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Micromechanically based stochastic finite elements

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Abstract. A stochastic finite element method for analysis of effects of spatial variability of material properties is developed with the help of a micromechanics approach. The method is illustrated by evaluating the first and second moments of the global response of a membrane with microstructure of a spatially random inclusion-matrix composite under a deterministic uniformly distributed load. It is shown that two mesoscale random continuum fields have to be introduced to bound the material properties and, in turn, the global response from above and from below. The intrinsic scale dependence of these two random fields is dictated by the choice of the finite element mesh.

Introduction

In elliptic boundary value problems there may be three different sources of randomness: distortion of the boundaries, fluctuation in the external force fields, and heterogeneity of the medium. All of these sources necessitate a stochastic generalization of the conventional solution methods. Such generalizations of the finite element method were attempted since the early eighties with a goal of grasping the randomness of either external force fields or medium's variability [1–6]. However, the latter aspect has been lacking a correct formulation in all the previous works, mainly due to purely hypothetical assumptions concerning the random field description of the material. That is, in the area of linear elastic structures, all these studies relied on a stochastic interpretation of the locally isotropic constitutive law

$$\sigma_{ij} = \lambda(\boldsymbol{x}, \omega)\epsilon_{kk}\delta_{ij} + 2\mu(\boldsymbol{x}, \omega)\epsilon_{ij}, \tag{1}$$

where the Lamé constants are taken to be random fields. In fact, most works considered the Young's modulus to be random field, oftentimes of Gaussian type, with the Poisson's ratio to be constant.

In this paper we develop a random continuum model using the micromechanics approach, and then use it as input for solution of a specific boundary value problem. As a starting point we take the fact that discreteness of materials is the key cause of their nondeterministic constitutive response. We follow [7], where the out-of-plane response of a two-dimensional linear elastic matrix-inclusion composite with a spatially random distribution of inclusions was studied; this gives, at the same time, information on in-plane conductivity of such a material. However, in contrast to [7], where a stochastic finite difference method was developed for the solution of a boundary value problem, the present paper develops, for the first time, a micromechanically based stochastic finite element method. The link between the microstructure and the finite element method is provided by a so-called *window* introduced in our previous works [8–10], which is shown to correspond to a single finite element cell.

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The micromechanical basis

A fundamental role in our formulation is played by the concept of a *random medium*, which, as is commonly done in stochastic mechanics [6], is taken as a family $\boldsymbol{B} = \{\boldsymbol{B}(\omega);\ \omega \in \Omega\}$ of deterministic media $\boldsymbol{B}(\omega)$, where ω indicates one specimen, and Ω is an underlying sample (probability) space. Formally, Ω is equipped with a σ-algebra F and a probability distribution P. In an experimental setting P may be specified by a set of stereological measurements, while in a theoretical setting P is usually specified by a chosen model of a microstructure. For example, in case of a polycrystalline material we may take every specimen $\boldsymbol{B}(\omega)$ to be modeled by a realization of a Voronoi tessellation (Fig. 1(a)), while in case of a matrix-inclusion composite we may take it as a certain planar point process with exclusion of overlapping of disks (Fig. 1(b)). We assume that these microstructures are linear elastic, and the statistics of microscale properties are space-homogeneous and ergodic. While, for simplicity and clarity of presentation, the discussion is conducted in two dimensions (2-D) here, a generalization to 3-D is quite straightforward.

Now, with the help of Fig. 1, we introduce a *window* of size

$$\delta = L/d. \tag{2}$$

Equation (2) defines a nondimensional parameter δ specifying the scale L of observation (and measurement) relative to a typical microscale d (i.e. grain size) of the material structure. In view of the fact that either one of the microstructures in Fig. 1 is a result of a certain random point process in plane, the window bounds a random microstructure $B_\delta = \{B_\delta(\omega);\ \omega \in \Omega\}$, where $B_\delta(\omega)$ is a single window realization from a given specimen $\boldsymbol{B}_\delta(\omega)$.

In order to define the effective moduli of B_δ, we introduce two types of boundary conditions on its boundary ∂B_δ: (1) displacement-controlled (essential) boundary conditions on ∂B_δ

$$u_i = \bar{\epsilon}_{ij} x_j, \tag{3}$$

and (2) stress-controlled (natural) boundary conditions on ∂B_δ

$$t_i = \bar{\sigma}_{ij} n_j. \tag{4}$$

It follows that in a continuum setting the effective stiffness tensor of any specific body $B_\delta(\omega)$ is either

$$\boldsymbol{C}^{\mathrm{e}}_\delta = \boldsymbol{C}^{\mathrm{e}}_\delta(\omega) \quad \text{or} \quad \boldsymbol{C}^{\mathrm{n}}_\delta = \boldsymbol{C}^{\mathrm{n}}_\delta(\omega), \tag{5}$$

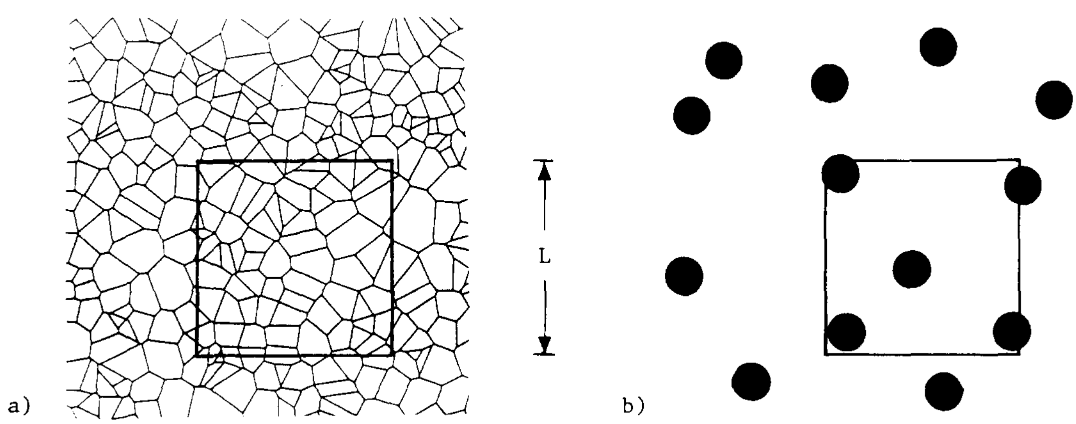

Fig. 1. Showing a window of size $\delta = L/d$ (a) in a Voronoi microstructure, and (b) in a matrix-inclusion composite.

depending on whether (3) or (4) is used; superscripts e and n indicate essential and natural boundary conditions, respectively. It follows from the principles of minimum potential energy and complementary energy that [#1]

$$C^{\mathrm{R}} \equiv \langle S_1^{\mathrm{n}} \rangle^{-1} \leqslant \langle S_{\delta}^{\mathrm{n}} \rangle^{-1} \leqslant \langle S_{\delta'}^{\mathrm{n}} \rangle^{-1} \leqslant C^{\mathrm{eff}} \leqslant \langle C_{\delta'}^{\mathrm{e}} \rangle \leqslant \langle C_{\delta}^{\mathrm{e}} \rangle \leqslant \langle C_1^{\mathrm{e}} \rangle \equiv C^{\mathrm{V}} \quad \forall \delta' > \delta, \tag{6}$$

where C^{eff} denotes the effective stiffness tensor of a deterministic continuum corresponding to the scale $\delta \to \infty$, and $\langle\ \rangle$ denotes ensemble averaging.

The principal conclusions to be made here are [7,10]:

(i) C^{R} and C^{V} are the Reuss and Voigt bounds, respectively.

(ii) The scatter in C_{δ}^{n} and C_{δ}^{e} is strongest at the scale $\delta = 1$, and it tends to 0 as $\delta \to \infty$.

(iii) For any finite δ, both these moduli are, in general, anisotropic.

(iv) Since for any $\delta > 1$, B_{δ} is a random rather than a deterministic medium, the window plays the role of a representative volume element (RVE) of a *continuous random medium* $B_{\delta} = \{B_{\delta}(\omega);\ \omega \in \Omega\}$; in view of (5), this continuum approximation is, generally, nonunique since we have two random tensor fields C_{δ}^{n} and C_{δ}^{e} at our disposal. This conclusion together with (iii) indicates that the locally isotropic unique random tensor field (1) should not be assumed.

(v) The scatter in both elasticity tensors becomes eventually negligible at some large, or very large $\bar{\delta}$, so that we arrive at an invertible constitutive law in the sense that

$$C_{\bar{\delta}}(\omega) \approx [S_{\bar{\delta}}(\omega)]^{-1} \approx C^{\mathrm{eff}} \quad \forall \omega \in \Omega, \tag{7}$$

where $C_{\bar{\delta}}$ and $S_{\bar{\delta}}$ are obtained from (3) and (4), respectively. $\bar{\delta}$ may then be taken as the scale of an RVE of a *continuous deterministic medium* $B_{\mathrm{det}} = B_{\bar{\delta}}$.

(vi) Definitions $(5)_1$ and $(5)_2$ are analogous to a *moving locally averaged random field*, although no direct straightforward averaging is possible, but, rather, computations must be carried out. It follows that the normalized *autocorrelation* (or *autocovariance*) *functions* of C_{ijkl}'s are δ-dependent. Thus, in contradistinction to the procedures employed by others – the "weighted integral method" [5], or the "spectral representation method" [6] – which have no connection to the material microstructure, the definition of the autocorrelation functions together with our method of windows outlined above provides a rigorous basis for determining the autocorrelation functions [8,9,11].

The above observations suggests a methodology of solution of stochastic boundary value problems. Three measuring levels may be introduced: microscale $\delta = 1$, mesoscale δ_{meso}, and macroscale δ_{M}, where δ_{M} = macroscopic dimension of the body $B(\omega)$. In case $\bar{\delta}$ of eqn. (7) is on the order of, or even greater than, the macroscale δ_{M}, one is forced to deal with spatial fluctuations on the macroscale. Thus, a statistical rather than a deterministic continuum approximation is applicable. Accordingly, a solution of the problem at hand is then conducted with a certain choice of a mesoscale δ_{meso} of an RVE of the statistical continuum. However, since two alternative definitions of boundary conditions are possible – displacement-controlled (3) and stress-controlled (4) – two different random anisotropic continua result!. Thus, a given boundary value problem may then be solved analytically or numerically – by, say, stochastic finite elements – to find the upper and lower bounds on response according as C_{δ}^{e} and C_{δ}^{n} are used.

[#1] For two fourth-rank tensors A and B, an order relation $B \leqslant A$ means
$t_{ij} B_{ijkl} t_{kl} \leqslant t_{ij} A_{ijkl} t_{kl} \quad \forall t \neq 0$

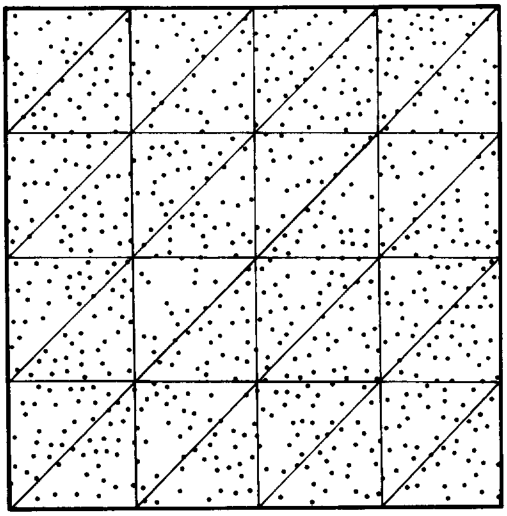

Fig. 2. Showing a membrane made of a matrix-inclusion composite with a finite element mesh of resolution δ.

The finite element formulation

A triangular finite element for analysis of various problems in mechanics is briefly described here. The basic steps in setting up the finite element equations for out-of-plane displacements of a membrane are outlined. We note, however, that the same methodology is applicable to more general cases of materials with elastic as well as inelastic microstructures, e.g. plane stress, plane strain, and three-dimensional problems.

With reference to Fig. 2, we start with a square-shaped finite element mesh, and for the sake of simplifying the algebra, we subdivide each such element into two right-sided triangles. However, the key point is that, in accordance with conclusion (v) of the previous section, each square element represents a window. Thus, in accordance with the statement following eqn. (2), δ is truly the lengthscale of a meso-type random continuum approximation which is dictated by the chosen finite element mesh. We make a reference to [12] for a discussion of these aspects and of the stochastic variational formulation.

Now, the nodal displacement vector for the element is (superscript e indicates an element)

$$\{\boldsymbol{u}^e\} = [u_1\ u_2\ u_3]^{\mathrm{T}}. \tag{8}$$

While, the displacement at any point inside the element is given in terms of the nodal displacement vector as

$$u^e = [N_1\ N_2\ N_3]\{\boldsymbol{u}^e\}, \tag{9}$$

where $[N]$ is the shape functions matrix given by

$$N_i = \frac{1}{A}(a_i + b_i x + c_i y) \quad \text{where } i = 1, 2, 3, \tag{10}$$

in which A is the element area and a, b, c are coefficients defined in terms of the nodal coordinates. The gradient vector of the displacement is given by

$$\mathrm{gr}\{u^e\} = [B]\{\boldsymbol{u}^e\}, \tag{11}$$

where

$$\mathrm{gr}\{u^e\} = \begin{bmatrix} \partial u/\partial x \\ \partial u/\partial y \end{bmatrix}, \qquad [B] = \begin{bmatrix} b_1 \; b_2 \; b_3 \\ c_1 \; c_2 \; c_3 \end{bmatrix}.$$

The stiffness matrix of each element can be calculated by

$$[K^e] = \int_A [B]^{\mathrm{T}}[C][B] \, \mathrm{d}A, \tag{12}$$

where $[C]$ is the material moduli matrix given by either C^{e}_{δ} or C^{n}_{δ} obtained in the previous section. At this stage, we synthesize the global stiffness matrix from those of the sub-elements over the entire region as

$$[K] = \sum_{e=1}^{n} [K^e], \tag{13}$$

in which n is the total number of finite elements. Finally, after applying the specified boundary conditions, the unknown quantities are obtained by solving a system of linear algebraic equations (by a Gausian method) in the form of

$$[K]\{U\} = \{F\}. \tag{14}$$

Here, $\{U\}$ and $\{F\}$ are the global displacement and force vectors, respectively.

Numerical results

The micromechanics-based stochastic finite element is used here to solve an elastostatic membrane problem. The microstructure is taken as a matrix-inclusion composite with both phases being locally isotropic. The out-of-plane deformation $u(x_1, x_2)$ governed by the partial differential equation

$$\frac{\partial}{\partial x_i}\left[C_{ij}(\boldsymbol{x}, \omega)\frac{\partial u}{\partial x_j}\right] = f(\boldsymbol{x}) \tag{15}$$

will be obtained by applying the stochastic finite element method of Section 3 corresponding first to a random continuum approximation $\boldsymbol{B}^{\mathrm{e}}_{\delta}$, and then to $\boldsymbol{B}^{\mathrm{n}}_{\delta}$, at a given scale δ. Thus, C_{ij} in (15) are components, and realizations, of the random tensor fields $\boldsymbol{C}^{\mathrm{e}}_{\delta}$ or $\boldsymbol{C}^{\mathrm{n}}_{\delta}$.

The microstructure is modeled under the following specifications:

(i) Inclusions are round nonoverlapping disks of the diameter $d = 5\Delta l$, where Δl is the unit length, and occupy 10% of the volume of the medium;

(ii) Both phases are locally isotropic homogenous continua;

(iii) The distribution of the inclusions corresponds to a planar Poisson process with the restriction that the minimal spacing between any two centers of 170% of the inclusion diameter to avoid the stress concentration problem;

(iv) The membrane problem is being expressed in the form of a Poisson equation (15), under Dirichlet boundary conditions $u = 0$ on $\delta \boldsymbol{B}$ of a square-shaped body domain of the size $400\Delta l \times 400\Delta l$, subjected to a uniform force distribution: $f = 10^{-2}/(\Delta l)^2$.

Now, solution of the problem may be summarized in the following steps:

(a) Generation, in a Monte Carlo sense, of one realization $\boldsymbol{B}(\omega)$ of the matrix-inclusion composite according to the assumptions stated above.

(b) Microstructure discretization: the domain is discretized into $n \times n$ square windows (RVE's) for the purpose of obtaining the upper and lower moduli. The calculation of these moduli is conducted for each window using a finite-difference type mesh representing the

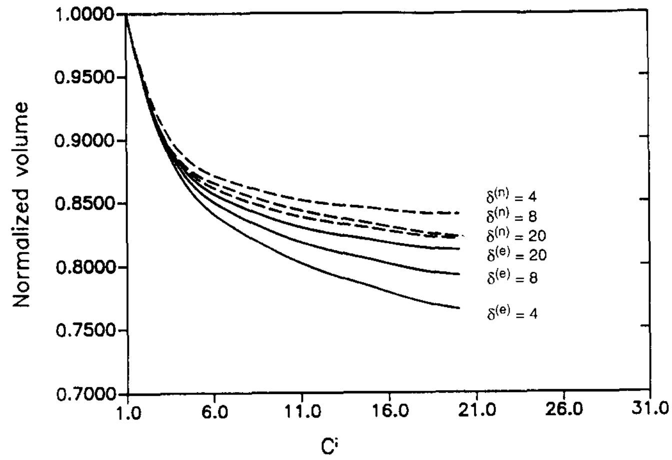

Fig. 3. Graph of the ensemble average "upper" and "lower" responses, normalized over the deterministic case $C^i = C^m = 1$. $\delta^{(e)}$ and $\delta^{(n)}$ correspond to C_δ^e and C_δ^n in eqn. (15), respectively.

continuous phases of the matrix and inclusions. The size of the finite difference mesh inside the window is $m \times m$, where m is related to the chosen scale factor δ by $m = 5\delta$. Here $n = 80\delta$, where n is the number of windows in the x_1 (and x_2) direction.

(c) Finite element discretization: for a given δ, the dimension of the problem is discretized by $2(n \times n)$ finite elements (see Fig. 2) for the purpose of obtaining the global response $u^{(e)}(x, \omega)$ and $u^{(n)}(x, \omega)$ of eqn. (15). For each finite element, the input of the upper moduli C_δ^e and lower moduli C_δ^n are those obtained via the micromechanical model under the conditions (3) and (4), respectively.

To take into account the randomness in the inclusions' distribution, ten different $\boldsymbol{B}(\omega)$'s are generated and the solution for the global response is obtained. As a measure of the global response of $\boldsymbol{B}(\omega)$, we choose the volume $V(\omega)$ under the membrane, so that we obtain a set of 10 "upper" estimates $V^{(e)}(\omega)$ and a set of 10 "lower" estimates $V^{(n)}(\omega)$. Figure 3 shows the ensemble averages $\langle V^{(e)} \rangle$ and $\langle V^{(n)} \rangle$ for three different values of δ plotted as functions of increasing stiffness C^i of the inclusion with C^m kept constant. Here C^m (matrix stiffness) is taken as unity for simplicity, so that C^i becomes a so-called *contrast* and all the plots are normalized by $V^{(e)} = V^{(n)}$ at $C^i = C^m = 1$, which is the purely deterministic case. As may be expected, the membrane deformation under essential boundary condition is smaller than that under the natural boundary condition, since the moduli C_δ^e are always stiffer than the C_δ^n. On the other hand, an increase in the stiffness of the inclusions leads to stiffening of the membrane, and hence, to the reduction of the deformation and consequently, of $V^{(e)}$ and $V^{(n)}$. Therefore, for a fixed δ, both curves are decreasing monotonically and diverging away from $C^i = C^m = 1$, with increasing C^i. In addition, for a fixed contrast, we see that the two responses (bounds) get closer with increasing δ, and have a tendency to converge to a unique value as $\delta \to \infty$, which corresponds to the deterministic case. However, we should note that this limit can only be attained in the approximate sense of eqn. (7), providing the fluctuations in stiffness disappear for such large finite elements. Thus, it is expected that, for a fixed contrast, the scatter in the responses (as measured here by the standard deviation) decreases when δ goes up, see Fig. 4. On the other hand, for any fixed δ, it increases with the contrast (i.e. microstructural randomness) increasing.

The membrane example problem presented here is a simple but generic one – it illustrates the essential features of a micromechanics-based approach in grasping the spatial heterogeneity of materials in stochastic finite element analyses. Two random fields have to be considered

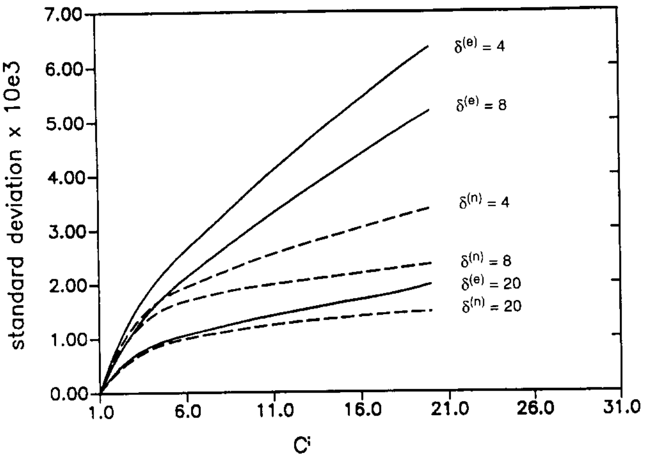

Fig. 4. Graph of standard deviation of the "upper" and "lower" responses.

in describing the microstructure and bounding the response of the heterogenous medium, with the choice of both fields being dictated by choice of a finite element mesh.

We end with a note that the finer the finite element mesh, the higher is the computational cost of a finite element solution, but the lower is the computational cost of a micromechanical specification of the material. These and other related issues are discussed in [12].

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