

Response statistics of composite structures with stochastic material properties based on microstructure

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Abstract

The stochastic finite element analysis of composite structures requires the accurate quantification of the random spatial variation of material properties at different scales [1]. In a recent paper by the authors [2], a Bayesian framework has been presented for determining the spatial variability of the apparent material properties of two-phase composites. Bayesian analysis allowed quantifying the uncertainty in the parameters of the respective mesoscale random fields through sampling from their posterior distribution. Moreover, it was shown that the exponential correlation model is the most plausible among different models belonging to the Matérn family through computing their respective posterior probabilities. In this paper, use is made of the above results to generate sample functions of the mesoscale random fields and to compute the probabilistic characteristics of the eigenfrequencies of composite structures. Parametric investigations are conducted to examine the effect of the identified random field parameters on structural response statistics.

1 Introduction

Composite materials display a random spatial variation of mechanical properties, attributed to the mismatch of the properties of their constituent materials. Structural analysis using the traditional Finite Element Method (FEM) in this case cannot account for all possible output scenarios. The Stochastic Finite Element Method (SFEM) [1] tackles this issue by taking the input uncertainty into account, propagating it through the system and assessing its stochastic response. This paper focuses on the response variability of composite structures as a continuation of the authors' previous work, since the parameters of the random input (material property fields) have been derived in [2].

In the case of composite materials, the macroscopic response of the structure is directly linked to the microscopic configuration, which is often plagued by uncertainty. Depending on the scale considered, the mechanical properties of a composite can display various degrees of spatial randomness, as shown in [3],[4]. Mesoscale random fields can be used to model this spatial variability [5], by applying homogenization in conjunction with the moving window technique [6], [7]. These fields will then serve as input in applying the SFEM and therefore identifying them is of paramount importance.

In [2], the authors applied Bayesian analysis to identify the parameters defining random property fields, given available composite microstructure data. In the Bayesian framework, field parameters are modelled as random variables and their full posterior distribution is obtained instead of a point estimate, while potential dependencies between these parameters are also revealed. In this particular case, the model parameters include the mean and standard deviation of the underlying field, as well as the correlation lengths in the x- and y- direction. Additionally, using the Bayesian approach, the most plausible correlation model belonging to the Matérn class was determined to be the exponential one, for the given microstructure data.

Having clearly defined the random mechanical properties of the composite structure, the next step would be to calculate the random structural response. Several recent papers have investigated the dynamic response variability of structures when material uncertainty is present. For example, the generalized variability response function (GVRF) methodology is employed in [8] to compute the displacement response and the effective compliance of linear plane stress systems. Geißendörfer et al. [9] proposed a stochastic multiscale method for the computation of the natural frequencies of metal foams, analyzing random field data derived from CT images. In [10], [11], random fields of the mesoscale elasticity tensor of polycrystalline materials are generated using Stochastic Volume Elements (SVEs) and SFE analysis is carried out, obtaining the resonance frequency of MEMS micro-beams using Monte Carlo Simulation (MCS) while establishing a link between the random field correlation and the SFE mesh size. In [12] random eigenvalue analysis is performed using MCS with an optimally selected start vector, while studying the effect of the material property field correlation length on the Coefficient Of Variation (COV) of the eigenvalue output. Naskar et al. [13] computed the stochastic natural frequencies of laminated composite beams with the Radial Basis Function (RBF) approach, considering randomness in the material properties and matrix cracking damage. A Spectral Stochastic Isogeometric Analysis method is proposed in [14] for free vibration analysis, obtaining the statistics of the eigenvalues and eigenvectors and showing its efficiency compared to MCS.

As an extension of previous publications by the authors [15], [4], the present work aims to compute the response variability of a composite structure, whose mechanical properties are modelled by random fields and their parameters have been obtained from Bayesian analysis for a given microstructure. Stochastic Finite Element analysis is carried out herein, studying the variability of the system eigenvalues (eigenfrequencies). The output variability is determined through MCS and the convergence of the eigenvalue statistics (mean, standard deviation) is investigated. Since the model parameters derived from Bayesian analysis are random variables, several combinations are tested, including fixing the parameters at their posterior values as well as accounting for their full uncertainty in assessing the posterior predictive random field. Random fields are generated with spectral covariance decomposition, which is a discrete form of the Karhunen-Loève (KL) expansion. The random eigenvalues of a simply supported and a cantilever beam are computed and results are also given at different scales, depending on the size of the moving window, which shows the amount of microstructure data taken into account.

The contents of this paper are as follows: In Section 2, the Bayesian approach for identification of random field parameters is explained and previous findings are reported. Section 3 contains a thorough description of the method adopted for the calculation of the structural response variability. Numerical results are presented and analyzed in Section 4, while useful conclusions are drawn in Section 5.

2 Bayesian identification of random material property fields

Before conducting a response analysis, it is vital to obtain accurate estimates of the random material property fields serving as model input. In the case of limited data, a Bayesian approach is well suited for the identification of the parameters of these random fields. In [4], starting with a computer simulated image of a two-phase composite, which can be seen in Fig.1, realizations of random fields of the elasticity tensor components are obtained, through homogenization and application of the moving window technique. Through this procedure, the composite is divided into Stochastic Volume Elements (SVEs) which are smaller than the Representative Volume Element (RVE) and possess random homogenized mechanical properties. The random field is then constructed from considering these properties at the center of the SVEs.

Different mesoscale random fields are obtained from the same composite image, depending on the moving window size. The non-dimensional scale factor $\delta = L/d$ is used to characterize each mesoscale model, where L is the moving window size, d is the inclusion diameter and $\delta \in [1, \infty]$. By adjusting the moving window size, random fields at two different scale factors are obtained, $\delta_1 = 11.21$ and $\delta_2 = 22.42$, leading to 3249 and 625 SVEs, respectively [5]. While using a larger scale factor can save computational cost from analyzing fewer SVEs, the modelling of the composite is considered less accurate.

The examined composite contains a volume fraction $v_f = 40\%$ of randomly dispersed circular inclusions with a diameter $d = 7.14 \mu m$, while it has a stiffness ratio $E_{incl}/E_m = 1000$. According to [4], a lognormal

marginal distribution is well suited for a property field with such a high stiffness ratio. The elasticity components investigated are the axial stiffness C_{11} and the shear stiffness C_{33} of the 2-D elasticity tensor, which, under the isotropy assumption, is given by the following equation:

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ & C_{22} & 0 \\ \text{symm} & & C_{33} \end{bmatrix} \quad (1)$$

with $C_{11} = C_{22}$ and $C_{12} = C_{11} - C_{33}$.

Figs.2, 3 show the computed realization of the random field, as well as its empirical marginal distributions and 2-D autocorrelation functions for the C_{11} and C_{33} components of the apparent elasticity tensor. As the scale factor increases, i.e. less microstructure data is taken into account, the correlation length is increased, leading to reduced spatial variability. In the limit case of $\delta \rightarrow \infty$, the random fields become fully correlated, as the moving window reaches the RVE size. Having obtained one realization of the random property fields and with no additional microstructure information available, Bayesian inference can be applied to learn the parameters of an adopted model of the mesoscale random fields.

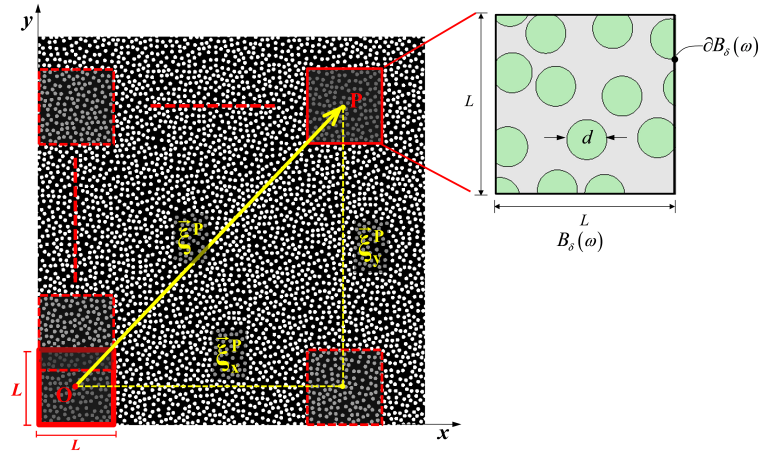


Figure 1: Illustration of the composite material and the moving window technique.

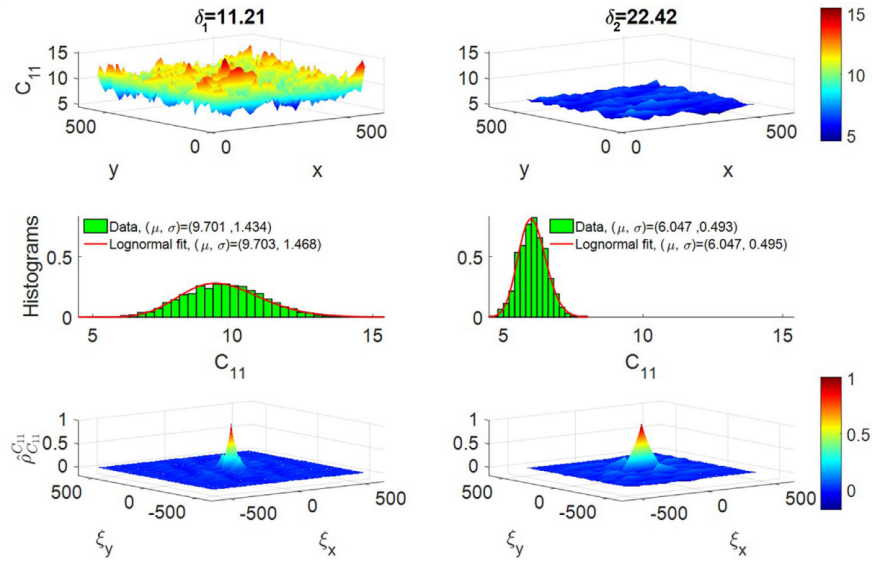


Figure 2: Mesoscale random fields of elasticity tensor component C_{11}

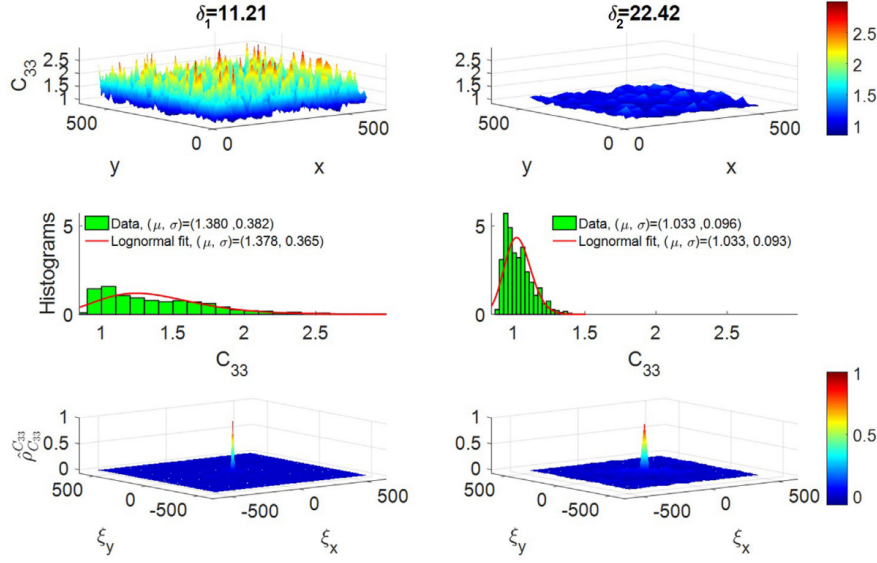


Figure 3: Mesoscale random fields of elasticity tensor component C_{33}

2.1 Bayesian identification of model parameters and model selection

In the Bayesian approach, model parameters are regarded as random variables and using Bayes' rule, their full posterior distribution is determined given available microstructure data, instead of a single point estimate. Consider a homogeneous random field $A(\omega, \mathbf{x})$, with $\mathbf{x} \in B_\delta$, defined in terms of a model M with parameter vector $\boldsymbol{\theta} \in \mathbb{R}^m$. B_δ is a SVE of the composite (see Fig.1) and ω denotes the randomness of a quantity. $A(\omega, \mathbf{x})$ models a component of the apparent elasticity tensor, for some mesoscale size δ . We are interested in learning the vector $\boldsymbol{\theta}$ using direct measurements of the random field $\mathbf{d} = [a^1; \dots; a^{n_d}]$ at locations $\mathbf{x}^1, \dots, \mathbf{x}^{n_d}$. The measurement locations refer to the midpoint positions of the moving window and the data \mathbf{d} refers to the corresponding homogenized property values. Bayesian analysis is employed to learn the vector $\boldsymbol{\theta}$. That is, a prior density $f(\boldsymbol{\theta}|M)$ given the model M is imposed, describing prior knowledge on the model parameters, i.e. before measurements become available, and Bayes' rule is applied to update the prior density given the data. Bayes' rule states:

$$f(\boldsymbol{\theta}|\mathbf{d}, M) = c_{E|M}^{-1} L(\boldsymbol{\theta}|\mathbf{d}, M) f(\boldsymbol{\theta}|M) \quad (2)$$

where $f(\boldsymbol{\theta}|\mathbf{d}, M)$ is the posterior density of the parameters given the data \mathbf{d} and model M , and $L(\boldsymbol{\theta}|\mathbf{d}, M)$ is the likelihood function, describing the measurement information. The reciprocal of the proportionality constant, $c_{E|M}$, is the evidence of model class M and is given by the integral:

$$c_{E|M} = \int_{\mathbb{R}^m} L(\boldsymbol{\theta}|\mathbf{d}, M) f(\boldsymbol{\theta}|M) d\boldsymbol{\theta} \quad (3)$$

Consider first the case where the random field $A(\omega, \mathbf{x})$ is Gaussian. Then, $\boldsymbol{\theta}$ includes the mean μ , standard deviation σ and parameters of the correlation kernel of the field $\rho(\boldsymbol{\xi}|\boldsymbol{\theta}_\rho)$, with $\boldsymbol{\xi} = (\xi_x, \xi_y)$ being the space lag; i.e. $\boldsymbol{\theta} = [\mu; \sigma; \boldsymbol{\theta}_\rho]$. If $A(\omega, \mathbf{x})$ is a non-Gaussian homogeneous translation field, then it is given by:

$$A(\omega, \mathbf{x}) = F^{-1} \cdot \Phi[U(\omega, \mathbf{x})] \quad (4)$$

where F^{-1} is the inverse of the marginal cumulative distribution function (CDF) of $A(\omega, \mathbf{x})$, $U(\omega, \mathbf{x})$ is a standard Gaussian field and Φ is the standard normal CDF. In such case, $\boldsymbol{\theta}$ includes the parameters $\boldsymbol{\theta}_F$ of the marginal distribution of $A(\omega, \mathbf{x})$ and the parameters $\boldsymbol{\theta}_\rho$ of the correlation kernel of $U(\omega, \mathbf{x})$, i.e. $\boldsymbol{\theta} = [\boldsymbol{\theta}_F; \boldsymbol{\theta}_\rho]$. We note that the finite dimensional distribution of the random field defined by Eq.4 is a

Gaussian copula model and its likelihood function can be found in [2]. For the case that the marginal distribution of translation field is of the lognormal type, Eq.4 takes the following form:

$$A(\omega, \mathbf{x}) = \exp[\mu_G + \sigma_G U(\omega, \mathbf{x})] \quad (5)$$

where $U(\omega, \mathbf{x})$ is an underlying Gaussian field and μ_G, σ_G are auxiliary parameters of the transform.

The posterior distribution is often obtained numerically, due to the difficulty in evaluating the normalizing constant c . An adaptive version of the BUS approach (Bayesian Updating with Structural reliability methods) combined with Subset Simulation (SuS) is adopted in [2], yielding a sample approximation of the posterior distribution along with an estimate of the model evidence. More details regarding the implementation of the BUS-SuS approach can be found in [16].

The Bayesian approach is not limited to parameter identification but can also be used for model selection by computing the posterior probabilities $\Pr(M_i|\mathbf{d}, \mathbf{M})$ of different candidate random field models M_i (with various correlation kernels or marginal distributions) given the data. The probabilities $\Pr(M_i|\mathbf{d}, \mathbf{M})$ provide a rational means for selecting the most appropriate (plausible) model among a set of models as the one that maximizes $\Pr(M_i|\mathbf{d}, \mathbf{M})$ with respect to i .

2.2 Bayesian analysis results

Bayesian analysis was first performed to obtain the most plausible correlation model, belonging to the Matérn class, by varying the smoothness parameter ν . The anisotropic version of the Matérn auto-correlation function adopted herein is given by the following equation [17]:

$$\rho_\nu(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}r\right)^\nu K_\nu\left(\sqrt{2\nu}r\right) \quad (6)$$

where Γ is the gamma function, K_ν is the modified Bessel function of the second kind, ν is a non-negative smoothness parameter and r is defined as:

$$r = \sqrt{\left(\frac{\xi_x}{b_x}\right)^2 + \left(\frac{\xi_y}{b_y}\right)^2} \quad (7)$$

with (ξ_x, ξ_y) being the space lags along the axes x, y and b_x, b_y the respective non-negative correlation length parameters. The exponential ($\nu = 1/2$), modified exponential ($\nu = 3/2$) and squared exponential ($\nu \rightarrow \infty$) models belong to the Matérn family of autocorrelation functions [18]. Results showed the most plausible model to be the exponential one ($\nu = 1/2$) for the C_{11} component. In that case, the autocorrelation function is reduced to the following equation:

$$\rho_{1/2}(r) = \exp(-r) \quad (8)$$

For the shear stiffness C_{33} , all correlation models were nearly equally matching, with a slight preference for the exponential one. As a result, this model is adopted for both tensor components in the present paper.

Following the correlation model selection, the posterior distributions of all model parameters are obtained, which are depicted in Fig.4 for stiffness components C_{11}, C_{33} and scale factors δ_1 and δ_2 . Note that Bayesian analysis revealed a positive correlation between the correlation lengths b_x, b_y and the standard deviation of the underlying Gaussian field σ_G (see [2]). Subsequently, characteristic values of these parameters can be drawn from the given PDFs and used in a response analysis. For instance, the mean values of all parameters can be used or even the posterior predictive random field can be derived through generating random fields conditional on samples from the posterior distribution. It is also worth noting that Bayesian analysis results are affected by the moving window size and a smaller window (smaller scale factor) will lead to less variable model parameters, since more microstructure data is taken into account.

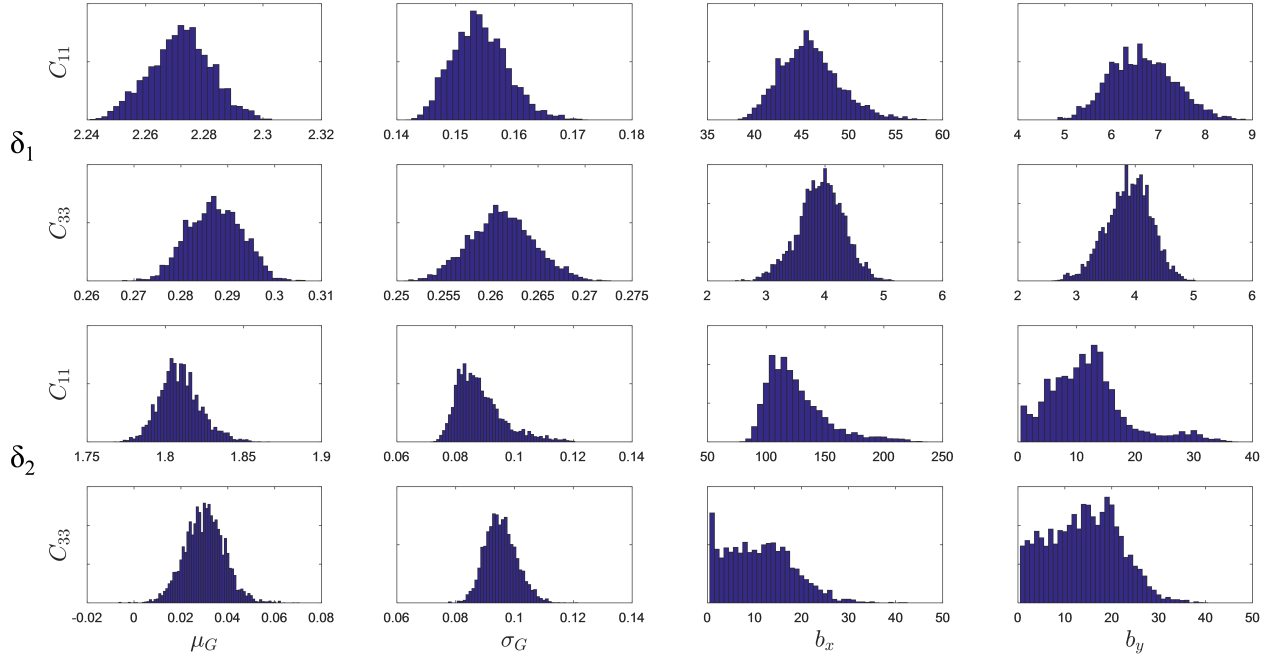


Figure 4: Random field parameter posterior distributions for elasticity tensor components C_{11} and C_{33} at mesoscale sizes $\delta_1 = 11.21$ and $\delta_2 = 22.42$

3 Computation of structural response variability

Following the random field parameter identification, response variability analysis of the composite structure is the next step in the SFEM approach. As the use of finite elements with random properties is involved, a technique for assigning discrete values of the random property fields is needed. In this paper the discrete form of the KL-expansion is applied to discretize the random fields, which is also called the covariance decomposition method. SFEM is conducted via MCS, meaning a large number of samples are generated and analyzed. The response variability is studied and the effect of the input random field parameters derived through Bayesian analysis is investigated across different scales.

3.1 Random field discretization using covariance decomposition

Uncertainty propagation and computation of the response requires not only identifying the parameters of the input random fields, but also their discretization and generation of respective sample functions. Among the existing methods used for random field discretization, a discrete form of the KL expansion is adopted in this work, which is also called spectral or modal covariance decomposition [19]. In the general case when the random field to be generated is non-Gaussian, covariance decomposition can be applied on an underlying Gaussian random field $U(\omega, \mathbf{x})$ and then realizations of the non-Gaussian random field can be obtained through the transformation of Eq.4. From this point on ω , which denotes the randomness of a quantity, will be omitted for simplicity.

Consider an approximation of a standard Gaussian random field $U(\mathbf{x})$, expressed in terms of the finite random vector $\mathbf{U} = [U_1, \dots, U_n]^T$, whose values are given, for instance, at the midpoints of a finite set of subdomains called stochastic elements [20]. The covariance matrix Σ_{UU} of the random vector \mathbf{U} can be obtained through evaluating the autocovariance of the random field $U(\mathbf{x})$ at the element midpoints. Since the covariance matrix is $n \times n$ bounded, symmetric and positive semi-definite, it has n real non-negative eigenvalues $\tilde{\lambda}_i$ and corresponding eigenvectors \mathbf{v}_i . Thus it can be decomposed as follows:

$$\Sigma_{UU} = \sum_{i=1}^n \tilde{\lambda}_i \mathbf{v}_i \mathbf{v}_i^T \quad (9)$$

The eigenvectors are orthogonal and we further assume that they have been normalized. Therefore, they form a basis in \mathbb{R}^n , meaning every element of \mathbb{R}^n can be expressed as a linear combination of the eigenvectors \mathbf{v}_i . Since the random vector \mathbf{U} is an element of \mathbb{R}^n , it can be represented as a linear combination of the eigenvectors \mathbf{v}_i multiplied by random amplitudes. As a result, the random vector can be expressed as follows:

$$\mathbf{U} = \sum_{i=1}^n \sqrt{\tilde{\lambda}_i} \mathbf{v}_i \zeta_i \quad (10)$$

where $\zeta_i, i = 1, \dots, n$ are random variables, which due to the orthonormality of the eigenvectors are given by:

$$\zeta_i = \frac{1}{\sqrt{\tilde{\lambda}_i}} \mathbf{v}_i^T \mathbf{U} \quad (11)$$

From Eq.11 it becomes apparent that the variables ζ_i have zero mean and are orthonormal, i.e., it holds:

$$E[\zeta_i] = 0, \quad E[\zeta_i \zeta_j] = \delta_{ij} \quad (12)$$

Since \mathbf{U} is Gaussian, the random variables ζ_i are independent standard normal random variables. As a result, simulation of the standard Gaussian random field $U(\mathbf{x})$ can be achieved by drawing realizations of ζ_i and applying Eq.10.

3.2 Structural response variability

Stochastic finite element analysis of 2-D composite structures is carried out herein. The input uncertainty is limited to the elastic tensor components, which are described by random fields. These fields are homogeneous, have lognormal distributions and their correlation structure is of the Matérn class. Through Bayesian analysis, the parameters defining these fields have been identified from given computer generated microstructure data. Subsequently, sample functions of these fields are generated with the covariance decomposition method. As a result, input uncertainty can be propagated through the structure with a suitable technique and the macroscopic response can be computed.

Response variability analysis is therefore conducted with MCS. A number of samples of the material property fields are generated, finite element analysis is carried out for each sample and the statistics of the eigenvalues are examined. The convergence of the estimated response statistics is observed through plotting the mean and COV of the response quantity against the number of MCS samples. The effect of random field parameter variability derived from Bayesian analysis is investigated. Results are reported at two different scales, corresponding to scale factors δ_1 and δ_2 .

According to [1], care must be taken, in order to match the stochastic element mesh size with the spatial variability of the random fields and as a result, the element length should lie between $b/4$ and $b/2$, where b is the correlation length. In the present work, since the property fields are statistically anisotropic, the minimum of both correlation lengths (x - and y - direction) is used to calculate the element length.

In all FE models analyzed, the plane stress assumption is made while using a unit thickness. The response variability is studied by conducting random eigenvalue analysis. The first 15 eigenvalues are computed, sorted in increasing order and their statistics are analyzed. Eigenvalues are vital in the calculation of the dynamic response of structures in the framework of modal analysis and it is crucial to investigate how they are affected by input uncertainty. It should be noted that this paper only focuses on uncertain mechanical properties and thus the composite density affecting the mass matrix is not considered spatially varying.

However, such an extension is possible through the authors' proposed multiscale framework and can be implemented in future works.

4 Results and discussion

This section contains the results of the SFE analysis. For each model, 1000 MCS are performed for different samples of the mesoscale random property fields and statistical convergence is achieved within this number of MCS. The parameters defining these fields, given by the random vector $\theta = [\mu_G, \sigma_G, b_x, b_y]$, are the mean and standard deviation of the marginal distribution of the underlying Gaussian field, as well as the correlation lengths in the x - and y - directions. Four different types of random field parameter combinations are examined: the *(mean)*, *(mean-COV · mean)*, *(mean + COV · mean)* as well as a predictive case, for which a random field realization is generated for posterior samples from the parameter vector θ . The difference in analyzing the microstructure in more detail (smaller scale factor δ_1) versus less detail (larger scale factor δ_2) is also visualized. It should be noted that random field parameters in the predictive case for δ_2 have been selected such that correlation lengths lower than $2 \mu m$ are excluded from MCS in order to achieve a reasonable finite element size and computational cost.

4.1 Simply supported beam

In this problem, the first 15 eigenvalues (eigenfrequencies) of a simply supported beam, which is shown in Fig.5, are calculated. Results are displayed in Figs.6 and 7.

For both scale factors, the means of the eigenvalues appear unaffected by the Bayesian analysis-derived random field parameters. The choice of parameters does affect the eigenvalue COV, however, and a more variable COV is observed in the higher mesoscale size δ_2 . This can be explained by the Bayesian analysis yielding random field parameters with more variability, as the moving window size increases, due to limited microstructure data being available. While the eigenvalue COV is more variable in the higher mesoscale size, for all parameter combinations examined, it is lower than the COV of the lower mesoscale size δ_1 . Additionally, the mean eigenvalues in the lower mesoscale size are higher than those of the higher mesoscale size. Increased variability of the response in the lower mesoscale sizes is expected due to the more detailed modelling of the heterogeneous microstructure and has also been observed in [4].

Regarding the specific parameter combinations, the COV appears to increase as parameters are chosen towards the right tail of their distributions. For instance, the response variability for the *(mean + COV · mean)* case is the largest compared to that of the other parameter combinations tested. This effect is also expected, since simultaneously increasing the correlation lengths and the point variance σ_G will lead to an increased output COV in the structural problem. Lastly, random selection of the random field parameters (predictive distribution) is shown to lead to a response resembling the one given by the mean parameters for both scale factors.

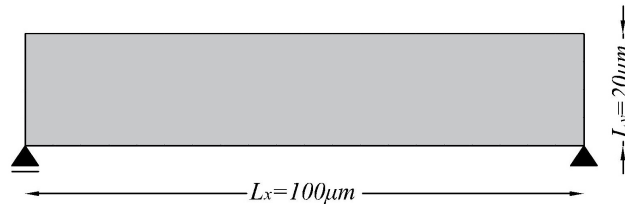


Figure 5: Simply supported beam

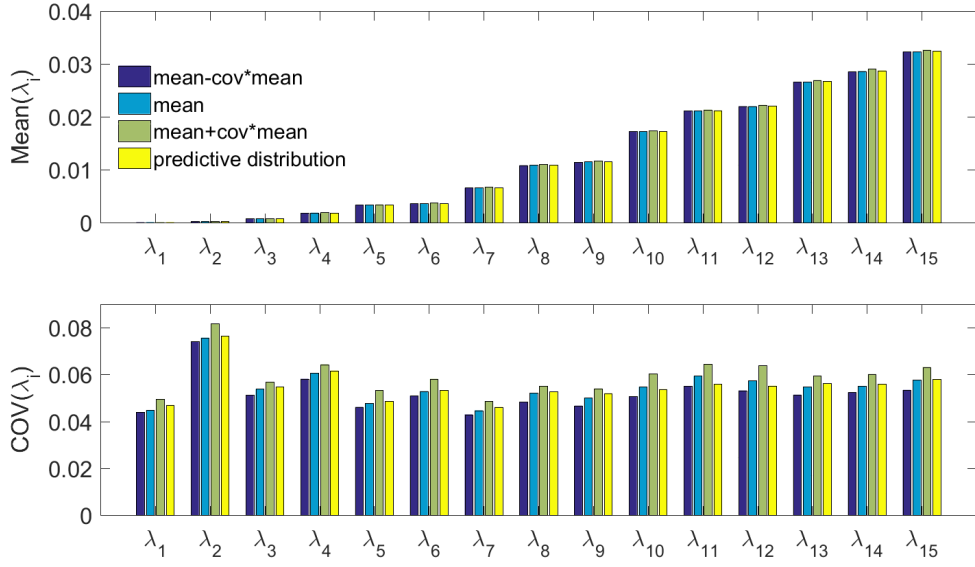


Figure 6: Mean, COV of eigenvalues for δ_1 , simply supported beam

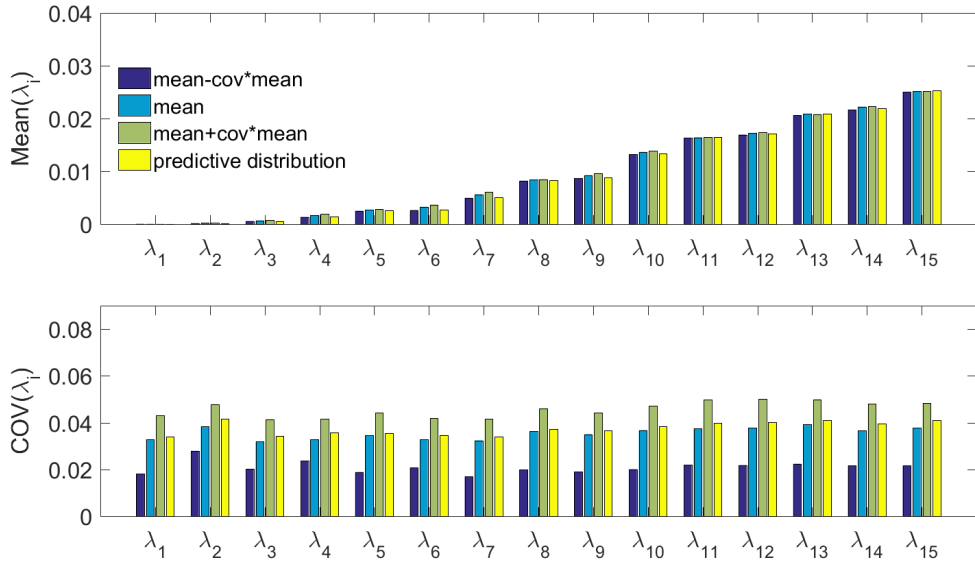


Figure 7: Mean, COV of eigenvalues for δ_2 , simply supported beam

4.2 Cantilever beam

In the second example, the eigenvalues of a cantilever beam, shown in Fig.8, are examined. Results are displayed in Figs.9 and 10.

Similarly to the previous results, the mean does not depend on the input field parameters chosen. Significant differences in the eigenvalue COV are observed for different field parameters for the higher mesoscale size δ_2 with the $(\text{mean} + \text{COV} \cdot \text{mean})$ parameter case again showing the highest COV among the selected parameters combinations. Nonetheless, the output COV for the higher mesoscale size δ_2 is lower than that of the lower mesoscale size δ_1 .

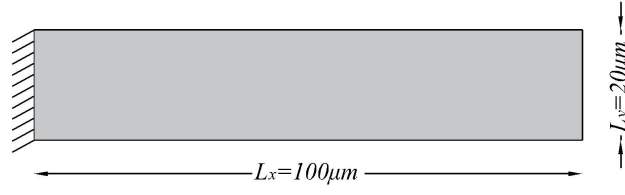


Figure 8: Cantilever beam

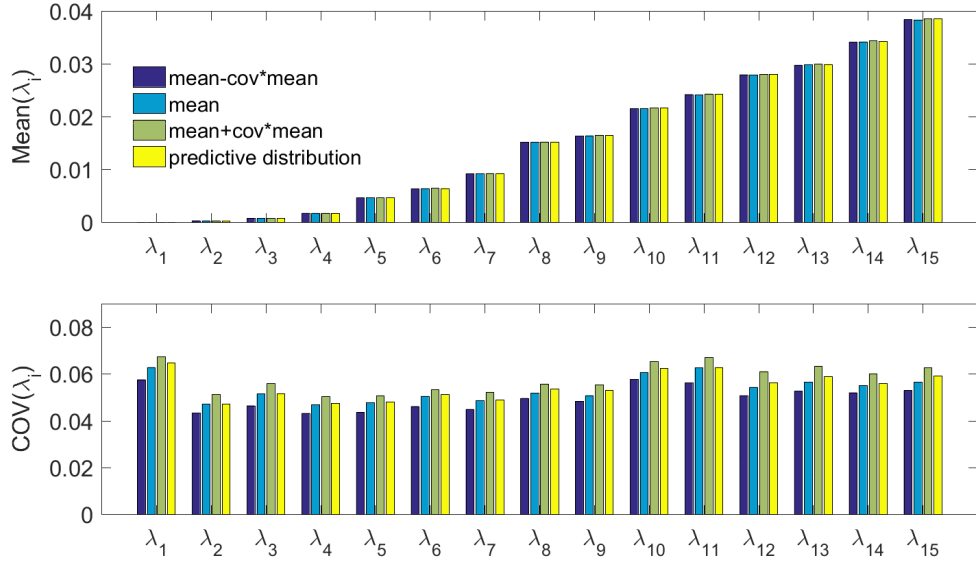


Figure 9: Mean, COV of eigenvalues for δ_1 , cantilever beam

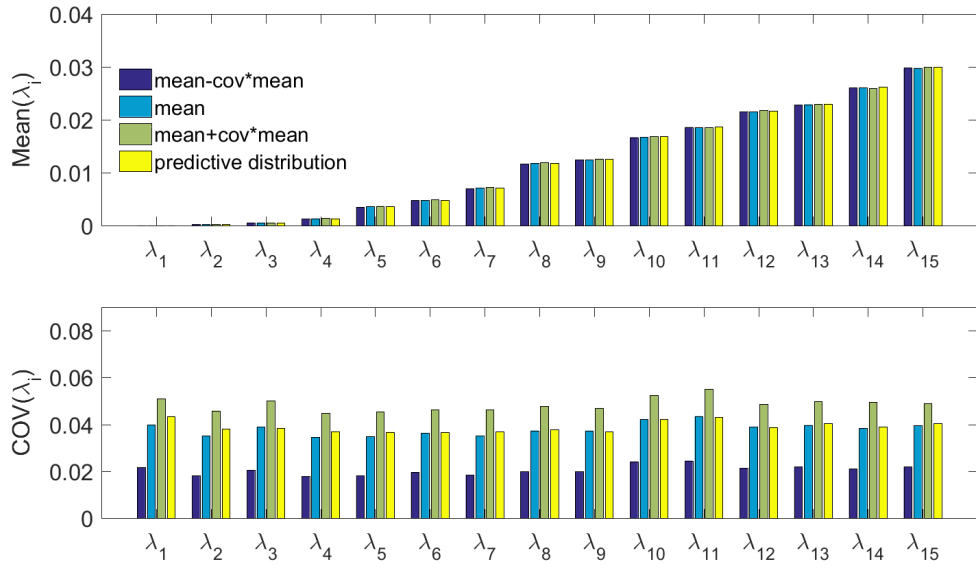


Figure 10: Mean, COV of eigenvalues for δ_2 , cantilever beam

5 Conclusions

In this paper, a complete link is established between composite microstructure and the dynamic response characteristics at the macroscale. The uncertain parameters of the mesoscale random fields describing the spatially variable material properties serve as input in the SFE analysis of composite structures and their effect on the statistical characteristics of the eigenvalues is examined.

In all cases studied, the means of the eigenvalues appear unaffected by the chosen random field parameters. For the smaller mesoscale size, the output COV is only slightly affected by the random field parameters. In the larger mesoscale size, however, different parameter choices have significant effect on the response COV. The substantial effect of uncertain random field parameters on the response variability observed in higher mesoscales can be explained by the fact that Bayesian analysis results are more variable in this case due to the smaller amount of microstructure data. Despite being less affected by the model parameters, the eigenvalue COV in the lower mesoscale size is shown to be larger than that in the higher mesoscale size. The methodology followed herein can be useful for the computation of the dynamic response (e.g. displacement) of composite structures using modal analysis.

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