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Stochastic micromechanics of composites

M. Kaminski
Division of Mechanics of Materials, Technical University of Lodz
Poland

Abstract

The main idea of the article is to present the recent development in probabilistic computational micromechanics of composite materials. The main directions in these discipline, i.e. homogenization method, reliability analysis as well as fatigue and fracture phenomena are discussed in the context of application of Monte-Carlo simulation technique as well as the stochastic second order perturbation technique. Numerical illustration shows how to calculate probabilistic state functions (displacements, for instance), third order reliability indexes as well as expected values and variances of the effective elastic parameters of the simple composite beam structure under tension.

1 Introduction

Composite materials become still more and more popular in numerous applications (automotive, biomechanical, civil and mechanical engineering, space technology) and since this fact designing, computational modeling and optimization of these materials and such structures dominate systematically engineering activity. Manufacturing thermomechanical processes, multicomponent character, interface and degradation phenomena as well as experimental measurement procedures results in effective significant random uncertainty of composite materials behavior and since that should be incorporated in theoretical and numerical studies on composites.

The application of different computational probabilistic methods (Monte-Carlo simulation, perturbation and spectral techniques) is still open research problem in the context of effective material properties, interface modeling, fatigue and fracture computational modeling as well as reliability analysis. The references on any of these subjects are very numerous today and since that their analysis is extremely complicated; the decisive problem is to collect the consistent general probabilistic model for composite materials rather. The main value of such a model would be the applicability to various classes of composites

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as well as to the materials with different number and types of constituents and, in the context of engineering computations, general capability of single computer program implementation. The considerations presented below give the general view how to build such a model and how to use it in engineering practice.

2 Composite material model

The composite material model applied below is as general as it possible - the randomness is considered both in geometry as well as in mechanical and physical properties; the only one exception is homogenization theory where the periodic composites (in terms of microgeometry) are considered. The randomness of different composite properties is introduced in the form of probabilistic moments - expected values, variances (or standard deviations), correlation function or matrix as well as higher order statistics and coefficients describing the skewness or concentration of the particular random variable. The order (or range) of probabilistic analysis must be corresponding to input statistical information, variation range of input random variables and available computational model or program (stochastic second order perturbation technique has limitation on the second order coefficients, for instance).

The composite can have any finite number of the constituents [6] in the macroscale or in the Representative Volume Element (RVE) if only such an element can be found in the plane section or within the composite volume. The interface geometry can be introduced as deterministic and then both FEM and BEM modeling is applicable as well. The randomness can be introduced in the form of single defects with random parameters [6] modeled by stochastic interface in FEM approach or, alternatively, identified by interface points with random location [7]. The boundary element technique in conjunction with the additional Monte-Carlo simulation tool seems to be the most appropriate in that case.

3 Probabilistic computational techniques

The main idea of numerical techniques is explained on the example of the equation $\mathbf{L}\,\mathbf{u}=\mathbf{f}$, where $\mathbf{L}$ is a stochastic linear operator (representing stiffness matrix, for instance), $\mathbf{u}$ is the random response of the composite while $\mathbf{f}$ denotes admissible excitation of the system. As it is known, the analytical solutions for such a class of partial differential equations are available for some specific cases only and since that various approximating numerical methods are used.

1. read input probabilistic moments $\mu_K(\mathbf{L}), \mu_K(\mathbf{u})$
2. generate random values **L**, **u** (i=1,...,M)
3. carry out sampling for $\mathbf{L}^{(i)}\mathbf{u}^{(i)}=\mathbf{f}^{(i)}$, i=1,...,M
4. estimate response statistical moments $\mu_K(\mathbf{u})$

Figure 1: Standard Monte-Carlo simulation algorithm

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The oldest computational technique - Monte-Carlo simulation [6,11] consists of numerical procedures shown above where M denotes the total number of random samples to be generated. Then, the following unbiased estimators are used to calculate probabilistic moments of the output:

$$E[\mathbf{u}]=\frac{1}{M}\sum_{m=1}^{M}\mathbf{u}^{(m)}\ ,\ \mathrm{Var}(\mathbf{u})=\frac{1}{M-1}\sum_{m=1}^{M}\left(\mathbf{u}^{(m)}-E[\mathbf{u}]\right)^{2}\ , \tag{1}$$

where higher order probabilistic moments can be written out starting from the following definition:

$$\mu_{k}(\mathbf{u})=m_{k}\left[(\mathbf{u})-m_{1}(\mathbf{u})\right], \tag{2}$$

what makes it possible to calculate the skewness as

$$S(\mathbf{u})=\frac{\mu_{3}(\mathbf{u})}{\sigma^{3}(\mathbf{u})}. \tag{3}$$

To illustrate the stochastic second order perturbation method [5,10] let us denote random variable of equilibrium problem as a vector **b** and its probability density as p(**b**). Then, the expected value of the variable is defined as

$$E[\mathbf{b}]=\int_{-\infty}^{+\infty}\mathbf{b}p(\mathbf{b})d\mathbf{b} \tag{4}$$

where r,s=1,...,R indexing the random variables of the problem; the covariance is given as

$$\mathrm{Cov}(b^{r},b^{s})=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left(b^{r}-E\left[b^{r}\right]\right)\left(b^{r}-E\left[b^{r}\right]\right)p(\mathbf{b})d\mathbf{b}\,. \tag{5}$$

Next, all composite material parameters of and the state functions being random fields are extended by the use of the stochastic second order expansion via the Taylor series as follows [10]:

$$\mathbf{L}=\mathbf{L}^{0}+\varepsilon\mathbf{L}^{,r}\Delta b^{r}+\frac{1}{2}\varepsilon^{2}\mathbf{L}^{,rs}\Delta b^{r}\Delta b^{s}. \tag{6}$$

where $\varepsilon\Delta b^{r}$ denotes the first order variation of Δb^{r} about its expected value $E\left[b^{r}\right]$ and $\mathbf{L}^{(n)}$ represents the n-order partial derivatives of **L** with respect to the random variables evaluated at their expected values. Further, inserting analogous extensions to eqn (1) and comparing the same order terms we obtain

- zeroth order equations:

$$\mathbf{L}^{0}\mathbf{u}^{0}=\mathbf{f}^{0}, \tag{7}$$

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- first order equations (for r=1,...,R):

$$\mathbf{L}^0\mathbf{u}^{,r} = \mathbf{f}^{,r} - \mathbf{L}^{,r}\mathbf{u}^0, \tag{8}$$

- second order equations (for r,s=1,...,R):

$$\mathbf{L}^0\mathbf{u}^{(2)} = \left\{\mathbf{f}^{,rs} - \mathbf{L}^{,rs}\mathbf{u}^0 - 2\mathbf{L}^{,r}\mathbf{u}^{,s}\right\}\mathrm{Cov}(b^r, b^s). \tag{9}$$

To obtain the probabilistic solution for the equilibrium problem considered, eqn (7) is solved for zeroth order of **u**, next - eqn (8) for the first order terms and finally, eqn (9) for the second order displacements. Using the definition of expected value and introducing second order expansion we obtain

$$E[\mathbf{u}] = \mathbf{u}^0 + \tfrac{1}{2}\mathbf{u}^{,rs}\mathrm{Cov}(b^r, b^s). \tag{10}$$

while the first order cross-covariances are derived as follows:

$$\mathrm{Cov}(\mathbf{u}) = \left(\frac{\partial u}{\partial b}\right)^2 \mathrm{Cov}(\mathbf{b}). \tag{11}$$

It should be underlined that analysis presented is independent from the numerical method proposed for computations and can be implemented in Finite Element, Volume, Difference as well as Boundary Element or meshless methods computer programs.

4 Homogenization

As it was mentioned in Introduction, the homogenization model presented briefly below deals with periodic media, however composites with random microgeometry can be analyzed by using of the Voronoi Cell Finite Element approach (combined with perturbation and simulation techniques for materials characteristics randomized).

Generally, the effective material tensors (elasticity of conductivity) are calculated as [4,6,16]

$$C_{ijkl}^{(eff)} = \left\langle C_{ijkl} + C_{ijmn}\chi_{m,n}^{kl}\right\rangle_{\Omega},\ i,j,k,l,m,n=1,2,3 \tag{12}$$

where $\langle.\rangle_{\Omega}$ denotes the spatial averaging operator. Usually, the main problem is to find the periodic homogenization functions $\chi_{m,n}^{kl}$. In the case of fiber-reinforced or fiber-like composites, the periodicity conditions are applied on external boundaries of the RVE and the difference of corresponding material tensor components is applied at the interface to compute the homogenization function.

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For any 1, 2 or 3D heterogeneous structures with isotropic homogeneous constituents distributed periodically along x_3 axis it is obtained as a solution for the following problem:

$$\left(C_{ijkl}\left(\frac{x_3}{\varepsilon}\right)\chi^{mn}_{k,l} + C_{ijmn}\left(\frac{x_3}{\varepsilon}\right)\right)_{,jy} = 0 . \tag{13}$$

If the components are isotropic then eqn (12) leads to the following algebraic equation describing effective Young modulus:

$$e^{(eff)} = \frac{|\Omega|}{\int_{\Omega} \frac{dx_3}{e(x_3)}} . \tag{14}$$

Such a formulation makes it possible to derive the closed form equations for the expected values and covariances of the Young modulus homogenized using classical definitions of probabilistic moments or, alternatively, starting from the perturbation theory [5]. Using analogous methodology, the expected values and variances of effective material properties can be derived when viscoelastic material model is applied [17]. In the case of homogenization of composites with elastoplastic constituents the Transformation Field Analysis (TFA) or Fast Fourier Transform (FFT) may be used in conjunction with MCS methodology, while the stochastic perturbation method has not any application in this field until now [2].

5 Fatigue and fracture analysis

It is known that computational modeling of fatigue and fracture of composites is a very complicated process since the fact that damage does not consist in growth of a single crack but is caused by volumetric defects accumulation (coalescence of microvoids and microcracks in larger defects) as well as by numerous complex mechanisms depending on applied stress rates and cycles. There are some homogenization based models [9] where effective damage parameters characterizing the whole composite are calculated and, on the other hand, the critical element concepts [15] where damage development concentrates around primary interface or near interface cracks (critical element is such a part of the composite controlling their fracture strength).

The probabilistic perturbation analysis shown above is used in the form of so-called enriched stochastic finite elements where displacement components near the crack-tip are calculated using the stress intensity factors in FEM models [1,7]; the crack length is treated as random variable and accounted for any corresponding finite element; greater effectiveness of corresponding BE models in the modeling of such phenomena is expected.

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In the case of fatigue analysis, analogous formulation based on the SFEM are proposed (so-called Modified Finite Integral Method) however then any fatigue crack growth (FCG) stochastic model must be introduced - Paris-Erdogan, Palmgren-Miner (PM) or discrete Markovian models [12,13].

Let us consider the Palmgren-Miner rule to illustrate the application of the second order perturbation technique for derivation of first two probabilistic moments of damage function D. Starting from the deterministic PM model, the damage parameter D is calculated as

$$D_i = \sum_{j=1}^{j=i} \frac{n_j}{N_j}, \tag{15}$$

where N_j and n_j denote material and loading variables, respectively. In the case of material parameters treated as independent random variables, the expected value and the variance can be calculated as follows [8]:

$$E[D_i] = D_i\left(N^0\right) + \frac{1}{2!}\sum_{j=1}^{j=i} \left.\frac{\partial^2 D}{\partial N_j^2}\right|_{N^0} \mathrm{Var}(N) + \frac{1}{3!}\sum_{j=1}^{j=i} \left.\frac{\partial^3 D}{\partial N_j^3}\right|_{N^0} E\left[(N - E[N])^3\right] + \ldots \tag{16}$$

and

$$\mathrm{Var}(D) = E\left(D^2\right) - E^2(D). \tag{17}$$

How it can be seen from eqn (16), higher than the second order perturbation technique can be applied to calculate probabilistic moments of damage function D, while analogous successive implementation complicates unproportionally together with an increase of the perturbation order in discrete numerical techniques.

The infinitesimal expected value and variance are calculated in stochastic models, however first, the probability function describing the transition from the state t_0 to t must be proposed (stochastic processes are used instead of random variables and fields). Let us consider simple random walk modeling the crack growth in the material. If the stochastic process is labelled by integer numbers and total number of the steps n and if $p_{ij}^{(n)}$ is the probability of transition from step 'i' to 'j' then Chapman-Kolmogorov equations is introduced as [13]

$$p_{ij}^{(n)} = p_{ij-1}^{(n-1)}\alpha_{j-1} + p_{ij}^{(n-1)}\left(1-\alpha_j - \beta_j\right) + p_{ij+1}^{(n)}\beta_{j+1}. \tag{18}$$

where α_j is the probability of a positive step at state 'j', β_j - the probability of a negative step at state 'j' and $1-\alpha_j-\beta_j$ is the probability of 'no step'. This equation is a basis to derive the Kolmogorov transition density $p(x, t|x_0, t_0)$ where x is a crack length with initial value x_0, while t and t_0 denote initial and final time of the step. Therefore, the forward equation is obtained as

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$$\frac{1}{2}\frac{\partial}{\partial x}\left[\sigma^2(x)p\left(x,t\middle|x_0,t_0\right)\right]-\frac{\partial}{\partial x}\left[E[x]p\left(x,t\middle|x_0,t_0\right)\right]=\frac{\partial p}{\partial t}, \tag{19}$$

while backward one in the form of

$$\frac{1}{2}\sigma^2\left(x_0\right)\frac{\partial^2}{\partial x_0^2}p\left(x,t\middle|x_0,t_0\right)+E\left[x_0\right]\frac{\partial}{\partial x_0}p\left(x,t\middle|x_0,t_0\right)=-\frac{\partial p}{\partial t_0}. \tag{20}$$

Therefore, the probabilistic moments are calculated as follows:

$$E[x,t]=\lim_{\tau\to 0}\frac{1}{\tau}E\left[X(t+\tau)-X(t)\middle|X(t)=x\right], \tag{21}$$

as well as

$$Var(x,t)=\lim_{\tau\to 0}\frac{1}{\tau}E\left\{\left[X(t+\tau)-X(t)\right]^2\middle|X(t)=x\right\}. \tag{22}$$

As it can be shown [13], the general Markovian process leads to Paris-Erdogan equation with randomized parameters. Taking into account the physical interpretation of these results it can be mentioned that the infinitesimal expected value corresponds to the rate of crack length change; the initial crack length can be derived starting from backward equation. Further, it should be underlined that the stochastic processes modeling does not have corresponding computational FEM or BEM-based implementations until now.

6 Reliability analysis

Numerous investigations on stochastic reliability models based either on MCS technique as well as Stochastic Finite Element Methods show that the main disadvantage of the first and second order approaches (FORM and SORM, respectively) is that these methods make it possible to analyze symmetric probability density functions (PDFs) only. It is sufficient in the case of Gaussian or lognormal PDF of the output where third order probabilistic moments are equal to 0, however in the case of Weibull statistics for instance, the second order but third moment (W-SOTM) method should be used. Having computed up to the second order state functions, their expected values, standard deviations and skewnesses can be calculated as follows [14]:

$$E[\mathbf{u}]=\mathbf{u}+\tfrac{1}{2}\sum_{i=1}^{n}\left(\frac{\partial^2\mathbf{u}}{\partial b_i^2}\right)\sigma_i^2, \tag{23}$$

$$\sigma^2(\mathbf{u})=\{\mathbf{u}\}^2+\sum_{i=1}^{n}\left[\left(\frac{\partial\mathbf{u}}{\partial b_i}\right)^2+\mathbf{u}\left(\frac{\partial^2\mathbf{u}}{\partial b_i^2}\right)\right]\sigma_i^2+\sum_{i=1}^{n}\left(\frac{\partial\mathbf{u}}{\partial b_i}\frac{\partial^2\mathbf{u}}{\partial b_i^2}\right)S_i\sigma_i^2-E^2[\mathbf{u}] \tag{24}$$

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$$S(\mathbf{u}) = \left\{ \{\mathbf{u}\}^3 + \tfrac{3}{2}\sum_{i=1}^{n}\left[2\mathbf{u}\left(\frac{\partial \mathbf{u}}{\partial b_i}\right)^2 + \mathbf{u}^2\left(\frac{\partial^2 \mathbf{u}}{\partial b_i^2}\right)\right]\sigma_i^2 + \right. \tag{25}$$
$$\left. + \sum_{i=1}^{n}\left[\left(\frac{\partial \mathbf{u}}{\partial b_i}\right)^3 + 3\mathbf{u}\frac{\partial \mathbf{u}}{\partial b_i}\frac{\partial^2 \mathbf{u}}{\partial b_i^2}\right]S_i\sigma_i^3 - E^3[\mathbf{u}] - 3E[\mathbf{u}]\sigma^2(\mathbf{u}) \right\}\frac{1}{\sigma^3(\mathbf{u})}$$

while

$$R = \exp\left[-\left(-\frac{\overline{x}}{\lambda}\right)^{\beta}\right] \tag{26}$$

is the reliability index where the parameters $\overline{x}$, β and λ of corresponding Weibull distribution are derived from the following equations:

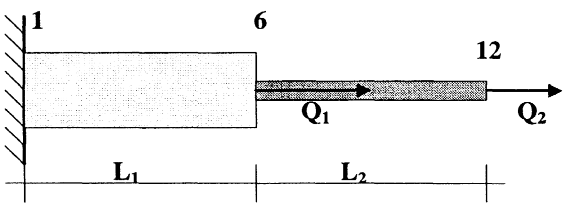
$$E[\mathbf{u}] = \lambda\Gamma\left(1+\frac{1}{\beta}\right) + \overline{x}, \quad \sigma(\mathbf{u}) = \lambda^2\left[\Gamma\left(1+\frac{2}{\beta}\right) - \Gamma^2\left(1+\frac{1}{\beta}\right)\right], \tag{27}$$
$$S(\mathbf{u}) = \lambda^3\left[\Gamma\left(1+\frac{3}{\beta}\right) - 3\Gamma\left(1+\frac{2}{\beta}\right)\Gamma\left(1+\frac{1}{\beta}\right) + 2\Gamma^3\left(1+\frac{1}{\beta}\right)\right]\frac{1}{\sigma^2(\mathbf{u})},$$

where $\Gamma(.)$ denotes the function Gamma values. It should be mentioned that the method of reliability index calculation proposed above is sensible if the material parameters of composite are random variables or fields. In the case of stochastic processes defining the composite behavior, more complicated models are necessary.

7 Numerical illustration

The following numerical example of two-component linear elastic bar is used to illustrate stochastic computational analysis of its reliability. The bar is built up with two homogeneous components with the following material and geometrical data: $E[e_1]=3000$, $A_1=4$, $l_1=15$, $E[e_2]=2500$, $A_2=2$, $l_2=10$ while the external loads $Q_1=200$ and $Q_2=250$ are applied to the structure; the input correlations and the homogenization results are collected in Tab. 1, while reliability studies using Stochastic Finite Element Method program - in Tab. 2.

Figure 2: Random composite bar under tension



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Tab. 1. Probabilistic data and results for computational experiments

Model	Expected values	Covariances
real	$E[e_1,e_2]=\{3000,2500\}$	$Cov(e_r,e_s)=\begin{bmatrix} 90.0 & 75.0 \\ symm. & 62.5 \end{bmatrix} \times 10^3$
effective	$E[e^{(eff)}]=2857,1437$	$Cov(e_r,e_s)=\begin{bmatrix} 41.649 & 16.659 \\ symm. & 6.663 \end{bmatrix} \times 10^3$

The reliability parameters presented in eqns (27) for nodes '6' and '12' are calculated using symbolic computations tool implemented in the mathematical package MAPLE V.

Tab. 2. Reliability calculations results

Variable	Node '6'	Node '12'
U	0.5625	1.0625
$\mathbf{u}^{,e}$	-0.0002	-0.0004
$\mathbf{u}^{(2)}$	0.0156	-0.0284
$E[\mathbf{u}]$	0.5781	1.0909
$Var(\mathbf{u})$	8.7891E-3	3.0189E-2
$\sigma(\mathbf{u})$	0.0937	0.1737
$S(\mathbf{u})$	-5.0180	-20.4089
$\beta(\mathbf{u})$	-4.1688	-3.2090
$\overline{x}(\mathbf{u})$	0.8121	1.3802
$\lambda(\mathbf{u})$	-0.1930	-0.2197
$R(\mathbf{u})$	0.9971	0.9972

8 Concluding remarks

All the considerations posed above make it possible to carry out probabilistic computational analyses of composite materials in terms of homogenization, fatigue and fracture as well as the reliability analysis. How it is shown, Monte-Carlo simulation method and stochastic second order perturbation technique have the wide range of applications in computational modeling of these phenomena. Stochastic computational mechanics of composite materials is still progressing discipline of engineering thanks to the great technological developments in this area as well as in computer technology what allows to carry out the very advanced deterministic and stochastic simulations and still more sophisticated theories and more precise experimental techniques. Special attention should be directed to the wavelets analysis which being developed quite recently is very effective in conjunction with FEM and eliminates the scale parameter problem in the case of homogenization approach which is common to all the methodologies worked out previously.

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