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MULTI-SCALE FRAMEWORK FOR MODELLING CARBON FIBRE WEAVES BASED ON STOCHASTIC REINFORCEMENT GEOMETRY

Andy Vanaerschot[1], Karen Soete[1], Stepan V. Lomov[2] and Dirk Vandepitte[1]

[1]KU Leuven, Department of Mechanical Engineering
Celestijnenlaan 300, 3001 Leuven, Belgium
e-mail: {andy.vanaerschot,karen.soete,dirk.vandepitte}@kuleuven.be

[2] KU Leuven, Department of Materials Engineering
Kasteelpark Arenberg 44, 3001 Leuven, Belgium
e-mail: stepan.lomov@kuleuven.be

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Abstract. *The internal geometry of textile composites is subjected to a significant amount of variability. An improved assessment of the quality of any composite material is achieved by identification and simulation of the inherent uncertainty in the reinforcement geometry. By following this strategy, many random realistic representations of the textile reinforcement can be generated based on experimental data of only a few textile samples. This work presents such a roadmap with its successive steps to characterise the spatial scatter in the internal structure of any textile composite (short- and long-range) and simulate random models possessing the measured statistical information on average. Three main steps can be distinguished: (1) collection of experimental data and statistical analysis, (2) stochastic multi-scale modelling of the reinforcement, and (3) construction of virtual specimens in a geometrical pre-processor such as WiseTex. The methodology is demonstrated for a typical carbon-epoxy 2/2 twill woven composite produced by resin transfer moulding, but is applicable to any woven textile or other topology with minor modifications.*

1 INTRODUCTION

The internal geometry of fibre-based composites is subjected to a significant amount of scatter. Variability in the macroscopic performance is dominated by the spatial randomness in the geometrical characteristics at the lower scale, especially for textile composites. By identifying the irregularity in the tow reinforcement, an improved assessment of the quality of a composite can be obtained and a virtual model with a more realistic representation of the reinforcement can be constructed. Among the different strategies for simulating variability in composites using appropriate scaling techniques [1, 2], those that will lead to the most accurate predictions of the statistical distributions of composite properties are calibrated by experimental quantification of the reinforcement variability. However, an inadequacy of experimental data on textile geometry is exists, while methods are lacking for reliable modelling of the effects of geometrical scatter on the randomness in the mechanical properties.

This article presents a stochastic modelling procedure for textile composites that enables to generate as many random virtual specimens as desired based on the statistical analysis of the reinforcement of only one or a few samples. The ensemble of virtual specimens possess the same statistical information on average as measured from the physical samples. The methodology consists of three steps: (1) collection of experimental data about reinforcement geometry, (2) multi-scale modelling of the reinforcement using advanced simulation strategies, and (3) creation of virtual specimens in a geometrical pre-processor such as WiseTex [3]. While step 1 is essential in replicating the real geometry, it is often omitted and researchers are forced to make assumptions about the input information for step 2 and 3.

Next sections describe the general approach and successive steps to build random virtual specimens, starting from the collection of experimental data till the generation of random samples. The methodology is applied on a carbon-epoxy 2/2 twill woven textile composite.

2 MULTI-SCALE FRAMEWORK

Scatter in the reinforcement is considered at the meso-scale (or the unit-cell scale) and macro-level (or the sub-component scale); variation in the matrix and fibre properties is not considered. The variability of each tow path is expressed in terms of its centroid coordinates (x, y, z), tow cross-sectional aspect ratio AR, tow cross-sectional area A and tow cross-sectional orientation θ. Three main steps can be distinguished in obtaining realistic descriptions of the internal geometry of textile composites:

1. **Collection of experimental data with statistical analysis**
   (a) Quantification of the short-range variation
   (b) Quantification of the long-range variation
   (c) Statistical analysis in terms of average trends, standard deviation and correlation information
2. **Stochastic multi-scale modelling of the reinforcement**
   (a) Combination of systematic and handling trends from the experimental data
   (b) Monte Carlo Markov Chain method for simulating auto-correlated deviations
   (c) Cross-correlated Series Expansion for simulating auto- & cross-correlated deviations

3. **Construction of virtual specimens in WiseTex**
   (a) Construction of the nominal model with manufacturer's data
   (b) Update tow path descriptions with generated instances

3 COLLECTION OF EXPERIMENTAL DATA WITH STATISTICAL ANALYSIS (STEP 1)

3.1 Methodology

Non-destructive inspection techniques are applied to measure the fabric architecture in a reliable and efficient way across the composite volume. Scatter in geometry is inspected on the short-range (meso-scale) and the long-range (macro-scale).

It is recommended to acquire short-range data on uncertain tow path parameters using X-ray micro-computed tomography (micro-CT). A three-dimensional (3-D) reconstructed volume is obtained, where from two-dimensional (2-D) slices are extracted in warp and weft direction. Tow cross-sectional shapes can be fitted with ellipses to extract data that fully describe the reinforcement: centroid coordinates (x, y, z), tow cross-sectional aspect ratio AR, tow cross-sectional area A and tow orientation θ in cross-section. After the collection of geometrical data, the reference period collation method [5] is applied. This approach groups tows that should be identical given the nominal periodicity of the textile, with such a representative tow named *genus*. Each tow parameter of each genus is decomposed in a non-stochastic, average trend and non-periodic stochastic fluctuations. These stochastic deviations are further quantified in terms of standard deviation and correlation length.

In addition to the short-range data, the collection of long-range can be advised when one or more tow path parameters have a correlation length ξ that exceeds the unit cell dimensions. Depending on the tow path parameter(s) that need such long-range quantification, additional micro-CT scans, optical imaging techniques or digital image correlation need to be performed.

The statistical information of all tow path parameters, from short- and long-range characterisation, are used as input to the next step for calibrating the reconstruction algorithms.

3.2 Application to a 2/2 twill composite

The methodology is applied to a 2/2 twill woven composite. The dry reinforcement is a fabric from Hexcel (G0986) [4] which is impregnated with epoxy in a Resin Transfer Moulding (RTM) process. It is a balanced textile with four warp (x-axis) and four weft (y-axis) tows. A virtual representation of the unit cell is given in figure 1 with λ_x=11.43 mm and λ_y=11.43 mm, respectively the periodic lengths of warp and weft tows. Considering the manufacturing of the 2/2 twill woven fabric, warp tows can be represented by one *genus*, and similar for the weft tows.

All tow parameters, with exception of the in-plane centroid position, vary within the unit cell dimensions. The latter centroid position is also subjected to the largest variability, indicated by the high standard deviation σ. The micro-CT procedure and derived statistical information is described in [6]. Additional long-range information is acquired for the in-plane centroid positions. An optical scan of the in-plane dimension of a single-ply composite, spanning a region of interest of 10 by 10 unit cells, is performed. A detailed discussion of the procedure and results are given in [8].

Figure 2 present the average reinforcement of the 2/2 twill woven composite. Deviations for all tow path parameters are approximately represented by a normal distribution, with a summary

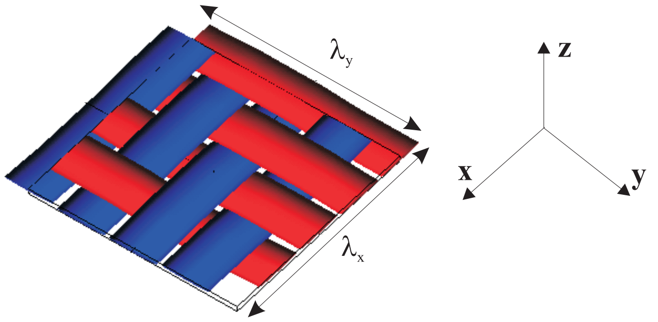


Figure 1: WiseTex model of a 2/2 twill woven reinforcement. The x-axis and y-axis of the coordinate system are respectively parallel to the warp and weft direction. The z-direction refers to the tickness direction.

of the statistical data given in table 3.2. Only the in-plane centroid position is cross-correlated between neighbouring tows.

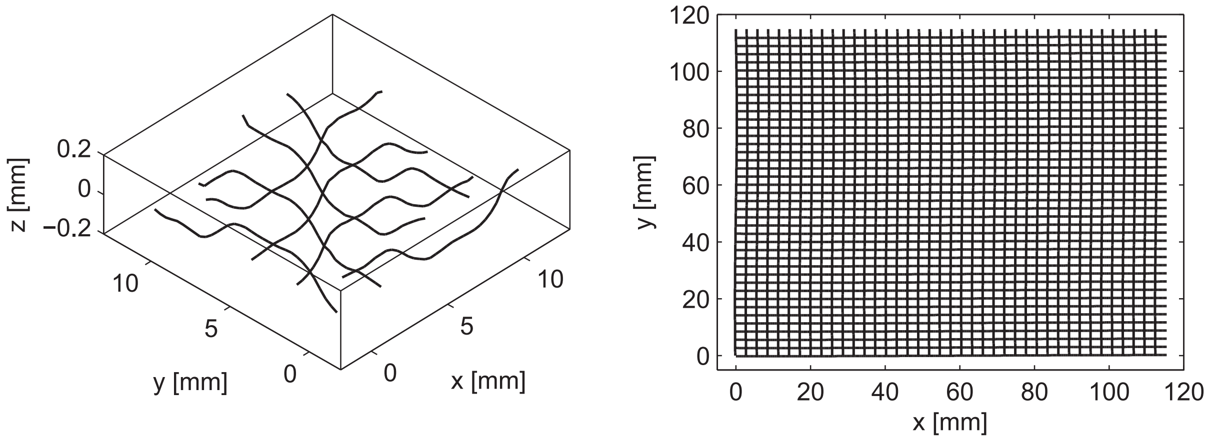


Figure 2: The average reinforcement description presented for the centroid coordinates of a 2/2 twill woven composite.

	x [mm]	**y [mm]**	**z [mm]**	AR **[-]**	A **[mm^2]**
σ^{warp} [mm]	-	0.106	0.014	1.774	0.023
ξ^{warp}_{auto} [mm]	-	114.89	1.78	7.26	2.53
ξ^{warp}_{cross} [mm]	-	4.49	-	-	-
σ^{weft} [mm]	0.615	-	0.015	1.440	0.024
ξ^{weft}_{auto} [mm]	52.89	-	1.62	5.48	1.01
ξ^{weft}_{cross} [mm]	13.16	-	-	-	-

Table 1: Statistical information of all tow path parameters: standard deviation, auto- and cross-correlation length.

4 STOCHASTIC MULTI-SCALE MODELLING OF THE REINFORCEMENT (STEP 2)

4.1 Methodology

A stochastic multi-scale modelling approach is developed to reproduce the measured variation in the tow reinforcement within the unit cell and between neighbouring unit cells. Random instances of tow paths are acquired by following successive steps:

1. Construct a 2-D lattice of straight tows, with rows representing the warp tows and columns representing the weft tows (other definition could be required for non-woven textiles).

2. On each row or column, define an equidistant grid consisting of locations i' and with a length $N_{i'}$ of which (1) the grid spacing is smaller than the shortest correlation length and (2) the length at least approximates the largest correlation length.

3. Interpolate the average trends of all tow path parameters to match the grid locations. Periodicity is exploited for the repetitive systematic trend of the short-range parameters.

4. Generate and add a set of zero-mean deviations $\{\tilde{\epsilon}^{sr}_{i'},\, i' = 1..N_{i'}\}$ along the grid of a single tow for each tow path property that exhibits a short-range trend. This step is performed continuously along an entire tow path spanning multiple unit cells and does not need to be limited per unit cell length.

5. Generate and add a set of zero-mean deviations $\{\tilde{\epsilon}^{lr}_{j'},\, j' = 1..N_{j'}\}$ along a second grid with locations j' of the same length but with a considerably larger grid spacing, with at least one point per periodic length. Afterwards interpolate the produced values to the short-range grid with locations i'.

A necessary condition for superposition of the short-range deviations onto the long-range deviations is that the short-and long-range deviations are not correlated with each other.

Zero-mean deviations which are only correlated along the tow path are produced by the Monte Carlo Markov Chain for textile structures [10], while uncertain quantities that are dependent along and between tow paths are generated using a cross-correlated Series Expansion method [11].

4.2 Monte Carlo Markov Chain algorithm

Tow path parameters which vary without any type of cross-correlation are generated using the Markov Chain algorithm for textile structures [10]. Deviations of a single tow path parameter are produced independently from other tow parameters in a single process. The Markovian operation is the core computation within the Monte Carlo based scheme and generates the distribution vector P^{ϵ}_{i+1} of the particular parameter ϵ at the next grid location $i+1$ using a probability transition matrix A^{ϵ}_{trans}:

$$P^{\epsilon}_{i+1} = A^{\epsilon}_{trans} P^{\epsilon}_{i} \tag{1}$$

Each tow parameter has a different transition matrix A^{ϵ}_{trans} that is calibrated with the experimental standard deviation and nearest-neighbour correlation information to reproduce the statistical information. A post-processing smoothing operation is required to reduce low-amplitude short-range spikes present in the discretized tow path. More details on this algorithm can be found in [10, 7].

4.3 Cross-correlated Series Expansion

A methodology proposed by Vořechovský [11] based on Series Expansion simulates tow path parameters that share the same auto-correlation and of which the cross-correlation can be represented by a single scalar, called cross-correlation coefficient. Each uncertain parameter is represented by a Gaussian random field H_i. The method is calibrated with the experimental standard deviation, auto-correlation and cross-correlation data, of which the correlation information is summarised in correlation matrices. A single realisation of tow parameter deviations for a certain tow path H_j, represented by $\tilde{H}_j$, is acquired using the Karhunen-Loève (K-L) Series Expansion [12], with λ and ϕ respectively the eigenvalues and -vectors of the auto-correlation matrix:

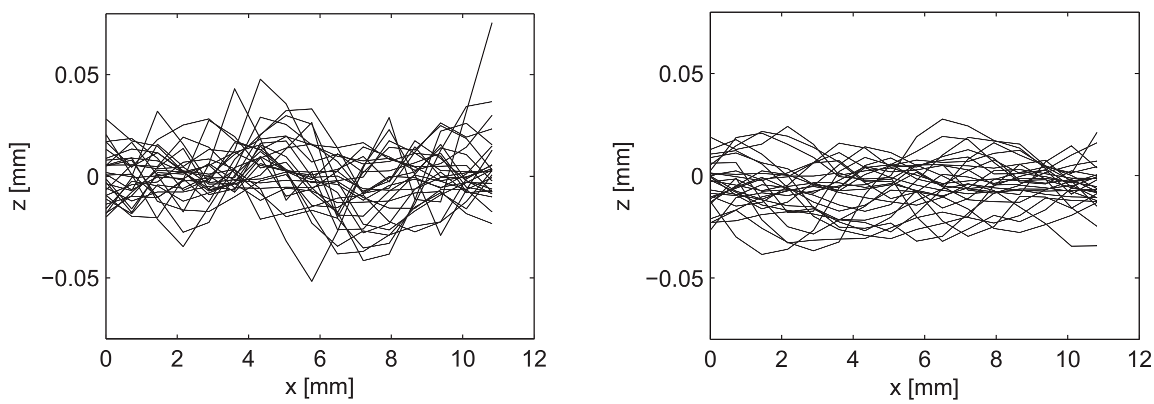
$$\tilde{H}_j(x) = \sum_{i=1}^{N_{KL}} \sqrt{\lambda_i^A} \chi_{j,i}^D \phi_i^A(x) \tag{2}$$

The random variables of χ^D are uncorrelated for each set of random variables that describe a single tow and at the same time cross-correlated between all sets of random variables belonging to different tows. Random fields of the in-plane centroids of warp and weft tows are simulated as a truncated series with N_{KL} terms. Only the largest eigenvalues and corresponding eigenvectors are considered in the procedure. A detailed discussion of the method is given in [9].

4.4 Application to a 2/2 twill composite

Stochastic instances of the 2/2 twill reinforcement are generated for a region spanning ten by ten unit cells, which is sufficiently large to represent the short- and long-range variation quantified in this composite. Each tow is discretised in 320 points, corresponding to 32 points per unit cell. The model is representative for one ply within a laminate which is stacked with 2/2 twill carbon fabrics on each ply.

The Monte Carlo Markov Chain method is employed for the generation of zero-mean deviations of the out-of-plane centroid z, area A and aspect ratio AR deviations. Smoothing is applied using information of ± 2 neighbouring grid points to obtain a realistic tow path, as demonstrated for the warp out-of-plane centroid for one periodic length in figure 3.



(a) Experiment (b) Simulation

Figure 3: Warp out-of-plane centroid deviations trend for 28 warp tows: (a) experimental vs. (b) smoothed deviations obtained from simulations.

Tow path deviations for thousand virtual specimens are generated with the Markov Chain to verify if the experimental statistics are reproduced. The standard deviations and auto-correlation lengths of single unit cells are centred around the experimental target values. Figure 4 shows the histogram of the unit cell statistics for the z-centroid of the warp tows. Smoothing has a limited effect on the standard deviation, while the correlation lengths are slightly shifted to higher values. Similar conclusions are made for the other tow parameters of the warp and weft genus.

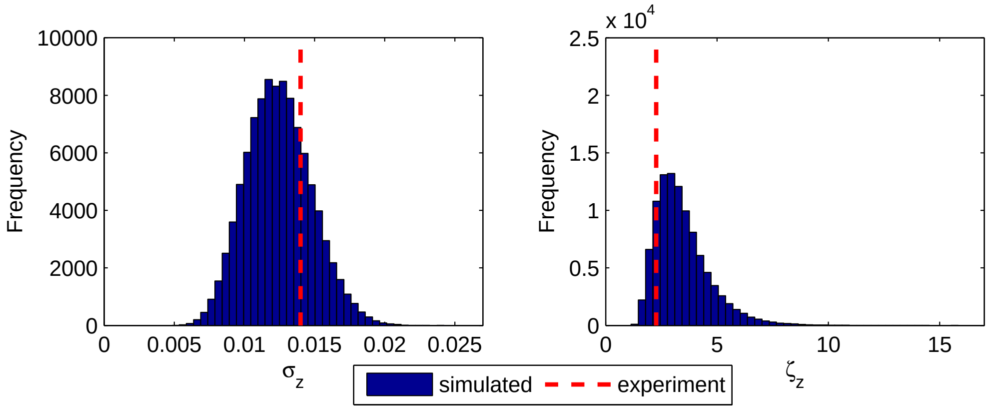
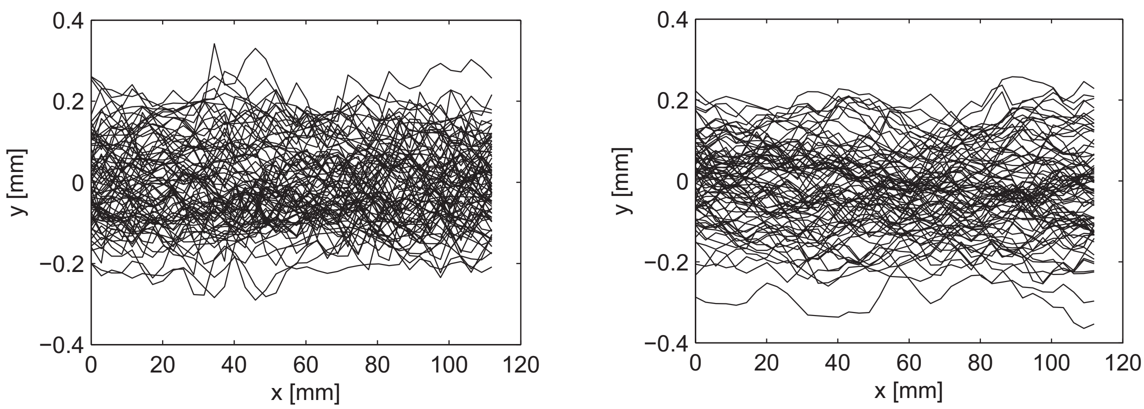


Figure 4: Unit cell standard deviations and correlation lengths of the out-of-plane warp centroid after smoothing.

All cross-correlated in-plane centroid deviations of the 2/2 twill woven composite are generated with the cross-correlated Series Expansion technique over a grid of 41 points. A good resemblance is found for the deviations pattern of the measured in-plane deviations and the produced deviation patterns, as demonstrated in figure 5 for the warp tows. The short wavelength of the experimental warp fluctuations and long wavelength of the measured weft deviations are reproduced without the need of an additional smoothing operation. As post-processing step, the generated deviations are interpolated over the grid of 320 points which is used for the short-range variations.

Comparison of the produced and target statistical information using the Series Expansion is demonstrated at the level of individual specimens. In figure 6, the histogram is presented of the generated auto- and cross-correlation lengths for the warp tows. The mean of the generated correlation lengths achieve the target statistics on average.



(a) Experiment (b) Simulation

Figure 5: Warp in-plane centroid deviations trend for 80 warp tows: (a) experimental vs. (b) simulated deviations.

5 CONSTRUCTION OF VIRTUAL SPECIMENS IN WISETEX (STEP 3)

5.1 Methodology

The last step of the multi-scale framework creates virtual textiles with random geometry. A virtual representation of the textile composite is obtained in WiseTex [3], which is a commer-

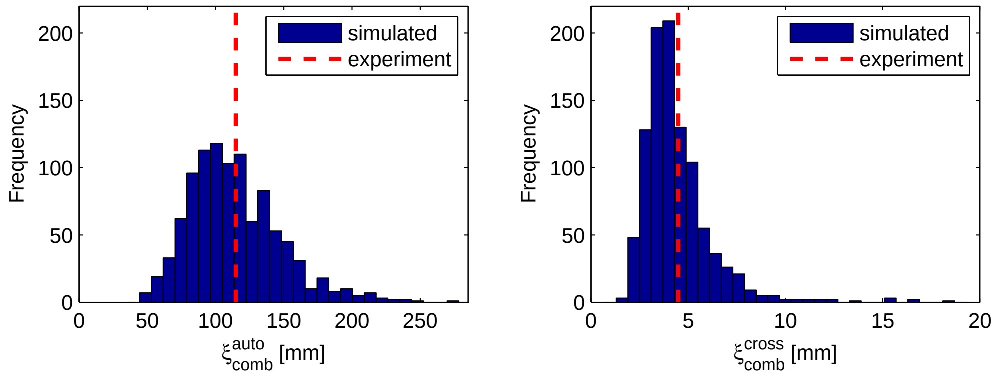


Figure 6: Auto- (left) and cross-correlation (right) lengths of produced warp in-plane positions.

cially available pre-processor for textile geometry. To obtain a random model, nominal tow path descriptions are overwritten with realistic tow representations obtained from the previous step, while preserving the original fibre mechanics and matrix properties.

5.2 Application to a 2/2 twill composite

A virtual specimen of the 2/2 twill woven composite is presented in figure 7, with warp and weft tows oriented respectively along the horizontal and vertical direction. The in-plane centroid position varies on the long-range with bundling behaviour appearing for the weft tows. The unit cell image demonstrates the variation in the out-of-plane centroid position and tow cross-sectional parameters.

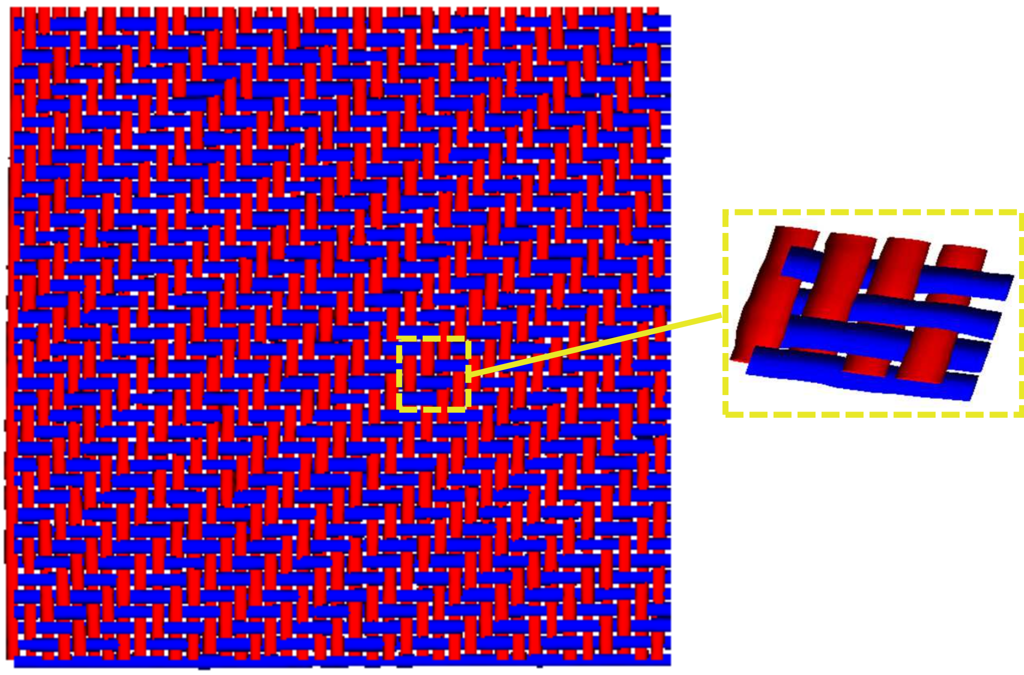


Figure 7: Virtual specimen in the WiseTex format. The in-plane dimension and a single unit cell is presented to demonstrate the short- and long-range variability.

6 CONCLUSIONS

A stochastic multi-scale strategy is presented to quantify and simulate the geometrical variability present in a textile composite. Three general steps are followed to acquire virtual specimens that possess the same statistical information on average as measured from experimental samples. In step 1, experimental data are collected on the centroid positions and cross-sectional dimensions over the short- and long-range distance. Step 2 continues with the construction of virtual tow paths as a combination of a mean trend with zero-mean deviations. If a tow path parameter is not cross-correlated with its adjacent tows, deviations for that parameter are produced with the Monte Carlo Markov Chain method. If cross-correlation is present, a cross-correlated Series Expansion technique is applied to generated the tow path properties. In the final step, random virtual specimens are created in the WiseTex software. These geometrical models will support material design in predicting a more realistic range in which the mechanical properties vary.

The methodology is demonstrated on a carbon-epoxy 2/2 twill woven composite. The in-plane centroid positions show the largest standard deviation of all tow properties with a correlation length exceeding the unit cell dimensions. Therefore, additional data are gathered by optical imaging of the in-plane dimension of multiple unit cell one-ply composites to inspect the in-plane positions over a larger distance. Virtual reinforcements are simulated that span a region of ten by ten unit cells and are representative for a ply within a laminate. Deviations of the out-of-plane centroid coordinate, aspect ratio and area are produced using the Markov Chain method, while the cross-correlated in-plane centroid position is generated by the Series Expansion procedure. A good comparison in terms of wavelengths and extreme values is obtained between the experimental and simulated deviations trends for all properties. Further, all simulated tow deviations achieve the target statistics on average. The virtual WiseTex model reflects the variation observed and quantified from the 2/2 twill composite sample.

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