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A MULTISCALE FRAMEWORK FOR THE STOCHASTIC ASSIMILATION AND MODELING OF UNCERTAINTY ASSOCIATED NCF COMPOSITE MATERIALS (ECCOMAS CONGRESS 2016)

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Abstract. *A multiscale framework to construct stochastic macroscopic constitutive material models is proposed. A spectral projection approach, specifically polynomial chaos expansion, has been used to construct explicit functional relationships between the homogenized properties and input parameters from finer scales. A homogenization engine embedded in Multiscale Designer, software for composite materials, has been used for the upscaling process. The framework is demonstrated using non-crimp fabric composite materials by constructing probabilistic models of the homogenized properties of a non-crimp fabric laminate in terms of the input parameters together with the homogenized properties from finer scales.*

1 INTRODUCTION

Conventional approaches to perform multiscale designs have been to average over the fluctuations of the material properties throughout the scales. In these approaches it is possible to deduce the constitutive material properties at the macroscopic scale from information available at finer scales [1], where the properties are computed by averaging over fluctuations in the stress response of the material. For instance, to deduce the material properties of continuous non-crimp fabric (NCF) composite materials, the averaged homogenized properties of a unit cell of a unidirectional lamina (consisting of a tow surrounded by resin within a bounded volumetric unit), at the so-called meso-scale are required. These meso-scale properties of the tow are in turn homogenized properties from its constituents at a finer scale, i.e., micro- scale.

Robust designs for such complex systems, where properties across scales matter, require reliable accounting of the material features as well as the fluctuations and uncertainties associated with the description and the performance of the constitutive representations at the various scales of interest. The main objective of this work is to propose a multiscale framework that is able to account for uncertainties associated with finer scales explicitly. The multiscale framework is demonstrated by performing stochastic modeling of an NCF composite material across multiple scales. Specifically, the uncertainties associated with three hierarchical scales have been assimilated from available measurements and propagated throughout the scales. A Polynomial Chaos (PC) spectral projection approach [2] has been used to construct the hierarchical functional relationships throughout the scales. The hierarchy of the scales starts at the scale of the fibers and resin within the tows and goes upward to construct stochastic constitutive models of a laminate or a structure composed of composite laminates. A homogenization engine embedded in Multiscale Designer [3], software for composite materials, has been used for the upscaling process. The proposed framework (i) is suitable for the modeling and analysis of composite materials, (ii) can be generalized to account for the behavior of physical systems containing composite parts, and (iii) can be incorporated in inverse calibration frameworks.

2 DEFINITION OF THE COMPOSITE MATERIALS

The proposed multiscale framework is used to construct probabilistic models of composite laminates that are up-scaled across multiple scales. The composite laminates consist of eight laminae made of continuous non-crimp fabric (NCF). That is, each lamina is composed of continuous unidirectional tows and resin. The carbon fiber tows are made of 12K fibers (T700SC 12000 50C). The laminate is designed to be symmetric such that the laminae are oriented as $[0/45/-45/90/90/-45/45/0]$.

3 DEFINITION OF THE SCALES AND THE RESPECTIVE ASSOCIATED PARAMETERS

The NCF laminate, used in this study, is composed of 8 laminae. Each lamina is composed of unidirectional tows and resin. The tows are composed of fibers with resin filling the space between the fibers. Thus, the properties of the fibers and resin are required to predict the constitutive properties of the tows. Then, the properties of the composite tows and those of the resin again are required to predict the constitutive properties of the NCF unidirectional lamina, which in turn together with other laminae, being oriented according to a certain layout, are required to predict the constitutive properties of the eight-layer laminate. The chart depicted in Figure 1 defines the multiple scales involved in the aforementioned upscaling process.

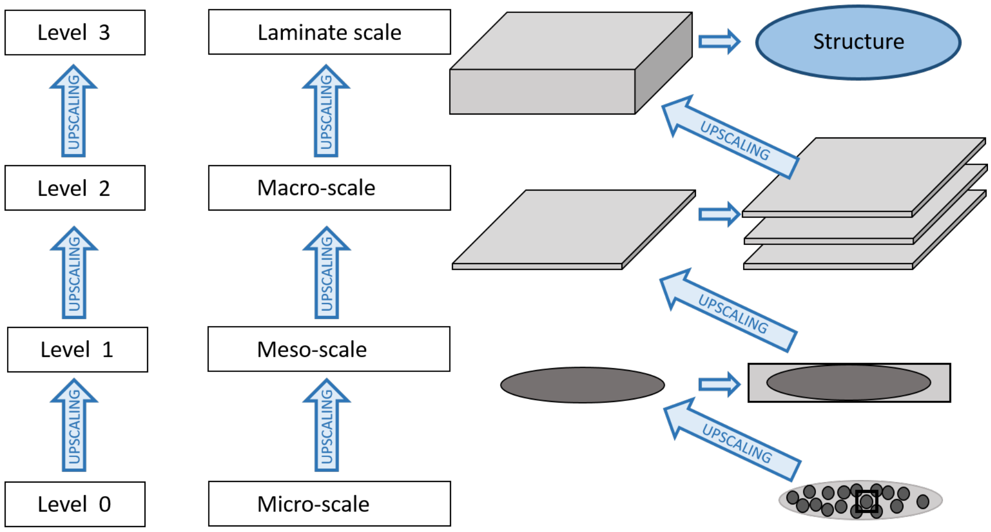

Figure 1: Schematic definition of the multiple scales.

The input parameters at each scale are grouped as (a) the parameters introduced at the scale (l) and which are characterized from available data at this scale, and (b) the parameters that are up-scaled from level ($l-1$). The parameters belonging to the first group are denoted by $\mathbf{P}^l$, where l refers to the respective scale. These groups are specific inputs to each level l; i.e., $\mathbf{P}^0$ is a group of inputs at level 0, and so on. The parameters belonging to the second group are denoted by $\mathbf{Q}^l$. The parameters from this group are input parameters at level l that have been obtained via an upscaling process from level $l-1$ to level l. The parameters from both groups are defined in the following subsections at each level.

3.1 Input parameters associated with level $l = 0$

The set of input parameters at level $l = 0$, $\mathbf{P}^0$, consists of three groups $\mathbf{P}^0_g$, $\mathbf{P}^0_f$,and $\mathbf{P}^0_m$ representing the parameters associated with the geometry of the unit cell, the material properties of transverse isotropic fibers, and the material properties of isotropic matrix, respectively.

Group	Parameter	Description
$\mathbf{P}^0_g$	$V_f^{F,T}$ %	Volume fraction of fiber within the tow
$\mathbf{P}^0_f$	$E_{f,A}$	Axial Young's modulus of fibers
	$E_{f,T}$	Transverse Young's modulus of fibers
	$G_{f,A}$	Axial shear modulus of fibers
	$\nu_{f,A}$	Axial Poisson's ratio of fibers
	$\nu_{f,T}$	Transverse Poisson's ratio of fibers
$\mathbf{P}^0_m$	E_m	Young's modulus of the matrix
	ν_m	Poisson's ratio of the matrix

Table 1: Input parameters $\mathbf{P}^0$ at level $l = 0$.

These parameters are modeled by uniform random variables. The volume fraction of fibers within the tow is denoted by $V_f^{F,T}$. The subscripts A and T, used with the tow material properties, denote the axial and transverse properties, respectively.

3.2 Input parameters associated with level $l = 1$

The set of input parameters at level $l = 1$, $\mathbf{P}^1$, consists of two groups $\mathbf{P}^1_g$ and $\mathbf{P}^1_m$ representing the parameters associated with the geometry of the unit cell in a NCF lamina and the material properties of an isotropic matrix, respectively. These parameters are modeled by uniform random variables.

Group	Parameter	Description
$\mathbf{P}^1_m$	E_m	Young's modulus of the matrix
	ν_m	Poisson's ratio of the matrix
$\mathbf{P}^1_g$	D_a	Major diameter of the tow
	d_a	Free distance along the major axis
	D_b	Minor diameter of the tow

Table 2: Input parameters $\mathbf{P}^1$ at level $l = 1$.

The geometry parameters define the dimensions of the unit cell of a NCF unidirectional lamina and are listed in Table 2. These are illustrated by the drawing in Figure 2, where D_a and D_b refer to the diameters of the tow along the major and minor directions, d_a and d_b refer to the gap between the tows along the major and minor directions, which are filled in by the matrix. Here, d_b is assumed to be constant and equal to $0.1\ mm$. The dimensions of the unit cell are denoted by $S_a = D_a + d_a$ and $S_b = D_b + d_b$.

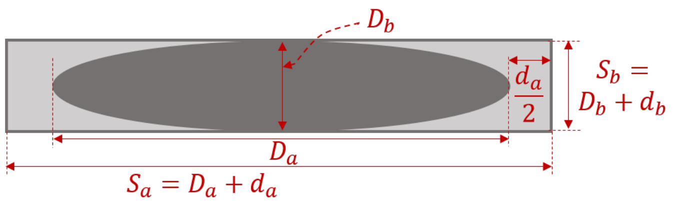

Figure 2: A schematic drawing of a unit cell in a NCF unidirectional lamina.

In addition, another set of input parameters at this scale is $\mathbf{Q}^1$, the set of homogenized material properties of the tow. These are the outcome of the homogenization H_1 associated with the upscaling process from level $l = 0$ to level $l = 1$.

Group	Parameter	Description
$\mathbf{Q}^1$	$E_{t,A}$	Axial Young's modulus of tow
	$E_{t,T}$	Transverse Young's modulus of tow
	$G_{t,A}$	Axial shear modulus of tow
	$\nu_{t,A}$	Axial Poisson's ratio of tow
	$\nu_{t,T}$	Transverse Poisson's ratio of tow

Table 3: Input parameters $\mathbf{Q}^1$ at level $l = 1$.

The material properties of the homogenized tow, which manifest a transverse isotropic symmetry, are denoted by $\mathbf{Q}^1 = (E_{t,A},\ E_{t,T},\ G_{t,A},\ \nu_{t,T},\ \nu_{t,A})$; where the subscript t refers to the tow and the subscripts A and T refer to the axial and transverse properties, respectively.

3.3 Input parameters associated with level $l = 2$

The input parameters at level $l = 2$, $\mathbf{P}^2$, consists of the geometry layout of the laminae within the eight-layer laminate, $\mathbf{P}_g^1$. The orientation of the unidirectional laminae is defined as $[0/45/-45/90]_s$, where the upper and lower laminae are oriented along the 0^o axis. The number of laminae is fixed for the laminate analyzed in this paper. The orientation of each lamina is also considered constant at this stage.

Moreover, the other set of input parameters at this scale, $\mathbf{Q}^2$, is the set of homogenized material properties of a unidirectional NCF lamina. These are the outcome of the homogenization H_2 associated with the upscaling process from level $l = 1$ to level $l = 2$. The material properties of the homogenized lamina, which are expected to manifest a transverse isotropic symmetry, are denoted by $\mathbf{Q}^2 = (E_{l,A},\ E_{l,T},\ G_{l,A},\ \nu_{l,T},\ \nu_{l,A})$; where the subscript l refers to the lamina and the subscripts A and T refer to the local axial and transverse properties, respectively.

Group	Parameter	Description
$\mathbf{Q}^2$	$E_{l,A}$	Axial Young's modulus of NCF lamina
	$E_{l,T}$	Transverse Young's modulus of NCF lamina
	$G_{l,A}$	Axial shear modulus of NCF lamina
	$\nu_{l,A}$	Axial Poisson's ratio of NCF lamina
	$\nu_{l,T}$	Transverse Poisson's ratio of NCF lamina

Table 4: Input parameters $\mathbf{Q}^2$ at level $l = 2$.

3.4 Output parameters associated with level 3

The layout of the laminate, $[0/45/-45/90]_s$, is designed to have quasi-isotropic material properties. These are grouped in $\mathbf{Q}^3$ and are: (1) $E_{xx} = E_{yy}$, (2) E_{zz} , (3) $G_{yz} = G_{xz}$, (4) G_{xy}, (5) $\nu_{xy} = \nu_{yx}$, (6) $\nu_{xz} = \nu_{yz}$, and (7) $\nu_{zx} = \nu_{zy}$.

4 HOMOGENIZATION APPROACH

A homogenization engine embedded in Multiscale Designer, software for composite materials, has been used for the upscaling process [3]. The multiscale design system enables the analysis and design of material systems, such as composite materials given their microstructure. An appropriate unit cell morphology is selected for each of the tow homogenization and the lamina homogenization, respectively.

5 MULTI-SCALE STOCHASTIC ASSIMILATION USING A SPECTRAL PROJECTION APPROACH

The homogenized properties of the laminate are obtained by upscaling the material and geometry parameters of the ordered laminae. The material properties of a lamina are obtained using a homogenization protocol that upscales the material and geometry parameters of a unit cell representing a lamina and consisting of a unidirectional tow. The homogenized material properties of a tow are also obtained using a similar homogenization protocol that upscales the geometry and material properties of a unit cell of fibers and resin.

This hierarchy of upscaling processes is addressed in this current work by propagating uncertainties associated with parameters from each scale to construct probabilistic models of the homogenized material properties of the laminate. It is worth noting that the proposed hierarchical framework is not confined to the eight-layer laminate addressed in this paper. It is a general framework that can be applied to other composite materials or any heterogeneous material where fluctuations observed at coarse scales are influenced by fluctuations present at multiple finer scales.

The propagation of uncertainties across the scales has been carried out using a Non-Intrusive Spectral Projection (NISP) approach [4]. The NISP approach enables probabilistic models of the engineering constants representing the homogenized material properties of a laminate as well as the homogenized properties at lower levels. In other words, stochastic surrogate models could be constructed to approximate the functional relationship of the parameters $\mathbf{Q}^l$, l denotes the corresponding level, in terms of the input parameters at the finer scales (lower levels); i.e., $\mathbf{Q}^3$ can be expressed in terms of $\mathbf{P}^0$, $\mathbf{P}^1$, and $\mathbf{P}^2$ instead of $\mathbf{P}^2$ and $\mathbf{Q}^2$. This is achieved by projecting the stochastic properties $\mathbf{Q}^l$ on a finite-dimensional stochastic space, Θ, through an orthogonal projection. The dimension of this stochastic space equals the dimension of the grouped input variables $\mathbf{P} = \{\mathbf{P}^0,\ \mathbf{P}^1,\ \cdots,\ \mathbf{P}^{l-1}\}$. To do so, a mapping of $\mathbf{Q}^l$ to a probability space, Θ, can be expressed in terms of a truncated polynomial chaos (PC) expansion [2] as,

$$\mathbf{Q}^l\,(\xi) = \sum_{j=0}^{N_{pc}} \mathbf{q}_j^l\ \Psi_j(\xi), \tag{1}$$

where, $l = 1,\ 2,\ or\ 3$ refers to the level of upscaled parameters $\mathbf{Q}^l$, and $\Psi_j(\xi)$ is the PC basis which consists of a set of normalized multi-dimensional orthogonal polynomials in ξ; ξ is a vector grouping normalized standard variables. The mapping between ξ and the independently-assumed random variables $\mathbf{P}^i$, introduced in the previous sections at the finer scales i, is defined such that $\Phi^\xi\big(\boldsymbol{\xi}\big) = \Phi^P\big(\mathbf{P}\big)$. The parameters $\mathbf{q}_j^l$ are the projection coefficients and $N_{pc}+1$ is the dimension of the PC terms, which can be defined in terms of the PC order q and the stochastic dimension N_{rv} denoting the size of vector ξ.

The orthogonality condition can be expressed in terms of the inner product, defined on the stochastic space Θ, as,

$$\langle \Psi_i(\xi), \Psi_j(\xi)\rangle = \langle \Psi_j(\xi), \Psi_j(\xi)\rangle\ \delta_{ij}, \tag{2}$$

where,

$$\langle u, v\rangle = \int_\Theta u(\xi)\ v(\xi)\ p_\xi(\xi)\ d\xi, \tag{3}$$

The projection coefficients $\mathbf{q}_j^l$ at level l can be expressed, given the orthogonality of the basis, in terms of the following inner products,

$$\mathbf{q}_j^l = \frac{\big\langle \mathbf{Q}^l(\xi), \Psi_j(\xi)\big\rangle}{\langle \Psi_j(\xi), \Psi_j(\xi)\rangle},\ j = 0, 1, ..., N_{pc}. \tag{4}$$

To estimate $\left\langle \mathbf{Q}^l(\xi), \Psi_j(\xi) \right\rangle$, a sparse grid cubatures (SGC) approach could be used [4]. According to this approach, N_{sgc} sets of ξ realizations and associated weights are generated; $\xi^{(i)}$ and $w_i,\ i = 1,\ \cdots,\ N_{sgc}$ [5]. The dimension of each set N_{sgc} is a function of the stochastic dimension N_{rv} and the level of the sparse grid cubatures L. Thus,

$$q_j^l = \sum_{i=1}^{N_{sgc}} w_i \, \mathbf{Q}^l(\xi^{(i)}) \, \Psi_j(\xi^{(i)}) \ , \ j = 1,\ \cdots,\ N_{pc}. \tag{5}$$

The spectral representation defined in eqation 1 is then fully identified in terms of the PC coefficients. The mean values, $\overline{\mathbf{Q}}^l$, and variances, $Var\left[\mathbf{Q}^l\left(\xi\right)\right]$, of the projected quantities of interest can be estimated, given the orthogonality of the basis, respectively, as,

$$\overline{\mathbf{Q}}^l = \mathbf{q}_j^0. \tag{6}$$

$$Var\left[\mathbf{Q}^l\left(\xi\right)\right] = \sum_{j=1}^{N_{pc}} {\mathbf{q}_j^l}^2. \tag{7}$$

6 EXAMPLE AND DISCUSSION

As explained in the previous section, it is possible to express the homogenization output at multiple scales ($\mathbf{Q}^l$, $\mathbf{Q}^2$, and $\mathbf{Q}^3$) using the same set of SGC nodes. First, the quantities of interest are computed at a set of SGC nodes, each of which consists of a combination of input parameters reported earlier for each scale. The process is repeated for increasing values of the SGC level in order to determine the appropriate SGC level. Second, at each of the given SGC levels, a set of respective polynomial chaos coefficients are estimated using equation 5. The estimated coefficients of (i) the axial modulus of a homogenized tow, $E_{t,A}$ from level $l = 1$, (ii) the axial modulus of a homogenized NCF lamina, $E_{l,A}$ from level $l = 2$, and (iii) the axial modulus of a homogenized NCF laminate E_{xx} from level $l = 3$ are plotted in Figures 3 to 5, respectively. The x-axis represents the index of the terms in the polynomial chaos expansion while the y-axis represents the value of the coefficients. The axial indices 1 to 11 correspond to the coefficients of the linear terms in the polynomial chaos representation. The coefficients are plotted for a set of polynomial chaos orders ranging from 1 to 3.

It is clearly shown that the nodes associated with SGC level 3 are sufficient to identify the coefficients $\mathbf{q}_j^l$. It can also be concluded that the contributions of some second order terms and possibly third order terms in the expansion are important for accurate representation of some homogenized properties at the different scales. To corroborate this conclusion, the probability density functions (PDFs) of the homogenized axial moduli at homogenization levels $l = 1$, $l = 2$, and $l = 3$ are plotted in Figure 6. The Figures show that the axial modulus of the homogenized tow at level $l = 1$ could be expressed as a linear combination of some of the input variables since the PDF curves associated with orders 1 to 3 are converged. However, the PDF curves of the axial moduli of the lamina, $l = 2$, and the laminate, $l = 3$, show that a second order polynomial chaos representation is appropriate, which indicates that some second order terms in the expansion contribute to these homogenized properties.

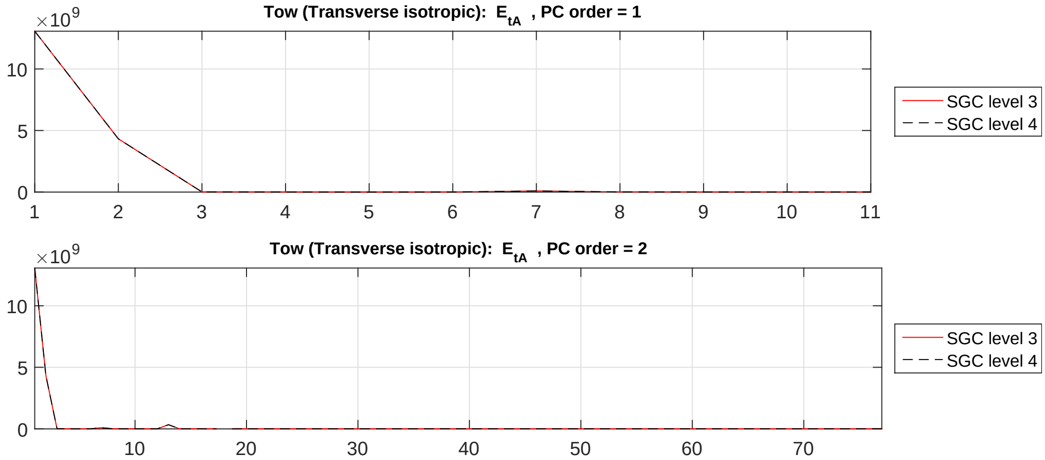

Figure 3: The PC coefficients q_j^1 for $E_{t,A}$.

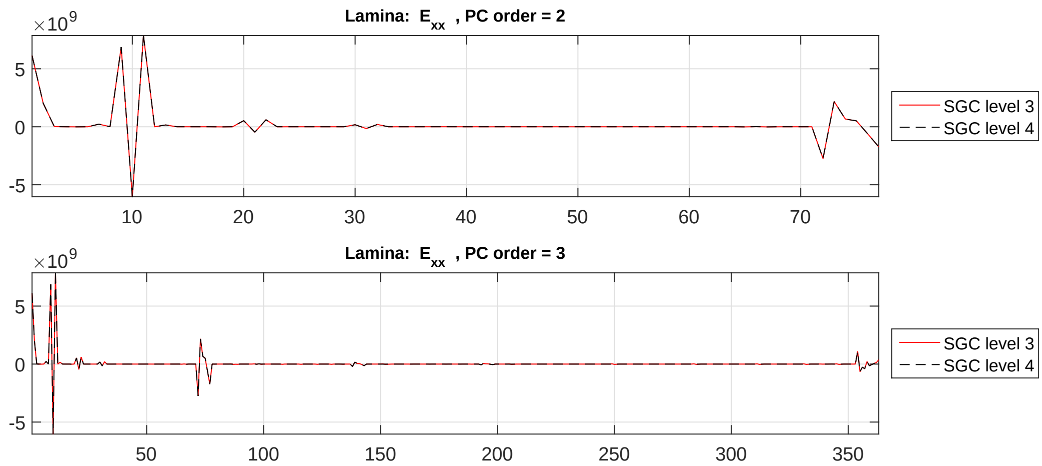

Figure 4: The PC coefficients q_j^2 for $E_{l,A}$.

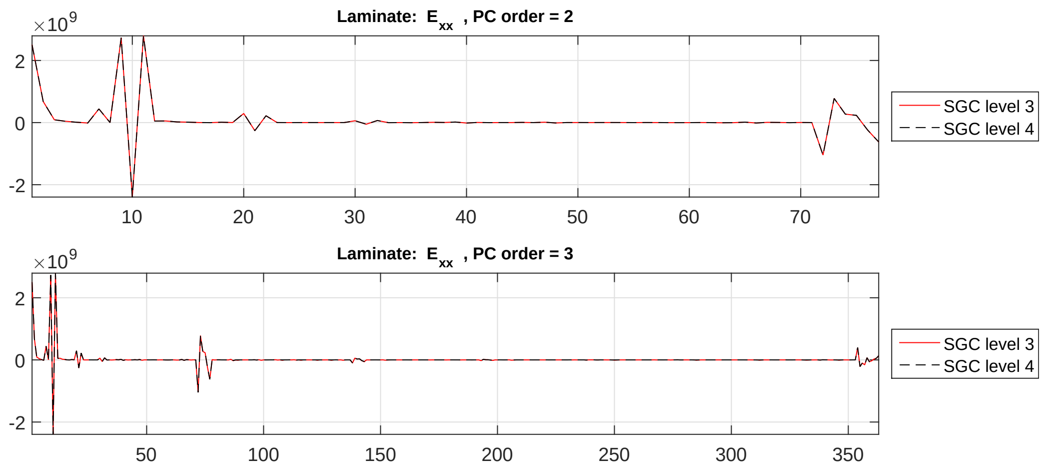

Figure 5: The PC coefficients q_j^3 for $E_{xx} = E_{yy}$.

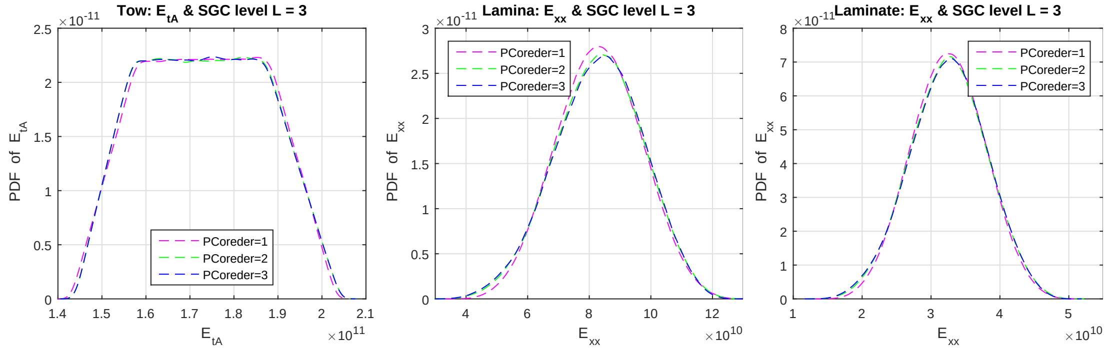

Figure 6: PDF curves for the axial elastic moduli: (left) $E_{tA} \in \mathbf{Q}^1$ (middle) $E_{lA} = E_{xx} \in \mathbf{Q}^2$ (right) $E_{xx} \in \mathbf{Q}^3$

7 CONCLUSIONS

It is shown that polynomial chaos expansion is able to characterize properties at a coarse scale in terms of fluctuations associated with properties from one or more finer scales. This characterization is achieved in terms of an analytical form of functional relationships with the underlying variables at the finer scales.

It is worth noting that the proposed hierarchical framework is not confined to the eight-layer laminate addressed in this paper. It is a general framework that can be applied to other composite materials or any heterogeneous material where fluctuations observed at coarse scales are influenced by fluctuations present at multiple finer scales.

The proposed framework (i) is suitable for the modeling and analysis of composite materials, (ii) can be generalized to account for the behavior of physical systems containing composite parts, (iii) enables analytical forms that can be readily used in sensitivity analyses, and (iv) can be incorporated in inverse calibration frameworks.

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