



Towards the probabilistic simulation of discontinuous ultra-thin Randomly Oriented Strands: Meso-macro modelling and uncertainty quantification

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ABSTRACT

This study introduces a hierarchical two-scale methodology to effectively simulate the mechanical behaviour of Randomly Oriented Strands (ROS) of ultra-thin discontinuous thermoplastic prepreg tapes. The mesoscopic model accounts for the stochastic morphology of the ROS composites, from which homogenised material properties, such as modulus and strength, are derived and incorporated into an isotropic macroscopic model. A comparative analysis of macro-models with spatially varying inputs versus single sets of inputs demonstrates that homogeneous modelling yields 20% higher accuracy in relation to experimental measurements. Additionally, we outline how this approach enables the application of uncertainty quantification to inform the meso-model about the target mean and standard deviation from experimental observations. The two-scale simulation framework paves the way to virtually analyse large-scale structures made from discontinuous composites by considering mesoscopic material properties.

1. Introduction

The recycling of composite materials is challenging due to their heterogeneous architecture, particularly the integration of a polymer matrix with reinforcing fibres [1]. A promising approach for repurposing high-quality continuous fibre composites involves converting them into Randomly Oriented Strands (ROS) [2]. In this process, continuous fibres are chopped into short segments and randomly dispersed within a resin system, resulting in composites with enhanced formability. This characteristic makes ROS well-suited for manufacturing complex geometries potentially from recycled materials such as prepreg off-cuts. Their use is growing in industries like automotive — for example, in the Toyota GR Yaris roof — and aerospace, such as Boeing 787 window frames. Despite these advantages, ROS composites are often perceived as low-strength and uncertain materials, limiting their wider applications.

Combined with Ultra-thin (UT) thermoplastic prepreps, these UT-ROS materials can have excellent mechanical properties [3,4], with comparable modulus and strength to equivalent quasi-isotropic laminates made from continuous fibres. They have the potential for wider applications in load-bearing structures, in addition to the existing applications e.g. in automotive [5] and aerospace [6] structures.

Considering costly (raw) materials and labour-intense manufacturing processes of composites, it is important to provide computational strategies for the design UT-ROS composites, including capabilities to

simulate stiffness and strength of real-world large-scale components. One typical computational method to predict the mechanical properties of ROS composites is Finite Element (FE) analysis [7]. Ideally, the FE simulations are performed by engineers using commercial software packages with standard built-in tools.

To ensure the safety and reliability of composite structures, it is important to incorporate progressive damage simulations into the design process. However, simulating progressive damage in composites remains a significant challenge due to the multiscale nature of these materials and the complex interactions among their constituents across different length scales (e.g. [8]). To effectively capture the structural response of large-scale composite components, FE models must account for their intricate nature across different spatial resolutions: micro, meso, and macro scales. However, the computational expense of doing so remains prohibitive for current computing capabilities. As a result, researchers and engineers often focus on one of these scales to examine the damage behaviour of the material or structure [8].

Microscale models typically focus on examining the interactions between fibres and the matrix at the length of a few hundred microns (e.g. [9]). Moving up the length scales, the most widely adopted method for numerically analysing composite structures involves assessing their behaviour at the meso/ply level. Mesoscale models consist of

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multiple layers of elements that represent individual plies within composite laminates (e.g. [10–13]). Additionally, composites can be represented as an equivalent homogeneous material using either stacked or single-layer element configurations. Macroscale models are employed for effectively simulating large-scale structures [14,15].

In order to combine the mechanical behaviour across different length scales, multi-scale techniques have been developed (e.g. [16, 17]). Hierarchical modelling employs homogenisation to translate predicted behaviour from a lower scale, such as a microscale, to a higher length scale. The macroscopic behaviour is governed by the underlying micromechanical constitutive relations, which dictate the stress–strain behaviour at an integration point of a macroscale FE model. These techniques are capable of predicting the macroscopic elastic response of materials with complex fibre architectures at the microscale [18]. A particular subclass of hierarchical multi-scale methods is recursive modelling, where a model utilises its own outputs to generate subsequent predictions or increasingly detailed representations [19]. In the context of composite materials, NASA's Multiscale Analysis Tool (NAS-MAT) is a good example how material behaviour can be recursively linked across several length scales [20,21]. Despite their predictive capability, hierarchical modelling approaches can be cumbersome to implement, as each scale must typically be analysed separately and the resulting information manually transferred between models.

In contrast, concurrent multiscale models enhance model resolution by explicitly accounting for multiscale features. FE² methods often use micro- or mesoscale Representative Volume Elements (RVEs) that are assigned to each integration point of the mesh representing a larger length scale [22]. One advantage of this method is that the base material properties of the RVE constituents are sufficient for in-situ updating the macroscale constitutive behaviour as the loading condition and material properties evolve. Despite some recent progress in simplifying the FE² method [23], the substantial computational cost associated with multiscale models has impeded their widespread adoption in practical applications. In addition, most of these sophisticated models require complex implementation schemes as user subroutines in commercial software.

The majority of the previously mentioned computational methods consider a single set of deterministic material properties, without accounting for the inherent uncertainty of composite materials. Recent studies have demonstrated the potential of combining physics-based FE simulations with data-driven surrogate models [24–26] to account for uncertainty in damage progression within composites [27,28]. This is particularly important for UT-ROS composites made from randomly oriented prepreg tapes due to their stochastic nature of tape placements and fibre orientations.

This paper aims to provide an efficient model to combine meso and macro simulations of UT-ROS composites with random fibre orientations. The proposed modelling framework can be conducted in every standard FE software without the need for in-depth coding skills. It highlights the critical role of fibre orientation distribution in determining structural response and offers a robust strategy for predicting failure in UT-ROS-based structures. By recursively incorporating uncertainty from mesoscale simulations, the framework also enhances reliability in structural performance assessments.

2. Material & testing

2.1. Material

TR 50S carbon fibre tows (Mitsubishi Chemical Co., Japan), were impregnated with DIAMIRON™ C polyamide-6 resin (Mitsubishi Chemical Co., Japan) to form 44 μm thick prepreg sheets [29]. The prepreg sheets were then chopped and randomly dispersed before being compression moulded at 250 °C and 5 MPa pressure for 10 minutes [29]. The moulded Ultra-thin Randomly Oriented Strands (UT-ROS) have their geometric features and the material properties listed in Table 1.

Table 1

Geometrical and material properties of individual tapes used in UT-ROS composites as inputs into meso-model described in Section 3.1.

Property [30]	Value
Orientation angle [°]	0–180
Tape width [mm]	5
Tape length [mm]	18
Tape thickness [mm]	0.044
Property [31]	Value
Young's modulus E_1 [GPa]	105
Young's modulus E_2 [GPa]	4
Shear modulus G_{12} [GPa]	1.2
Poisson's ratio ν_{12}	0.3
Poisson's ratio ν_{21}	0.01

2.2. Test results

Specimens made from UT-ROS plates with tape volume fraction of 55% and laminate thickness, $l_t = 3.1$ mm, exhibited fibre-dominant failure in standard tensile and bending tests [29,30,32]. The brittle tensile failure mode was examined through stress–strain responses, acoustic emission and fractography by Wan et al. [29]. Up to ultimate failure, the stress–strain curves were observed to be approximately linear. Acoustic emission indicated limited presence of damage until approaching the end of the tests [29]. Furthermore, the broken specimens exhibited distinctive brittle fracture surfaces after tensile tests as shown in Fig. 1 [29]. Similar observations were made at the tension side after four-point bending tests [32].

3. Simulation models

The proposed hierarchical multi-scale approach uses information from a meso-scale model and feeds it into a macro-model to simulate 4-point bending. The meso and macro models will be described in Section 3.1 and Section 3.2, respectively. Fig. 2 illustrates the workflow how the meso-model accounts for the presence of discontinuous tapes, while two different macro-modelling approaches are examined considering spatially varying inputs and constant inputs throughout the specimen for bending testing. Furthermore, Section 4 demonstrates how uncertainty quantification can be applied to inform the mean and standard deviation of ideal macroscopic properties derived from the meso-model.

3.1. Meso-modelling

A meso-model was developed in MATLAB (MathWorks, US) to represent each chopped tape within the UT-ROS composites. The model is based on a stochastic morphological modelling framework for tensile [33] and flexural [34] failure predictions.

The following assumptions were made:

1. The movements of chopped tapes, potentially resulting in defects (e.g. voids and wrinkles) and change of fibre orientations [35] during compression moulding, are ignored;
2. The chopped tapes can overlap without changing their morphology e.g. through the thickness;
3. Chopped tapes are perfectly bonded, and the failure is fibre-dominated brittle failure based on experimental observations by Wan et al. [29];

The moulding area, where chopped tapes are randomly distributed, is a rectangle offset by the length of one tape l_t from the boundary of the laminate, as displayed in Fig. 3(a). The coordinates of each tape centre, x and y and its rotation angle θ , cf. Fig. 3(b), follow uniform distributions with

$$X \sim \mathcal{U}(0, l_w) \quad Y \sim \mathcal{U}(0, l_h) \quad \Theta \sim \mathcal{U}(0^\circ, 180^\circ) \quad (1)$$

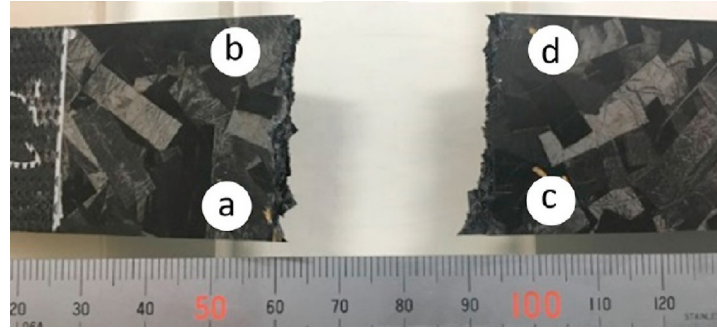


Fig. 1. Photo of a typical fracture surface after tensile testing of UT-ROS composites, indicating fibre-dominated failure [29].

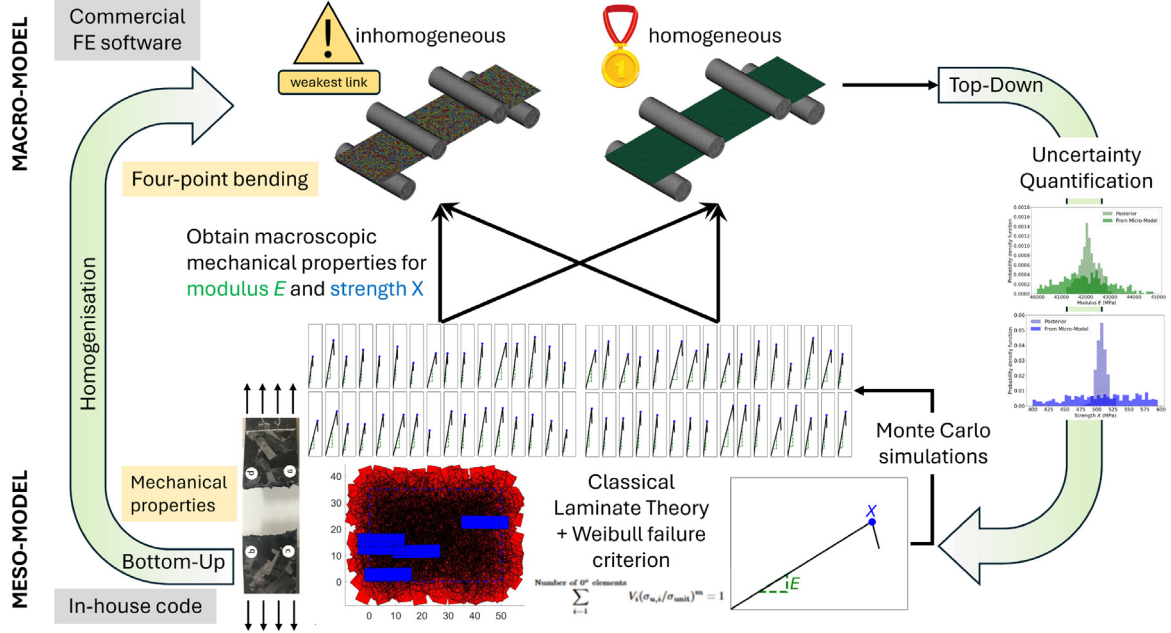


Fig. 2. Graphical overview illustrating how information is transferred from the meso- to the macro-model, and how uncertainty quantification links back to the meso-model.

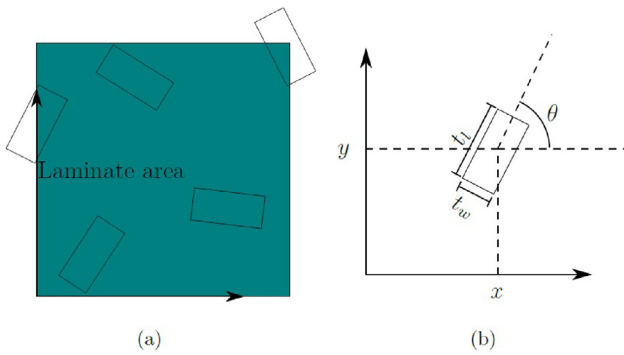


Fig. 3. Geometrical information [33] for (a) moulding and specimen areas (b) a tape.

where l_w, l_h are the width and height of the UT-ROS laminate. Note that only the chopped tapes that fall wholly or partially inside of the laminate area are considered for further calculations.

To calculate the mechanical behaviour of UT-ROS composites with respect to extension and bending, classical laminate theory [36] is applied.

The stiffness matrix of an individual tape is defined as

$$\mathbf{K} = \frac{1}{(1 - \nu_{12}\nu_{21})} \begin{bmatrix} E_1 & \nu_{21}E_1 & 0 \\ \nu_{12}E_2 & E_2 & 0 \\ 0 & 0 & G_{12}(1 - \nu_{12}\nu_{21}) \end{bmatrix} \quad (2)$$

where the material properties are listed in Table 1.

Eq. (3) calculates the transformed elastic matrix $\bar{\mathbf{K}}$ by axis rotation depending on the orientation of the tape such that

$$\bar{\mathbf{K}} = \mathbf{T}^{-1} \mathbf{K} \mathbf{R} \mathbf{T} \mathbf{R}^{-1} \quad (3)$$

where $\mathbf{T}$ is the transformation matrix, and $\mathbf{R}$ is the Reuter's matrix defined as

$$\mathbf{T} = \begin{bmatrix} c^2 & s^2 & 2sc \\ s^2 & c^2 & -2sc \\ -sc & sc & c^2 - s^2 \end{bmatrix} \quad \mathbf{R} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad (4)$$

where $c = \cos(\theta)$ and $s = \sin(\theta)$.

The transformed elastic matrices of each tape are summed up and normalised by the number of tapes N_{tpl} in Eq. (5) such that

$$\bar{\mathbf{K}}_n = \frac{1}{N_{tpl}} \sum_{l=1}^{N_{tpl}} \mathbf{T}^{-1} \mathbf{K} \mathbf{R} \mathbf{T} \mathbf{R}^{-1}. \quad (5)$$

To account for the through-thickness behaviour, ABD matrices can be formulated considering the through-thickness location z_k and the

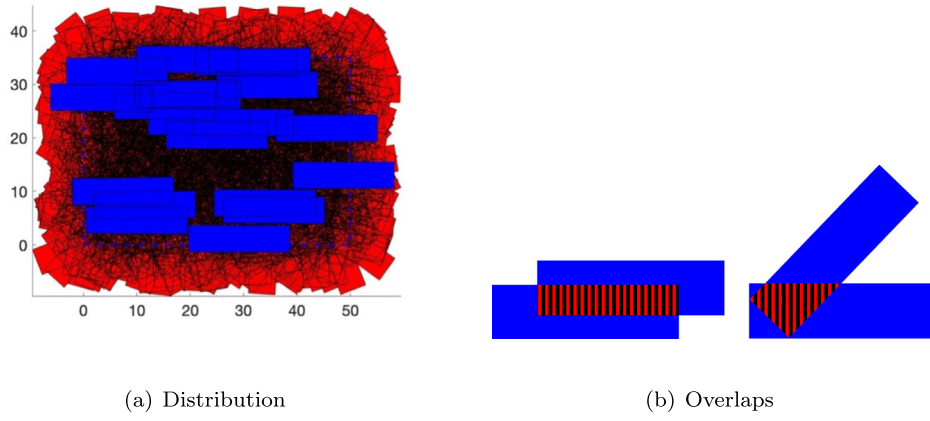


Fig. 4. “Critical tapes” [34] (a) distribution shown in blue in the gauge section of a specimen and their (b) overlaps.

average stiffness matrix $\bar{\mathbf{K}}_n$ such that

$$\mathcal{A} = \sum_{k=1}^{N_l} \bar{\mathbf{K}}_n (z_{k+1} - z_k), \quad (6)$$

$$\mathcal{B} = \frac{1}{2} \sum_{k=1}^{N_l} \bar{\mathbf{K}}_n (z_{k+1}^2 - z_k^2), \quad (7)$$

$$\mathcal{D} = \frac{1}{3} \sum_{k=1}^{N_l} \bar{\mathbf{K}}_n (z_{k+1}^3 - z_k^3). \quad (8)$$

where N_l is the total number of through-thickness calculations. $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{D}$ are the extensional, coupling and bending matrices, respectively.

A force F or a moment M applied to the specimen is then related to its mid-plane strain ϵ and curvature κ by

$$\begin{Bmatrix} F \\ M \end{Bmatrix} = \begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B} & \mathcal{D} \end{bmatrix} \begin{Bmatrix} \epsilon \\ \kappa \end{Bmatrix} \quad (9)$$

The Young's modulus of the laminate can then be derived from the $\mathcal{A}$ matrix such that

$$E = \frac{\mathcal{A}_{11}}{l_t} \quad (10)$$

where l_t is the laminate thickness.

To evaluate stresses and failure, Eq. (9) is used to find the corresponding mid-plane strain ϵ and curvature κ , which is converted into the fibre-directional stress σ_u of the chopped tapes according to Eq. (11) in which z is the through-thickness location of the tapes.

$$\sigma_u = \bar{\mathbf{K}}\epsilon + z\bar{\mathbf{K}}\kappa \quad (11)$$

A Weibull failure criterion can predict the probabilistic failure of materials, in particular brittle materials [37]. It is based on the concept that brittle failure of the material is controlled by the weakest link. In the context of continuous fibre composites [38], the Weibull criterion is often used to relate the probability of failure to the fibre-direction stresses and the volume under stress such that

$$\sum_{i=1}^{\text{Number of } 0^\circ \text{ elements}} V_i (\sigma_{u,i} / \sigma_{\text{unit}})^m = 1 \quad (12)$$

where $\sigma_{u,i}$ is the fibre-directional stress in the 0° elements (aligned with loading direction), V_i is the volume of the 0° elements, σ_{unit} is the tensile strength of a unit volume of material, and m is the Weibull modulus. When Eq. (12) is satisfied, fibre failure is considered to be reached.

For continuous IM7/8552 carbon/epoxy laminates (Hexcel Co., US), it has been shown that the parameters $\sigma_{\text{unit}} = 3131$ MPa and $m = 41$ can represent the scaling of tensile strength [39]. While the same parameters are adequate for the simulation of the discontinuous UT-ROS material considered here [33,34], some modifications to Eq. (12)

are required to address fibre discontinuity. These modifications are outlined in the following according to [33,34].

First, chopped tapes with certain small angles with respect to the horizontal alignment (in loading direction) are identified (Fig. 4(a)). They are referred to as “critical tapes”. Here, a critical angle of 10° was chosen [34]. These “critical tapes” are expected to have the highest stress in the loading direction, so most likely to fail. According to Weibull theory, the failure of these “critical tapes”, the weakest link, will trigger the failure of the laminate.

Within the range of these “critical tapes”, they are considered continuous. The other angled tapes adjacent to these “critical tapes” are treated as discontinuous [33,34]. The forces carried by these tapes need to be transferred to the “critical tapes”. The contribution of these forces to a given “critical tape”, F_a , is calculated by their loading-directional stress, σ_x , times their projected area normal to the load-direction, A_x , times an overlapping area ratio, R , such that

$$F_a = \sum_{j=1}^{N_a} \sigma_x^j A_x^j R^j, \quad (13)$$

where N_a is the number of angled adjacent tapes, and the overlapping area ratio, R , is the overlapped area within the “critical tapes” (red hatched), as shown in Fig. 4(b), over the area of the “critical tape”.

The total force, F_t , includes the contribution of angled tapes adjacent to the “critical tapes”, F_a , and the force taken by the “critical tapes” themselves [33,34]. The resultant loading-directional stress in the “critical tape” can then be calculated via the total force, F_t , in a “critical tape” divided by its cross-sectional area:

$$\sigma_u = \frac{F_t}{A_c} = \frac{F_t}{l_w l_t} \quad (14)$$

For each “critical tape”, its fibre-directional stress is considered as a “ 0° element” in Eq. (12). Then all “critical tapes” are summed up to assess failure. Once the condition in Eq. (12) is fulfilled, the flexural strength of the laminate, X , can be determined at the instant of failure moment as follows.

To determine the flexural stress, the applied moment, M , is ramped up via a series of moment increments per unit width, and translated into an applied nominal stress σ_B , via the second moment of area of the specimen:

$$\sigma_B = \frac{6M}{l_t^2}. \quad (15)$$

Once the condition in Eq. (12) is met, the flexural strength X is determined by

$$X = \sigma_B |_{\text{Eq. (12) is met}}. \quad (16)$$

Since the meso-model incorporates material variability, multiple simulations are necessary to capture the range of possible behaviours.

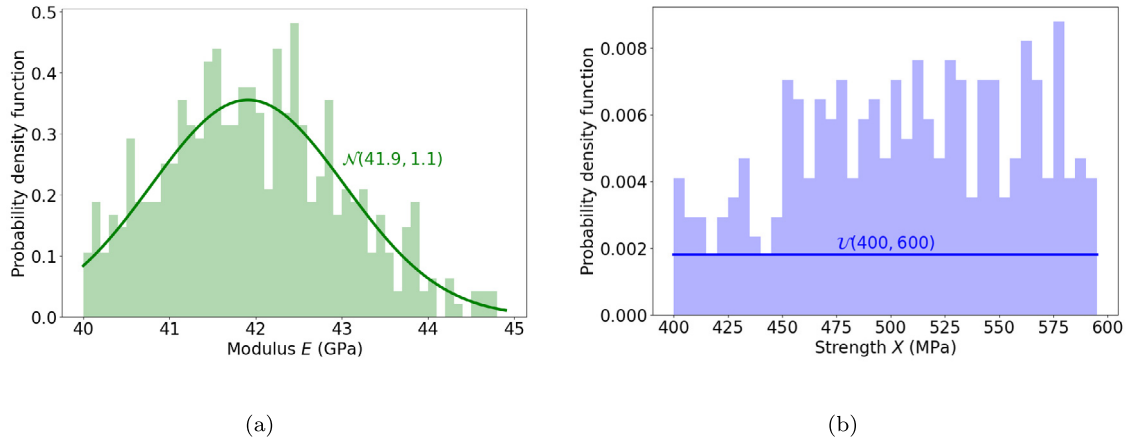


Fig. 5. Resulting mechanical properties from 2000 meso-model simulations. These values serve as input into the macro-model described in Section 3.2.

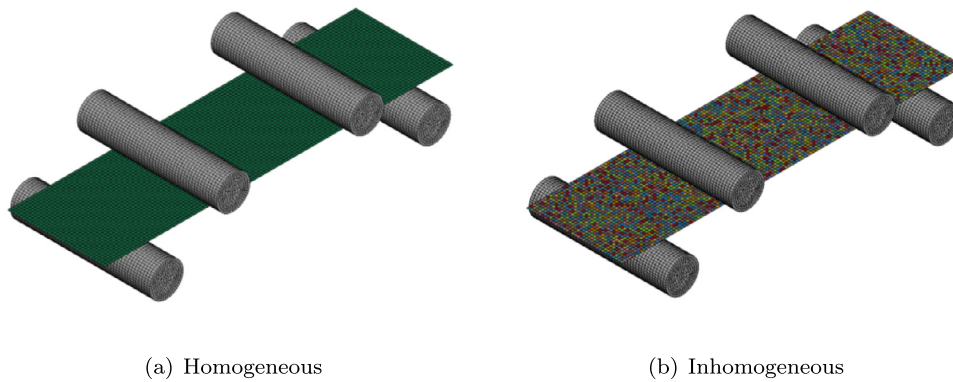


Fig. 6. Two different macro-models for the FE simulation of UT-ROS composites subjected to four-point bending tests. Each colour within the composite plate represents a set of input parameters (E, X).

Each individual meso-model evaluation takes approximately 80 seconds, allowing for the efficient execution of a large number of simulations. Here, 2000 simulations were performed, from which the modulus E (see Eq. (10)) and flexural strength X (see Eq. (16)) were extracted for each case. Fig. 5 shows the resulting distributions of these two mechanical properties. The moduli E follow a normal distribution $\mathcal{N}$ with mean value of 41.9 GPa and standard deviation of 1.1 GPa, while the strength values are uniformly distributed, denoted by $\mathcal{U}$, within the range from 400 MPa to 600 MPa.

3.2. Macro-modelling

The macro-model for the simulation of a four-point bending test uses the modulus E and flexural strength X properties derived from the meso-model shown in Fig. 5 to effectively bridge the length scales between the two models. In the following, two distinct macro-models, as depicted in Fig. 6, will be examined. The homogeneous approach shown in Fig. 6(a) consistently applies a single set of input parameters (E, X) to model the UT-ROS material. In contrast, the inhomogeneous model, shown in Fig. 6(b), features spatially varying inputs with 20 different sets of parameters (E, X) assigned randomly from the distributions shown in Fig. 5.

The simulation of the macro-models is conducted in the explicit FE software LS-DYNA [40]. Shell elements with a single element through the thickness of the UT-ROS composite are used, and the material response is characterised by a simple isotropic material model comprising modulus E and Poisson's ratio $\nu = 0.3$. Elements are eroded when the effective von Mises stress exceeds the flexural strength X . It is appropriate to use the flexural strength from the meso-model because it enables

the single shell elements to represent failure with a stress gradient under bending. Rigid pins (depicted in grey in Fig. 6) interact with the UT-ROS composite through surface-to-surface contacts, assuming a friction coefficient of 0.2 [41]. A prescribed displacement is applied to the top pins, while all degrees of freedom are constrained in the bottom pins. In accordance with the experimental procedure [32], the shell thickness is $t_s = 3.1$ mm, the total width and length of the UT-ROS beam are $b = 35$ mm and 125 mm, respectively, with the support length $L = 96$ mm between the two bottom pins.

Additional settings, such as the in-plane element size and the number of through-thickness integration points, were determined by sensitivity analyses. The results presented in Appendix A indicate that element sizes of $1 \text{ mm} \times 1 \text{ mm}$, combined with eight through-thickness integration points, produce consistent bending results that are independent of the FE settings.

One simulation takes approximately 1–2 minutes on a conventional computer. Thanks to such efficiency, 500 simulations of each macro-model were evaluated.

3.3. Results & analysis

The transition from the meso-model described in Section 3.1 to the macro-model described in Section 3.2 is achieved through the exchange of the laminate modulus E and flexural strength X . The collection of pairs (E, X) obtained from 500 meso-model evaluations serve as input parameters into the macro-models.

The macro-model simulations measure the pin displacement δ and the resulting forces P during four-point bending. The bending strain ϵ

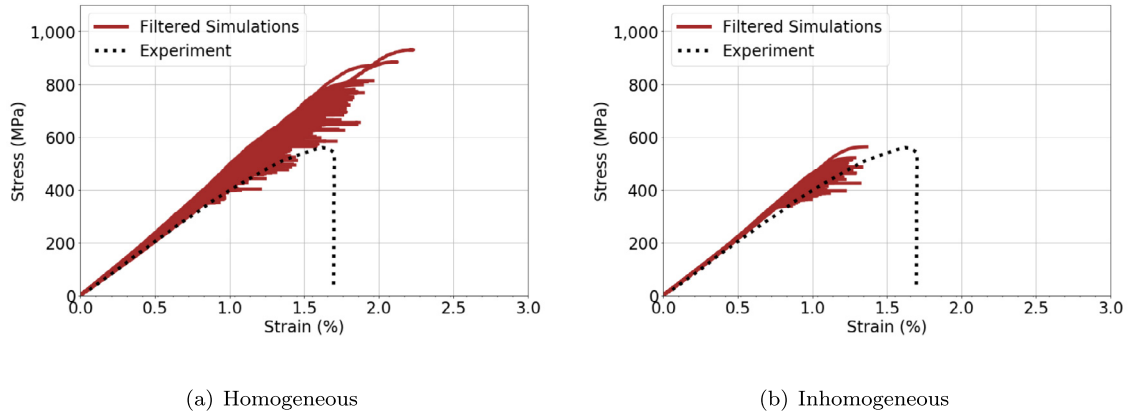


Fig. 7. Comparison of stress vs strain response between experiment [32] and 500 macro-model simulations of four-point bending tests of UT-ROS composites.

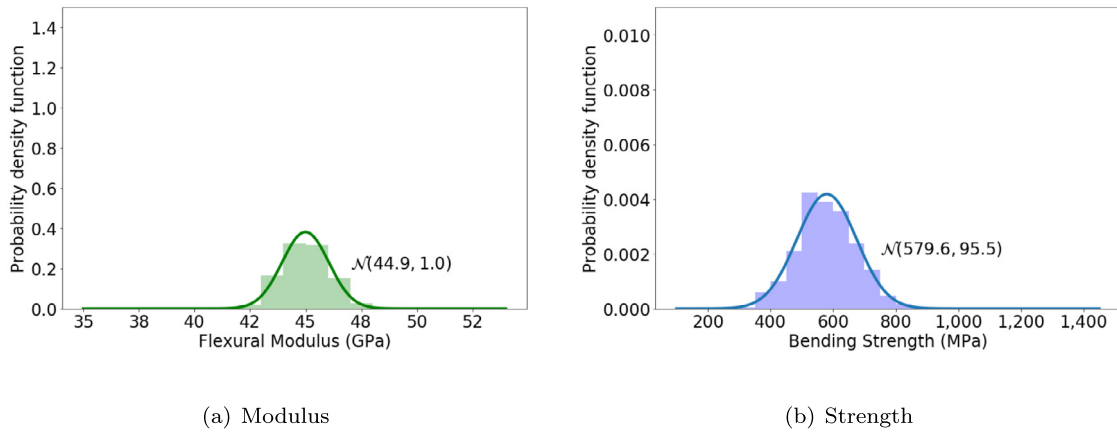


Fig. 8. Distributions of modulus and strength obtained from homogeneous macro-models.

and stress σ can be calculated according to ASTM standard D7264 [42] by:

$$\epsilon = \frac{4.36\delta l_f}{L^2} \quad (17)$$

and

$$\sigma = \frac{3PL}{4bl_f^2} \quad (18)$$

respectively.

Due to significant noise present in the force, and hence the stress response, within the explicit FE analysis of the four-point bending tests, a third-order Butterworth filter with critical frequency of 0.01 was applied to all results. Fig. B.3 in Appendix B shows a raw stress–strain response directly extracted from a macro simulation in comparison to the filtered response. The high filter scores in Fig. B.4 for both simulation datasets demonstrate that filtering maintains the characteristics of the raw data.

Fig. 7(a) and (b) compare one representative stress–strain curve obtained from experiments [32] with the filtered simulation results from the homogeneous and inhomogeneous macro-model, respectively. It can be seen that the results from the homogeneous modelling approach in Fig. 7(a) cover a wide range, with maximum stress values both below and above the experimentally measured peak stress. In contrast, the results obtained from the inhomogeneous approach shown in Fig. 7(b) consistently fall below the experimental peak stress. To further quantify these observations, Figs. 8 and 9 show the distributions of the flexural moduli (slope of the stress–strain curve) and the flexural strength values (peak of the stress–strain curve) as determined from the stress–strain curves obtained from the homogeneous and inhomogeneous macro-models, respectively. The distributions of both the modulus and flexural

strength are narrower in the results from the inhomogeneous macro-model in Fig. 9 compared to the homogeneous counterpart shown in Fig. 8. Furthermore, the mean values of both measurements are equal or lower in these instances.

These results of the mean simulated modulus and flexural strength are compared to experimental measurements [32] in Fig. 10. The height of each bar represents the mean value, while the error bars correspond to the standard deviation of each property. Table 2 presents the associated quantitative data. The results in Fig. 10(a) show that both homogeneous and inhomogeneous macro-models are capable of predicting the mean and standard deviation of the modulus measured in UT-ROS composites subjected to four-point bending tests. Table 2 reveals that the mean flexural moduli vary by approximately 10% when compared to experimental measurements. Similarly, the homogeneous macro-model predicts a mean bending strength of 579.6 MPa, which is 5%–6% higher than the experimental measurements. Conversely, the inhomogeneous model yields a mean bending strength that is 25% lower than the experimentally determined value. The rationale for this finding will be discussed in Section 5, and these findings will preclude the inhomogeneous macro-model from further analysis. Additionally, it can be seen that the standard deviations in flexural strength obtained from both simulations are significantly higher than the experimental counterpart. This raises the question of what the range and distribution of the homogeneous input values generated by the meso-model should be to match experimental mean and standard deviation values. It is important to note, however, that the experimental data are based on only six tests. To achieve statistically robust conclusions and better inform model calibration and validation, a substantially larger number of repetitions is necessary.

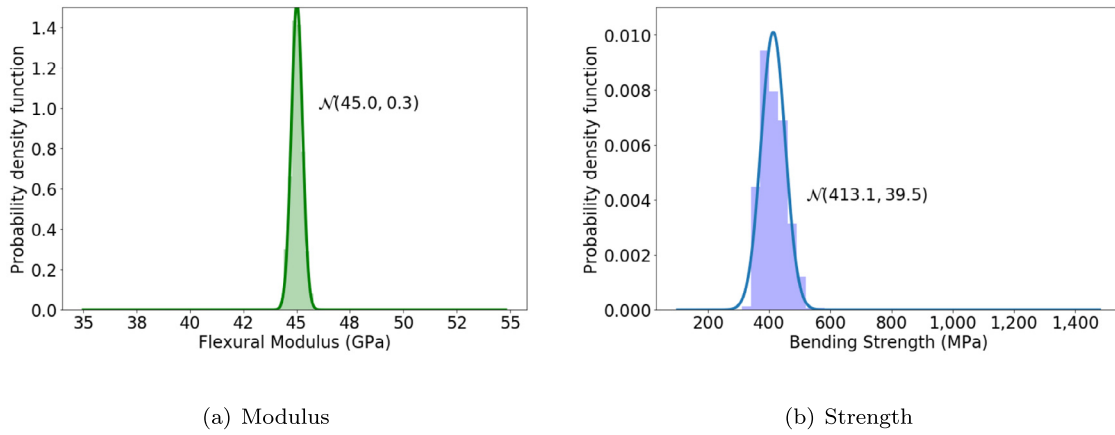


Fig. 9. Distributions of modulus and strength obtained from inhomogeneous macro-models.

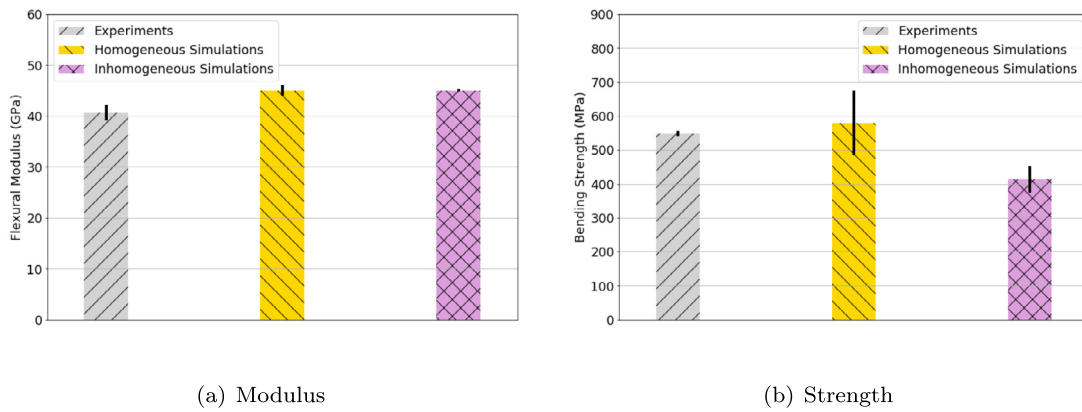


Fig. 10. Comparison of bending properties of UT-ROS composites between experiments [32] and macro-model simulations.

Table 2

Quantitative comparison of properties derived from four-point bending tests and simulations of UT-ROS composites.

	Macro-model simulations ^a		Experiments ^b [32]
	Homogeneous	Inhomogeneous	
Flexural modulus (GPa)	44.9 (± 1.0)	45.0 (± 0.3)	40.7 (± 1.5)
Strength (MPa)	579.6 (± 95.5)	413.1 (± 39.5)	548.0 (± 8.2)

^a based on 500 simulations

^b based on 6 tests

4. Uncertainty quantification

The findings from the previous section indicate that the homogeneous macro-model is capable of predicting certain, though not all, properties obtained from the UT-ROS composites subjected to four-point bending. The objective of this section is to determine the appropriate range and distribution of the homogeneous macro-model inputs (E, X), as generated by the meso-model, necessary for accurately simulating all properties. This objective can be achieved through uncertainty quantification.

4.1. Data analysis & machine learning

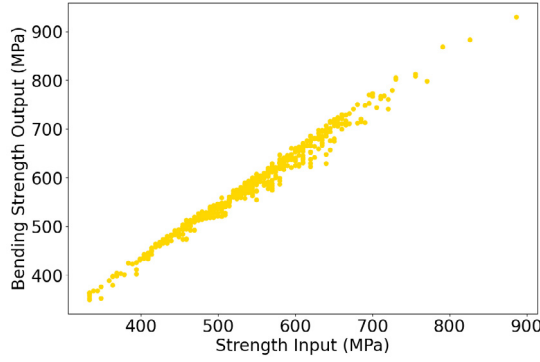
The bending strength analysis in Fig. 10 showed that the standard deviation of 95.5 MPa derived from the homogeneous macro-model is significantly higher than the 8.2 MPa deviation observed in experiments. With the aim to reduce this discrepancy, Fig. 11(a) shows the

relationship between the strength input X from the meso-model and the resulting bending strength from the macro-model.

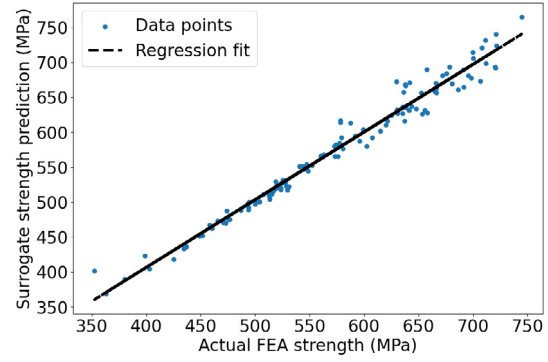
For the purpose of uncertainty quantification, it is essential to develop a fast surrogate model $\mathcal{M}$ capable of mapping the meso-model inputs (E, X) to the flexural strength from macro-models. Here, machine learning in form of Gaussian Process Regression (GPR) is employed with a rational quadratic kernel of length scale $l = 0.1$ and scale mixture $\alpha = 1.0$. GPR has been proven efficient in engineering applications with relatively small datasets [43]. Following the normalisation of the meso-model inputs (E, X) to a range of 0 to 1, the dataset of 500 datapoints is divided into 75% training and 25% testing subsets. Fig. 11(b) shows the testing results, comparing the actual flexural strength obtained from the macro-model with the strength predicted by the GPR regression. The r^2 score of 98.8% indicates a high confidence in the established surrogate model $\mathcal{M}(E, X)$, which effectively relates the inputs (E, X) from the meso-model to the resulting flexural strength.

4.2. Markov chain Monte Carlo

The developed fast surrogate model $\mathcal{M}(E, X)$ is the foundation to conduct uncertainty quantification in form of Markov Chain Monte Carlo (MCMC). Given the input $\theta = (E, X)$ and experimentally determined flexural strength y_{test} shown in Table 2, MCMC aims to determine the posterior probability density function (pdf) $p(\theta|y_{\text{test}})$ of the meso-model outputs θ conditioned on experimental test data y_{test} , meaning that the algorithm aims to find distributions for E and X to match the distribution of the experimental flexural strength. The



(a) Data analysis



(b) Regression results

Fig. 11. Data analysis of flexural strength outputs and strength inputs into macro-models, and results of Gaussian Process Regression (GPR) for surrogate modelling.

posterior density can be calculated by Bayes' rule [44] such that

$$\underbrace{p(\theta|y_{\text{test}})}_{\text{posterior}} \propto \underbrace{p(\theta)}_{\text{prior}} \underbrace{p(y_{\text{test}}|\theta)}_{\text{likelihood (model evaluation)}} \quad (19)$$

where $p(\theta)$ is the prior density, called the prior, and $p(y_{\text{test}}|\theta)$ the likelihood function.

Under the assumption that the experimental data follow a normal distribution $y_{\text{test}} \sim \mathcal{N}(\mu_{\text{test}}, \sigma_{\text{test}})$, with mean $\mu_{\text{test}} = 548$ MPa and standard deviation $\sigma_{\text{test}} = 8.2$ MPa, the likelihood function becomes

$$p(y_{\text{test}}|\theta) = \mathcal{N}(y_{\text{test}} - \mathcal{M}(\theta), \sigma_{\text{test}}), \quad (20)$$

where $\mathcal{M}(\theta)$ is the surrogate model obtained from GPR. To solve Eq. (19), a stochastic process is evaluated to generate a Markov chain of samples. MCMC iteratively draws samples that are accepted or rejected based on their posterior probability. In this study, the EMCEE Hammer [45] implementation of the Affine Invariant Ensemble Sampler (AIES) [46] in Python is chosen to conduct MCMC. The number of interacting random walks, referred to as the number of chains, within one step is set to 50. It is assumed that the meso-model inputs $\theta = (E, X)$ are stochastically independent with prior distributions $p(E) \sim \mathcal{N}(44.5, 4.5)$ and $p(X) \sim \mathcal{U}(350, 1, 000)$, where $\mathcal{U}(x_1, x_2)$ denotes a uniform distribution ranging from x_1 to x_2 .

The MCMC algorithm terminates after 2000 steps. With 50 walks within each step, a total of $2,000 \times 50 = 100,000$ model evaluations $p(y_{\text{test}}|\theta)$ were required. Thanks to the highly efficient surrogate model $\mathcal{M}$, the algorithm only takes approximately 30 seconds to complete on a computer equipped with an Intel Xeon Gold 522R CPU @ 2.90GHz (2 processors), 192 GB RAM, and a NVIDIA Quadro RTX 500 GPU operating on a 64-bit Windows Server 2019 Standard Operating System.

Fig. 12 shows the posterior distributions obtained for the two inputs E and X . Table 3 compares the assumed prior with the resulting posterior distributions. The shifts in the posterior distributions relative to their assumed priors indicates that the Bayesian inference process using MCMC effectively optimised the two mechanical properties to replicate the experimentally observed variability. By comparing the posterior distributions with the meso-model outputs in Fig. 12, it can be seen that both posteriors differ significantly from the data derived from the meso-modelling approach. In contrast to the meso-model outputs, both posterior distributions exhibit a distinct peak at approximately 42–43 GPa and 500–525 MPa for the modulus E and flexural strength X of the UT-ROS composites, respectively. Notably, the variation in strength inputs shown in Fig. 12(b) is vastly different, with a narrow posterior range obtained from the MCMC analysis. These results explain the large discrepancy in the standard deviations of strength measurements between the homogeneous simulation and experiments shown in Table

Table 3

Comparison of prior and posterior distributions within MCMC analysis.

Property	Prior	Posterior
Modulus (GPa)	$\mathcal{N}(44.5, 4.5)$	$\mathcal{N}(42.1, 0.4)$
Strength (MPa)	$\mathcal{U}(350, 1, 000)$	$\mathcal{N}(507.2, 7.9)$

2. To match the experimental data, these results suggest that the meso-model should generate outputs similar to the posterior distributions shown in Fig. 12. To enhance confidence in these results, the calculated posterior distributions shown in Fig. 12 are used as inputs into the GPR surrogate model $\mathcal{M}$. Fig. 13 demonstrates that the obtained flexural strength closely matches the target experimental data, indicating that the MCMC analysis was successful.

5. Discussion

Section 3 presented a direct approach for transitioning from a meso-scale model — considering individual tapes within UT-ROS composites — to different macro-scale models. The uncertainty quantification discussed in Section 4 identified the distributions of key input parameters that the meso-model must provide to enable accurate macro-model predictions in comparison to experimentally measured data. The following section builds on these findings, including a discussion of the associated benefits, limitations, and challenges.

5.1. Homogeneous vs inhomogeneous macro-models

One key finding from the macro-model analysis was that the inhomogeneous model produced significantly lower flexural strength values compared to its homogeneous counterpart. The inhomogeneous model randomly assigns twenty sets of input parameters (E, X) across the geometry of the UT-ROS beam with the goal to replicate the material's spatial inhomogeneity. To understand the reasons behind the low flexural strength estimations of the inhomogeneous model, Fig. 14 presents a plot of flexural strength (y-axis) against the weakest strength (x-axis) derived from the twenty meso-model informed input pairs. A clear linear correlation is evident, indicating that the weakest element dictates the overall flexural strength simulation. The comparison with the experimental measurements shown in Fig. 10(b) suggests that the inhomogeneous macro-model, along with the resulting weakest link principle, provides overly conservative strength estimations, with a discrepancy of approximately 25%. In contrast, the homogeneous macro-model yielded bending strength estimations that are only 5%–6% higher than average experimental measurements. In addition, unlike the inhomogeneous macro-model, the homogeneous approach allows for uncertainty analyses as demonstrated in Section 4.2.

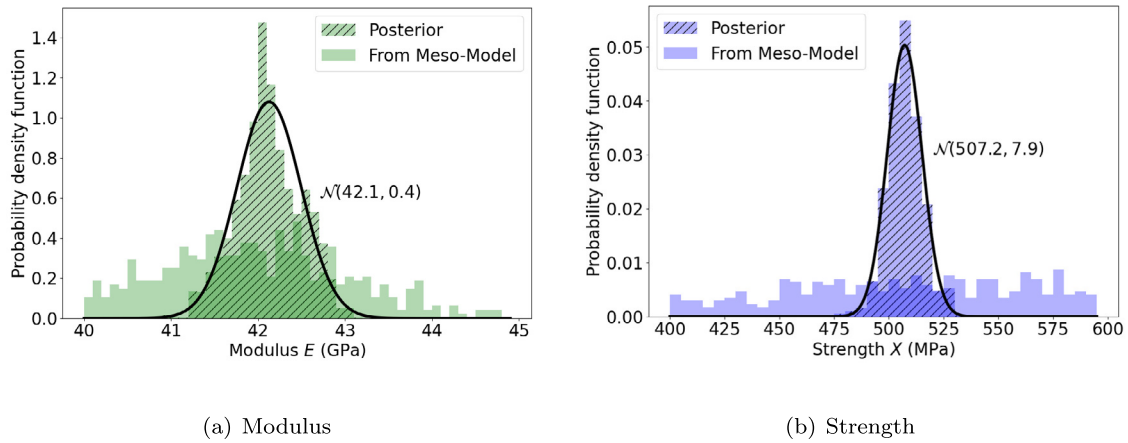


Fig. 12. Posterior distributions of E and X to match experimental bending behaviour $y_{\text{test}} \sim \mathcal{N}(\mu_{\text{test}}, \sigma_{\text{test}})$ compared to input data obtained from meso-models.

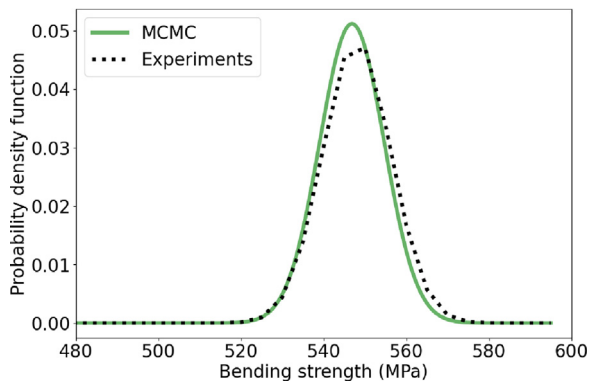


Fig. 13. Validation of MCMC results and GPR surrogate model against experimental measurements [32].

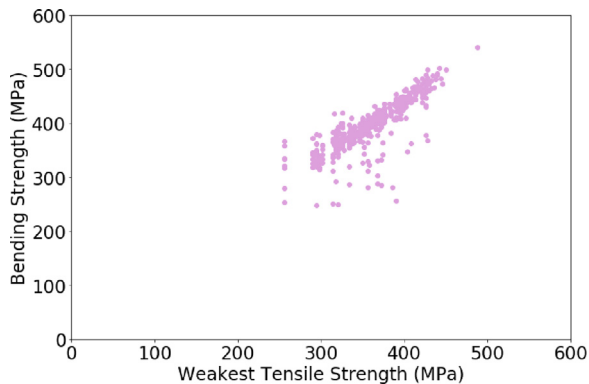


Fig. 14. Confirmation of weakest link principle in inhomogeneous macro-models by comparing the weakest strength element with the resulting bending strength.

5.2. Implications of uncertainty quantification

The uncertainty analysis presented in Section 4.2 identified the optimal distributions of input pairs (E, X) , ensuring that the macro-model matches the experimentally measured mean and standard deviation. Given that these input pairs (E, X) are directly derived from the meso-model, as outlined in Section 3.1, this raises the question of how to adjust the meso-model settings to yield the ideal distributions for modulus E and flexural strength X , as depicted in Fig. 12.

These findings motivate the need for further investigation into the sensitivity of the various input parameters within the meso-model, with the aim of identifying those that most significantly influence the predicted flexural properties (E, X) . For example, the Weibull parameters σ_{unit} and m , derived from continuous IM7/8552 laminates as described in Section 3.1, may require recalibration to more accurately reflect the characteristics of UT-ROS composites. Another example is the orientation of individual tapes. While Table 1 assumes a uniform distribution of orientation angles between 0° and 180° , X-ray computed tomography conducted by Zhao et al. [35] revealed that the actual distribution in UT-ROS composites may deviate from uniformity. By treating the inputs as random variables, another MCMC analysis, similar to the one conducted in Section 4.2, is required to quantify the distributions of each influential input parameters so that the target distributions shown in Fig. 12 are achieved.

5.3. Benefits

The presented framework on the transition from meso- to macroscale offers three key advantages:

1. **Simplicity and Accessibility:** The macro-model requires only basic isotropic material parameters (E, X) , along with a strength-based element erosion criterion. These features are readily available in standard commercial FE software, making the approach broadly accessible and easy to implement.
2. **Scalability and Efficiency:** The framework provides a pathway for upscaling mesostructurally informed properties to large-scale UT-ROS composite structures using conventional FE tools. This ensures both computational efficiency and practical relevance for industrial applications.
3. **Reverse Analysis:** The uncertainty analysis presented in Section 4.2 enables reverse engineering of the meso-model. This allows for targeted refinement of specific parameters and settings to better align with desired macroscopic behaviour.

5.4. Limitations & challenges

The proposed framework considers flexural behaviour of UT-ROS composites. This focus is primarily motivated by the use of very thin UT-ROS composite sheets, where failure is predominantly brittle and tensile in nature. In such configurations, first ply failure tends to govern the overall mechanical response, which explains the findings about the weakest link in inhomogeneous macro-models as shown in Fig. 14 and discussed in Section 5.1. The fibre-dominated nature of first ply failure further justifies the use of classical laminate theory combined with a stress-based Weibull failure criterion described in

Section 3.1. In addition, the assumptions about the meso-modelling stated at the beginning of Section 3.1 have minimal impact on the fibre-dominated response and, consequently, do not significantly influence the mechanical behaviour of UT-ROS composites.

For the simulation of thicker components, compressive and shear properties become increasingly relevant, and dominant failure modes may shift toward progressive failure mechanisms. Addressing these behaviours may require modifications to both the meso- and macro-models, including the relaxation of the stated meso-modelling assumptions and the incorporation of delamination effects. Such modifications, while potentially improving model fidelity, would also substantially increase computational costs, thereby limiting the framework's capacity for rapid predictions.

In the context of scaling up to larger structural components, the Weibull modulus used in Eq. (12) may require attention to account for the correct size effects, commonly observed in composite materials. Experimental investigations across specimens of varying sizes are essential to characterise these effects and to inform potential adjustments to the Weibull parameters.

6. Conclusion

This work establishes a practical and scalable pathway for computationally connecting mesostructural variability in ultra-thin randomly oriented strand (UT-ROS) composites with their macroscopic mechanical performance. A comparison between homogeneous and inhomogeneous macro-models revealed that the homogeneous approach, despite its simplified representation, more accurately captures the experimentally observed flexural properties. In contrast, the inhomogeneous model, while conceptually closer to the material's spatial variability, consistently underestimates flexural strength due to the dominance of the weakest-link effect.

The integration of the macro-model with surrogate-assisted Bayesian inference further illustrates how probabilistic methods can inform which mesostructural parameters truly govern macroscopic behaviour. This opens the door not only to more reliable simulation workflows, but also to data-informed reverse optimisation of manufacturing parameters, ultimately enabling the targeted tuning of variability.

Looking forward, the framework developed here provides a foundation for expanding the simulation of UT-ROS composites beyond tensile-dominated bending. Incorporating compressive, shear, and progressive failure mechanisms will be essential for thicker structures and more complex loading scenarios. Equally, refining the mesostructural input distributions using advanced characterisation methods, such as X-ray computed tomography, orientation reconstruction, and Weibull calibration, will enhance both fidelity and predictive confidence.

Overall, this methodology points toward a broader vision: a unified, uncertainty-aware modelling ecosystem in which mesostructural randomness is not a limitation but a quantifiable, exploitable design variable for the next generation of tape-based discontinuous-fibre composite structures.

CRediT authorship contribution statement

Johannes Reiner: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Xiaodong Xu:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

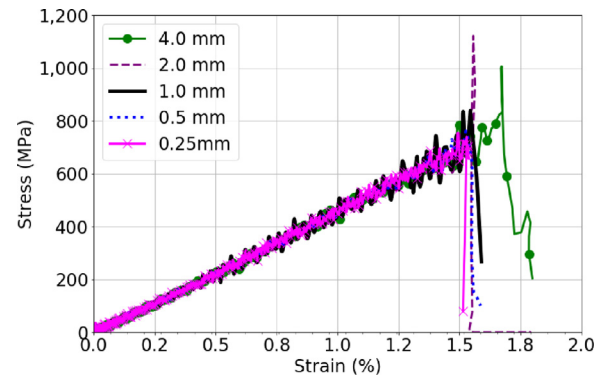


Fig. A.1. In-plane mesh size sensitivity analysis of macro-models to simulate four-point bending of UT-ROS composites.

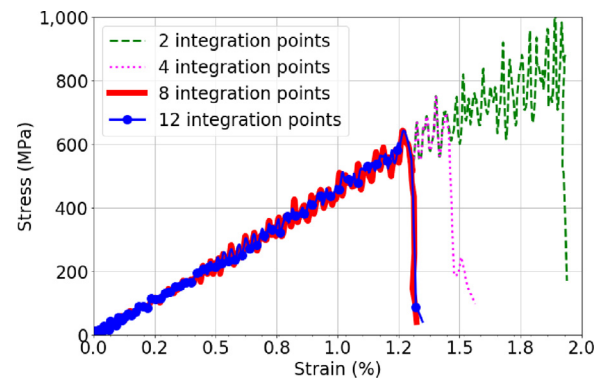


Fig. A.2. Analysis of through-thickness integration points to simulate four-point bending of UT-ROS composites.

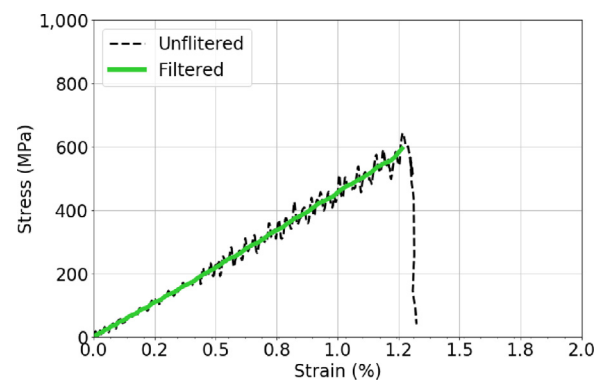


Fig. B.3. Example of unfiltered and filtered stress vs strain response obtained from the macro-model.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used Microsoft Copilot for proofreading and improving readability. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the article.

Appendix A. Sensitivity analyses of macro-models

The macro-model simulations of the four-point bending tests, depicted in Fig. 6, consist of a single shell element through the thickness of the UT-ROS composite. To ensure that the simulation outcomes are

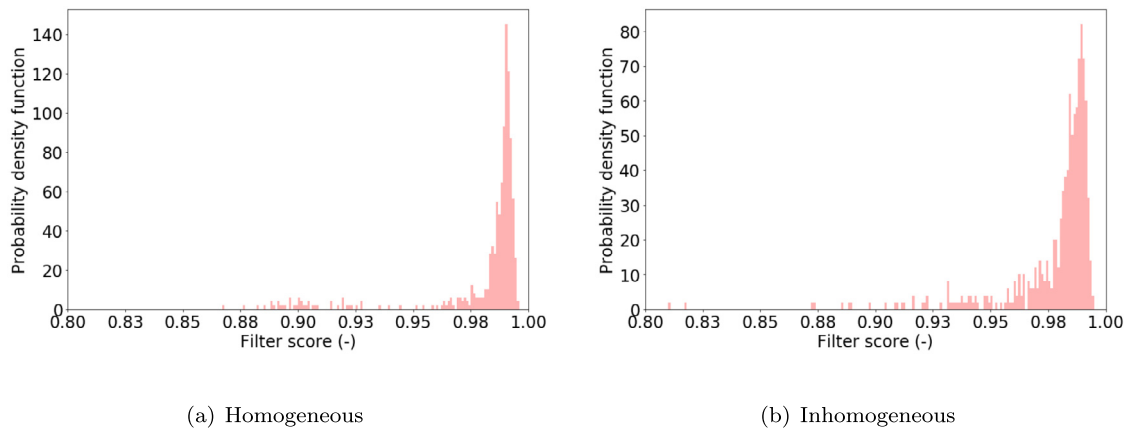


Fig. B.4. Evaluation of filtering quality across all 500 macro-models.

independent of the mesh size and the number of through-thickness integration points, two sensitivity analyses were conducted. Fig. A.1 presents the results obtained from different in-plane element sizes ranging from coarse $4.0 \text{ mm} \times 4.0 \text{ mm}$ sizes to fine meshes with dimensions of $0.25 \text{ mm} \times 0.25 \text{ mm}$. Four through-thickness integration points are kept constant. The results in Fig. A.1 demonstrate that mesh convergence is achieved with an element size of $1.0 \text{ mm} \times 1.0 \text{ mm}$. Similarly, Fig. A.2 shows the sensitivity with respect to the number of through-thickness integration points. The mesh size is kept constant at $1.0 \text{ mm} \times 1.0 \text{ mm}$. The results indicate that 8 integration points are sufficient to accurately simulate the mechanical behaviour of UT-ROS composites subjected to four-point bending.

Appendix B. Filtering

The analysis of the stress vs strain responses from the macro-model simulations is based on filtered curves. Fig. B.3 shows an example of an unfiltered and filtered stress vs strain response. Details about the filtering process can be found in Section 3.3.

To evaluate the quality of the filtering process, the regression score function (`r2_score` in Python) was applied to all 500 stress vs strain curves generated from the homogeneous and inhomogeneous macro-models. The optimal filtering score is 1.0, indicating a perfect regression fit to the original, unfiltered curve. For example, the filtering shown in Fig. B.3 results in a `r2_score` of 0.994. Fig. B.4 presents the filter scores across all macro-model results. It can be seen that the majority of filter scores are close to 1.0, demonstrating the high quality of the filtering. It is interesting to note that the inhomogeneous macro-models show lower filter scores, suggesting a higher level of noise in their stress-strain responses compared to the homogeneous counterparts.

Data availability

Data will be made available on request.

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Towards the probabilistic simulation of discontinuous ultra-thin Randomly Oriented Strands: Meso-macro modelling and uncertainty quantification

Reiner, Johannes; Xu, Xiaodong

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