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Stochastic Macro Material Properties, Through Direct Stochastic Modeling of Heterogeneous Microstructures with Randomness of Constituent Properties and Topologies, by Using Trefftz Computational Grains (TCG)

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Abstract: In this paper, a simple and reliable procedure of stochastic computation is combined with the highly accurate and efficient Trefftz Computational Grains (TCG), for a direct numerical simulation (DNS) of heterogeneous materials with microscopic randomness. Material properties of each material phase, and geometrical properties such as particles sizes and distribution, are considered to be stochastic with either a uniform or normal probabilistic distributions. The objective here is to determine how this microscopic randomness propagates to the macroscopic scale, and affects the stochastic characteristics of macroscopic material properties. Four steps are included in this procedure: (1) using the Latin hypercube sampling, to generate discrete experimental points considering each contributing factor (material parameters and volume fraction of each phase, etc.); (2) randomly generating Representative Volume Elements (RVEs) of the microstructure for each discrete experimental point, and compute the effective macro-scale material properties at these points, using the computationally most efficient Trefftz Computational Grains; (3) relating the macro-scale material properties to the microscale random variables using the Kriging method; (4) taking advantage of the approximate macro-micro relation, and using the Monte Carlo simulation, to establish the probabilistic distribution of the macro-scale material properties. By considering the Al/SiC composite as an example, we give step-by step demonstration of the procedure, and give some comparisons with experimental results. The obtained probabilistic distributions of the effective macro-scale material properties have fundamental engineering merits, which can be used for reliability-based material optimization, and integrated-design of micro- as well as macro-structures. The

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studies in this paper are germane to the concepts of the Materials Genome Initiative (MGI), and Integrated Materials Science, Mathematics, Modeling, and Engineering (IMSMME).

Keywords: Trefftz Computational Grains, Direct Numerical Modeling, Microstructure, Material Uncertainty, Monte Carlo Simulation, Kriging method, Latin Hypercube

1 Introduction

Increasing applications of heterogeneous materials, such as alloys with precipitates/pores, composites with fiber/whisker/particulate reinforcements, have been experienced in both civil and military engineering in the past few decades, because of their superior mechano/thermo/electro/electromagnetic multi-physical properties. In fact, any material can be considered as heterogeneous if the scale is fine enough, with its randomly distributed local complexities such as pores, inclusions, micro-cracks, grain boundaries, dislocations, foreign atoms, atom vacancies, etc. However, a simple, affordable, and reliable analytical/computational method to model the complex heterogeneous microstructures, to rapidly estimate the macro-level stiffness, strength, fracture toughness, and thermo/electro/electromagnetic properties of various heterogeneous materials, given those of the constituent materials, are still under development. This will only be the basis of micro-, meso-, and macro- multi-scale modeling of dynamic response and damage of heterogeneous complex materials and structures, which is at the heart of the Materials Genome Initiative (MGI), and Integrated Materials Science, Mathematics, Modeling, and Engineering (IMSMME).

The recent pioneering work on Trefftz and SGBEM Computational Grains [Dong and Atluri (2011, 2012a-e, 2013)], each of which can model, with the highest mathematical precision, a single grain of the constituent/composite microstructure, with arbitrary embedded inclusions, pores, and micro-cracks, can be regarded as the first step in the authors' efforts to eventually achieve this goal of stochastic multi-scale modeling for IMSMME. The Trefftz and SGBEM Computational Grains are more powerful than the several analytical and semi-analytical methods, such as due to [Eshelby (1957); Hashin and Shtrikman (1963); Hill (1965); Mori and Tanaka (1973); Nemat-Nasser and Hori (1999)], because a truly representative material element, such as a polyhedron, with many micro-complexities such as inclusions, voids, and microcracks, can be directly modeled. ***Indeed, the work in Dong and Atluri (2012 d), is essentially an advancement to the Eshelby's (1957) celebrated work on an ellipsoidal inclusion in an infinite body, in that Dong and Atluri (2012 d) essentially provide a solution for an ellipsoidal inclusion in a 3 dimensional***

grain of arbitrary polyhedral shape, with each face of the polyhedron being an arbitrary polygon. The Trefftz and SGBEM Computational Grains are shown to lead several orders of higher mathematical accuracy as well as computational efficiency than the traditional, FEM-based models [Christman, Needleman and Suresh (1989), Bao, Hutchinson, McMeeking (1991), Guedes and Kikuchi (1991)], because no meshing is needed for each grain, which greatly saves the human-labor as well as computational burden. Compared to the VCFEM by [Ghosh and Mallett (1994); Ghosh, Lee and Moorthy (1995)], the Trefftz and SGBEM computational grains are not only mathematically much more correct and computationally more efficient, but can also correctly and accurately capture the local stress concentrations and interfacial/intergranular stress states which are microcrack precursors and are germane to the studies of damage initiation and propagation.

However, for realistic heterogeneous materials, various micro-scale uncertainties may exist, such as the material properties of each of the constituents, the particle sizes and distributions of each constituent in the microstructure, the microcrack lengths and density, etc. How this microscale randomness propagates to the macroscale, and affects the stochastic material properties of the macro-structure, is the main scope of the present study. In order to achieve this, the previous deterministic analyses by using Trefftz Computational Grains (TCG) are extended to include microscopic randomness, with certain probabilistic distributions. A four-step procedure is presented here: (1) generate discrete samples of these uncertainties using the Latin Hypercube; (2) compute the macro-scale material properties at discrete experiment points by using TCG; (3) relate the macroscale material properties to the microscale uncertainties by using the Kriging method; (4) compute the probabilistic distributions of the macro-scale material properties, by using a Monte-Carlo simulation, and the approximate macro-micro relation. The entire procedure is very simple and efficient, and is much more accurate than the recent few studies of stochastic homogenization, using semi-analytical methods or FEM-based unit cell models [Kamiński and Kleiber (2000); Xu and Graham-Brady (2005); Sakata, Ashida, Kojima and Zako (2008)].

This paper is organized as follows. In sections 2-5, the detailed discussion of each step of the procedure is given, accompanied by numerical examples for Al/SiC composites. In section 6, some comparisons with experimental results, and other semi-analytical methods, are given. In section 7, a simple example of using the computed stochastic material properties, to perform a macro-structure reliability analysis is presented. In section 8, we complete this study with some concluding remarks.

2 Generation of Experimental Points Using a Latin Hypercube

Suppose we use the vector $X \in R^n$ to denote the microscale random variables, for which the probabilistic distributions are already known. We use $Y \in R^p$ to denote the macroscale material properties, the probabilistic distributions of which are to be determined, and are assumed to depend on those of X. In order to relate Y to X through statistical regression, a sufficient number of experimental points $x_1, x_2, ...x_m$, and the responses $y_1, y_2, ..., y_m$ at these experimental points are needed. Out of the many methods to generate experimental points, the Latin hypercube sampling is a strategy for generating random experimental points while ensuring that all portions of the vector space is represented, see [McKay, Conover and Beckman (1979)] for details.

Consider the case where one wants to sample $m$points in the n-dimensional vector space. The Latin hypercube sampling strategy is as follows:

(1) Divide the interval of each dimension into $m$non-overlapping intervals having equal probability;

(2) Sample a point randomly from a uniform distribution in each interval in each dimension;

(3) Pair randomly the points from each dimension.

Table 1: Material Properties of Each Constituent of the Al/SiC Composite

E_{Al}	Normal Distribution, $\mu_{E_{Al}} = 74GPa, \sigma_{E_{Al}} = 5\%\mu_{E_{Al}}$
E_{SiC}	Normal Distribution, $\mu_{E_{SiC}} = 410GPa, \sigma_{E_{SiC}} = 5\%\mu_{E_{SiC}}$
v_{Al}	Deterministic, $v_{Al} = 0.33$
v_{SiC}	Deterministic, $v_{SiC} = 0.19$

In this study, we take Al/SiC composite as an example. The distribution of material properties of each constituent in the composite is listed in table 1. The Young's modulus of both Al and SiC are considered to be random variables subject to independent normal distributions. According to [Chawla, Sidhu and Ganesh (2006)], we assume the expectations μ and standard deviations σ, respectively, of these two random variables as : $\mu_{E_{Al}} = 74GPa$, $\sigma_{E_{Al}} = 5\%\mu_{E_{Al}}$, $\mu_{E_{SiC}} = 410GPa$, $\sigma_{E_{SiC}} = 5\%\mu_{E_{SiC}}$. The coefficients of variations are thus $C_V(E_{Al})$=5% and $C_V(E_{SiC})$=5%. On the other hand, the Poisson's ratio of each constituent in the composite are considered as constants, i.e. $v_{Al} = 0.33$, $v_{SiC} = 0.19$, because they are relatively stable. We also consider that the volume fractions of the SiC particles are distributed from 10% to 30%. From these variables, the vector $X = [E_{Al}, E_{SiC}, SiC\%]$ belongs to a

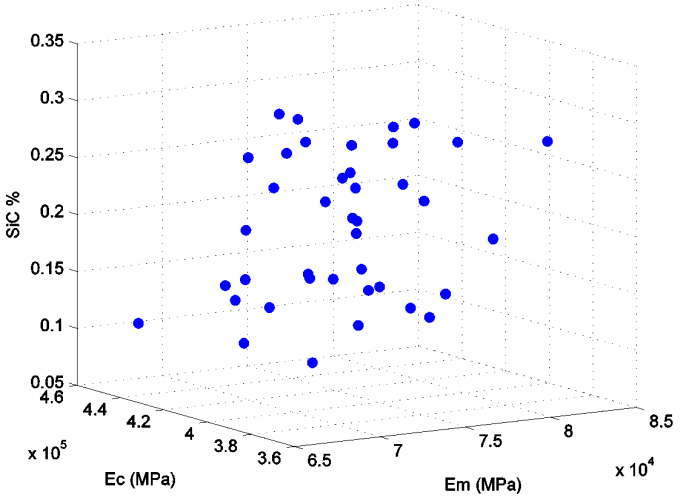

Figure 1: The Latin sampling of 40 data points in 3-dimensional space

three dimensional space, and we can use the above mentioned procedure to generate experimental points. In this study, 40 experimental points are randomly generated using Latin hypercube, and their locations are shown in figure 1.

3 Predicting the Macroscale Material Properties at Discrete Points Using Trefftz Computational Grains

For each generated experimental point x_i, we use the Trefftz Computational Grains to determine the macroscale material properties of the heterogeneous composite. In order to do this, a truly representative material element needs firstly to be generated. For example, in this study, the particle diameters are assumed to have a uniform distribution from $6\mu m$ to$10\mu m$, with an average size of $8\mu m$. The sizes of the particles are randomly sampled, subjected to a specific volume fraction of the experimental point x_i, and are distributed into a $40\mu m \times 40\mu m \times 40\mu m$ cube. The locations of the particles are also randomly generated, using a "take and place" procedure similar to the one used by [Bazant, Tabbara, Kazemi and Pijaudier-Cabot (1990)]. 3 out of the 40 randomly generated representative material elements are shown in figure 2, with different volume fractions of SiC.

Each representative material element is thereafter discretized into many Trefftz Computational Grains, each of which includes a single SiC particle, using the code of Dirichlet Tessellation by [Rycroft, Grest, Landry, Bazant (2006)]. For each Tre-

fftz Computational Grain as shown in figure 3, a polynomial type of displacement field $\tilde{\mathbf{u}}$ is assumed at the grain boundary $\partial\Omega^e$, and a complete Trefftz trial displacement field is assumed in both the matrix material Ω_m^e as well as the inclusion Ω_c^e, i.e. $\mathbf{u}_m$ and $\mathbf{u_c}$. From [Lurie (2005)], these complete Trefftz solutions can be expressed as the Papkovich-Neuber solution:

$$\mathbf{u} = \left[4(1-\nu)\mathbf{B} - \nabla(\mathbf{R}\cdot\mathbf{B} + \mathbf{B_0})\right]/2G \tag{1}$$

where the potentials $\mathbf{B}$, B_0 are harmonic functions depending on the shape of the inclusion. For example, spherical harmonics λ_p for internal problems and λ_k for external problems are respectively:

$$\begin{aligned}
\lambda_p &= \sum_{n=0}^{\infty} R^n \left\{ a_0^0 YC_0^0(\theta,\phi) + \sum_{m=1}^{n} \left[a_n^m YC_n^m(\theta,\phi) + b_n^m YS_n^m(\theta,\phi) \right] \right\} \\
\lambda_k &= \sum_{n=0}^{\infty} R^{-(n+1)} \left\{ c_0^0 YC_0^0(\theta,\phi) + \sum_{m=1}^{n} \left[c_n^m YC_n^m(\theta,\phi) + d_n^m YS_n^m(\theta,\phi) \right] \right\}
\end{aligned} \tag{2}$$

The stiffness matrix can be developed for each Trefftz Computational Grain, using the stationarity of the variational functional:

$$\begin{aligned}
\pi(\tilde{u}_i^m, u_i^m, u_i^c) = &\sum_e \left\{ -\int_{\partial\Omega^e + \partial\Omega_c^e} \frac{1}{2} t_i^m u_i^m dS + \int_{\partial\Omega^e} t_i^m \tilde{u}_i^m dS - \int_{S_t^e} \bar{t}_i \tilde{u}_i^m dS \right\} \\
&+ \sum_e \left\{ \int_{\partial\Omega_c^e} t_i^m u_i^c dS + \int_{\partial\Omega_c^e} \frac{1}{2} t_i^c u_i^c dS \right\}
\end{aligned} \tag{3}$$

For detailed algorithmic formulations, see [Dong and Atluri (2012c,d)].

By assembly of the stiffness matrices of all Trefftz Computational Grains comprising the RVE, the displacement, strain, and stress fields of RVE can be directly computed. And the material properties y_m at each experimental point x_m can be computed by relating the average stress to the average strain.

We should emphasize that, the Trefftz method used here does not need any further discretization of each grain, as opposed to FEM-based methods. This procedure would be too difficult for FEM, if not impossible, because enormous effort has to be spent to develop a high-quality and compatible mesh for each of the many randomly generated RVEs, as well as spend several orders of more computational time. For this reason, the only few published FEM-based stochastic analyses of composites use unit-cell models, see [Kamiński and Kleiber (2000); Sakata, Ashida, Kojima and Zako (2008)], which is too simplistic to be representative for the complex random microstructural topologies of heterogeneous materials.

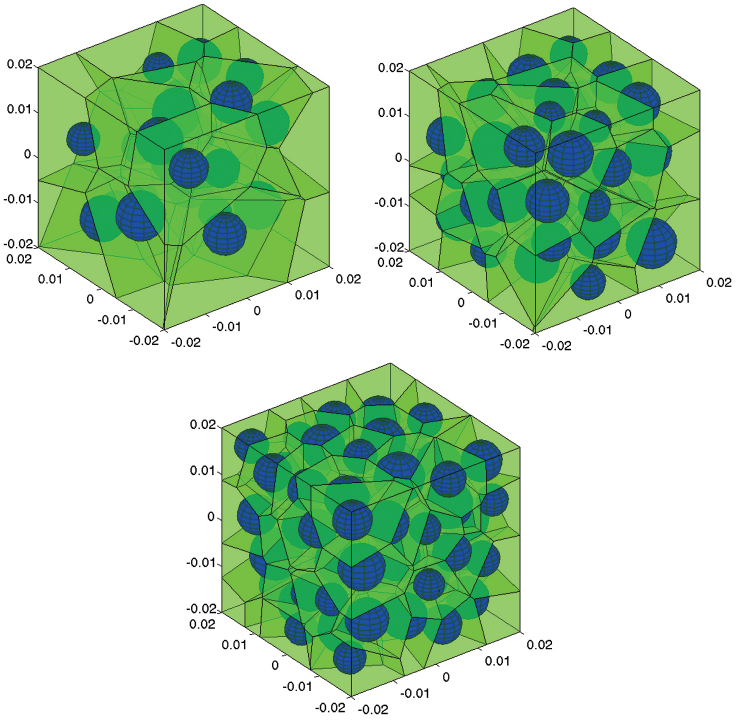

Figure 2: Three of the 40 RVEs with randomly distributed SiC particles, modeled by Trefftz Computational Grains

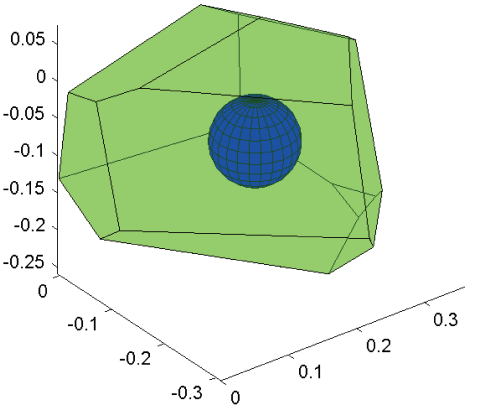

Figure 3: A Trefftz Computational Grain

4 Building up the Macro-Micro Relation using the Kriging Method

After the computation of the macro-scale material properties $y_1, y_2, ..., y_m$ at different experimental points $x_1, x_2, ..., x_m$, one can relate Y to X by statistical regression. One of the most commonly-used methods is the Kriging method. It starts by assuming:

$$y(x) = f^T(x)\beta + z(x) \tag{4}$$

where $f(x)$ is the vector of polynomial basis, and $z(x)$ is a random process, with zero mean and covariance:

$$E[z(x_1)z(x_2)] = \sigma^2 \Re(\theta, x_1, x_2) \tag{5}$$

σ^2 is the variance of the process, and $\Re(\theta, x_1, x_2)$ is a pre-defined correlation model with undetermined parameter θ. In this study, the Gaussian correlation model is used.

By appending the conditions of un-biasness and minimum mean square error, the following estimation of the regression coefficients can be obtained:

$$\hat{\beta} = \left(F^T R^{-1} F\right)^{-1} F^T R^{-1} G \tag{6}$$

with

$$\begin{aligned} F &= [f(x_1) f(x_2) \cdots f(x_m)]^T \\ G &= [y(x_1) y(x_2) \cdots y(x_m)]^T \\ R &= \begin{pmatrix} \Re(x_1, x_1) & \dots & \Re(x_1, x_m) \\ \vdots & \ddots & \vdots \\ \Re(x_m, x_1) & \cdots & \Re(x_m, x_m) \end{pmatrix} \end{aligned} \tag{7}$$

and the estimated $z(x)$ is:

$$\hat{z}(x) = r^T(x) R^{-1} \left(G - F\hat{\beta}\right) \tag{8}$$

with

$$r(x) = [\Re(x, x_m), \Re(x, x_m), ..., \Re(x, x_m)]^T \tag{9}$$

It should be noted that, in this process, the parameter θ is obtained by maximum likelihood estimation, see [Lophaven, Nielsen, Søndergaard (2002)] for further details.

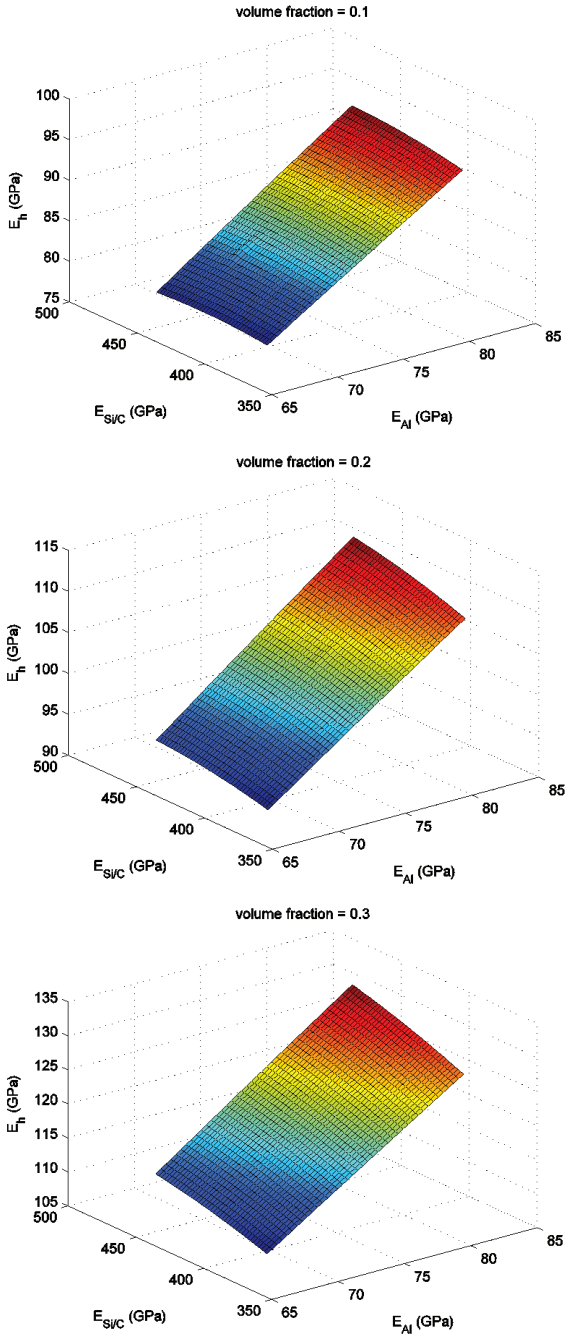

Figure 4: Response surface of the E_h (effective Young's Modulus) with respect to E_{Al} and E_{SiC}, with different volume fractions of SiC

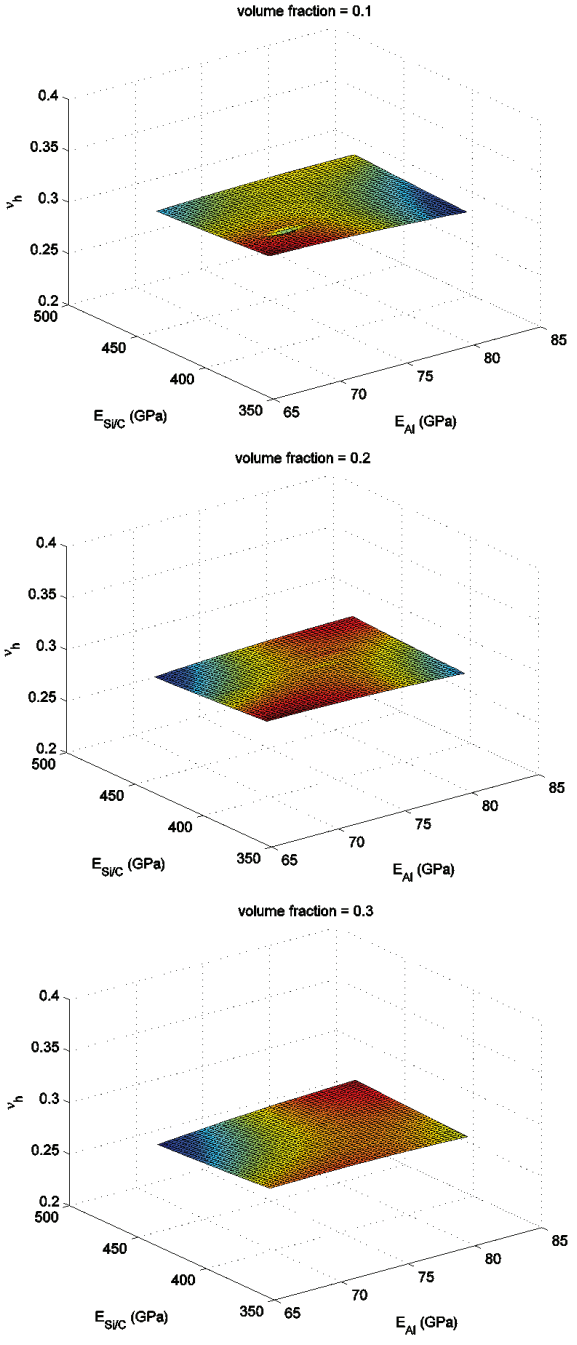

Figure 5: Response surface of the v_h (effective Poisson's ratio) with respect to E_{Al} and E_{SiC}, with different volume fractions of SiC

In this study, we are interested in the effective macro-scale Young's modulus E_h, and Poisson's ratio of the Al/SiC material. Each of them can be related to the vector X, which includes the Young's modulus of Al and SiC respectively, and the volume fraction of SiC particles. Because it is relatively difficult to visualize a four-dimensional space, and because naturally one is interested the macro-material properties with specific volume fractions of SiC (volume fractions are relatively deterministic), we plot the regressed model of both E_h and v_h at three specific volume fractions: 10%, 20%, 30%. As can be seen from figure 4 and figure 5, at specific volume fractions of SiC particles, E_h demonstrates significant variation with respect to E_{Al} and E_{SiC}, while the v_h is relatively stable.

5 Compute the Probabilistic Distribution of Macroscale Material Properties Using Monte Carlo Simulation

With the probabilistic distribution of X, and the relation between Y and $X_{established}$, the distribution of Y can be easily obtained by Monte-Carlo simulation. This procedure can be described as:

(1) Randomly generate a large sample $x_1, x_2, ..., x_q$ according to the probabilistic distribution of X;

(2) Predict the effective macro-scale material properties at these sample points: $y_1, y_2, ..., y_q$ using the established Kriging model;

(3) Fit the empirical distribution of Y to an appropriate probabilistic distribution.

For Al/SiC material, we go through the above-mentioned steps at specific volume fractions, and determine the probabilistic distribution of E_h. As shown in figure 6-8. The effective modulus E_h is subject to normal distribution for different volume fractions. The distributions of the effective material parameters are given in table 2.

Table 2: Material Properties of Al/SiC at different volume fractions of SiC, with $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%

10% SiC	E_h	Normal Distribution, $\mu_{E_h} = 87.3GPa, \sigma_{E_h} = 3.96GPa$
	v_h	Deterministic, $v_h = 0.3182$
20% SiC	E_h	Normal Distribution, $\mu_{E_h} = 102.9GPa, \sigma_{E_h} = 4.45GPa$
	v_h	Deterministic, $v_h = 0.3026$
30% SiC	E_h	Normal Distribution, $\mu_{E_h} = 121.2GPa, \sigma_{E_h} = 4.99GPa$
	v_h	Deterministic, $v_h = 0.2905$

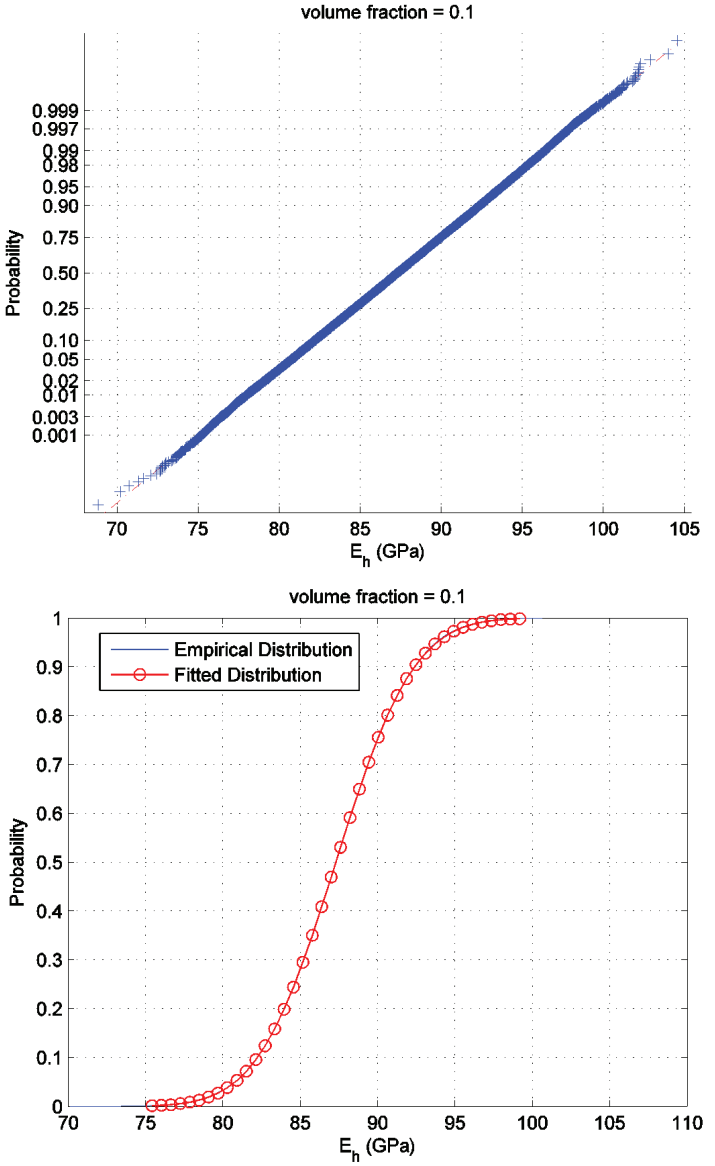

Figure 6: Fit the cumulative distribution of E_h with 10% SiC, when $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%

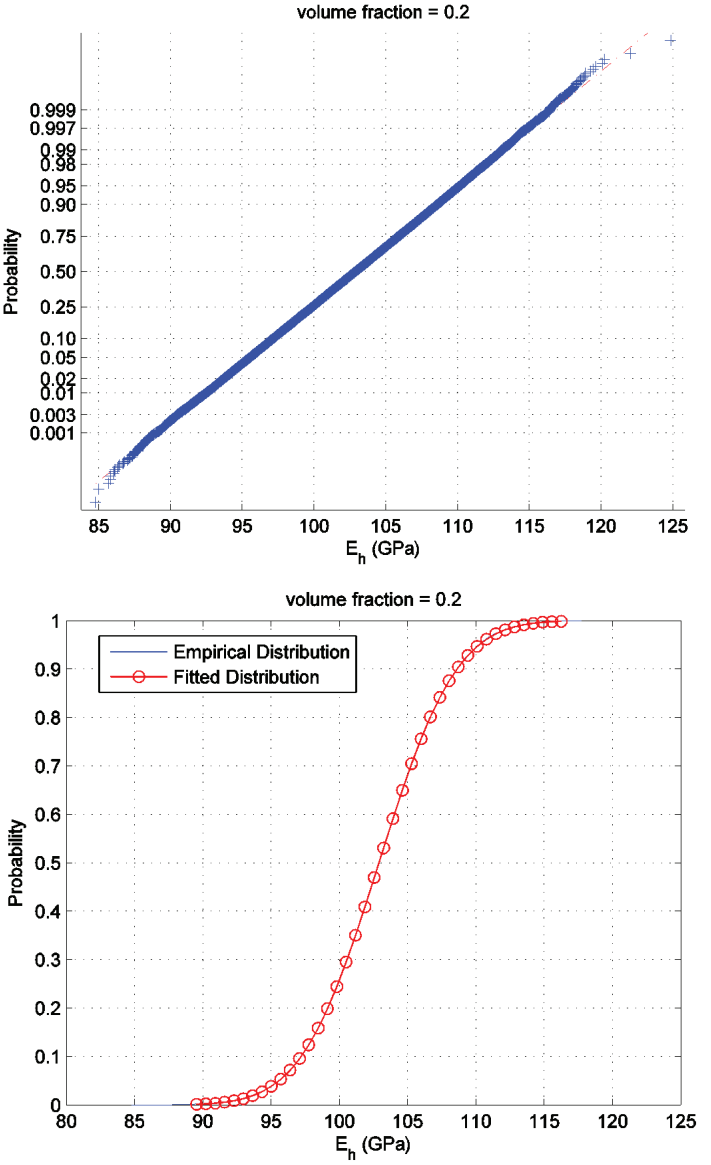

Figure 7: Fit the cumulative distribution of E_h with 20% SiC, when $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%

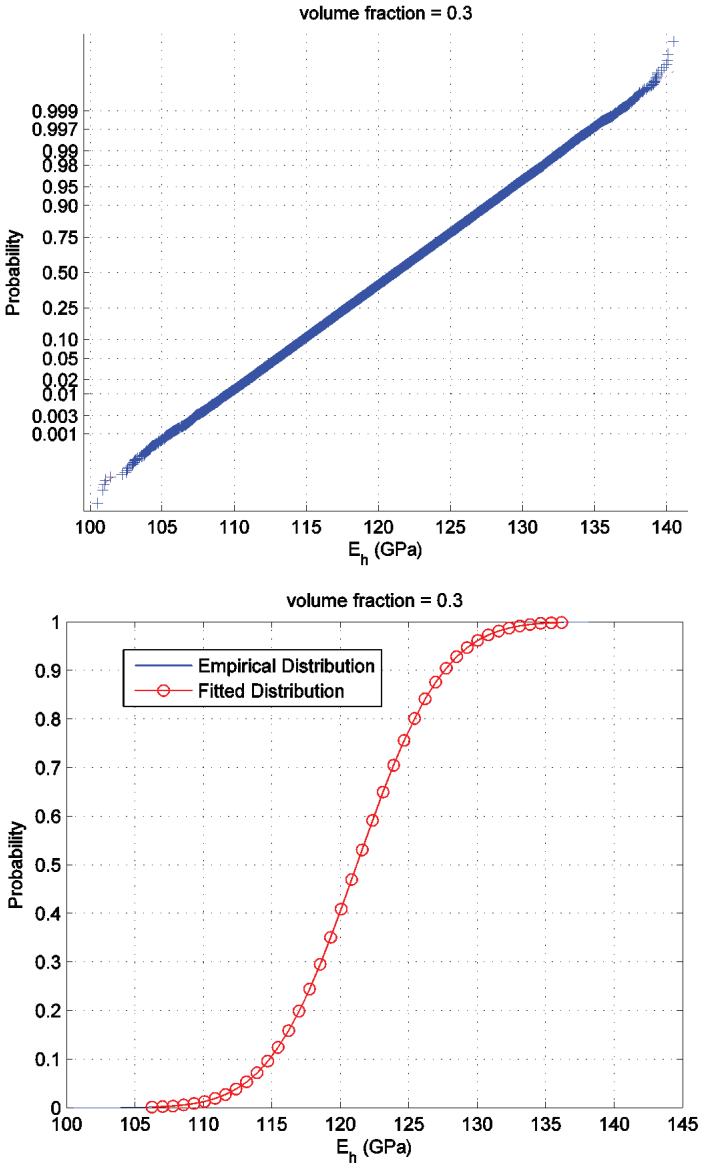

Figure 8: Fit the cumulative distribution of E_h with 30% SiC , when $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%

6 Discussion of the Al/SiC Experimental Results

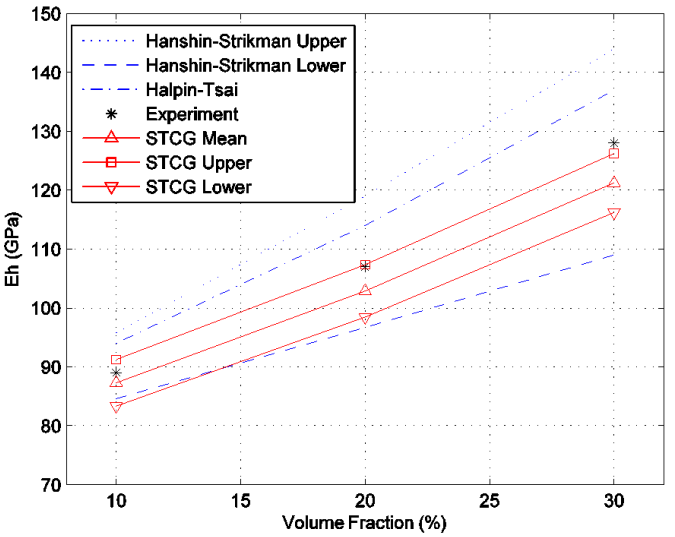

Figure 9: Calculated mean value (μ_{E_h}) and bounds ($\mu_{E_h} \pm \sigma_{E_h}$) of the effective Young's Modulus with different volume fractions of SiC, with $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%

In figure 9, we plot the mean value (μ_{E_h}) and bounds ($\mu_{E_h} \pm \sigma_{E_h}$) of the computed modulus together with other semi-analytical models and experimental results. It can be seen that present computation is very close to the experimental results. On the other hand, semi-analytical models such as Hashin-Strikman variational bounds and Halpin-Tsai method deviate much from the experimental results. For this reason, stochastic simulations based on semi-analytical models will be much less reliable, (if not completely useless), than the present method, as computed by Trefftz Computational Grains.

We also repeat the procedures of section 2-5 with different distributions of E_{Al} and E_{SiC} to analyze the sensitivity of the effective modulusE_h. In figure 10 and 11, we plot the calculated bounds of E_h, with two cases: (1) $C_V(E_{Al})$=2.5%, $C_V(E_{SiC})$=5%; (2) $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=2.5% . It is found that much smaller bounds are given for case 1. Therefore, the uncertainty of E_h is more sensitive to the uncertainty ofE_{Al} at 10%-30% volume fractions of SiC particles.

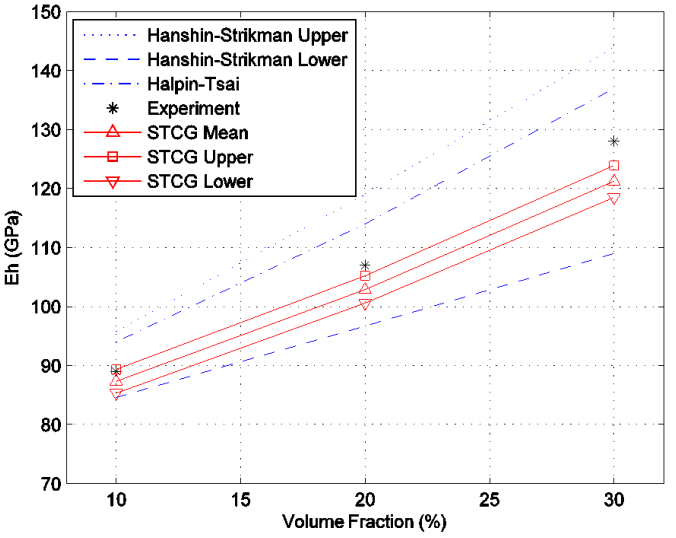

Figure 10: Calculated mean value (μ_{E_h}) and bounds ($\mu_{E_h} \pm \sigma_{E_h}$) of the effective Young's Modulus with different volume fractions of SiC, with $C_V(E_{Al})$=2.5%, $C_V(E_{SiC})$=5%

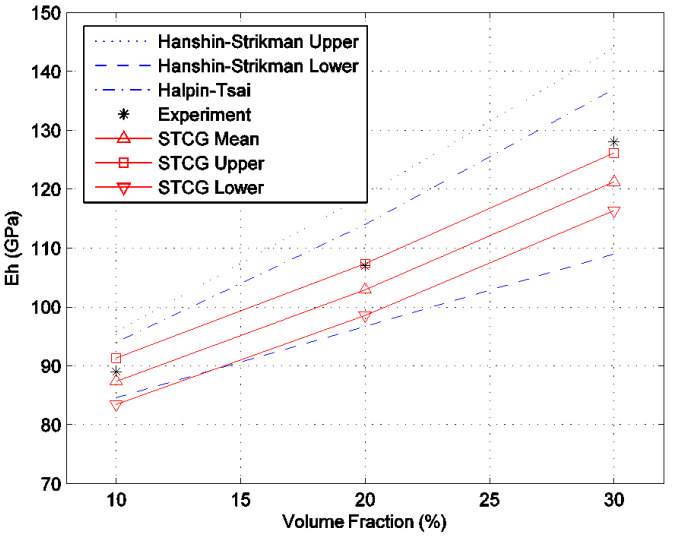

Figure 11: Calculated mean value (μ_{E_h}) and bounds ($\mu_{E_h} \pm \sigma_{E_h}$) of the effective Young's Modulus with different volume fractions of SiC, with $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=2.5%

7 Using the Obtained Stochastic Material Properties to Analyze the Reliability of Global Structures

As is mentioned earlier, the computed probabilistic distribution of the effective macro-scale material properties can be used for reliability-based material optimization, and integrated-design of micro- as well as macro-structures. In this section, we give a simple example by using the obtained stochastic material properties to analyze the reliability of global structures.

Consider a simple cantilever beam as shown in figure 12. A shear force $P = 30N$ is applied to the free-end of the beam. The geometry parameters of the beam is $L = 240mm,\ c = 10mm$. The analytical solution for this problem with deterministic Young's modulus and Poisson' ratio is given by [Timoshenko and Goodier (1970)]:

$$
\begin{aligned}
u_x &= -\frac{Py}{6\overline{E}I}[3x(2L-x)+(2+v)(y^2-c^2)] \\
u_y &= \frac{P}{6EI}[x^2(3L-x)+3v(L-x)y^2+(4+5v)c^2x] \\
I &= \frac{2c^3}{3}
\end{aligned}
\tag{10}
$$

We assume that the beam is made of 20% SiC reinforced Al composite, with material properties given in table 2. Then the empirical distribution of the maximum deflection u_y can be obtained by Monte Carlo simulation, as shown in figure 12. If we consider a design criterion, which states that u_y should be no larger than 2.1 mm, then from the cumulative distribution of u_y, we can obtain that the reliability of the structure is 79.6%.

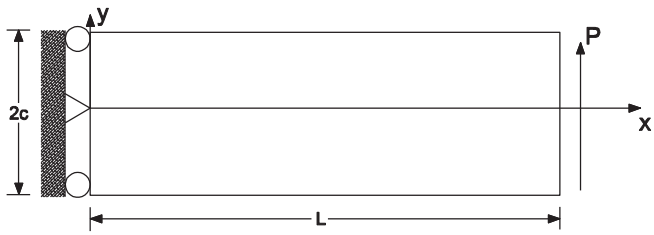

Figure 12: A cantilever beam subjected to shear load at the free end, made of Al/SiC material, with 20% SiC, $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5 %

8 Conclusions

A simple four-step reliable procedure of stochastic modeling is combined with the Trefftz Computational Grains (TCG), for the direct numerical simulation (DNS)

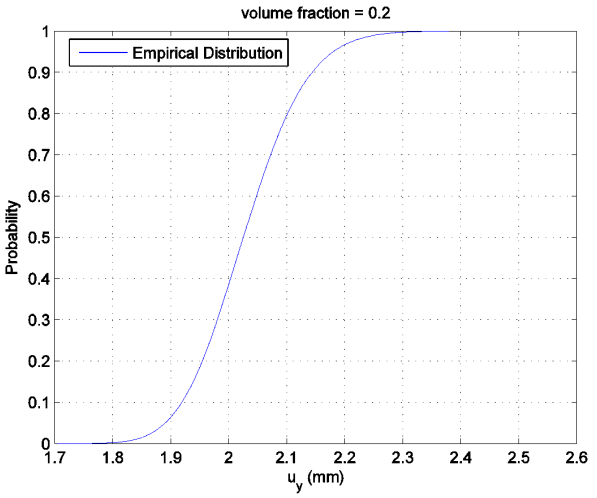

Figure 13: The cumulative distribution of maximum beam deflection u_y with 20% SiC , when $C_V(E_{Al})$=5%, $C_V(E_{SiC})$=5%.

of heterogeneous materials with microscopic randomness. In this procedure, truly random and representative material elements are automatically generated, and are directly solved by using Trefftz Computational Grains. The direct numerical simulation (DNS) is made possible because no meshing of any grain is needed, as opposed to the cumbersome FEM-based models. And because the randomly generated RVEs can account for the uncertain complex microstructural topologies, the current method is much more realistic and reliable than semi-analytical methods such as the Hanshin-Strikman bounds and Mori-Tanaka Method. This method can also be used to compute the macro-level multifunctional material properties, by taking advantage of the multi-physical computational grains by [Bishay and Atluri (2012,2013)]. The present procedures are seminal to the micro-, meso-, macro-multiscale dynamic and damage analyses of stochastic heterogeneous materials, which are germane to the Materials Genome Initiative (GMI) and Integrated Materials Science, Mathematics, Modeling, and Engineering of microscopically heterogeneous multifunctional materials.

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