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Catalanotti, G., & Sebaey, T. A. (2019). An algorithm for the generation of three-dimensional statistically Representative Volume Elements of unidirectional fibre-reinforced plastics: Focusing on the fibres waviness. *Composite Structures*, 227, [111272]. <https://doi.org/10.1016/j.compstruct.2019.111272>

Published in:
Composite Structures

Document Version:
Peer reviewed version

Queen's University Belfast - Research Portal:
[Link to publication record in Queen's University Belfast Research Portal](#)

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Journal Pre-Proof

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PII: S0263-8223(19)32196-8

DOI: <https://doi.org/10.1016/j.compstruct.2019.111272>

Reference: COST 111272

To appear in: *Composite Structures*

Received Date: 7 June 2019

Accepted Date: 26 July 2019

Please cite this article as: Catalanotti, G., Sebaey, T.A., An algorithm for the generation of three-dimensional statistically Representative Volume Elements of unidirectional fibre-reinforced plastics: Focusing on the fibres waviness, *Composite Structures* (2019), doi: <https://doi.org/10.1016/j.compstruct.2019.111272>

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An algorithm for the generation of three-dimensional statistically Representative Volume Elements of unidirectional fibre-reinforced plastics: Focusing on the fibres waviness

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Abstract

An algorithm for the generation of periodic three-dimensional statistically Representative Volume Elements (RVEs) of unidirectional (UD) fibre-reinforced plastics (FRPs) is reported. Fibres are modelled as Bézier curves, which control points are moved in a semi-random fashion, in order to introduce waviness along the fibres. Spatial descriptors, able to statistically characterise the fibre waviness, are proposed, and their probability distributions are optimized for possible matching with experimental measurements. The developed procedure is able to generate the fibre geometry in an effective and fast way. This represents the first step in the generation of high-fidelity micromechanical models for UD FRPs.

Key words: A. Representative Volume Elements (RVEs), B. Micromechanical modelling, C. Fibre waviness, D. Statistical analysis

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1 Introduction

A high-fidelity representation of the microstructure of heterogeneous materials is essential to predict their homogenised properties. This has given rise to the appearance, in the scientific literature, of a substantial number of works that have dealt with the generation of Representative Volume Elements (RVEs) for heterogeneous materials, and of which an extensive compendium can be found in [1].

Although numerous works have been devoted to unidirectional (UD) fibre-reinforced plastics (FRPs), the majority of them have dealt with the generation of two-dimensional (2D) RVEs where the focus has been on defining the fibre distribution [2,3]. Three-dimensional (3D) RVEs, are usually generated by simply extruding 2D RVEs in the fibre direction, consequently obtaining RVEs with perfectly aligned fibres.

The fact that fibres have a waviness is known, but so far it has been simply neglected, due to the difficulty in characterising and/or modelling such waviness. In addition, taking the fibre misalignment into account might not provide a substantial improvement over modelling the fibres as perfectly straight.

The latter assertion might be justified for some stress states. If, for example, a tensile stress state is considered in the longitudinal direction of the material (parallel to the fibres), the initial misalignment of each fibre will not play any major role in the formation of a kink band. However, in some cases, the effect of the misalignment is considerable, e.g. when a compressive stress state in the longitudinal direction is considered. It is well known that, in this case, the fibre misalignment plays a notable role (as an initial kinking), and therefore the consideration of the fibre waviness is crucial.

Focusing on 3D RVEs for composites with fibrous reinforcement, waviness has been implemented as *regular* waviness, for which an analytical expression exists, and *random* waviness, for which the fibre path is determined through a stochastic process. Disregarding the cases for which a *regular* waviness has been implemented, few works, yet impressive, have reported the implementation of *random* waviness for carbon nanotubes [4,5], natural fibres [6], and general fibrous materials [7,8]. Despite the fact that the aforementioned algorithms could be somehow adapted to the case of UD FRPs with high volume fractions (after making appropriate modifications), an issue remains unresolved: how is it possible to ensure that the geometry of the RVEs (fibre

distributions and waviness) is statistically representative of the actual microstructure of the material?

In the following, an answer to this question is sought, with particular emphasis on FRPs, proposing a semi-stochastic algorithm where the fibre waviness is resolved combining stochastic processes with an optimisation procedure.

2 Spatial descriptors for fibre waviness

Before proposing an algorithm able to generate the desired RVEs with fibre misalignments, it is necessary to choose which spatial descriptors are worth analysing in order to account for the fibre waviness. Although different approaches have been proposed [9–14], the usual one consists in *slicing* the composite along the planes perpendicular to the nominal natural axes of the composite material, and measuring the angle between the projection of the fibres tangent vector and a given direction.

Let x , y , and z be the natural axes in the longitudinal, transverse and through-thickness directions, and $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$, $\hat{\mathbf{k}}$ the unit vectors parallel to x , y , and z , respectively. Hence, the following angles can be defined (Fig. 1):

- ϕ_{zx} , the angle that the projection of the tangent vector $\mathbf{v}$ onto the plane of normal $\hat{\mathbf{k}}$ (plane in green in Fig. 1),

$$\text{proj}_{\hat{\mathbf{k}}}(\mathbf{v}) = \mathbf{v} - (\mathbf{v} \cdot \hat{\mathbf{k}}) \hat{\mathbf{k}} \quad (1)$$

forms with the nominal direction of the fibre, $\hat{\mathbf{i}}$,

$$\phi_{zx} = \arccos \frac{\text{proj}_{\hat{\mathbf{k}}}(\mathbf{v}) \cdot \hat{\mathbf{i}}}{\|\text{proj}_{\hat{\mathbf{k}}}(\mathbf{v})\|} \quad (2)$$

- ϕ_{yx} , the angle that the projection of the tangent vector $\mathbf{v}$ onto the plane of normal $\hat{\mathbf{j}}$ (plane in blue in Fig. 1),

$$\text{proj}_{\hat{\mathbf{j}}}(\mathbf{v}) = \mathbf{v} - (\mathbf{v} \cdot \hat{\mathbf{j}}) \hat{\mathbf{j}} \quad (3)$$

forms with the nominal direction of the fibre, $\hat{\mathbf{i}}$,

$$\phi_{zx} = \arccos \frac{\text{proj}_{\hat{\mathbf{j}}}(\mathbf{v}) \cdot \hat{\mathbf{i}}}{\|\text{proj}_{\hat{\mathbf{j}}}(\mathbf{v})\|} \quad (4)$$

Fig. 1. Angles that characterize the fibre misalignment.

- α_{xy} , the angle that the projection of the tangent vector $\mathbf{v}$ onto the plane of normal $\hat{\mathbf{i}}$ (plane in red in Fig. 1),

$$\text{proj}_{\hat{\mathbf{i}}}(\mathbf{v}) = \mathbf{v} - (\mathbf{v} \cdot \hat{\mathbf{i}}) \hat{\mathbf{i}} \quad (5)$$

forms with the transverse direction, $\hat{\mathbf{j}}$,

$$\alpha_{xy} = \arccos \frac{\text{proj}_{\hat{\mathbf{i}}}(\mathbf{v}) \cdot \hat{\mathbf{j}}}{\|\text{proj}_{\hat{\mathbf{i}}}(\mathbf{v})\|} \quad (6)$$

The angles ϕ_{zx} and ϕ_{yx} , defined as in-plane and out-of-plane misalignment angles, may easily be measured slicing the composite and using appropriate experimental techniques [15]. These angles assume a substantial importance when modelling the RVE, especially in the presence of particular stress states, such as when a longitudinal compressive stress is applied.

Depending on the manufacturing process used, it is unusual to experimentally measure different distributions for ϕ_{zx} and ϕ_{yx} . However, it should be observed that if the material is supposed to be transversely isotropic, for the symmetry of the problem, both ϕ_{zx} and ϕ_{yx} must have identical distributions ($\phi = \phi_{zx} = \phi_{yx}$). Hence, in the following, without loss of generality, ϕ will denote both the in- and out-of-plane angles, unless otherwise specified.

The distribution of the other angle, α_{xy} , is not of any practical interest because it does not have a substantial impact on the homogenised properties of

65 the composite in compression. Also note that it is not easy to measure α_{xy}
66 experimentally. It should be observed that if the fibre misalignment is com-
67 pletely random, the cumulative distribution function (cdf) of α_{xy} should be
68 a straight line passing through the points $(-\pi, 0)$ and $(\pi, 1)$. This information
69 could be used to check if the algorithm is working properly when a transversely
70 isotropic RVE is modelled.
71 The methodology proposed here does not necessarily require the assumption
72 of a specific analytical distribution for the fibre misalignment, as will be shown
73 in the following Section.

74 3 Algorithm for RVE generation

75 3.1 Modelling the waviness of the fibres

76 In order to introduce fibre waviness via a stochastic process, the fibres were
77 modelled as Bézier curves whose control points can be moved in a random
78 fashion in order to introduce the desired misalignment. The main advantage of
79 this modelling strategy is that the fibres have a precise analytical description;
80 this will give an advantage when imposing periodicity, and when importing
81 the RVE into a CAD or FEM software.

82 The *initial RVE* (before introducing the fibre misalignment) consists of straight
83 fibres that are placed randomly. In order to achieve this, two-dimensional (2D)
84 fibre distribution of the straight fibres was calculated using the methodology
85 proposed in [16,17], and is not reported here for the sake of conciseness.

86 With reference to the coordinate system presented in Section 2 (where x is
87 the nominal fibre longitudinal direction, and y and z are the transverse and
88 through-thickness directions, respectively), let the RVE be prismatic and have
89 the dimensions of H_x , H_y , and H_z .

90 Suppose that the RVE contains n_F fibres, which is related to the dimensions
91 of the RVE, as shown in [16], and that each fibre is modelled as a Bézier curve
92 with n control points (from 0 to $n-1$). The analytical expression of this curve
93 reads:

$$\mathbf{B}(t) = \sum_{i=0}^n \binom{n}{i} (1-t)^{n-i} t^i \mathbf{P}_i, \quad 0 \leq t \leq 1 \quad (7)$$

94 where $\mathbf{P}_i = \{x_i, y_i, z_i\}^T$ are the coordinates of the i -th control point. It can
95 also be supposed that the control points are equally spaced in the x direction

and that they can only be moved in the plane perpendicular to x . By moving the control points in this plane, waviness can be introduced.

If every fibre has n control points, there will be $n \cdot n_F$ control points in the RVE, from 0 to $n_F \cdot n - 1$. Therefore, this label identifies a unique control point in the RVE. All these points can be moved randomly, and this process can be repeated until the desired misalignment has been achieved.

At the I -th iteration, the order of the control points to be moved is calculated by computing a vector, π_I , containing the randomised sequence of integers from 0 to $n_F \cdot n - 1$.

Iterating through the elements of π_I , with $J = 1, \dots, n \cdot n_F$, the J -th control point of the sequence, $K = \pi_I(J)$, can be selected and moved.

If the position of this control point at the end of the iteration $I - 1$ is $\mathbf{P}_K^{I-1}$, its position at the end of the I -th iteration, $\mathbf{P}_K^I$, can be computed as:

$$\mathbf{P}_K^I = \mathbf{P}_K^{I-1} + \mathbf{u}_K^I \quad (8)$$

where the displacement $\mathbf{u}_K^I$ reads:

$$\mathbf{u}_K^I = \rho_K^I \{0, \cos \theta_K^I, \sin \theta_K^I\}^T \quad (9)$$

being θ_K^I and ρ_K^I the angular and polar coordinates of the control point at the iteration I in the polar coordinate system that lies on the plane perpendicular to x and with the origin on the position of the same control point at the iteration $I - 1$, $\mathbf{P}_K^{I-1}$, as shown in Figure 2.

The angular coordinate, θ_K^I , is chosen as:

$$\theta_K^I = 2\pi \mathcal{U} \quad (10)$$

where $\mathcal{U}$ is a continuous random variable uniformly distributed in the interval $[0, 1]$.

The polar coordinate, ρ_K^I , is obtained with a more complex stochastic process. Firstly, the maximum possible value of the radial coordinate $\bar{\rho}_K^I$ is evaluated, which satisfies the condition of no-contact/no-intersection between the fibre that owns the control point and the other surrounding fibres. Secondly, the value of the radial coordinate is chosen to be in the range $[0, \bar{\rho}_K^I]$, following a stochastic process which details will be presented in Section 3.3. It is worth to point-out that, to calculate the value of $\bar{\rho}_K^I$, it is necessary to calculate the

Fig. 2. Schematic representation of a fibre as a Bézier curve and relative control polygon (the black and red circles indicate the position of the control point at iteration $I - 1$ and I , respectively. The blue circle is the centre of the intersection between the fibre and the plane of normal $\hat{\mathbf{z}}$. The star indicates the furthest position that could be assumed by the control point K at iteration I).

123 contact between the fibre whose control point is moved, and the neighbour fi-
 124 bres in the RVE. The contact is detected when the minimum distance between
 125 the fibres results to be equal or smaller than 2 times the radius R of the fibre
 126 (that is considered, for simplicity, to be constant in the RVE).

127 3.2 Periodicity of the RVE

128 Numerical homogenisation requires the use of appropriate Periodic Boundary
 129 Conditions (PBCs). Therefore, the RVE needs to be periodic along the three
 130 directions. The first implication of this necessity is that the distance between
 131 two points of different fibres, with coordinates $\mathbf{l}$ and $\mathbf{m}$, is not simply given
 132 by the Euclidean distance:

$$d_{lm} = \|\mathbf{l} - \mathbf{m}\| = \sqrt{\sum_{j=1}^3 [l(j) - m(j)]^2} \quad (11)$$

133 but it should be calculated as [16]:

$$d_{lm} = \sqrt{\sum_{j=1}^3 (\min \{|l(j) - m(j)|, H(j) - |l(j) - m(j)|\})^2} \quad (12)$$

134 where $\mathbf{H} = \{H_x, H_y, H_z\}^T$. If this is the distance between two points, the
 135 distance between two adjacent fibres can be calculated as the minimum value
 136 assumed by d_{lm} . Therefore, in order to calculate $\bar{\rho}_K^I$, the control point K is
 137 incrementally moved of $\Delta\rho$ until when, after s times, the contact between two
 138 fibres has been detected ($\min(d_{lm}) < 2R$). When this occurs, $\bar{\rho}_K^I$ is estimated
 139 as $\bar{\rho}_K^I = s\Delta\rho$.

140 The use of Bézier curves makes it easy to impose the geometrical periodicity
 141 of the RVE in the longitudinal direction, that is ensured providing both C^0
 142 and C^1 continuities between the first (or the n -th) control point of a fibre
 143 and the n -th (or first) control point of the same fibre when translated in the
 144 longitudinal direction by $-H_x\hat{\mathbf{i}}$ (or $H_x\hat{\mathbf{i}}$).

145 Let the first control point of the fibre have coordinates $\mathbf{P}_0$ and the last (n -th)
 146 control point of the same fibre have coordinates $\mathbf{P}_{n-1}$. Keeping in mind the
 147 end point interpolation property of the Bézier curves (i.e. the curve begins at
 148 $\mathbf{P}_0$ and ends at $\mathbf{P}_{n-1}$), to ensure C^0 continuity the projections of the first and
 149 last control points on any plane of normal $\hat{\mathbf{i}}$ must coincide. If we consider the
 150 plane of normal $\hat{\mathbf{i}}$ passing for $\mathbf{P}_0$, the previous mathematical condition can be
 151 written as:

$$\mathbf{P}_0 = \mathbf{P}_{n-1} - (\mathbf{P}_{n-1} \cdot \hat{\mathbf{i}})\hat{\mathbf{i}} \quad (13)$$

152 To ensure C^1 continuity, it is required to resort to the end point derivative
 153 property (i.e. the k -th derivative at the start (or the end) of a Bézier curve
 154 depends only on the first (or the last) $k + 1$ control points). Therefore, re-
 155 membering also that Bézier curves are tangent to the start (or the end) of the
 156 Bézier polygon, C^1 continuity is assured if:

$$\{\mathbf{P}_1 - \mathbf{P}_0\} \times \{\mathbf{P}_{n-1} - \mathbf{P}_{n-2}\} = 0 \quad (14)$$

157 Hence, when the first and second control points ($\mathbf{P}_0$ and $\mathbf{P}_1$, respectively)
 158 move, the last and penultimate control points ($\mathbf{P}_{n-1}$ and $\mathbf{P}_{n-2}$, respectively)
 159 need to move accordingly, and vice versa, in order to satisfy both Equations
 160 (13) and (14).

161 3.3 Determination of the radial coordinate ρ_K^I

162 The aforementioned stochastic process was used to perturb perfectly straight
 163 fibres, as shown in Figure 3. However, an appropriate choice of the radial

164 coordinates ρ_K^I needs to be done in order to obtain the desired misalignment.
 165 In order to achieve this, the distribution of ϕ , obtained numerically (calculating
 166 the tangent at several equispaced points on the fibres), needs to be compared
 167 to the experimental one.

(a) Initial configuration.

(b) Perturbed configuration.

Fig. 3. Fibre misalignment through the perturbation process.

168 Since the value of ρ_I^K needs to be in the range $[0, \bar{\rho}_I^K]$, it can be written:

$$\rho_I^K = \lambda_I^K \bar{\rho}_I^K \quad (15)$$

169 where λ_I^K is a scalar in the range $[0, 1]$.

170 It could be thought to chose $\lambda_I^K = \mathcal{U}$, as done in Equation (10), but, if this
 171 would be the case, one would not have any control on the distribution of
 172 ϕ that will be obtained by the algorithm. Moreover, the distribution of ϕ
 173 will depend on the counter I , as shown in Figure 4(a). It is observed that
 174 increasing I results in a reduction of the kurtosis of the distribution of ϕ while
 175 its skewness remains virtually unchanged, as expected. Figure 4(b) shows also
 176 the cdf of α_{xy} which is virtually a straight line passing from the point $(-\pi, 0)$
 177 and $(\pi, 1)$, as expected, since there is no preferential direction. It is evident
 178 that there is a need to choose λ_I^K in order to have the numerical distribution
 179 (generated by the algorithm) to match the experimental distribution. To do
 180 this, the experimental distribution needs to be used as an input, and the value
 181 of λ_I^K should be the result of an optimisation process. Here, to achieve this
 182 objective, two different ways are proposed: minimizing either the difference
 183 between the likelihood or the probability functions between the experimental
 184 and numerical distributions.

Fig. 4. Distribution of ϕ and α_{xy} when $\rho_I^K = \bar{\rho}\mathcal{U}$.

3.4 Minimisation of the standard error of the likelihood

If the first method is used, the value of λ_I^K is chosen in order to minimize the standard error of the maximum likelihood estimate (MLE).

If $\hat{\boldsymbol{\vartheta}}$ is the vector that contains the MLE parameters for $\boldsymbol{\vartheta}$, the standard error $SE(\hat{\boldsymbol{\theta}})$ can be expressed as:

$$SE(\hat{\boldsymbol{\vartheta}}) = \sqrt{\text{Var}(\hat{\boldsymbol{\vartheta}})} \quad (16)$$

where $\text{Var}(\hat{\boldsymbol{\vartheta}})$ is the asymptotic covariance matrix estimated as the inverse of the Fisher information matrix $\mathcal{I}(\boldsymbol{\vartheta})$. Therefore, at the I -th iteration, the standard error can be written as $SE(\hat{\boldsymbol{\vartheta}}(\lambda_I^K))$ and λ_I^K can be chosen in order to minimise the standard error.

To illustrate the methodology developed in this work, let assume that the misalignment angles follow the general von Mises distribution, $\mathcal{M}(\mu, \kappa)$, whose probability density function (pdf) [18] reads:

$$g(\phi; \mu, \kappa) = \frac{1}{2\pi I_0(\kappa)} e^{\kappa \cos(\phi - \mu)} \quad (17)$$

where μ is the mean direction, $\kappa \geq 0$ the concentration parameter, and I_p is the modified Bessel function of the first kind and order p .

If it is assumed that $(\phi_1, \dots, \phi_j, \dots, \phi_N)$ is a random sample from a von Mises distribution¹, the MLE for the mean direction is simply $\hat{\mu} = \bar{\phi}$ where $\bar{\phi}$ is

¹ Despite the fact that the method is general and any circular distribution can, in principle, be used, the von Mises distribution is assumed here as normally is done in presence of circular data.

201 the circular mean of ϕ_j , while for the concentration parameter, the Maximum
 202 Likelihood estimate $\hat{\kappa}$ of κ is the solution of $A(\hat{\kappa}) = \bar{R}$, where the function A
 203 reads:

$$A(\kappa) = I_1(\kappa) / I_0(\kappa) \quad (18)$$

and $\bar{R}$ is the *mean resultant length* defined as:

$$\bar{R} = \sqrt{\bar{C}^2 + \bar{S}^2}; \quad \bar{C} = \frac{1}{N} \sum_{j=1}^N \cos \phi_j; \quad \bar{S} = \frac{1}{N} \sum_{j=1}^N \sin \phi_j \quad (19)$$

Therefore, the estimate for κ reads:

$$\hat{\kappa} = A^{-1}(\bar{R}) \quad (20)$$

204 where A^{-1} is the inverse of A that has to be computed numerically.

205 Because x is the axis aligned with the direction of the fibre, the mean direction
 206 of Equation (17) is known and equal to $\mu = 0$; in this case the concentration
 207 parameter κ is the only parameter that characterises the angular distribution
 208 and its MLE reads $\hat{\kappa} = A^{-1}(\bar{C})$.

209 Since $\hat{\mu} = 0$, because the nominal longitudinal direction is obtained for $\phi = 0$,
 210 the only MLE parameter that will be taken into account will be $\hat{\kappa}$. Therefore,
 211 minimising iteratively the standard error, $SE(\hat{\kappa}(\lambda_I^K))$, provides the desired
 212 numerical distribution (Fig. 5).

Fig. 5. Experimental and numerical distributions obtained by minimising the SE of the likelihood.

213 3.5 Minimisation of the standard error of the probability

214 The experimental and numerical distributions can be compared not only in
 215 terms of likelihood, but also in terms of probability. Let $Q(p)$ be the quantile
 216 function, defined as $Q(p) := Pr(X < x) = p$, and let $\mathbf{Y}$ and $\hat{\mathbf{Y}}$ be the vec-
 217 tors containing the p-quantiles calculated at the values $\{1/p, 2/p, \dots, (p-1)/p\}$,
 218 for the experimental and numerical angles distributions. The stochastic op-
 219 timisation process in this case will force the two distributions to match by
 220 minimising the standard error calculated as:

$$SE = \sqrt{\frac{1}{p} \sum_i^p [Y(p) - \hat{Y}(p(\lambda_I^K))]^2} \quad (21)$$

221 Since the p-quantiles could be calculated for any distribution, it will not be
 222 necessary to assume any analytical formulation for the experimental distribu-
 223 tion. If the p-quantiles are reported in a Q-Q plot, the optimization process
 224 will force the points to lie along the bisector of the first and third quadrant
 225 (Fig. 6(a)) Once again the match of the pdf is remarkable (Fig. 6(b)).

Fig. 6. Experimental and numerical distributions obtained by minimising the SE of the probability.

226 3.6 Further considerations on the proposed methodology

227 3.6.1 Transverse orthotropy

228 The methodology proposed above could easily be extended to the case of non
 229 transversely isotropic FRPs. It is not uncommon that, because of the manu-

facturing process used, composites exhibit different misalignment distribution of the in-plane, ϕ_{zx} , and out-of-plane, ϕ_{yx} , angles [14].

If the actual transverse orthotropy of the material has to be taken into account, one must minimise the standard errors (of Equations (16) or (21) depending on whether the likelihood or probability are used) of the in-plane, ϕ_{zx} , and out-of-plane, ϕ_{yx} , angles. Although several approaches can be used, one easy way, that has been tested here, consists in choosing a combined cost function defined as the sum of the standard error for the two distributions. The value of λ_I^K at the I -th iteration is therefore chosen as:

$$\lambda_I^K = \underset{\lambda_I^K \in [0,1]}{\operatorname{argmin}} \{SE(\phi_{zx}) + SE(\phi_{yx})\} \quad (22)$$

This approach allows to obtain distinct distributions for the in-plane and out-of-plane angles as shown in Fig. 7.

Fig. 7. Optimised distributions for the in-plane and out-of-plane angles.

3.6.2 Duration of the algorithm

Equations (16), (21), and (22) need to be solved in a numerical sense, until when an error threshold, SE_{min} , or a maximum number of iterations, I_{max} has been reached. The easiest way to implement this is to use a *while loop* and exiting the loop when $I > I_{max}$ or $SE < SE_{min}$.

The duration of each run depends on several parameters, namely, the number of fibres, n_F , the number of control points for each fibre, n , the volume fraction, v_F , and the threshold SE_{min} . The duration of each run also depends on the entity of the misalignments that need to be introduced. It is obvious that

larger the entity of this misalignment, more difficult is the convergence of the algorithm.

Suppose that under the same conditions, it is required to generate two RVEs whose misalignment can be assumed to follow a von Mises distribution with concentration parameters κ' and κ'' , respectively. If κ' is a very large number ($\kappa' > 3000$) and κ'' is a relatively small number ($\kappa'' \approx 500$), the first RVE is characterised by fibres that are almost rectilinear, while the second RVE shows fibres substantially misaligned. The algorithm will quickly converge in the first case, while in the second case it will converge after a substantial amount of time, or will never converge (depending on the actual value of the volume fraction that has been used) and, in that case, it will be stopped because the maximum number of iterations, I_{max} , has been reached.

3.6.3 Amplitude, wavelength and number of control points

Two more parameters that characterise the misalignment are the amplitude and the wavelength of the fibre that, as reported by several authors (see [19] among others), play a substantial role on the compressive response of the composite. These parameters are linked to the geometry of the RVE, the number of control points and the misalignment angle distribution.

It has been reported an amplitude in the range of 3-10 times the fibre diameter and a wavelength in the range of 300-800 times the fibre diameter for APC-2/AS4 [20]; similar values have been reported by other authors [19].

While the amplitude of the fibre could be easily controlled (imposing that the maximum distance between the fibre and the line that connects the first and last control point be in the aforementioned range), more complicated is to obtain the desired wavelength. It should be observed that the wavelength will be equal to H_x , since the RVEs are periodic, and that the power spectral density of the wavelength (between 0 and H_x) will depend on the number of control points. To impose an average wavelength of 300-800 times the fibre diameter is not feasible since it will require an extremely large RVE. Therefore, it is appropriate to perform some preliminary calibration analysis in order to choose the correct number of control points. Since fibres are not very flexible, it is suggested to use the minimum number of control points to achieve a given misalignment angle distribution.

283 *3.6.4 Combining the stochastic processes*

284 In order to increase the randomness of the misalignment angle distribution,
285 and to improve the convergence of the algorithm, the value of λ_I^K was chosen
286 combining the stochastic process discussed in Section 3.3, with the quasi-
287 random optimisation process reported in Sections 3.4 or 3.5. Therefore, in the
288 first 30 iterations, the value of λ_I^K was randomly chosen in the interval $[0, 1]$,
289 while after the 30-th iteration was calculated by solving the Equations (16) or
290 (21) .

291 **4 Generation of the RVEs in Rhino and Abaqus**

292 The coordinates of the control points obtained at the end of the stochastic
293 process allow to generate simply the RVE by using commercially available
294 software.

295 Using Python [21], a script was implemented to import the control points in
296 Rhino 5 [22] and automatically create the geometry of the fibres and, using
297 appropriate Boolean operations, that of the matrix as shown in Fig. 8. For an
298 RVE of this size, the generation of the two parts (i.e. fibres and matrix), takes
299 less than one minute.

Fig. 8. Rhino model for matrix (on the left) and fibre (on the right).

300 The two parts were exported (using the same script) as SAT (Standard ACIS
301 Text format) files and imported in Abaqus [23]. Another Python script was
302 used to import, mesh, assemble, and apply appropriate boundary conditions.

303 For the model shown in Fig. 9, the generation of the mesh took few minutes
 304 (on a Dell OptiPlex 7040 Desktop, depending on the mesh size) while the
 305 application of PBCs may take up to 2 hours on the same system depending on
 306 the complexity of the model. Since Abaqus does not have a built-in method to
 307 apply PBCs, this task needs to be performed using a Python script. It should
 308 be observed that if the misalignment is not substantial, the fibres and matrix
 309 could be meshed using hexahedral elements, which simplifies the application
 310 of PBCs. If the misalignment is substantial, as in Fig. 9, the mesh will fail
 311 using hexahedral meshing, and only tetrahedral meshing will work. In this case
 312 the application of PBCs is more complicated. A possible solution is to export
 313 the native mesh as orphan mesh and, in that framework, modify the position
 314 of the nodes in order to be able to apply the appropriate PBCs.

Fig. 9. RVE generated in Abaqus CAE ($v_f = 0.5$, $n = 6$, von Mises distribution with $\kappa = 1500$).

315 Finally, a very time consuming task is the assignment of the material proper-
 316 ties and orientation to the elements of the fibres, since: (i) the strength of the
 317 elements is not taken constant (but following a Weibull or Weibull of Weibull
 318 distribution), and (ii) the material orientation of each element is taken to vary
 319 accordingly with the fibre misalignment.
 320 The first task is solved simply by iterating through the elements of the fi-

321 bre and assigning to each of them the value of the strength generated by a
 322 given statistical distribution. For the second task, the calculations involved are
 323 slightly more complicated. Assuming that the fibres are transversely isotropic,
 324 the longitudinal direction for each element was found as following:

- 325 i) for the i -th element, the coordinates of the centroid $\mathbf{C}_i = \{x_i, y_i, z_i\}^T$ is
 326 calculated;
- 327 ii) the nearest point of the middle line of the fibre to $\mathbf{C}_i$ is found. This point
 328 has coordinate $\mathbf{C}_f = \{x_f, y_f, z_f\}^T$;
- 329 iii) the unit vector tangent to the fibre in $\mathbf{C}_f$, $\hat{\mathbf{f}}$, is calculated and it is applied
 330 as the longitudinal direction of the element i .

331 5 Conclusions

332 A numerical algorithm for the generation of high-fidelity periodic RVEs for
 333 UD FRPs was proposed. The fibres are modelled as Bézier curves whose con-
 334 trol points are moved in a semi-random fashion in order to introduce wavi-
 335 ness/misalignment. The algorithm generates the angle misalignment distri-
 336 bution combining a stochastic process with an optimisation procedure which
 337 decreases the Standard Error obtained when comparing the experimental dis-
 338 tribution with the numerical one generated by the algorithm.

339 The Standard Error is calculated in two ways, namely by comparing the like-
 340 lihood and/or the probability of the distribution. Both methodologies provide
 341 excellent results. The only difference is that the procedure based on the likeli-
 342 hood requires the assumption of a given analytical distribution for the circular
 343 data experimentally collected.

344 The use of an analytical expression for the fibre, based on Bézier curves, allows
 345 to easily impose the periodicity of the RVE. Moreover, each fibre has a very
 346 precise analytical description and exporting the geometry is as simple as ex-
 347 porting the coordinates of the control points. These coordinates are imported
 348 to Rhino 5 where the models of the matrix and fibres are generated. These
 349 are imported to Abaqus, where the Finite Element model is built. All these
 350 procedures are automatised by means of Python scripts.

351 The proposed methodology represents the first step in the generation of 3D
 352 periodic RVEs of UD composites with randomly misaligned fibres.

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