real world balanced plain weave composites is the main subject of this contribution. The interested reader may also consult the works [3, 6] for similar studies in case of dimensionally-reduced models of woven composites.

In the following text, a and $\boldsymbol{a}$ denote a scalar or a vectorial quantity, respectively. In addition, for all vectors, the C programming language-style indexing is used, i.e., the first component of a vector $\boldsymbol{a}$ with the dimension N is denoted a_0 while the last entry denoted as a_{N-1}. Other notation is introduced in the text as needed.

2 Elements of quantification of microstructure morphology

The advocated approach to the definition of optimal periodic unit cells essentially relies on a proper choice of description of the morphology of the studied material system. This means, in particular, that instead of describing a position of individual constituents within the sample in every detail, an attention is paid to the determination of quantities that incorporate the most important topological and geometrical features of the microstructure. In the present work, we restrict our attention to the characterization by two specific descriptors: one- and two-point probability functions S_r and S_{rs} and refer an interested reader to [14, 21] for more details. To that end, consider a two-phase heterogeneous material formed by phases r and s and denote the characteristic function of the domain occupied by the r-th phase as χ_r, $r \in \{m, b\}$.[1] Then, the one-point probability function $S_r(x)$ is defined as the probability that a point $\boldsymbol{x}$ will be found in a given phase r while the two-point probability function $S_{rs}(\boldsymbol{x}, \boldsymbol{y})$ stands for the probability that points $\boldsymbol{x}$ and $\boldsymbol{y}$ will be located in phases r and s, respectively:

$$S_r(\boldsymbol{x}) = P(\chi_r(\boldsymbol{x}) = 1), \tag{1}$$

$$S_{rs}(\boldsymbol{x}, \boldsymbol{y}) = P(\chi_r(\boldsymbol{x}) \cdot \chi_s(\boldsymbol{y}) = 1), \tag{2}$$

with the expression $P(A)$ denoting the probability that a statement A is true. For the case of statistically *homogeneous* and *ergodic* media, information contained in the one-point probability function reduces to the volume fraction of a given phase. In addition, the two-point probability function then depends on the difference between points $\boldsymbol{x}$ and $\boldsymbol{y}$ only (see, e.g., [14] for more details) and can be obtained from the relation

$$S_{rs} = \frac{1}{|\Omega|} \mathcal{F}^{-1} \left(\widehat{\chi}_r \cdot \overline{\widehat{\chi}_s} \right), \tag{3}$$

where $|\Omega|$ denotes the area (or volume) of the analyzed domain and $\overline{\widehat{f}}$ stands for the complex conjugate to the Fourier transform of f. Note that in actual implementation, Eq. (3) is approximated using the Fast Fourier Transform, see [21, 24] for further discussion.

3 Statistically optimized periodic unit cell definition

A particular parametrization of the idealized unit cell, considered in this work, is derived from the geometrical model proposed by Kuhn and Charalambides [5]. In the original form of an one-layer unit cell, the model is fully determined by four geometrical parameters: the spacing of warp and fill tows a, the height of the tows b, the height of the unit cell h and the gap between the tows g, see Fig. 2b).

For the transverse cross-sectional plane located in the middle of the weave, the bundle surface functions s_{low} and s_{up}, see Fig. 2b), can be expressed as

$$s_{\mathrm{low}}(x) = \begin{cases} \dfrac{b}{2}\left(\sin\left(\dfrac{\pi x}{a}\right) - \dfrac{x(1-\delta)}{g} - \dfrac{1}{2}(1+\delta)\right) & 0 \leq x < \dfrac{g}{2} \\ -\dfrac{b}{2}\left(1 + (1+\beta)\sin\left(\dfrac{\pi(2x-g)}{2(a-g)} - \beta\right)\right) & \dfrac{g}{2} \leq x \leq \dfrac{a}{2} \end{cases}, \tag{4}$$

$$s_{\mathrm{up}}(x) = \begin{cases} \dfrac{b}{2}\left(\sin\left(\dfrac{\pi x}{a}\right) - \dfrac{x(1-\delta)}{g} + \dfrac{1}{2}(1+\delta)\right) & 0 \leq x < \dfrac{g}{2} \\ \dfrac{b}{2}\left(\sin\left(\dfrac{\pi x}{a}\right) + \delta\right) & \dfrac{g}{2} \leq x \leq \dfrac{a}{2} \end{cases}, \tag{5}$$

[1] Note that in the following text, the subscript m will be reserved for the matrix phase while the symbol b will be used to denote the part of a material occupied by warp and fill tows.

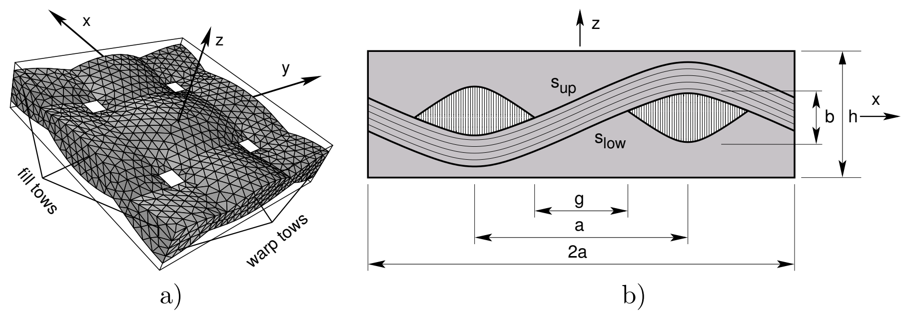


Figure 2: Scheme of a one-layer idealized unit cell: (a) three-dimensional scheme, (b) geometrical parameters

where coefficient β is defined as

$$\beta = \sin\left(\frac{\pi g}{2a}\right)$$

and $\delta = (1 + \beta)\cos(\beta)$. Values of function $s_{\rm low}$ and $s_{\rm up}$ for $x > a/2$ and $x < 0$ follow from obvious symmetry of the PUC. An interested reader is again referred to [5] for the three-dimensional variant of the model.

Even though this model is fully capable of describing the geometry of real-world single-layer woven composites [5, 20] or even multi-layered composites with specific types of imperfections [24] its applicability to complex multi-layered composite systems exhibiting substantial shift and nesting of individual layers is rather limited. In particular, extensive numerical experiments performed in [24] showed the necessity of considering at least two-layer unit cell when dealing with multi-layered composite systems with important relative shifts of individual layers. This naturally leads to enhanced geometrical model, see Fig. 3, where, in addition to basic geometrical parameters a, b, g and h, relative shifts of individual layers in the x, y and z directions Δ_x, Δ_y and Δ_z are introduced as independent parameters. The configuration of the upper layer then directly follows from an appropriate change of the coordinate system together with application of periodicity of the structure. With this type of enrichment, the geometrical model is fully described by seven geometrical parameters,

$$\boldsymbol{x} = (a, b, g, h, \Delta_x, \Delta_y, \Delta_z).$$

The statistically optimal values of the parameters $\boldsymbol{x}$ of the SEPUC then follow from the minimization of the least square error

$$E(\boldsymbol{x}) = \sum_{i=0}^{W-1} \sum_{j=0}^{H-1} \left(S_{bb}^0(i,j) - S_{bb}(\boldsymbol{x}, i, j) \right)^2, \tag{6}$$

where S_{bb}^0 is the bundle-bundle two-point probability function related to the original microstructure while S_{bb} stands for the two-point probability function

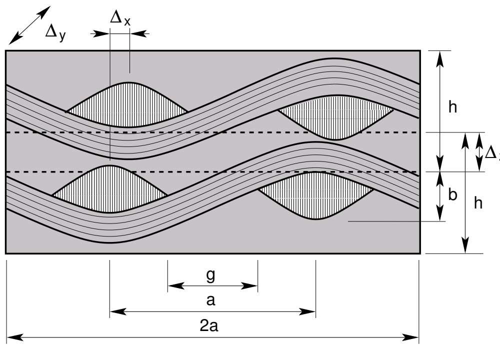


Figure 3: Scheme of a two-layer idealized unit cell

of the idealized unit cell described by parameters $\boldsymbol{x}$; H and W are the height and the width of the bitmap, respectively. A closer inspection reveals that the objective function E is non-convex, multi-modal and discontinuous due to the effect of limited bitmap resolution. Based on our experience with such difficult optimization problems, a stochastic global optimization algorithm **RASA** combining the real-valued genetic algorithms and the simulated annealing method, described in [8], is employed to solve this optimization problem.

4 Image processing and analysis of C/C composites

As already suggested in the introductory part one of the major steps in the analysis is preparation of images of real microstructures. Although not explicitly required in the present approach an image analysis may provide a valuable data on the morphology of real structures (shape and distribution of individual structural components, its size and volume fraction, etc.). This step requires both carefully prepared specimen and a skilled worker for image acquisition and analysis.

The present contribution is concerned with the plain weave balanced C/C composites. For the purpose of image analysis a C/P laminated plate was first manufactured by molding together eight layers of carbon fabric Hexcel G 1169 composed of carbon multifilament Torayca T 800 HB and impregnated by phenolic resin Umaform LE. A set of twenty specimens having dimensions 25×2.5×2.5 mm were then cut out of the laminate and subjected to further treatment (carbonization, reimpregnation, recarbonization, second reimpregnation and graphitization) to create the C/C composite, Fig. 4. The selected specimens were then fixed into the epoxy resin and after curing subjected to final surface grounding and polishing using standard metallographic techniques. This part of the specimen preparation should deserve a special attention as it significantly influences the quality of final structural images.

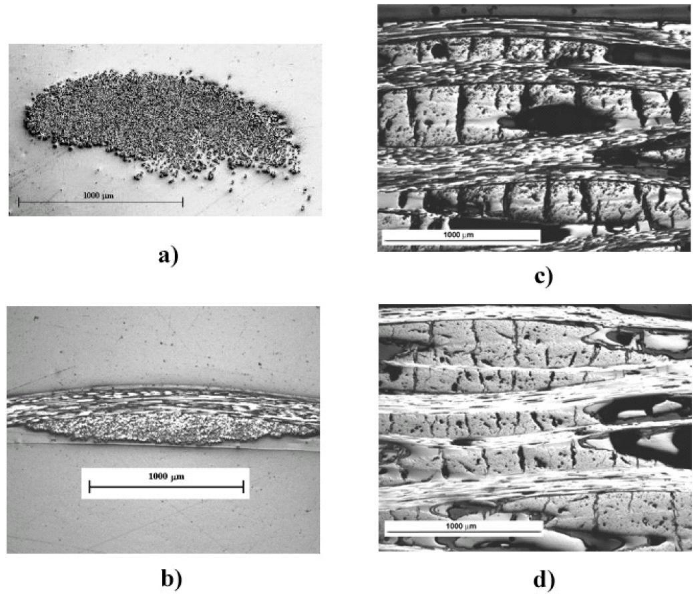


Figure 4: Examples of scanned structures: a) virgin carbon tow, b) carbon woven fabric, c) carbonized composite, d) graphitized composite

The actual image analysis device required for structural image acquisition and analysis consists of NIKON ECLIPSE E 600 microscope, Märzhauser motorized scanning stage, digital monochrome camera VDC 1300C and image analysis software LUCIA G[2]. Note that carbon specimen high reflectance allows relatively good visual resolution of individual parts of a composite structure as depicted in Fig. 4. Unfortunately, an automatic separation of individual objects is disabled by low color contrast of reinforcement (carbon fabric) and matrix, which calls for manual preprocessing of images. **LUCIA G** offers several ways of image editing. Here, the distinction between the fiber tow and matrix is done by marking the borders of the selected object with the help of `ImageEdit` function, Fig. 5.

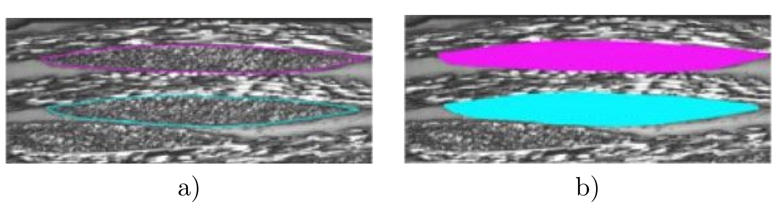


Figure 5: Image editing: a) object editing by manual marking of object borders, b) automatic marking of selected objects

[2] `http://www.laboratory-imaging.com/index.php`

Further image analysis and object measurement is fully automatic. For the purposes of microstructural quantification discussed in the next section it is required to transform the preprocessed color images into their binary counterparts as shown in Fig. 6. It should be emphasized that the binary image of real microstructure plotted in Fig. 6c is essentially the only input data needed in the construction of the desired PUC.

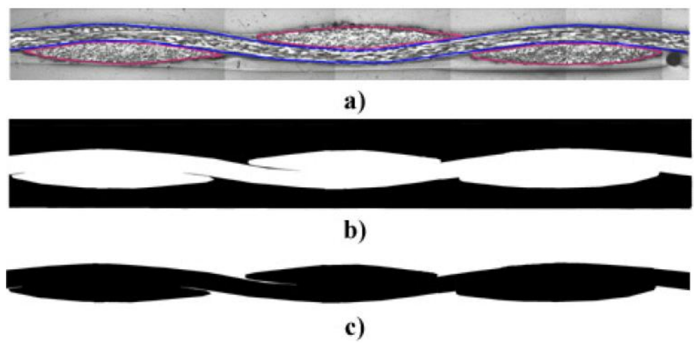


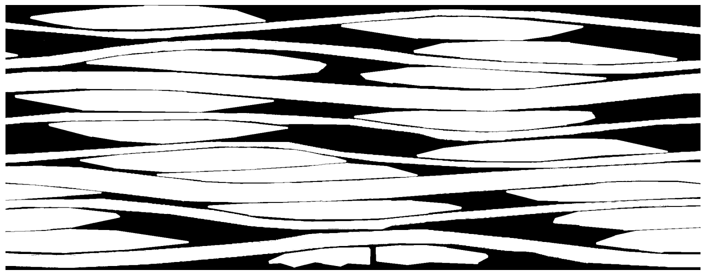
Figure 6: Creation of plain weave binary image: a) preprocessing of original image, b) conversion to binary image, c) inversion of binary image

5 Example of the statistically optimal unit cell

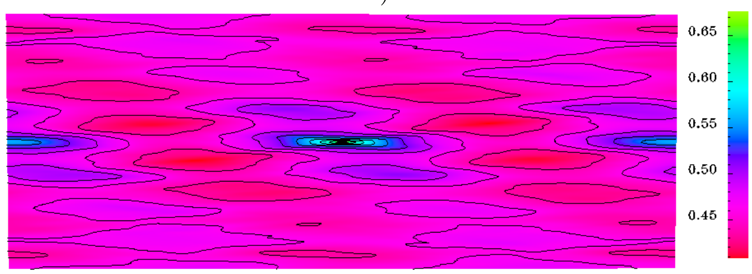
In this section we focus on the application of the previously introduced methodology to the eight-layer woven C/C composite. Using the image processing operations briefly discussed in the previous section, the binary image of a planar section of laminate with resolution 2262×861 pixels has been constructed, see Fig. 7a). A strong nesting of individual layers as well as relative shift in all directions is clearly visible and hence one cannot expect that a one-layer unit cell can be used as a concise geometrical model of the analyzed material. To this end, the bundle-bundle two-point probability function of the target microstructure was computed, see Fig. 7b), as an input for the optimization procedure. As can be observed, the two-point probability function is highly anisotropic and encodes the information of both fill and warp tows position and connectivity.

The optimization algorithm was executed ten times to check, whether the global optimum of the problem was found. The maximum number of function evaluations for each optimization run was set to $25,000$, the target value of the objective function was selected as 10^{-6}. In addition, in order to decrease computational complexity of the problem, the dimensions of the bitmap 7a) were reduced to 766×292 pixels. This step does not introduce significant errors as the two-point probability function is not very sensitive to bitmap resolution.

The lower and upper bounds on individual parameters, summarized in Tab. 1, were determined on the basis of direct measurement of the digitized micrograph.



a)

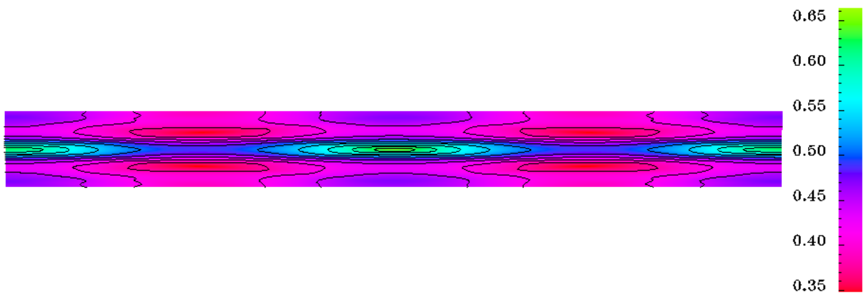


b)

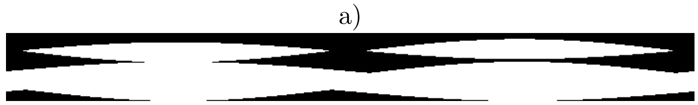
Figure 7: Target microstructure. a) binary image, b) two-point probability function

The resulting optimal parameters of the statistically optimized unit cell are presented in Tab. 1. Note that the scatter in reported values corresponds to ten independent results of the optimization procedure. The average value of these data was used as the most reliable value of the SOPUC geometrical parameters. Corresponding optimal two-point probability function and three-dimensional SOPUC model are shown in Fig. 8.

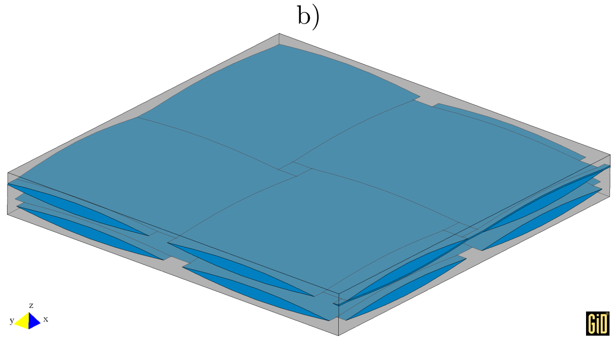
From the presented data, it can be concluded that the precision of identified parameters is more than sufficient from the point of view of practical requirements. From the qualitative point of view, it seems that the statistically optimized unit cell tries to reproduce the matrix rich regions together with the strong nesting of individual layers as close as possible with the constraints of the selected geometrical model. From the character of the two-point probability function, it can be concluded that the optimal unit cell captures well the volume fraction of the microstructure (bitmap Fig. 7a) has the tow volume fraction equal to 67.6 %, the optimized bitmap 66.4 %). In addition, the values of the two-point probability function for small values of argument correspond rather well in both horizontal and vertical directions (Fig. 8a). These effects are, at least from the point of view of selected objective function E, stronger then the relative shift of individual layers observed in the original binary image.



a)



b)



c)

Figure 8: Statistically optimal periodic unit cell, a) two-point probability function, b) three-dimensional model

Parameter	***Lower bound*** [pixel]	***Upper bound*** [pixel]	***Optimal value*** [pixel]
a	350	380	360 ± 0
b	10	40	21 ± 0
g	10	100	40 ± 0
h	30	60	42 ± 0
Δ_x	-200	200	3 ± 1
Δ_y	-200	200	33 ± 1
Δ_z	-30	30	8 ± 1

Table 1: Parameters of the statistically optimal unit cell

6 CAD models of statistically optimal unit cells

Once the parameters of the SEPUC are determined from the optimization procedure point of view, they need to be converted into an appropriate three dimensional model complying with the assumption of periodicity of the analyzed material sample. Note that in the previous study [24] we used a robust three-dimensional advancing front mesh generator **T3D**[3] for this step of the analysis; see also [7, 11] for a detailed discussion of related algorithms. This was possible thanks to working with relatively simple geometries, which allowed a manual of a SOPUC into the **T3D** code. Unfortunately, this approach is no longer feasible for the current, quite general, statistically optimized unit cells and needs to be replaced with a more flexible technique.

To this end, we employ elements of CAD operations [12] combined with volumetric modeling capabilities of the **ANSYS**[4] package to generate the finite element mesh using the mapped meshing technique introduced in [19]. In order to ensure the symmetry of the resulting FEM mesh, a primitive block of the tow is modeled first, see Fig. 9a). Subsequently, using mirroring, copying and merging operations, the whole volume of one reinforcement layer is generated (Fig. 9b). The second layer is then directly obtained by re-generating and moving of a layer similar to the one produced in the previous step according to parameters Δ_x, Δ_y a Δ_z. Note that to ensure the periodicity of the model, the volume correspoding to one layer is suitably enlarged, see Fig. 9c). Finally, the volume corresponding to matrix is generated using the subtraction of the body of reinforcements and the parallelepiped defining the SEPUC (Fig. 9d). Then, the surfaces has been meshed using the Advancing Front Technique and copied to corresponding periodically extended objects. Finally, the tetrahedral elements corresponding to tows and matrix are generated based on the data created in the previous steps. The corresponding finite element mesh is finally shown on Fig. 9e)–f). Such a mesh can be directly used for the numerical modeling of overall behavior of real world composite systems in elastic and inelastic range.

[3] `http://mech.fsv.cvut.cz/~dr/t3d.html`
[4] `http://www.ansys.com`

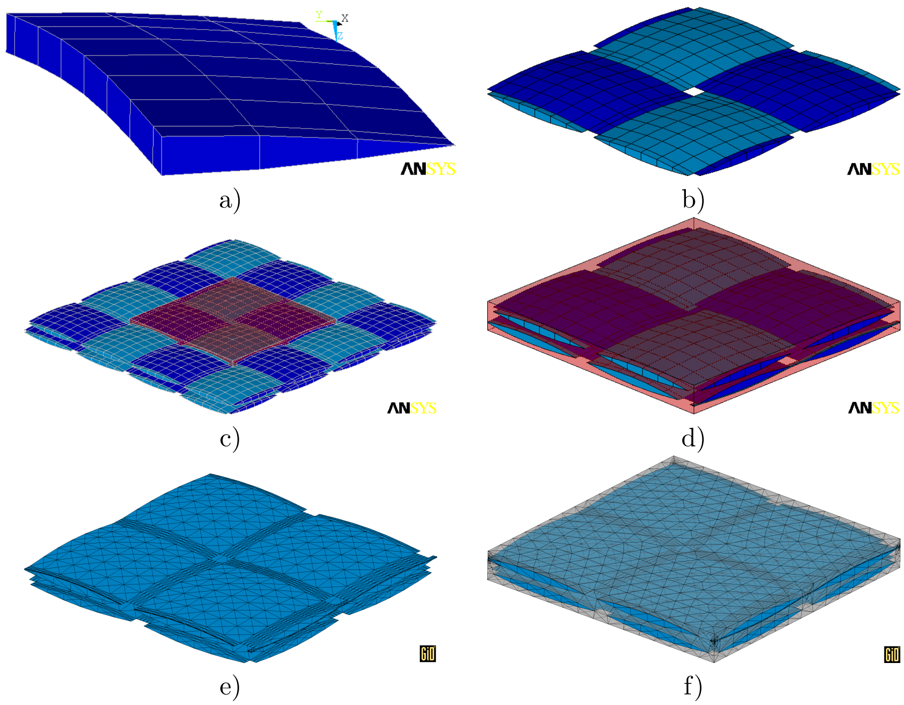


Figure 9: Finite element mesh generation. a) primitive volume, b) one layer of reinforcements, c) two layers of reinforcements, d) CAD model of PUC, e) FEM mesh of tows, f) FEM mesh of SOPUC

7 Conclusions

In summary, the present results seem to confirm the applicability of the proposed approach to the modeling of real material systems with various imperfections in terms of a SOPUC. Combining material statistics up to second order statistical moments with a genetic algorithm based optimizer provides a powerful tool in the search for such a unit cell, which is computationally more simple when compared to an equivalent sample of a real composite but still able to incorporate the most important geometrical characteristics of actual material. It can be expected that SOPUCs that geometrically resemble the real material systems will provide an "identical" mechanical response when subjected to the same boundary and loading conditions. Once the geometrical finite element mesh is combined with an appropriate numerical simulation method it can be used to predict linear as well as non-linear properties of woven composite materials directly on the basis of digitized images of real world structures. Possible generalization of this study include a more detailed statistical characterization of the composite using, e.g., lineal path functions used in [24]. This will be the subject of the future work.

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