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Development of a Multi-scale Surrogate-based Tool for Composite Property Estimation

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Abstract. In this study a numerical-based surrogate model is proposed to estimate the effective elastic properties of unidirectional composite lamina, while accounting for geometric and material property uncertainties at both micro and meso scales. In the multi-scale build-up nature of composites many uncertainties occur, mainly in material properties and geometric characteristics. These uncertainties present a challenge in estimating composite material properties. The currently available property estimation/homogenisation tools are mainly in two categories: analytical equations based on an assumed model configuration and finite element homogenisation methods that are more flexible and accurate, but computationally expensive. Hence, this study develops surrogate models capable of representing various uncertainties based on established numerical homogenisation. This tool significantly decreases analysis duration compared with frequent use of full FEA. Thus, represents many composite uncertainties in an efficient way. This tool is particularly useful for developing reliability-based composite structures design approaches.

Keywords: Composites; Uncertainty; Homogenisation; Elastic properties; Surrogates.

1 INTRODUCTION

Composite structures are commonly used in modern transportation, construction and renewable energy applications because of improved stiffness/weight properties compared with alloys. However, the heterogeneous nature and the manufacturing process of composites open the door to many material and geometrical uncertainties to occur within all scales [1, 2]. In addition, due to uncertainties, engineering with composites is more challenging than with metals. As a result, the use of composite materials is still limited to advanced products in aerospace, transportation and wind energy [3]. Therefore, uncertainties representation and quantification is a vibrant topic in composites research.

The traditional method of representing uncertainties within any engineering system is by the use of safety factors in the form of a deterministic design approach to account for known and unknown uncertainties. As a result, it is not possible to quantify structure's reliability [4]. Additionally, the use of safety factors is considered conservative and leads to restricted use of the composite [5]. For that reason, probabilistic representation that can account for such uncertainties are widely used [6, 7].

On the other hand, a reliability-based approach forms a more realistic representation. Several tools are available to achieve this approach, including both theoretical and numerical techniques, i.e. Monte Carlo Simulation (MCS) and First/Second order reliability methods (F/SORM) [8]. F/SORM is widely employed to account for composite constituent materials, strength, and loading uncertainties [4].

Due to the fact that a finite element analysis (FEA) homogenisation method is capable of accounting for more geometrical uncertainties such as fibre cross-sectional shape and fibre stacking uncertainties [9], MCS is often used. Yet, the use of FEA in a MCS probabilistic framework leads to high computational cost. Therefore, our previous studies aimed to develop surrogate models to replace expensive FEA with analytical terms feasible for MCS frameworks [9, 10]. This study aims to extend our approach to include more uncertainties and produce reliable/realistic material representation at the meso-scale.

This study is structured to construct surrogate models that accounts for the effect of several micro-scale geometric and material uncertainties on the lamina scale elastic properties. In section 2, the methodology is explained. Section 3 presents and discusses results using the developed surrogate models, compared with FEA results. Section 4 draws conclusions from the observations and results, highlighting the key findings and future work.

2 METHODOLOGY

Micro-scale uncertainties propagate to higher scale effecting stiffness and mechanical properties. Thus, it is important to capture their effect using a probabilistic framework. Sadik et al. [9] developed a chain of computationally cheap FEA-based surrogate models to improve the efficiency of the reliability analysis by minimising the use of FEA homogenisation. This framework accounts for micro-scale geometric and material uncertainties at the RVE scale. In addition, this study will extend that framework to include more uncertainties, namely fibre-volume ratio (V_f) and generate a more realistic meso-scale representation.

The existing framework extracts the homogenised elastic properties from an RVE using the FEA data points obtained using the periodic RVE homogenisation tool EasyPBC [11]. The framework uses polynomial regression fits to form the relationship between uncertainties and their effect on all elastic properties using data points obtained by the FEA homogenisation. A second surrogate model is developed to sum the individual effects from all uncertainties Eq.1:

$$E_i = \bar{E}_i + \sum_{j=1}^{N} f_i(x_j) \qquad \text{Eq. 1}$$

Where E_i is one of the approximated elastic properties, $\bar{E}_i$is the deterministic value, N the number of uncertain parameters (x_j) and $f_i\,(x_j)$ is a polynomial that links the value of uncertain parameter j with the change in elastic property i (relative to deterministic value).

However, the previous framework only used RVEs with 2 fibres (e.g. a “small RVE”). Thus, it was not possible to represent spatial variation of within a lamina, as illustrated in Fig. 1. Also, V_f uncertainty was not included in the previous framework.

In order capture a more realistic representation, a second scale of RVEs is added to the previous framework. The added scale is constructed using small RVEs with their assigned random variable uncertainties. This framework creates a larger RVEs (LRVEs) instead of small RVEs, although reference to scale here is a relative expression.

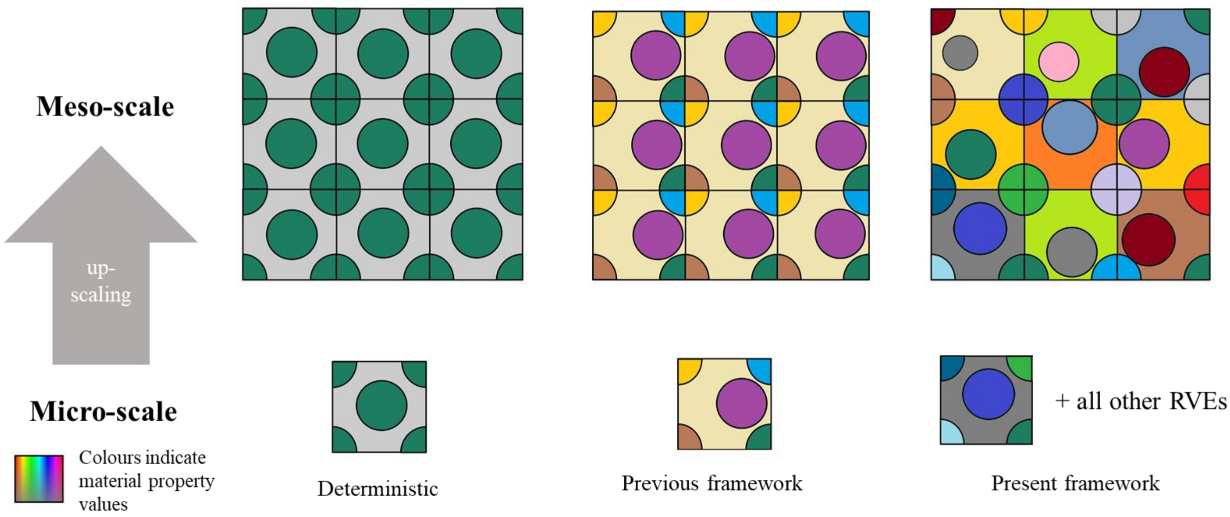


Fig. 1. The current and previous micro-meso upscaling approach.

A key aspect of the upscaling process is a correlated arrangements of fibres within the LRVE. It is assumed that fibres are divided into two types: fixed and non-fixed. Fixed fibres are represented by the four quarter corner fibres of the RVE. Geometrically speaking, these quarters need to remain in place to maintain periodic boundaries of the RVE. Whereas the central fibre, can shift within the RVE representing stacking uncertainty without violating periodicity. As for correlation, fibre material uncertainty is assigned to the five parts of the RVEs' fibre individually (see Fig. 1 and Fig. 2). However, the same uncertainty value of each quarter is used in its neighbouring quarters as shown Fig 1 and 2 colour mapping.

There are three proposed approaches to analyse the new two-scale RVE framework shown in Fig. 1 and Fig. 2: a) an established full FEA analysis (Yellow route), starting with periodic homogenisation of all RVE, constructing a LRVE and applying FEA homogenisation. b) Surrogate-FEA based (Green route), the LRVE is constructed from RVEs homogenised using surrogate models explained earlier. The constructed LRVE is then homogenised numerically as yellow rout, but with a less expensive FEA. c) Full surrogate-based (except data points, Blue route), this approach uses the surrogate model developed at the micro-scale and an additional surrogate model for LRVE to sum up the effects of all small RVEs replacing FEA homogenising of the green rout. The developed surrogate model is explained in the next section.

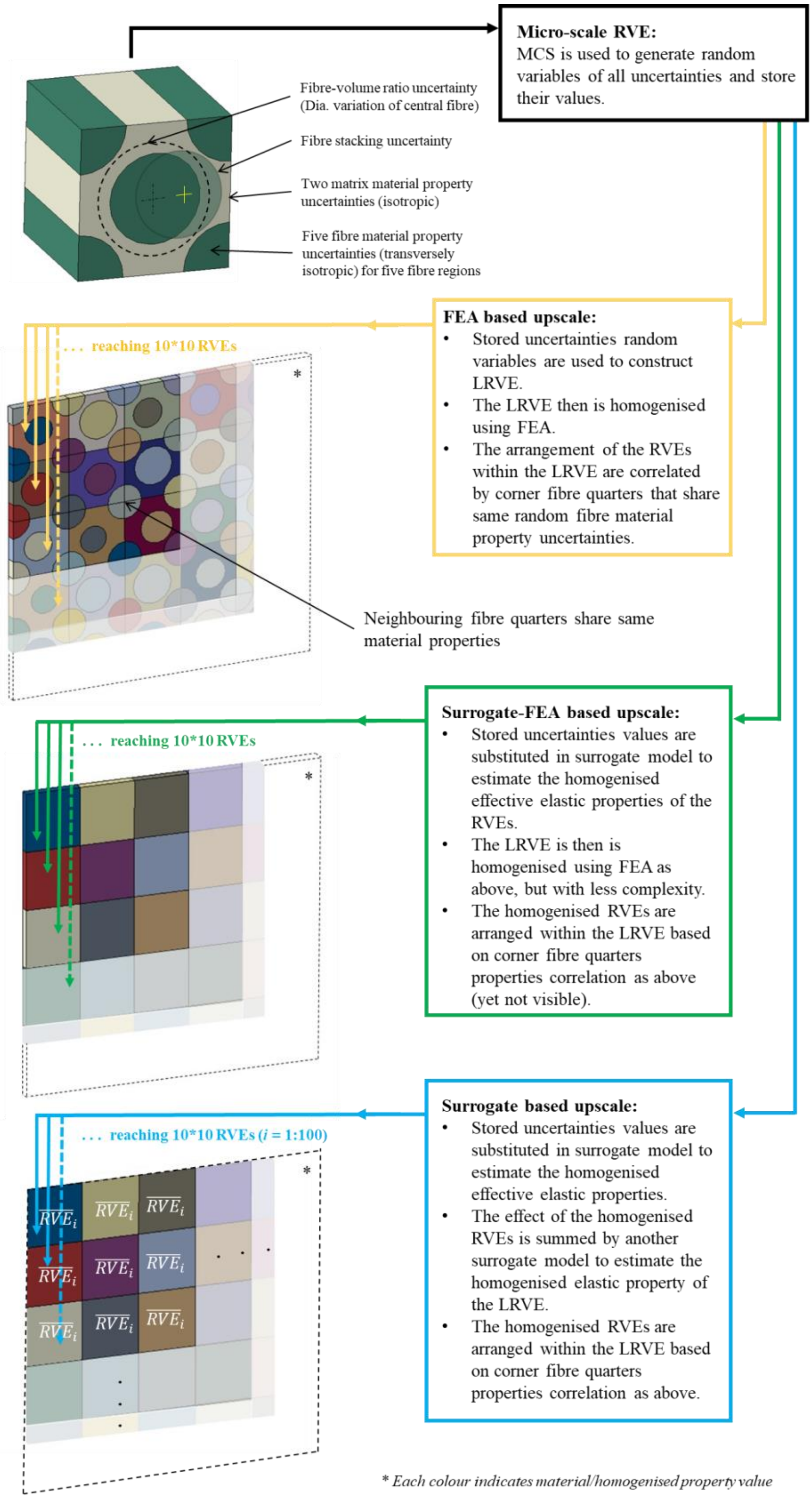


Fig. 2. The proposed frameworks to estimate the effective elastic properties of unidirectional composite lamina.

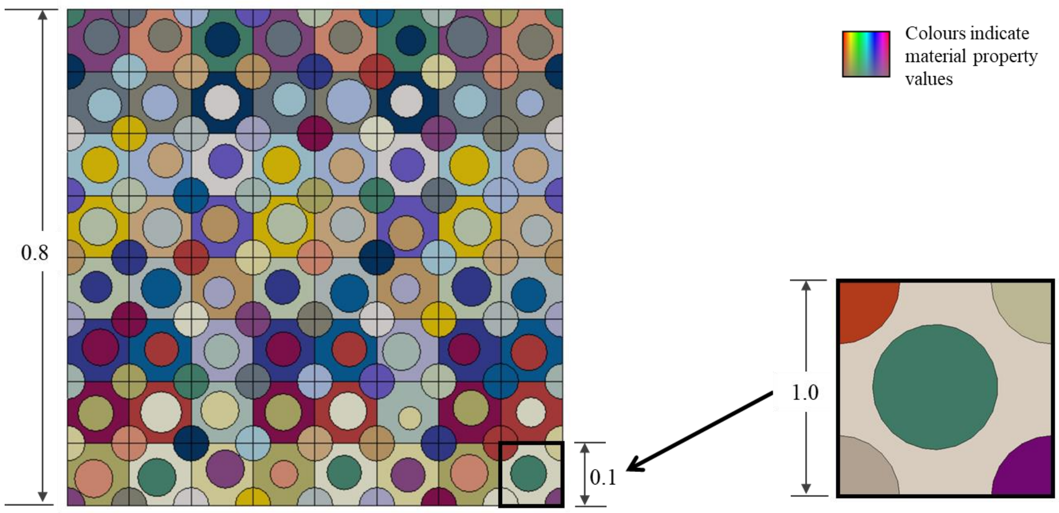
3 RESULTS AND DISCUSSIONS

In this study, *E*-glass fibre and Epoxy composite material properties are used to investigate the proposed frameworks. Properties are adopted from [12] and based on engineering assumptions for the statistical distribution. In addition, two geometric uncertainties are included, fibre stacking represented by radial displacement (r) with its direction (θ), and V_f ratio as shown in Table 1.

Table 1. Material properties and uncertainties.

Property/uncertainty	Fibre (E-glass)		Matrix (Epoxy)		Fibre-volume ratio V_f	Fibre stacking (r and θ)
	E (GPa)	υ (ratio)	E (GPa)	υ (ratio)		
Mean/lower limit	72.45	0.25	4.0	0.3	0.52	RVE centre, 0°
Distribution	Normal	Normal	Normal	Normal	Normal	Uniform
CoV/higher limit	10%	10%	10%	10%	10%	0.12, 360°

Based on the above, the three identified routs are constructed to establish a comparison. Initially, 64 RVEs (8*8) are randomly generated. All of which were placed in a specific arrangement within the LRVE based on fibre quarters correlation (as illustrated in Fig. 1 and Fig. 2). The generated LRVE is shown in Fig. 3.



Random LRVE ($\overline{RVE}_1, \overline{RVE}_2, \ldots, \overline{RVE}_{64}$) First small RVE ($\overline{RVE}_1$)

Fig. 3. A randomly generate LRVE with showing the first small RVE.

To validate the previously developed micro-scale surrogate model, the first generated RVE ($\overline{RVE}_1$) is investigated. The homogenised properties of this RVE are estimated by analysing it individually using EasyPBC; its properties are compared with the deterministic model (using mean values) showing considerable effect due to random uncertainties, see Table 2 (3). In the previous framework, this RVE is considered as an outputs and its properties are assigned to the macro-scale (see Fig. 1). Using the micro-scale surrogate models developed earlier, the elastic properties of this RVE can be estimated using FEA data points and uncertainty values without the need to directly analyse the modelled RVE. The associated error is low, as shown in Table 2 (5), except for v_{21} which requires further investigation.

Table 2. First small RVE FEA and surrogate model homogenised elastic properties.

Elastic property	Unit	(1) Deterministic model (FEA)	*(2)* $\overline{RVE}_1$ elastic properties (FEA)	(3) Effect % between (1)&(2)	(4) Micro-scale surrogate models	(5) Error % between (2)&(4)
E_{11}	GPa	39.57	43.91	11.0%	43.91	0.0%
E_{22}		9.37	11.73	25.3%	11.69	0.3%
E_{33}		9.37	11.56	23.4%	11.53	0.2%
G_{12}	GPa	4.34	5.38	23.9%	5.36	0.3%
G_{13}		4.34	5.25	21.0%	5.24	0.1%
G_{23}		4.89	5.94	21.4%	5.93	0.2%
v_{12}	ratio	0.270	0.269	-0.2%	0.270	0.2%
v_{13}		0.270	0.271	0.4%	0.271	0.2%
v_{21}		0.064	0.072	12.6%	0.073	1.2%
v_{23}		0.433	0.438	1.2%	0.438	0.1%
v_{31}		0.064	0.071	11.6%	0.072	0.6%
v_{32}		0.433	0.431	-0.3%	0.430	0.2%

Moving to the constructed LRVE, in the full FEA route the 64 RVEs form a LRVE are homogenised using EasyPBC. At which, three size of FEA wedge element are presented (0.004, 0.008, and 0.016 with a LRVE edge length of 0.8). The homogenised properties obtained are shown in Table 3. It is important to note that the 0.004 mesh size took more than 12 hours to complete using 6 CPU cores.

On the other hand, the Surrogate-FEA based route substitutes stored uncertainties values into the developed micro-scale surrogate models. The extracted homogenised properties are then assigned to construct a low fidelity LRVE model (only 64 FEA Hex elements as shown in Fig. 4). This model is analysed by EasyPBC to extract the homogenised elastic properties as explained earlier in Fig. 2 and shown in Table 3. Processing time of this model is significantly smaller than the previous, including the time required to prepare FEA data points used to develop the micro-scale surrogate models.

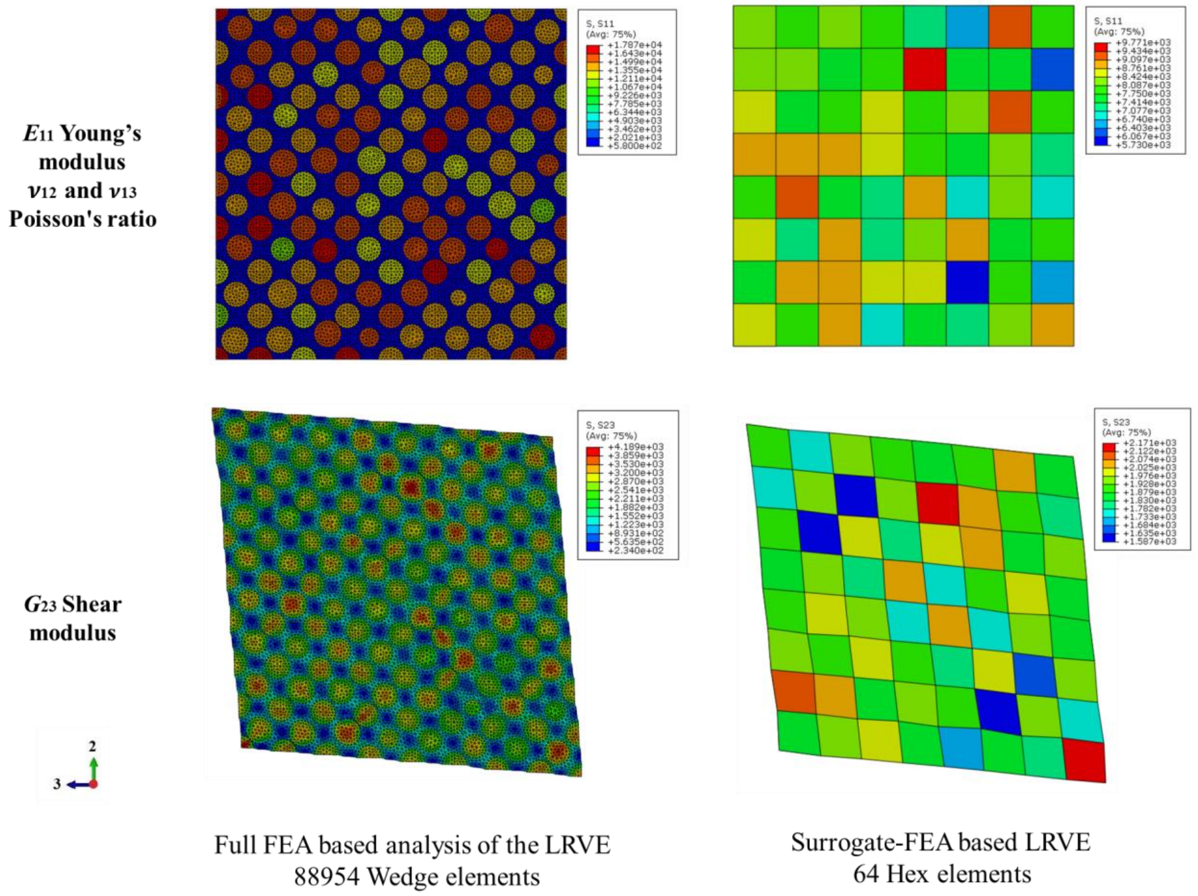


Fig. 4. Illustration of the numerical models for FEA based and surrogate-FEA based framework.

As for the Surrogate based route, the micro-scale surrogate models used above are employed to extract the homogenised elastic properties of all RVEs. In addition, a developed surrogate model replaces the low fidelity LRVE FEA analysis. This model is a polynomial-based fit that estimates the effect of small RVE property variation on the LRVE. This is done using three low fidelity LRVE FEA data points: an increased, deterministic, and decreased elastic properties of a single small RVE within the remaining 63 RVEs at the deterministic properties, fitted to form the macro-scale polynomial surrogate model. This surrogate model is implemented by substituting the homogenised properties of each RVE, then their corresponding effects are summed up to form the elastic properties of the LRVE as explained in Eq. 2 below:

$$E^{i}{}_{LRVE} = \sum\left(E^{i}{}_{\overline{RVE}_1}, E^{i}{}_{\overline{RVE}_2}, \ldots, E^{i}{}_{\overline{RVE}_N}\right) - (N-1) * E^{i}{}_{Det} \qquad \text{Eq. 2}$$

Where $E^{i}{}_{LRVE}$ is one of the approximated elastic properties of the LRVE, $E^{i}{}_{\overline{RVE}_{1,2,..N}}$is uncertainties effect of each RVE on the LRVE using macro-scale polynomial, N the total number RVEs within a LRVE, and $E^{i}{}_{Det}$ is the deterministic value of elastic property *i*. It is important to note that this technique ignores the effect of RVE location in relation to other RVEs within the LRVE. Results of implementing the above for the selected randomly generate LRVE are shown in Table 3. Furthermore, this approach is computationally cheap and thus feasible for reliability analysis using MCS.

In order to examine the results of all three routes, the fully FEA run of the randomly generated LRVE (mesh size of 0.004) is used as a reference value to measure the error for the other routes. Error magnitude of both surrogate-FEA based and surrogate based routes is relatively small. However, for this particular randomly generated example (and assumed distributions in Table 1), the difference between the reference and the deterministic homogenised elastic properties is low, and comparable to the observed error of the other methods (see Table 3). A possible reason is numerical error due to the fact that the mico-scale models and the deterministic run are developed using a different mesh size (0.02 with an RVE size of 1.0) compared with the 0.004 reference FEA. In addition, the developed technique to calculate the effective elastic properties in the third route did account for the effect of RVEs location within the LRVE. Therefore, further investigation is needed to address the accuracy and establish clear understanding using more LRVE samples.

Table 3. The Homogenised elastic properties and error for the proposed approaches.

Elastic property	Unit	Deterministic model (FEA)	Full FEA				Surrogate-FEA based		Surrogate based	
			0.016 mesh	0.008 mesh	0.004 mesh	Effect % between 0.004 mesh & Det. FEA	Estimated Properties	Error %	Estimated Properties	Error %
E_{11}	GPa	39.57	38.42	39.70	40.02	1.1%	40.12	0.2%	40.12	0.2%
E_{22}		9.37	9.66	9.54	9.46	1.0%	9.46	-0.1%	9.45	-0.1%
E_{33}		9.37	9.69	9.54	9.47	1.1%	9.47	0.0%	9.45	-0.3%
G_{12}	GPa	4.34	4.35	4.38	4.38	1.1%	4.41	0.5%	4.40	0.3%
G_{13}		4.34	4.35	4.38	4.38	1.0%	4.38	0.1%	4.39	0.2%
G_{23}		4.89	5.01	4.88	4.82	-1.5%	4.74	-1.6%	4.74	-1.6%
v_{12}	ratio	0.270	0.267	0.267	0.266	-1.3%	0.266	0.0%	0.267	0.2%
v_{13}		0.270	0.267	0.267	0.267	-1.1%	0.267	0.1%	0.267	0.1%
v_{21}		0.064	0.067	0.064	0.063	-1.4%	0.063	-0.4%	0.064	1.2%
v_{23}		0.433	0.394	0.413	0.419	-3.1%	0.416	-0.6%	0.417	-0.6%
v_{31}		0.064	0.067	0.064	0.063	-1.2%	0.063	-0.2%	0.064	0.6%
v_{32}		0.433	0.395	0.414	0.419	-3.1%	0.417	-0.6%	0.416	-0.8%

4 CONCLUSIONS

In this study, two surrogate-based methods are proposed and investigated for estimating the elastic properties of composite material with the presence of several uncertainties. A previously developed micro-scale surrogate model, which is used as a backbone for the proposed methods, is capable of generating relatively accurate property estimations (less than 1.0% error, except v_{23} and v_{32}). Correspondingly, the proposed surrogate-based methods deliver similar inherited error. However, this is considered relatively high as it is comparable to the effect of the uncertainties on the properties of a particular LRVE.

Due to the fact that the full FEA approach is not feasible for probabilistic reliability problems, the main advantage of both proposed methods is the reduction of processing time. However, there is a need to improve the accuracy of proposed methods by optimising the selection of data points, polynomial fits used, meshing, and considering the effect of RVE placement within the LRVE.

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