THE ROLE OF MICROSTRUCTURE UNCERTAINTY IN STOCHASTIC FINITE ELEMENT ANALYSIS

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Abstract. *The linking of microstructure uncertainty with the random variation of material properties at the macroscale has gained considerable attention in recent years. This linking is particularly needed in the framework of the stochastic finite element method (SFEM) where arbitrary assumptions are usually made regarding the probability distribution and correlation structure of the macroscopic mechanical and geometric properties. To highlight this need, the effective properties of random two-phase media can be computed by exploiting the excellent synergy of the extended finite element method (XFEM) and Monte Carlo simulation (MCS). The homogenization is based on Hill's energy condition and involves the generation of a large number of random realizations of the microstructure geometry based on a given volume fraction of the inclusions and other parameters (shape, number, spatial distribution and orientation). The mean value, coefficient of variation and probability distribution of the effective elastic modulus and Poisson ratio of the random medium are computed and used in the framework of SFEM to obtain the response variability of a composite structure.*

1 INTRODUCTION

A powerful tool in computational stochastic mechanics is the stochastic finite element method (SFEM). SFEM is an extension of the classical deterministic FE approach to the stochastic framework i.e. to the solution of stochastic problems whose (material and geometric) properties are random with the FE method. The considerable attention that SFEM received over the last two decades can be mainly attributed to the understanding of the significant influence of the inherent uncertainties on systems behavior and to the dramatic increase of the computational power in recent years, rendering possible the efficient treatment of large-scale problems with uncertainties [1]. In most SFEM applications, the description of macroscopic material properties using random variables/fields is based on arbitrary assumptions of the respective probability distribution [2-4]. In addition, the correlation structure of the random field is often arbitrarily assumed and the correlations of different material parameters are typically ignored in the random field model. This is mainly due to the fact that insufficient experimental evidence is usually available to validate all of the detailed characteristics of a macro-random field.

The mechanical behavior of heterogeneous and in particular of composite materials is governed by the mechanical properties of their individual components, their volume fractions and other parameters defining their spatial and size distribution. As mentioned before, only the macroscopic mechanical behavior is of interest in many cases. However, the microstructure attributes of this type of materials are extremely important for a better understanding of their intrinsic properties. This is the reason for which the linking of micromechanical characteristics with the random variation of material properties at the macroscale has gained particular attention in recent years. In [5], the quantitative characterization of the microstructure of random heterogeneous materials is treated in detail and the connection between material properties and microstructure is established for several cases. In [6], a process for the evaluation of stochastic formulations for modeling the constitutive behavior of heterogeneous solid materials is proposed. A FEM incorporating microstructural material randomness below the level of a single (mesoscale) finite element is described in [7]. A moving-window micromechanics technique is applied in [8] to produce material property fields associated with the random microstructure of particulate reinforced composites. A homogenization procedure for determining effective properties of composite structures with stochastic material characteristics is considered in [9]. Auto- and cross-correlations of material properties are estimated in [10] using simple micromechanical models and homogenization. The effect of microstructural randomness on the fracture behavior of composite cantilever beams is investigated in [11] through the application of cohesive zone elements with random properties. The generalized variability response function (GVRF) methodology is used in [12] to compute the displacement response and the effective compliance of linear plane stress systems. The influence of a microscopic random variation of the elastic properties of component materials on the mechanical properties and stochastic response of laminated composite plates is investigated in [13].

Despite the aforementioned efforts, the number of publications highlighting the role of microstructure uncertainty in the framework of SFEM is still very limited. As a step forward in this direction, the effective properties of random two-phase media are computed in this paper by exploiting the excellent synergy of the extended finite element method (XFEM) and Monte Carlo simulation (MCS). The homogenization is based on Hill's energy condition and involves the generation of a large number of random realizations of the microstructure geometry based on a given volume fraction of the inclusions and other parameters such as shape, number, spatial distribution and orientation (section 2). The mean value, coefficient of variation and probability distribution of the effective elastic modulus and Poisson ratio of the random medium are computed in section 3. In section 4, the effective properties are used in the framework of SFEM to obtain the response of a composite structure and useful conclusions are derived regarding the effect of random microstructure geometry on the probabilistic characteristics of the response.

2 HOMOGENIZATION OF RANDOM COMPOSITES USING XFEM AND MCS

Effective homogeneous properties of composite materials can be extracted through appropriate homogenization techniques, e.g. [5,9,10,13,14-17]. A novel homogenization approach was presented in [18] where extended finite element analysis of microstructure coupled with MCS was used. This MCS based stochastic homogenization approach involves the computational analysis of a large number of randomly generated realizations of the composite medium using XFEM. The results derived from the micromechanical analysis are then used in the calculation of the effective properties of an equivalent homogeneous medium, where Hill's energy condition is satisfied. These effective properties will serve as a basis for the stochastic finite element analysis of structures made from random composites, as explained in section 3.

It is worth noting that in [18], the influence of inclusion shape on the effective Young modulus and Poisson ratio of the homogenized medium was demonstrated through histograms of the corresponding properties, along with the statistical convergence of their mean and coefficient of variation (COV). In section 2.3 of this paper, the effect of inclusion shape on the effective properties of the random composites will also be quantified in terms of the inclusion surface to volume ratio with regard to the mean values of the stochastic material properties for various volume fractions.

2.1 Problem formulation

Consider a medium which occupies a domain $\Omega \subset R^2$ whose boundary is represented by Γ. Let prescribed traction $\overline{t}$ applied on surface $\Gamma_t \subset \Gamma$ (natural boundary conditions) and prescribed displacements $\overline{u}$ applied on $\Gamma_u \subset \Gamma$ (essential boundary conditions). The medium contains an inclusion which occupies the domain Ω^+ and is surrounded by the internal surface $\Gamma_{incl} \subset \Gamma$ such that $\Omega = \Omega^+ \cup \Omega^-$ and $\Gamma = \Gamma_t \cup \Gamma_u \cup \Gamma_{incl}$ (Fig. 1). The governing equilibrium and kinematic equations for the elastostatic problem of the medium is:

$$div(\sigma) + b = 0 \text{ in } \Omega \tag{1}$$

$$\sigma = \mathbb{C} : \varepsilon \tag{2}$$

where b are the body forces acting on the medium, $\varepsilon = \frac{1}{2}\left(\nabla u + \nabla u^T\right)$ is the second order tensor of the measured strains and $\mathbb{C}$ is the fourth order elasticity tensor. The essential and natural boundary conditions are:

$$u = \overline{u} \text{ in } \Gamma_u \tag{3}$$

$$\sigma \cdot n = \overline{t} \text{ in } \Gamma_t \tag{4}$$

where n is the unit outward normal to Γ_t.

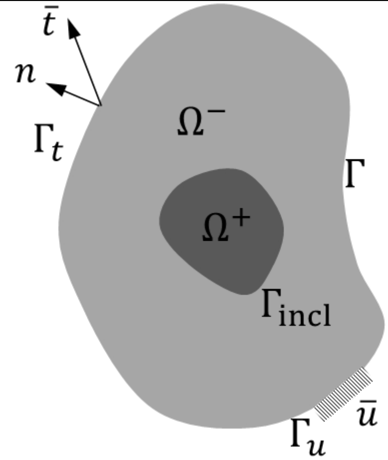

Figure 1. Schematic of a medium which occupies a domain $\Omega = \Omega^+ \cup \Omega^-$, contains an inclusion (Ω^+) and is subjected to essential and natural boundary conditions on surfaces Γ_u and Γ_t, respectively.

In the context of XFEM, weak discontinuities (material interfaces) can be captured by a discontinuous approximation of the displacement function $u^h(x)$. This function can be decomposed into a continuous (fem) and a discontinuous (enriched) part as follows:

$$\begin{aligned} u^h(x) &= u^h_{fem}(x) + u^h_{enr}(x) \\ &= \sum_{i\in I} N_i(x) u_i + \sum_{j\in J} N_j(x)\left(\sum_{k=1}^{n_0} \psi_k(x)\alpha_{jk}\right) \end{aligned} \tag{5}$$

where I is the set of all nodes in the mesh, J is the set of nodes that are enriched with the enrichment functions ψ_k and α_{jk} are the enriched nodal variables corresponding to node j whose support is cut by the k^{th} inclusion. To improve the accuracy and convergence of XFEM solution, Moës et al. [19] have proposed the following enrichment function:

$$\psi_k(x) = \sum_{i\in I} N_i(x)\left|\phi_i^k\right| - \left|\sum_{i\in I} N_i(x)\phi_i^k\right| \tag{6}$$

This ridge function is centered on the interface, has discontinuous first derivative and zero value on the elements which are not crossed by the interface. ϕ_i^k are the nodal values of a level set function corresponding to the k^{th} inclusion. The level set function is used here to represent inclusions of arbitrary shape ("rough circle") and is expressed as a random function of the form:

$$\phi(x,\theta) = \|x-c\| - R(\alpha(x),\theta) \tag{7}$$

where x is the spatial location of a point in the meshed domain, c is the center of a "rough circle" inclusion which has radius $R(\alpha(x),\theta)$ expressed as a random field, $\alpha(x) \in [0,2\pi]$ is the polar angle at position x and θ denotes the randomness of a quantity (Fig. 2). The iso-zero of Eq. (7) defines the location of the inclusion interface $\Gamma_{incl}(\theta)$. The radius of the rough circle is taken as [20]:

$$\begin{aligned} R(\alpha,\theta) = 0.2 + 0.03Y_1(\theta) + 0.015\{&Y_2(\theta)\cos(k_1 a) + \\ Y_3(\theta)\sin(k_1 a) + Y_4(\theta)\cos(k_2 a) &+ Y_5(\theta)\sin(k_2 a)\} \end{aligned} \tag{8}$$

where the i.i.d. uniform random variables $Y_i(\theta) \in U\left(-\sqrt{3},\sqrt{3}\right),\ i = 1,\ldots,5$. Note that the first random variable controls the "mean" reference radius while the other four control its amplitude. k_1, k_2 are deterministic constants which define the period of oscillations of the random rough circle around the shape of the reference (perfect) circle. Fig. 3 presents four different inclusion shapes obtained by substituting different pairs of k_1 and k_2 values in Eq. (8).

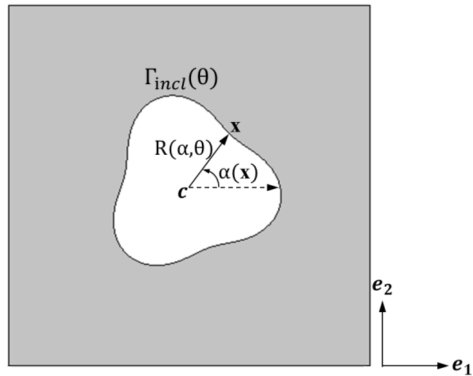

Figure 2. Schematic representation of a rough circle.

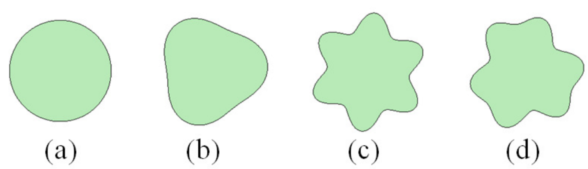

Figure 3. Inclusions of arbitrary shape constructed using: a) $k_1 = 0$, $k_2 = 0$, b) $k_1 = 0$, $k_2 = 3$, c) $k_1 = 0$, $k_2 = 6$ and d) $k_1 = 3$, $k_2 = 6$.

2.2 Homogenization in the framework of MCS

The homogenization of microstructural behavior is performed based on the fundamental assumption of statistical homogeneity of the heterogeneous medium [21]. This means that all statistical properties of the state variables are the same at any material point and thus a representative volume element (RVE) can be identified. Effective homogeneous material properties, corresponding to the random microstructures generated by the algorithm presented in [18], are obtained by MCS. For this purpose, a sufficiently large number of elastic analyses are conducted where the RVEs were subjected to displacement boundary conditions (Fig. 4). Although there is a constant homogenized material property within the RVE, this property changes from realization to realization making it a random variable. The effective Young modulus E_{eff} and Poisson ratio ν_{eff} are determined through the stochastic homogenization procedure by assuming that the resulting homogeneous material is linear and isotropic in an average sense.

Homogenization is based on Hill's energy averaging theorem which states that the strain energy of the homogenized macro-continuum has to be equal to that of the microstructured RVE, as follows:

$$\bar{\sigma} : \bar{\varepsilon} = \frac{1}{|V|} \int_{\Omega} \sigma : \varepsilon \, dY \tag{9}$$

where $\bar{\sigma}$ and $\bar{\varepsilon}$ are the macroscopic stress and strain tensors, σ and ε are the corresponding microscopic quantities, V is the volume of the RVE and Y are the microstructural spatial coordinates.

Miehe and Koch [15] proposed a computational procedure to exclusively define the overall macroscopic stresses and tangent moduli of a typical microstructure from the discrete forces and stiffness properties on the boundary nodes of the meshed RVE model. Following this procedure, a prescribed strain tensor $\bar{\varepsilon}$ is applied on the boundary of the microstructure models through displacement boundary conditions of the form (Fig. 4):

$$u_q = D_q^T \bar{\varepsilon} \tag{10}$$

where D_q is a geometric matrix that depends on the coordinates of the nodal point q which lies on the boundary of the model, defined by

$$D_q = \frac{1}{2}\begin{bmatrix} 2x_1 & 0 \\ 0 & 2x_2 \\ x_1 & x_2 \end{bmatrix} \tag{11}$$

where $(x_1, x_2) \in Y$. The overall macroscopic stress $\bar{\sigma}$ is then calculated in an average manner from the nodal reaction forces f_q obtained by XFEM analysis as

$$\bar{\sigma} = \frac{1}{|V|}\sum_{q=1}^{M} D_q f_q \tag{12}$$

where M is the number of boundary nodes q. As mentioned previously, the macroscopic stress is related to the imposed macroscopic strain by a linear isotropic elastic constitutive matrix in the form

$$\begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{12} \end{bmatrix} = \begin{bmatrix} C_{eff} & D_{eff} & 0 \\ D_{eff} & C_{eff} & 0 \\ 0 & 0 & G_{eff} \end{bmatrix}\begin{bmatrix} \bar{\varepsilon}_{11} \\ \bar{\varepsilon}_{22} \\ \bar{\varepsilon}_{12} \end{bmatrix} \tag{13}$$

where

$$C_{eff} = \begin{cases} \dfrac{E_{eff}}{1-v_{eff}^2} & \text{plane stress} \\ \dfrac{\left(1-v_{eff}\right)E_{eff}}{\left(1+v_{eff}\right)\left(1-2v_{eff}\right)} & \text{plane strain} \end{cases}, \quad D_{eff} = \begin{cases} \dfrac{v_{eff}E_{eff}}{1-v_{eff}^2} & \text{plane stress} \\ \dfrac{v_{eff}E_{eff}}{\left(1+v_{eff}\right)\left(1-2v_{eff}\right)} & \text{plane strain} \end{cases}$$

and $$G_{eff} = \frac{E_{eff}}{2\left(1+v_{eff}\right)} \tag{14}$$

The computation of the effective Young modulus and Poisson ratio is accomplished by imposing the macrostrain vector $\bar{\varepsilon} = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}^T$ in form of displacements (see Eq. (10)). Thus $C_{eff} = \bar{\sigma}_{11} / \bar{\varepsilon}_{11}$ and $D_{eff} = \bar{\sigma}_{22} / \bar{\varepsilon}_{11}$ can be calculated from which E_{eff} and v_{eff} are derived for each Monte Carlo sample.

2.3 Effect of microstructure geometry on the effective properties

The amount of inclusion shape roughness can be quantified by the surface to volume ratio variable λ, which in 2-dimensional space can be calculated as the fraction of inclusion perimeter length over its surface area. This variable is calculated numerically for each RVE sample in the MCS. Fig. 5 demonstrates the effect of the mean λ variable on mean E_{eff} for composites with E_m = 1 GPa, E_{incl} = 1000 GPa, $v_m = v_{incl}$ = 0.3 and volume fraction vf=0.2, 0.3 and 0.4. As shown, mean E_{eff} is increased with increasing λ in each vf case. As the total area of the inclusions in the RVE for a given vf remains constant, it can be concluded that the roughness of the inclusions shape, which is interpreted by the length of their perimeter, is responsible for the increase of the effective properties of the composite material. Another important observation is that the rate of increase of E_{eff} becomes larger as vf increases. This means that the effect of inclusion shape roughness on the effective properties of the composite is more significant when large volume fractions of inclusions are considered.

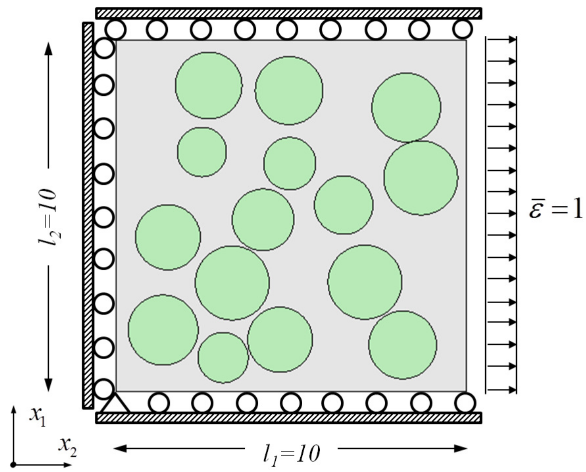

Figure 4. RVE with displacement boundary conditions used in the process of homogenization (dimensions in mm).

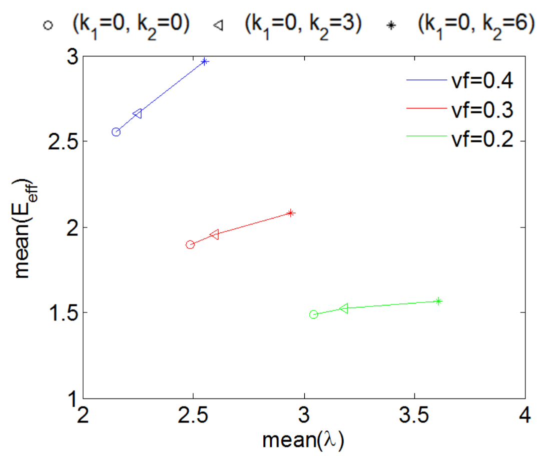

Figure 5. Effect of surface to volume ratio of the inclusions on the mean E_{eff} of the homogenized material for three cases of vf=0.2, 0.3 and 0.4 (composite with 15 inclusions).

3 STOCHASTIC FINITE ELEMENT ANALYSIS BASED ON MATERIAL MICROSTRUCTURE

A fundamental issue in the stochastic finite element method is the modeling of the uncertainty characterizing the macroscopic system properties. In the framework of SFEM, the uncertainty is quantified by using random variables/fields with specific probability distribution and correlation structure. These statistical characteristics are in most cases arbitrarily assumed and parametric investigations are performed in order to examine the effect of each assumption on random system response. However, in the case of heterogeneous (composite) materials, an arbitrary assumption of the statistical characteristics of the macroscopic (effective) properties can be incompatible with the underlying microstructure as it may violate Hill's energy averaging theorem (Eq. 9). In this paper, effective properties that are compatible with the material microstructure are computed and their probability distributions are obtained using the XFEM-MCS based homogenization approach described in section 2. This approach leads to a constant homogenized material property within each realization of the RVE, which is a random variable (random field with very large correlation length) and thus the resulting SFE formulation is greatly simplified as discussed in detail in [22].

The probability distributions of the effective elastic modulus and Poisson ratio of the composite material defined in section 2.3 are obtained from the respective histograms of [18]. The selected PDF fits are shown in Fig. 6 for a random composite containing 15 inclusions. A lognormal distribution is well suited to the effective

Young modulus whereas a normal distribution is a very good choice for the Poisson ratio. In the case of a composite with two inclusions, the asymmetry of the lognormal distribution and the scatter of the elastic modulus values are substantially increased, as shown in [22].

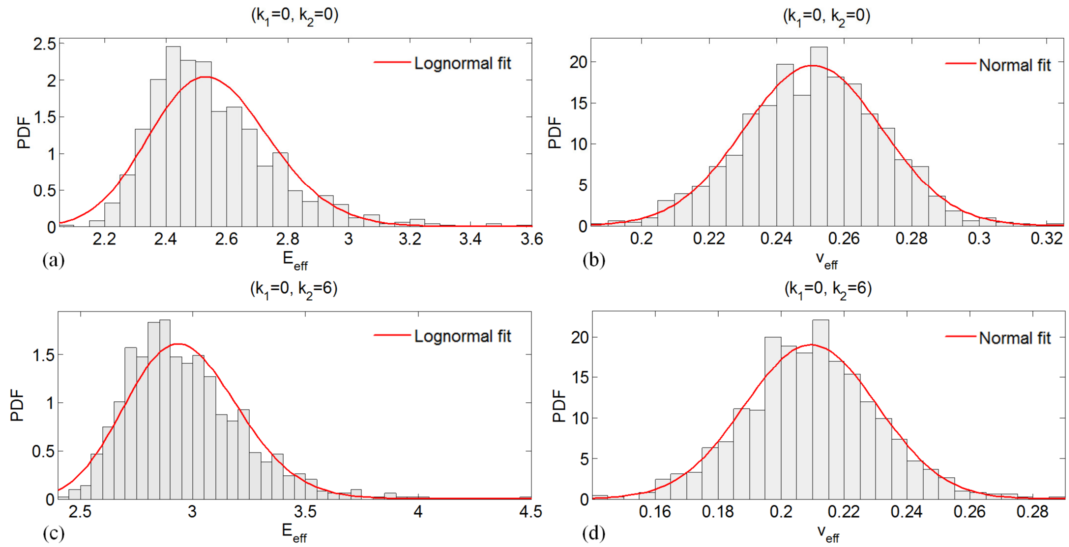

Figure 6. Histograms and fitted PDFs of the effective material properties of the random composite containing 15 inclusions (vf = 0.4).

4 NUMERICAL EXAMPLE

In this section, the effect of material microstructure on the response variability of a plane stress plate shown in Fig. 7 is investigated using the SFE approach. The plate has unit thickness and random material properties with probability distribution, mean and COV computed in section 3. A total of 1000 Monte Carlo simulations are performed for each different case of composite material. The examined response quantities are the vertical and horizontal displacement v, u of the upper right corner of the plate.

Figs. 8-9 illustrate the statistical convergence of the mean and COV of the examined response quantities for the four cases of material microstructure considered. As expected, the effective elastic modulus has a dominant effect on the response variability. The largest mean value of vertical displacement v is observed in the case of the composite material with 15 circular inclusions (which has the smallest mean effective Young modulus), whereas the higher COV(v) is obtained for the random composite with 2 circular inclusions (which has the largest dispersion of E_{eff}). Since the material properties obtained using the underlying microstructure are random variables, the response COV tends to the input COV. A magnification of uncertainty is observed in the case of the horizontal displacement where the computed COV is approx. 1.25 times larger than the COV of E_{eff} (for the composite with 2 circular inclusions). This can be attributed to the additional contribution of the Poisson ratio variation on the horizontal displacement.

The histograms of the monitored displacement v along with two fitted PDFs (lognormal and Gaussian) are presented in Fig. 10 for the same four cases of material microstructure. It can be observed that both PDFs offer an accurate representation of the displacement especially in the case of 15 inclusions. The lognormal fit offers the same accuracy in the approximation of the first two moments but leads to a better representation of the shape of the histogram [22].

5 CONCLUSIONS

In this paper, the statistical characteristics (mean value, coefficient of variation and probability distribution) of the effective elastic modulus and Poisson ratio of random composites have been computed taking into account the material microstructure. The excellent synergy of the extended finite element method and Monte Carlo simulation has been exploited to this purpose. An arbitrary assumption of the statistical characteristics of the macroscopic properties can be incompatible with the actual microstructure as it may violate Hill's energy averaging theorem used in the homogenization. This proves the need of linking microstructure uncertainty with the random variation of material properties at the macroscale in the framework of the stochastic finite element method. The stochastic finite element analysis of a composite structure using the computed effective properties has shown that the response variability can be significantly affected by the random microstructure.

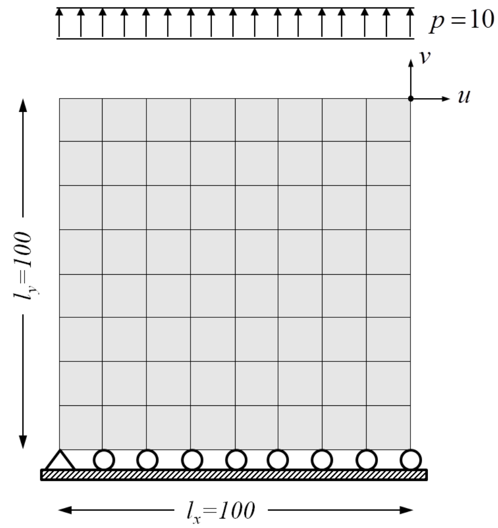

Figure 7. Plane stress plate under uniform tension (dimensions in mm and load in GPa).

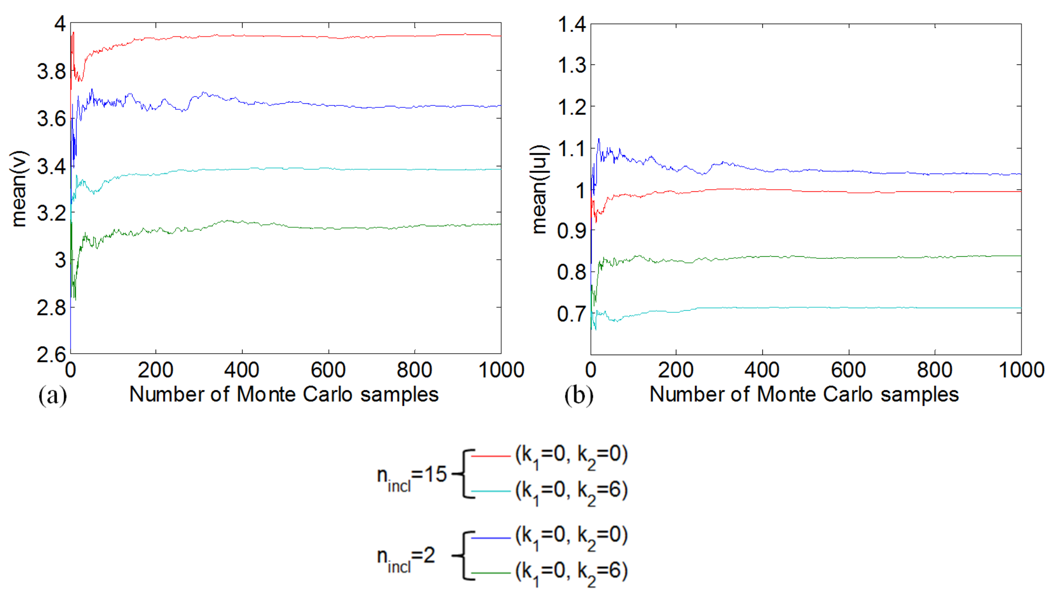

Figure 8. Mean value of (a) vertical displacement v, (b) horizontal displacement u vs. number of MC samples for two cases of inclusion shape and number.

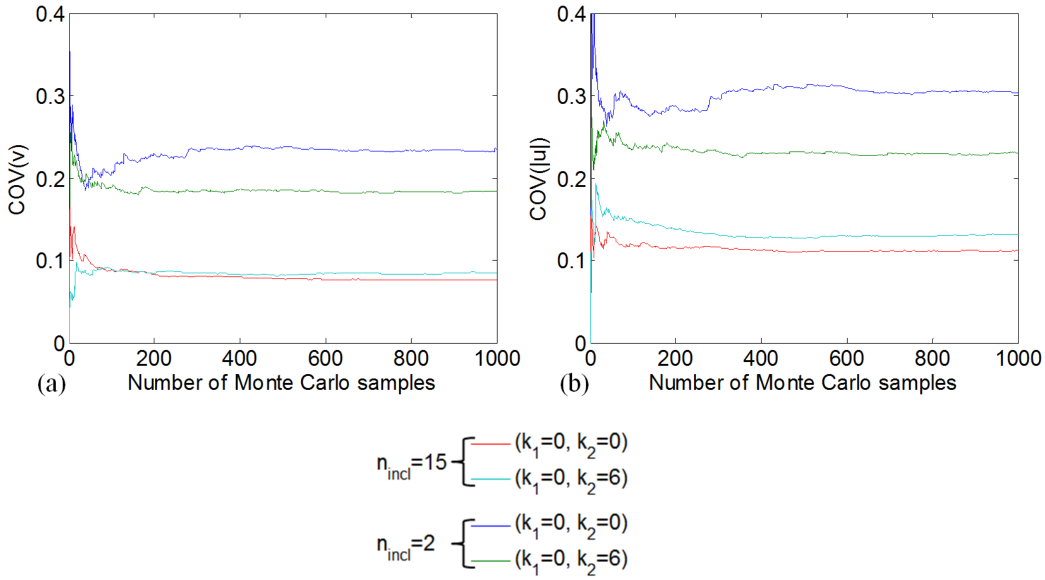

Figure 9. COV of (a) vertical displacement *v*, (b) horizontal displacement *u* vs. number of MC samples for two cases of inclusion shape and number.

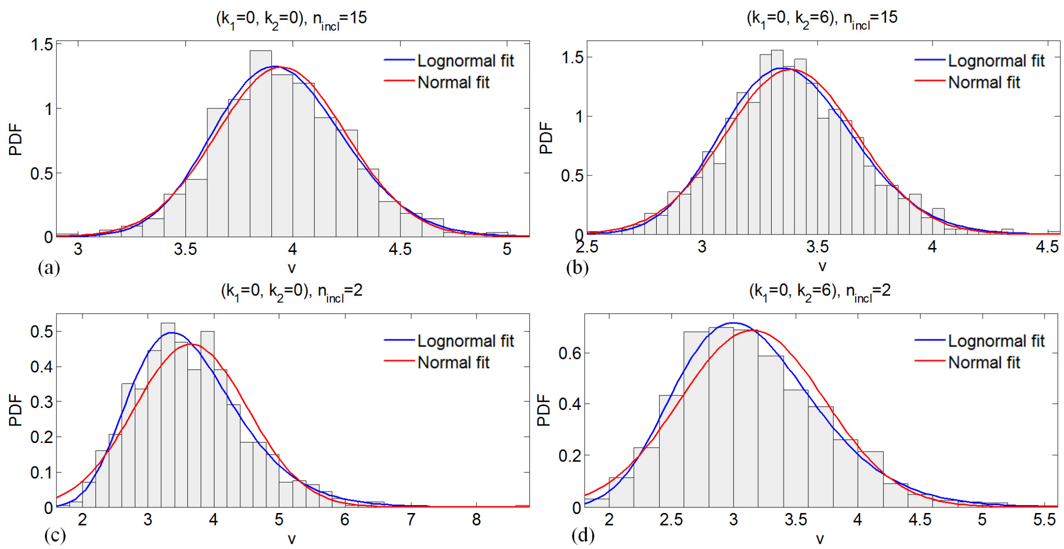

Figure 10. Histograms and fitted PDFs of the vertical displacement *v* for two cases of inclusion shape and number.

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