SPECTRAL STOCHASTIC HOMOGENIZATION OF COMPOSITES WITH RANDOMNESS IN CONSTITUENT MATERIAL PROPERTIES

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ABSTRACT

Stochastic analysis of heterogeneous materials starting from the constituent level directly is necessary and shows a promising prospect in the application of material design. In this paper, spectral stochastic homogenization method is developed by combining asymptotic expansion homogenization and spectral stochastic method, which is further implemented in a commercial finite element package. The probability distribution of stochastic effective properties, including transverse moduli and thermal expansion coefficient are predicted with the developed method, the result of which shows a matching accuracy with that of Monte Carlo simulation, but the spectral stochastic homogenization method is much more computationally efficient.

1 INTRODUCTION

Composites have exceptional stiffness and strength properties and thus are extensively applied in aerospace industry as high performance structural materials. Unlike metallic materials, composites consist of multiple constituents, such as matrices and reinforcements. Uncertainties as the properties of each constituent usually show, stochastic effective or overall properties are needed in the reliability analysis of a structure component in engineering applications [1]. To this end, different micro-mechanics approaches combined with stochastic methods have been proposed. Bounds prediction and refined estimates have been conducted in analytical framework [2, 3]. The corresponding development in numerical aspect, computational homogenization, as one ingredient in multiscale technology, has been extensively studied in recent decades [4].

Combined with computational homogenization method, various stochastic methods can be utilized to predict stochastic effective properties of composites arising from the randomness of constituent material properties. Monte Carlo simulation, known as a universal stochastic method, was carried out to assess the uncertainty of the equivalent properties due to not only the randomness of constituent moduli [5] but also microstructural morphology [6]. The demand of computational efficiency impels the development of non-sampling based methods. Perturbation methods, among the most popular ones, were applied in two-dimensional and three-dimensional asymptotic homogenization of composites [7, 8]. A stochastic multi-scale computational homogenization method have been developed recently [9] and applied to woven textile composites [10].

Good results though perturbation methods can obtain for the first two statistical moments under condition of small variation, probability distribution prediction and the case of large variation are beyond their capability. Another method mentioned in [11], spectral stochastic method, emerges as a powerful alternative. Related research on the application of this method in homogenization remains few [12]. Recently, the authors have developed a novel method for the implementation of the spectral stochastic method within commercial finite element (FE) packages [13]. In this paper, the method is extended for the spectral stochastic homogenization of composites with randomness in constituent material properties and stochastic effective thermo-elastic properties are predicted.

2 SPECTRAL STOCHASTIC HOMOGENIZATION METHOD

2.1 Description of stochastic homogenization formulation

Computational homogenization method has been a research hotspot over the past decades. So-called representative volume element (RVE) is solved to calculate effective properties based on asymptotic method [7] or Hill-Mandel macrohomogeneity condition [9]. Asymptotic homogenization, the focus of this paper, aims at solving partial differential equation (PDE) with rapidly oscillating coefficients, the corresponding physical phenomenon of which can be found in many engineering and scientific problems, such as fibre reinforced composites, laminated plates and so on [14]. An approximation with much smoother coefficients can be derived with asymptotic homogenization, resulting a two-scale problem.

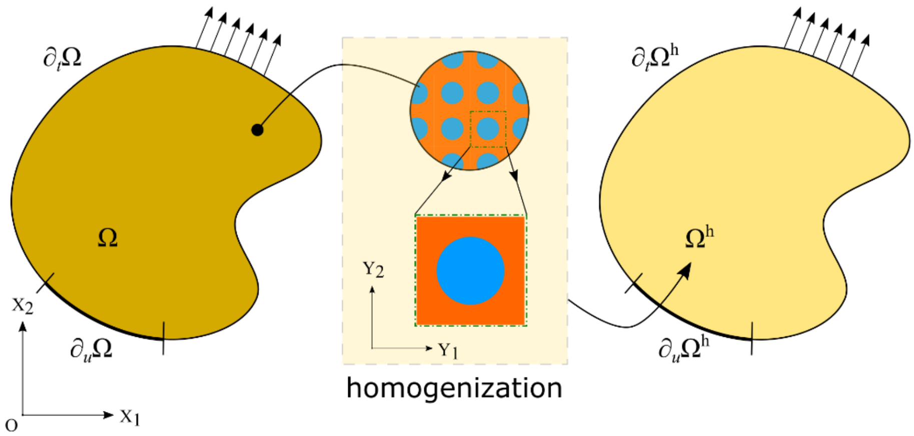

Figure 1: Illustration of homogenization method.

As shown in Fig. 1, besides the original scale $\boldsymbol{x}$, another length scale $\boldsymbol{y} = \boldsymbol{x}/\zeta$ ($\zeta \ll 1$) is introduced to describe the fast variable, corresponding to macroscale and microscale in the context of composites, respectively [14]. With the assumption of periodic microstructure, the stiffness tensor and thermal expansion tensor of material properties only depend on the microscale

$$\begin{aligned} \mathbb{D}^{\zeta}(\boldsymbol{x}) &= \mathbb{D}(\boldsymbol{y}) = \mathbb{D}(\boldsymbol{x}/\zeta), \\ \boldsymbol{\alpha}^{\zeta}(\boldsymbol{x}) &= \boldsymbol{\alpha}(\boldsymbol{y}) = \boldsymbol{\alpha}(\boldsymbol{x}/\zeta), \end{aligned} \tag{1}$$

where superscript ζ denotes the ζ Y-periodicity in the system of coordinates $\boldsymbol{x}$. Considering randomness in the stiffness tensor, the strong form of original boundary value problem can be written as

$$\begin{gathered} \boldsymbol{\nabla}^{\zeta} \cdot \boldsymbol{\sigma}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) + \boldsymbol{b} = 0, \text{ in } \Omega; \\ \boldsymbol{\sigma}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) = \mathbb{D}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) : \boldsymbol{\epsilon}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) - \boldsymbol{\beta}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi})(T - T_0), \text{ in } \Omega; \\ \boldsymbol{\epsilon}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) = \left(\left(\boldsymbol{\nabla}^{\zeta}\boldsymbol{u}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi})\right)^{T} + \boldsymbol{\nabla}^{\zeta}\boldsymbol{u}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi})\right)/2, \text{ in } \Omega; \\ \boldsymbol{u}^{\zeta} = \hat{\boldsymbol{u}} \text{ on } \partial_u\Omega, \boldsymbol{\sigma}^{\zeta} \cdot \boldsymbol{n} = \hat{\boldsymbol{t}} \text{ on } \partial_t\Omega, \end{gathered} \tag{2}$$

where $\boldsymbol{\xi}$ is random variable or vector, $\boldsymbol{\beta}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) = \mathbb{D}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) : \boldsymbol{\alpha}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi})$ and $\boldsymbol{\nabla}^{\zeta} = \boldsymbol{\nabla}_{\boldsymbol{x}} + \boldsymbol{\nabla}_{\boldsymbol{y}}/\zeta$ according to the chain rule.

A double-scale asymptotic expansion of displacement field is expressed as

$$\boldsymbol{u}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) = \boldsymbol{u}^{(0)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \zeta\boldsymbol{u}^{(1)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \zeta^2\boldsymbol{u}^{(2)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + O(\zeta^3), \tag{3}$$

where $\boldsymbol{u}^{(0)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) = \boldsymbol{u}^{(0)}(\boldsymbol{x},\boldsymbol{\xi})$ can be proved. Then strain and stress can be easily derived as

$$\begin{aligned} \boldsymbol{\epsilon}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) &= \zeta^{-1}\boldsymbol{\epsilon}^{(0)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \boldsymbol{\epsilon}^{(1)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \zeta^{1}\boldsymbol{\epsilon}^{(2)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + O(\zeta^2), \\ \boldsymbol{\sigma}^{\zeta}(\boldsymbol{x},\boldsymbol{\xi}) &= \zeta^{-1}\boldsymbol{\sigma}^{(0)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \boldsymbol{\sigma}^{(1)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + \zeta^{1}\boldsymbol{\sigma}^{(2)}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) + O(\zeta^2). \end{aligned} \tag{4}$$

With these expansions, the two-scale problem can be derived directly by substituting Eq. (3) and (4) into Eq. (2) or through a variational form, details of which refer to literatures [4]. The homogenized problem can then be given by

$$\begin{gathered} \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{\sigma}^h(\boldsymbol{x},\boldsymbol{\xi}) + \boldsymbol{b} = 0, \text{ in } \Omega^h; \\ \boldsymbol{\sigma}^h(\boldsymbol{x},\boldsymbol{\xi}) = \mathbb{D}^h(\boldsymbol{x},\boldsymbol{\xi}) : \boldsymbol{\epsilon}^h(\boldsymbol{x},\boldsymbol{\xi}) - \boldsymbol{\beta}^h(\boldsymbol{x},\boldsymbol{\xi})(T - T_0), \text{ in } \Omega^h; \\ \boldsymbol{\epsilon}^h(\boldsymbol{x},\boldsymbol{\xi}) = \left(\left(\boldsymbol{\nabla}_{\boldsymbol{x}} \boldsymbol{u}^h(\boldsymbol{x},\boldsymbol{\xi})\right)^T + \boldsymbol{\nabla}_{\boldsymbol{x}} \boldsymbol{u}^h(\boldsymbol{x},\boldsymbol{\xi})\right)/2, \text{ in } \Omega^h; \\ \boldsymbol{u}^h = \hat{\boldsymbol{u}} \text{ on } \partial_u \Omega^h, \ \boldsymbol{\sigma}^h \cdot \boldsymbol{n} = \hat{\boldsymbol{t}} \text{ on } \partial_t \Omega^h, \end{gathered} \tag{5}$$

where superscript h denotes homogenization and $\boldsymbol{\beta}^h(\boldsymbol{x},\boldsymbol{\xi}) = \mathbb{D}^h(\boldsymbol{x},\boldsymbol{\xi}) : \boldsymbol{\alpha}^h(\boldsymbol{x},\boldsymbol{\xi})$.

Effective properties of composites can be derived from the homogenized stiffness tensor $\mathbb{D}^h(\cdot,\boldsymbol{\xi})$ and thermal expansion tensor $\boldsymbol{\beta}^h(\cdot,\boldsymbol{\xi})$, which have expressions as

$$\begin{aligned} \mathbb{D}^h(\cdot,\boldsymbol{\xi}) &= \frac{\mathbf{1}}{|\mathrm{Y}|}\int_{\mathrm{Y}} \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \left(\mathbb{I} - \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\chi}(\boldsymbol{y},\boldsymbol{\xi})\right)^T \mathrm{d}y, \\ \boldsymbol{\beta}^h(\cdot,\boldsymbol{\xi}) &= \frac{\mathbf{1}}{|\mathrm{Y}|}\int_{\mathrm{Y}} \left(\boldsymbol{\beta}(\boldsymbol{y},\boldsymbol{\xi}) - \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\gamma}(\boldsymbol{y},\boldsymbol{\xi})\right) \mathrm{d}y, \end{aligned} \tag{6}$$

where $\boldsymbol{\chi}(\boldsymbol{y},\boldsymbol{\xi})$ is the mechanical characteristic displacement tensor of third-order and $\boldsymbol{\gamma}(\boldsymbol{y},\boldsymbol{\xi})$ is the thermomechanical characteristic displacement tensor of first-order, which is solved by

$$\begin{aligned} \boldsymbol{\nabla}_{\boldsymbol{y}} \cdot \left(\mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \left(\mathbb{I} - \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\chi}(\boldsymbol{y},\boldsymbol{\xi})\right)^T\right) &= 0, \\ \boldsymbol{\nabla}_{\boldsymbol{y}} \cdot \left(\boldsymbol{\beta}(\boldsymbol{y},\boldsymbol{\xi}) - \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\gamma}(\boldsymbol{y},\boldsymbol{\xi})\right) &= 0. \end{aligned} \tag{7}$$

For the purpose of numerical solution, weak formulations can be written as

$$\begin{aligned} \int_{\mathrm{Y}} \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{v} : \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \left(\boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\chi}(\boldsymbol{y},\boldsymbol{\xi})\right)^T \mathrm{d}y &= \int_{\mathrm{Y}} \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{v} : \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi})\mathrm{d}y, \forall \boldsymbol{v} \in \widetilde{\mathrm{V}}_{\mathrm{Y}}, \\ \int_{\mathrm{Y}} \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{v} : \mathbb{D}(\boldsymbol{y},\boldsymbol{\xi}) : \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{\gamma}(\boldsymbol{y},\boldsymbol{\xi})\mathrm{d}y &= \int_{\mathrm{Y}} \boldsymbol{\nabla}_{\boldsymbol{y}}\boldsymbol{v} : \boldsymbol{\beta}(\boldsymbol{y},\boldsymbol{\xi})\mathrm{d}y, \forall \boldsymbol{v} \in \widetilde{\mathrm{V}}_{\mathrm{Y}}, \end{aligned} \tag{8}$$

where $\widetilde{\mathrm{V}}_{\mathrm{Y}}$ is the set of Y-periodic continuous and sufficiently regular functions with zero average in Y. Eq. (8) is usually solved by FEM, the matrix form of which is given by

$$\begin{aligned} \bigwedge_{e=1}^{n_{ele}}\left(\int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T}\boldsymbol{D}^e(\boldsymbol{\xi})\boldsymbol{B}^e \mathrm{d}y\, \boldsymbol{\chi}^e(\boldsymbol{\xi})\right) &= \bigwedge_{e=1}^{n_{ele}}\left(\int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T}\boldsymbol{D}^e(\boldsymbol{\xi})\mathrm{d}y\right), \\ \bigwedge_{e=1}^{n_{ele}}\left(\int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T}\boldsymbol{D}^e(\boldsymbol{\xi})\boldsymbol{B}^e \mathrm{d}y\, \boldsymbol{\gamma}^e(\boldsymbol{\xi})\right) &= \bigwedge_{e=1}^{n_{ele}}\left(\int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T}\boldsymbol{\beta}^e(\boldsymbol{\xi})\mathrm{d}y\right), \end{aligned} \tag{9}$$

where $\boldsymbol{\beta}^e(\boldsymbol{\xi}) = \boldsymbol{D}^e(\boldsymbol{\xi})\boldsymbol{\alpha}^e(\boldsymbol{\xi})$.

The solution of Eq. (9) is then substituted into Eq. (6) and the homogenized stiffness matrix and thermal expansion matrix can be obtained as

$$\begin{aligned} \boldsymbol{D}^h(\boldsymbol{\xi}) &= \sum_{e=1}^{n_{ele}} \frac{V_e}{V_{tot}} \boldsymbol{D}^e(\boldsymbol{\xi})\left(\boldsymbol{I} - \boldsymbol{B}^e\boldsymbol{\chi}^e(\boldsymbol{\xi})\right), \\ \boldsymbol{\beta}^h(\boldsymbol{\xi}) &= \sum_{e=1}^{n_{ele}} \frac{V_e}{V_{tot}} \left(\boldsymbol{\beta}^e(\boldsymbol{\xi}) - \boldsymbol{D}^e(\boldsymbol{\xi})\boldsymbol{B}^e\boldsymbol{\gamma}^e(\boldsymbol{\xi})\right), \end{aligned} \tag{10}$$

where V_{tot} is the volume of RVE and V_e is the volume of a single element. As seen from Eq. (9) and Eq. (10), the randomness of homogenized stiffness matrix originates in properties of fibre and matrix $\boldsymbol{D}^e(\boldsymbol{\xi})$, $\boldsymbol{\alpha}^e(\boldsymbol{\xi})$. To obtain the probability distribution of $\boldsymbol{D}^h(\boldsymbol{\xi})$ and $\boldsymbol{\beta}^h(\boldsymbol{\xi})$, repeatedly generating samples of $\boldsymbol{D}^e(\boldsymbol{\xi})$, $\boldsymbol{\alpha}^e(\boldsymbol{\xi})$ and solving Eq. (9) and Eq. (10) is a direct method but time-consuming. Thus, a non-sampling method is introduced in the following section.

2.2 Application of spectral stochastic method

Spectral stochastic method adopts Polynomial Chaos expansion to discretize random variables in stochastic space, which is usually combined with finite element method and thus also termed as spectral stochastic finite element method [11]. This method is initially developed to solve stochastic linear static problem and employed in this work to analyze stochastic homogenization problem. Suppose the input stochastic parameters can be expressed as a linear combination of random variables

$$\begin{gathered} \boldsymbol{D}^e(\boldsymbol{\xi}) = \textstyle\sum_{i=0}^{N-1} \boldsymbol{D}_i^e \xi_i, \\ \boldsymbol{\alpha}^e(\boldsymbol{\xi}) = \textstyle\sum_{i=N}^{M+N-1} \boldsymbol{\alpha}_{i-N-1}^e \xi_i, \end{gathered} \tag{11}$$

and approximation of solution variables can be expressed with truncated Polynomial Chaos expansion as

$$\begin{gathered} \boldsymbol{\chi}^e(\boldsymbol{\xi}) = \textstyle\sum_{j=0}^{P_\chi-1} \boldsymbol{X}_j^e \Psi_j(\boldsymbol{\xi}), \\ \boldsymbol{\gamma}^e(\boldsymbol{\xi}) = \textstyle\sum_{j=0}^{P_\gamma-1} \boldsymbol{R}_j^e \Psi_j(\boldsymbol{\xi}), \end{gathered} \tag{12}$$

where $\Psi_j(\boldsymbol{\xi})$ is orthogonal polynomials in terms of random variables [13].

Substitute the mechanical item of Eq. (11) and Eq. (12) into Eq. (9) and the approximation error can be minimized through Galerkin approach

$$\begin{gathered} \wedge_{e=1}^{n_{ele}}(\boldsymbol{k}^e\boldsymbol{X}^e) = \wedge_{e=1}^{n_{ele}}(\boldsymbol{f}^e); \\ \boldsymbol{k}_{jk}^e = \textstyle\sum_{i=0}^{N-1} \int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T} \boldsymbol{D}_i^e \boldsymbol{B}^e \mathrm{d}y\, \boldsymbol{c}_{ijk},\ \boldsymbol{c}_{ijk} = E\left[\xi_i \Psi_j(\boldsymbol{\xi}) \cdot \Psi_k(\boldsymbol{\xi})\right]; \\ \boldsymbol{f}_k^e = \textstyle\sum_{i=0}^{N-1} \int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T} \boldsymbol{D}_i^e \mathrm{d}y\, \boldsymbol{d}_{ik},\ \boldsymbol{d}_{ik} = E[\xi_i \cdot \Psi_k(\boldsymbol{\xi})]; \\ j,k = 0,1,\cdots,P_\chi - 1; \end{gathered} \tag{13}$$

where $E[x]$ denotes the expectation of random variable x. The same process can be applied to the thermomechanical item, which results

$$\begin{gathered} \wedge_{e=1}^{n_{ele}}\left(\bar{\boldsymbol{k}}^e\boldsymbol{R}^e\right) = \wedge_{e=1}^{n_{ele}}\left(\bar{\boldsymbol{f}}^e\right); \\ \bar{\boldsymbol{k}}_{jk}^e = \textstyle\sum_{i=0}^{N-1} \int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T} \boldsymbol{D}_i^e \boldsymbol{B}^e \mathrm{d}y\, \boldsymbol{c}_{ijk}; \\ \bar{\boldsymbol{f}}_k^e = \textstyle\sum_{i=0}^{N-1} \sum_{l=N}^{M+N-1} \int_{\mathrm{Y}^e} \boldsymbol{B}^{e^T} \boldsymbol{D}_i^e \boldsymbol{\alpha}_{l-N-1}^e \mathrm{d}y\, \boldsymbol{g}_{ilk},\ \boldsymbol{g}_{ilk} = E[\xi_i \xi_l \cdot \Psi_k(\boldsymbol{\xi})]; \\ j,k = 0,1,\cdots,P_\gamma - 1. \end{gathered} \tag{14}$$

Since Eq. (13) and (14) are two groups of deterministic linear equations, it can be easily solved with available FE packages. The solution $\boldsymbol{X}^e$ and $\boldsymbol{R}^e$ are then substituted into Eq. (12) and explicit expressions of $\boldsymbol{\chi}^e(\boldsymbol{\xi})$ and $\boldsymbol{\gamma}^e(\boldsymbol{\xi})$ in terms of simple random variables (e.g., normal random variable) can be obtained. However, the stochastic homogenized stiffness matrix still cannot be derived directly through Eq. (10), which contains two parts of randomness $\boldsymbol{D}^e(\boldsymbol{\xi})$and $\boldsymbol{\chi}^e(\boldsymbol{\xi})$ or $\boldsymbol{\gamma}^e(\boldsymbol{\xi})$.

Polynomial Chaos is employed to expand left hand side of Eq. (10)

$$\begin{gathered} \boldsymbol{D}^h(\boldsymbol{\xi}) = \textstyle\sum_{m=0}^{Q_\chi-1} \boldsymbol{D}_m^h \Psi_m(\boldsymbol{\xi}), \\ \boldsymbol{\beta}^h(\boldsymbol{\xi}) = \textstyle\sum_{m=0}^{Q_\gamma-1} \boldsymbol{\beta}_m^h \Psi_m(\boldsymbol{\xi}). \end{gathered} \tag{15}$$

For the sake of simplicity, $P_\chi = Q_\chi$ and $P_\gamma = Q_\gamma$ are assumed. Substitute Eq. (11), (12) and (15) into

Eq. (10) and the coefficients in Eq. (15) can be obtained similarly with those in Eq. (12)

$$\bar{\boldsymbol{c}}_{mm}\boldsymbol{D}_m^h = \sum_{e=1}^{n_{ele}}\frac{V_e}{V_{tot}}\left(\sum_{i=0}^{N-1}\boldsymbol{D}_i^e\boldsymbol{d}_{im} - \sum_{i=0}^{N-1}\sum_{j=0}^{P_\chi-1}\boldsymbol{D}_i^e\boldsymbol{B}^e\boldsymbol{X}_j^e\,\boldsymbol{c}_{ijm}\right),$$

$$\bar{\boldsymbol{c}}_{mm}\boldsymbol{\beta}_m^h = \sum_{e=1}^{n_{ele}}\frac{V_e}{V_{tot}}\left(\sum_{i=0}^{N-1}\sum_{l=N}^{M+N-1}\boldsymbol{D}_i^e\boldsymbol{\alpha}_{l-N-1}^e\,\boldsymbol{g}_{ilm} - \sum_{i=0}^{N-1}\sum_{j=0}^{P_\gamma-1}\boldsymbol{D}_i^e\boldsymbol{B}^e\boldsymbol{R}_j^e\,\boldsymbol{c}_{ijm}\right), \tag{16}$$

$$\bar{\boldsymbol{c}}_{mm}= E[\Psi_m(\boldsymbol{\xi})\cdot\Psi_m(\boldsymbol{\xi})].$$

With the explicit expressions by Eq. (15), the probability distribution of stochastic homogenized matrices can be obtained by sampling of $\boldsymbol{\xi}$. The effective properties can be derived from compliance matrix $\boldsymbol{S}^h(\boldsymbol{\xi}) = \left(\boldsymbol{D}^h(\boldsymbol{\xi})\right)^{-1}$ and

$$\boldsymbol{S}^h(\boldsymbol{\xi}) = \begin{bmatrix} \frac{1}{E_{xx}} & -\frac{\nu_{yx}}{E_{yy}} & 0 \\ -\frac{\nu_{xy}}{E_{xx}} & \frac{1}{E_{yy}} & 0 \\ 0 & 0 & \frac{1}{G_{xy}} \end{bmatrix}. \tag{17}$$

Meanwhile, the homogenized expansion coefficient can be obtained by

$$\boldsymbol{\alpha}^h(\boldsymbol{\xi}) = \boldsymbol{S}^h(\boldsymbol{\xi})\boldsymbol{\beta}^h(\boldsymbol{\xi}), \tag{18}$$

where $\boldsymbol{\alpha}^h(\boldsymbol{\xi}) = [\alpha_{xx} \quad \alpha_{yy} \quad 0]^T$.

3 A NUMERICAL EXAMPLE

To illustrate the spectral stochastic homogenization method, a 2D unit cell is utilized to analyze stochastic effective properties of composites in this section. The fiber volume fraction is 0.47. The mean properties of constituent material are listed in Table 1. Young's moduli and coefficient of thermal expansion are assumed to be Gaussian random variables with coefficients of variation C_v.

Constituent	Young's modulus [GPa]	Poisson's ratio	Coefficient of thermal expansion [10^{-6}/°C]
Fiber	379.3	0.1	8.1
Matrix	68.3	0.3	23.0

Table 1: Material properties of fiber and matrix in composites [15].

3.1 Numerical implementation

Traditionally, spectral finite element method (SSFE) is difficult to be implemented in a commercial FE package because its formulation is usually developed at a level of global stiffness matrix [11]. To overcome this difficulty, the authors have developed the formulation of SSFE at element stiffness level, which is realized in Abaqus FEA and then adopted to solve stochastic static problems with material properties considered as random field [13]. The idea of stochastic element is extended to solve stochastic homogenization problem, which is introduced as follows.

As shown in Fig. 2, standard finite element mesh is employed to discretize the unit cell. Similar with deterministic homogenization [16], periodic boundary condition is applied to four edges, AB/DC and AD/BC. Point A is constrained to eliminate rigid body motion. But stochastic element is used instead of traditional deterministic element. Extra sets of nodes are introduced in stochastic element to represent extra degrees of freedom in Eq. (12), which can be considered as discretization in the stochastic space. The total number of node sets is determined by the Polynomial Chaos terms, P_χ or P_γ in Eq. (12) and the extra nodes lie in the same coordinates with the original set of nodes, as shown in Fig. 2.

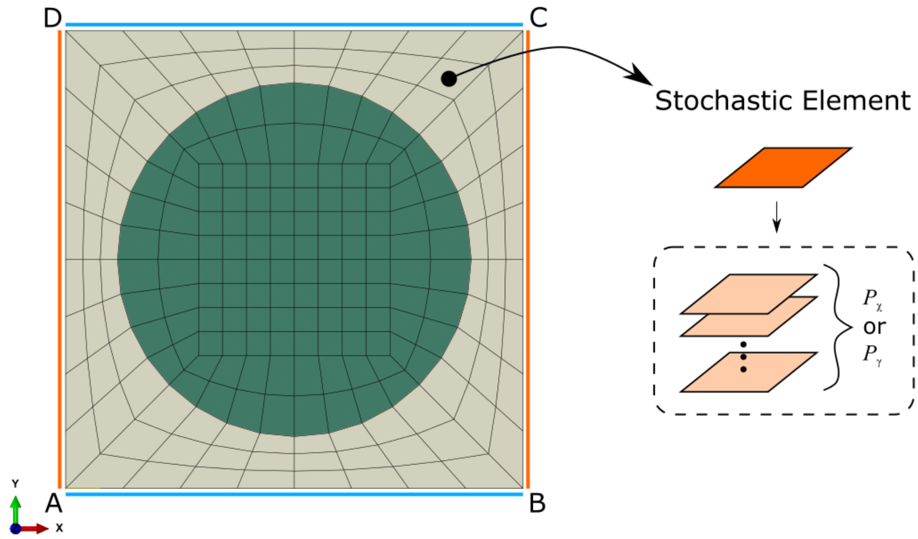

Figure 2: Finite element model of the unit cell.

This stochastic element is implemented in Abaqus FEA through UEL, a user subroutine to define an element, details of which refer to previous work [13]. Slight difference for this problem is that two kinds of materials are used. A unification expression of two materials for Eq. (10) can be written as

$$\begin{aligned} E(\boldsymbol{\xi}) &= \left(E_f + E_m\right) + C_v E_f \xi_1 + C_v E_m \xi_2, \\ \alpha(\boldsymbol{\xi}) &= \left(\alpha_f + \alpha_m\right) + C_v \alpha_f \xi_3 + C_v \alpha_m \xi_4, \end{aligned} \tag{19}$$

where E_m and α_m vanish for fiber material while E_f and α_f are zero for matrix material. Since the numbers of random variables in Eq. (13) and Eq. (14) are different, 2 and 4 respectively, they are solved with two jobs separately. Since there are three columns of load vectors at the right hand side of Eq. (13), a linear perturbation step with multiple load cases is employed [16]. After the coefficients in Eq. (15) are obtained, Monte Carlo simulation is adopted to generate the probability distribution of effective properties with MATLAB.

3.2 Results

Two cases with material properties of small variation ($C_v = 0.1$) and large variation ($C_v = 0.2$) are analyzed with spectral stochastic method, the results of which are further compared with those obtained by Monte Carlo simulation (MCS). The implementation of MCS-based homogenization is based on the deterministic homogenization [16], where the material parameters are inputted as sampling. Total 10^4 simulations were conducted. The total CPU time cost for MCS and spectral stochastic method are about 2900s and 7s, respectively. Since periodic square array is assumed for fiber distribution, material properties after homogenization are isotropic and thus only two transverse moduli and thermal expansion coefficient are examined.

Second order Polynomial Chaos is adopted to expand the mechanical and thermomechanical characteristic displacement in Eq. (9). The remained Polynomial Chaos terms in Eq. (12), P_χ and P_γ, are 6 and 15, respectively [13]. The results of the first term (i.e., $\boldsymbol{X}_0$ and $\boldsymbol{R}_0$), as plotted in Fig. 3, are actually the mean value of $\boldsymbol{\chi}(\boldsymbol{\xi})$ and $\boldsymbol{\gamma}(\boldsymbol{\xi})$, which show periodicity in terms of displacement and are consistent with the results of deterministic homogenization [16]. The results of higher terms, $\boldsymbol{X}_1 \sim \boldsymbol{X}_5$ and $\boldsymbol{R}_1 \sim \boldsymbol{R}_{15}$, are similar but smaller in magnitude. The solution variables are then substituted into Eq. (16), which derives the coefficients of stochastic homogenized matrices in Eq. (15), as shown in Fig. 4.

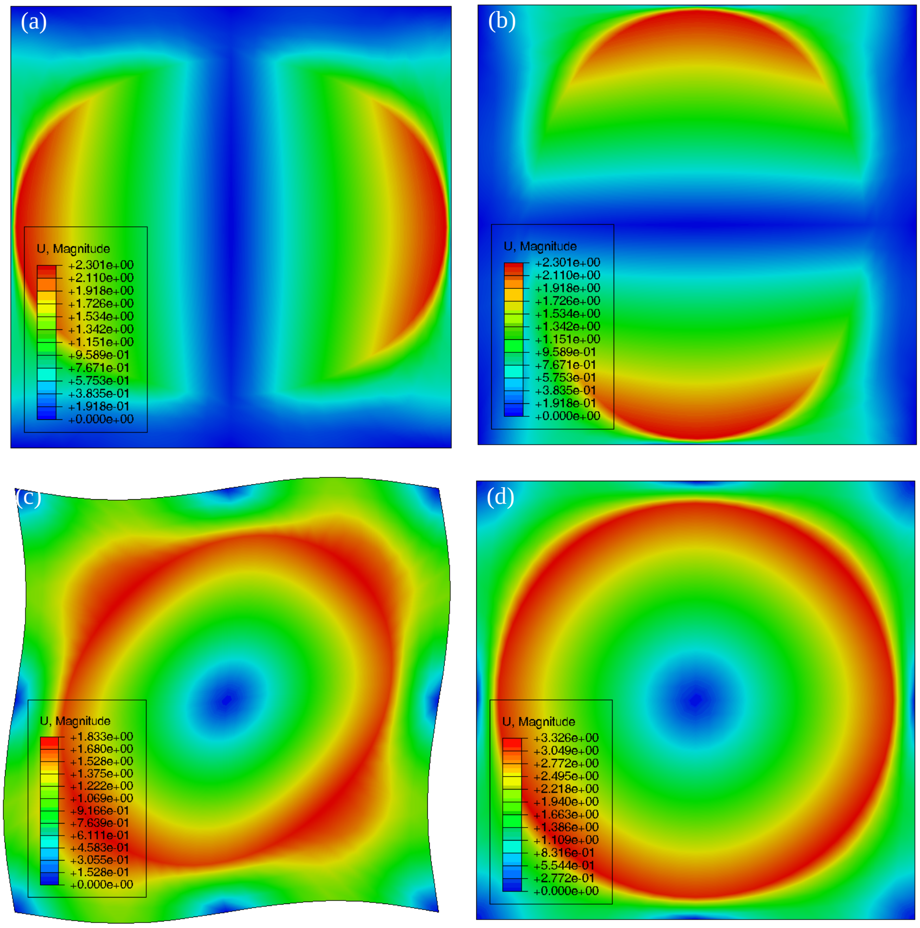

Figure 3: Mechanical and thermomechanical characteristic displacement ($C_v = 0.1$):
(a) $(\boldsymbol{X}_0)_1$; (b) $(\boldsymbol{X}_0)_2$; (c) $(\boldsymbol{X}_0)_3$; (d) $\boldsymbol{R}_0$.

$\boldsymbol{D}^{\mathrm{h}}_{\mathrm{m}}$	$(\boldsymbol{\beta}^{\mathrm{h}}_{\mathrm{m}})^{\mathrm{T}}$
m=0 ↓ m=5	m=0 ↓ m=15

$$\boldsymbol{D}^{\mathrm{h}}_{\mathrm{m}},\ \mathrm{m}=0 \rightarrow \mathrm{m}=5:\quad
\begin{bmatrix} 160.57 & 45.93 & 0.00 \\ 45.93 & 160.57 & 0.00 \\ 0.00 & 0.00 & 45.80 \end{bmatrix},
\begin{bmatrix} 4.72 & 1.27 & 0.00 \\ 1.27 & 4.72 & 0.00 \\ 0.00 & 0.00 & 0.69 \end{bmatrix},
\begin{bmatrix} 11.46 & 3.36 & 0.00 \\ 3.36 & 11.46 & 0.00 \\ 0.00 & 0.00 & 3.91 \end{bmatrix},
\begin{bmatrix} -0.30 & -0.09 & 0.00 \\ -0.09 & -0.30 & 0.00 \\ 0.00 & 0.00 & -0.06 \end{bmatrix},
\begin{bmatrix} 0.61 & 0.18 & 0.00 \\ 0.18 & 0.61 & 0.00 \\ 0.00 & 0.00 & 0.11 \end{bmatrix},
\begin{bmatrix} -0.30 & -0.09 & 0.00 \\ -0.09 & -0.30 & 0.00 \\ 0.00 & 0.00 & -0.06 \end{bmatrix}$$

$$(\boldsymbol{\beta}^{\mathrm{h}}_{\mathrm{m}})^{\mathrm{T}},\ \mathrm{m}=0 \rightarrow \mathrm{m}=15:\quad
\begin{array}{l}
[\,3129.44 \quad 3129.44 \quad 0.00\,] \\
[\,81.66 \quad 81.66 \quad 0.00\,] \\
[\,233.43 \quad 233.43 \quad 0.00\,] \\
[\,88.07 \quad 88.07 \quad 0.00\,] \\
[\,224.88 \quad 224.88 \quad 0.00\,] \\
[\,-5.37 \quad -5.37 \quad 0.00\,] \\
[\,10.70 \quad 10.70 \quad 0.00\,] \\
[\,3.02 \quad 3.02 \quad 0.00\,] \\
[\,5.06 \quad 5.06 \quad 0.00\,] \\
[\,-5.33 \quad -5.33 \quad 0.00\,] \\
[\,5.83 \quad 5.83 \quad 0.00\,] \\
[\,17.49 \quad 17.49 \quad 0.00\,] \\
[\,0.00 \quad 0.00 \quad 0.00\,] \\
[\,0.00 \quad 0.00 \quad 0.00\,] \\
[\,0.00 \quad 0.00 \quad 0.00\,]
\end{array}$$

Figure 4: Coefficients in Polynomial Chaos expansion of homogenized stiffness matrix and thermal expansion matrix ($C_v = 0.1$).

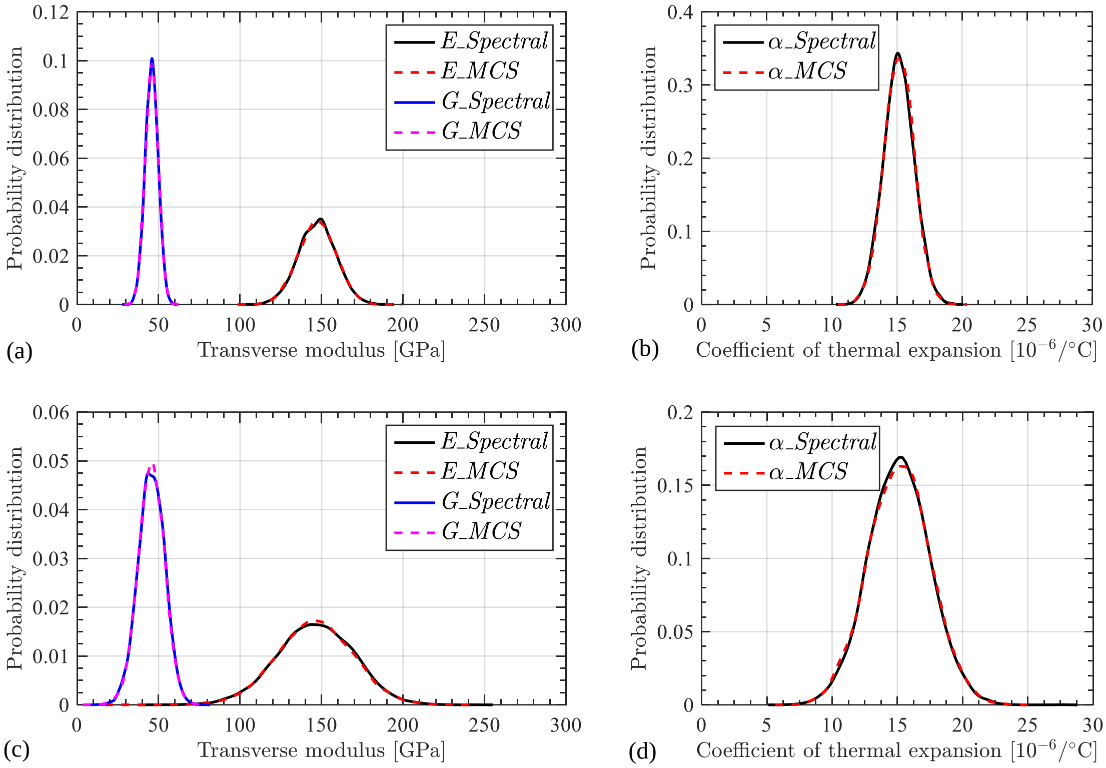

Figure 5: Probability distribution of effective properties:
(a) $C_v = 0.1$, mechanical properties; (b) $C_v = 0.1$, thermal property;
(c) $C_v = 0.2$, mechanical properties; (d) $C_v = 0.2$, thermal property.

C_v	Statistical results	Young's modulus [GPa]	Shear modulus [GPa]	Coefficient of thermal expansion [10^{-6}/°C]
	Mean	147.29/147.24*	45.76/45.74	15.15/15.16
0.1	Standard deviation	11.48/11.51	4.00/4.02	1.16/1.17
	Coefficient of variation	0.078/0.078	0.087/0.088	0.076/0.077
	Mean	146.03/145.66	45.56/45.45	15.16/15.15
0.2	Standard deviation	23.32/23.29	8.04/8.01	2.36/2.33
	Coefficient of variation	0.160/0.160	0.176/0.176	0.156/0.154

* Results by spectral stochastic method/MCS

Table 2: The statistical results of stochastic effective properties.

With the coefficients in Eq. (15) known, stochastic effective properties are further obtained with Eq. (17) and Eq. (18). As shown in Fig. 5, the probability distribution of mechanical properties and thermal property predicted by spectral stochastic method agree well with that by Monte Carlo simulation under both conditions of small variation and large variation. The statistical results are then extracted and listed in Table 2. It can be seen that the mean values of these properties predicted are almost the same for small variation and large variation while the standard deviation of the case with large variation is twice as large as that of small variation. Besides, the coefficient of variation in effective properties is slightly smaller than that in constituent material properties. Correlation analysis is also conducted on stochastic effective properties. As plotted in Fig. 6, strong and positive correlation can be observed between Young's modulus and shear modulus while almost no correlation between Young's modulus and thermal expansion coefficient.

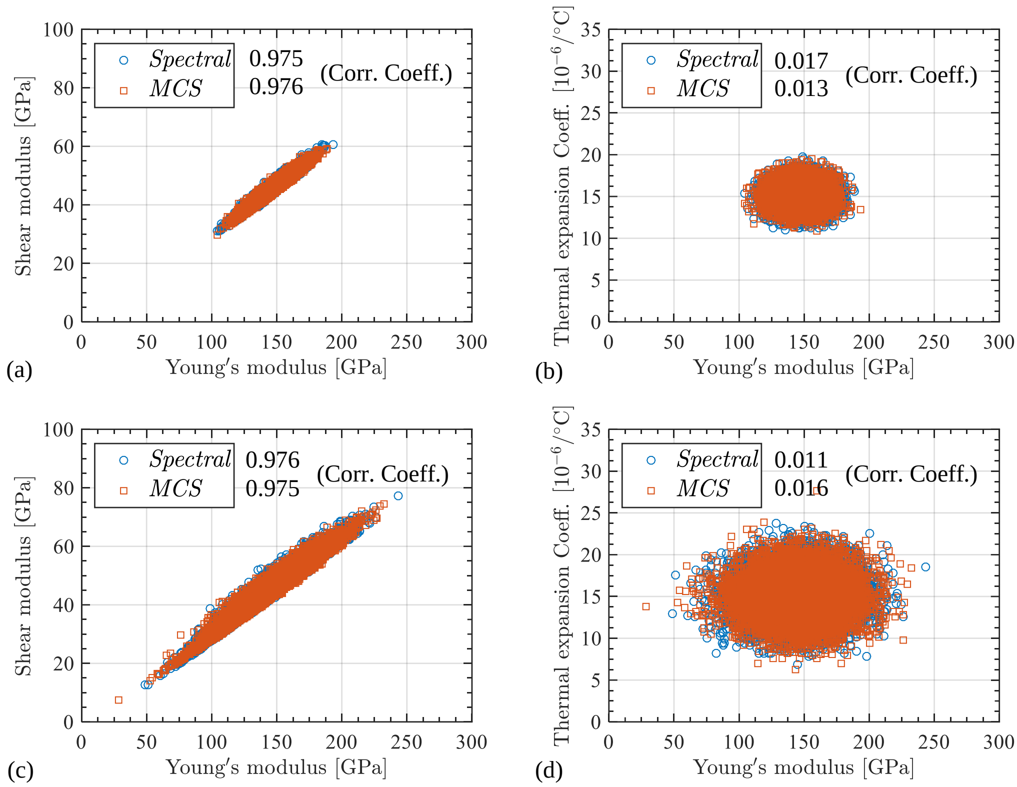

Figure 6: Correlation analysis results:
(a) $C_v = 0.1$, E vs G; (b) $C_v = 0.1$, E vs α;
(c) $C_v = 0.2$, E vs G; (d) $C_v = 0.2$, E vs α.

4 CONCLUSIONS

A spectral stochastic homogenization method is presented for the prediction of stochastic effective properties of composites by taking into account the randomness of constituent materials. As a combination of computational homogenization method and spectral stochastic method, this newly developed method presents many advantages. It is straightforward for the extension of this method to any heterogeneous material satisfying the two-scale assumption of asymptotic homogenization method, which provides an efficient method to examine many possible scenarios of material microstructure before real materials are fabricated. Since uncertainty analysis at multiple length scales is essential in Integrated Computational Materials Engineering (ICME), the spectral stochastic homogenization method shows an efficient way to link the randomness at two scales, which does not cost extensive computational fees. A numerical example with a simple 2D unit cell is adopted to validate the method. Both statistical moments and probability distribution of stochastic effective properties have been obtained. Besides, correlation analyses have also been conducted to calculate correlation coefficients between Young's modulus and shear modulus, Young's modulus and thermal expansion coefficient. All results show good agreements with those obtained by Monte Carlo simulation.

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