Probabilistic Engineering Mechanics **8** (1993) 107–114

Micromechanics as a basis of random elastic continuum approximations

Martin Ostoja-Starzewski

Department of Materials Science and Mechanics, Michigan State University, East Lansing, Michigan 48824-1226, USA

(Received April 1992; revised version received and accepted November 1992)

The problem of the determination of stochastic constitutive laws for input to continuum-type boundary value problems is analyzed from the standpoint of the micromechanics of polycrystals and matrix-inclusion composites. Passage to a sought-for random continuum is based on a scale dependent window playing the role of a Representative Volume Element (RVE). It turns out that an elastic microstructure with piecewise continuous realizations of random tensor fields of stiffness cannot be uniquely approximated by a random field of stiffness with continuous realizations. Rather, two random continuum fields may be introduced to bound the material response from above and from below. As the size of the RVE relative to the crystal size increases to infinity, both fields converge to a deterministic continuum with a progressively decreasing strength of fluctuations. Since the RVE corresponds to a single finite element cell not infinitely larger than the crystal size, two random fields are to be used to bound the solution of a given boundary value problem at a given scale of resolution. The method applies to a number of other elastic microstructures, and provides the basis for stochastic finite differences and elements. The latter point is illustrated by an example of a stochastic boundary value problem of a heterogeneous membrane.

1 INTRODUCTION

In recent years there has been a new development in computational mechanics: stochastic finite elements; see for example Refs 1–3. All the researchers in this area working with linear elastic structural responses rely, to the best of our knowledge, on a straightforward generalization of a continuum constitutive law, namely that the stiffness tensor is a random field with continuous realizations $\underset{\sim}{C}(x,\omega)(=C_{ijkl}(x,\omega))$ in the body domain*

$$\underset{\sim}{\sigma} = \underset{\sim}{C}(x,\omega)\underset{\sim}{\epsilon} \qquad \omega \in \Omega \qquad x - (x_1, x_2) \tag{1}$$

Here, in keeping with the terminology of random processes, ω indicates one realization from the underlying sample space Ω. The assumption (1) tacitly implies the invertibility of such a constitutive law in the sense of existence of its inverse

$$\underset{\sim}{\epsilon} = \underset{\sim}{S}(\underset{\sim}{x},\omega)\underset{\sim}{\sigma} \qquad \underset{\sim}{S}(\underset{\sim}{x},\omega) = \underset{\sim}{C}^{-1}(\underset{\sim}{x},\omega) \tag{2}$$

whereby $\underset{\sim}{\epsilon}$ in (1) and $\underset{\sim}{\sigma}$ in (2), respectively, are uniform fields applied to a hypothetical unspecified Representative volume Element (RVE) of a random medium. Furthermore, typically, an isotropic form is adopted

$$\sigma_{ij} = \lambda(\underset{\sim}{x},\omega)\delta_{ij}\varepsilon_{kk} + 2\mu(\underset{\sim}{x},\omega)\varepsilon_{ij} \tag{3}$$

by simply postulating the Lamé constants to be random fields.

While the effort in stochastic finite elements is on the development of efficient numerical methods for the solution of boundary value problems, the assumptions (1), (2) and (3) do not adequately account for the material microstructure. Thus, the present paper sets out to provide that missing link, and, as a byproduct, to examine the validity of (1), (2) and (3). At the same time, our results have applicability to stochastic finite difference methods, which do not yet appear to have been developed.

As a starting point we take the fact that discreteness of materials is the key cause of their nondeterministic constitutive response. Thus, the microstructure should provide the basis for the development of continuum type constitutive laws. We discuss this using the paradigm of

*Hereinafter, $\underset{\sim}{x}$ and $\underset{\approx}{x}$ denote second and fourth rank tensors, respectively.

Probabilistic Engineering Mechanics 0266-8920/93/$06.00

a medium with Voronoi geometry. One major advantage of choosing such a setting is the possibility to grasp both the geometrical and the physical microscale material randomness, while another is the possibility of assessing the statistics of fluctuations as a function of the scale of observation. The latter observation leads to the concept of a scale-dependent RVE, which forms the basis of a strategy for determination of effective constitutive laws of a class of linear elastic random microstructures, continuum random field characterizations of such microstructures, and methods involved in the solution of stochastic boundary value problems. We illustrate this approach, and especially this last point, with an example of a membrane with a random microstructure, where two random continuum approximations, an upper and lower a lower one, have to be employed in order to establish the bounds on response of an actual membrane.

2 MODEL OF A RANDOM MICROSTRUCTURE

A fundamental role in our formulation is played by the concept of a random microstructure, which, as is commonly done in mechanics of random media,[4] is taken as a family $\boldsymbol{B} = \{\mathbf{B}(\omega);\ \omega \in \Omega\}$ of deterministic media $\mathbf{B}(\omega)$, where ω indicates one specimen (realization), 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 the purpose

of further discussion, we take every specimen $\mathbf{B}(\omega)$ to be modeled by a realization of a Voronoi tessellation (Fig. 1(a)), which corresponds to one realization of a space-homogeneous planar Poisson process of a given density. Each cell of this tessellation, centered at x, is assumed to be occupied by a homogeneous continuum governed by a stiffness tensor $\underline{C}(x,\omega)$ following the same space-homogeneous probability distribution $P(\underline{C})$ and satisfying the so-called ellipticity conditions: $\exists\alpha,\beta > 0$ such that for any $\underline{\epsilon}$ the following inequalities hold

$$\alpha\underline{\epsilon}\underline{\epsilon} \leq \underline{\epsilon}\underline{C}\underline{\epsilon} \leq \beta\underline{\epsilon}\underline{\epsilon} \tag{4}$$

Thus, we have a realistic model of an ergodic polycrystalline medium without holes and rigid inclusions described by a random field $\underline{C} = \{\underline{C}(x,\omega); x \in \boldsymbol{B}, \omega \in \Omega\}$ with piecewise-constant realizations. In particular, we have for every component $C_{ijkl}(\omega)$ of $\underline{C}(\omega)$, for every $\omega \in \Omega$

$$\lim_{\delta\to\infty} \frac{1}{V_\delta} \int_{V_\delta} C_{ijkl}(x,\omega)\,\mathrm{d}V \equiv \overline{C}_{ijkl} = \langle C_{ijkl}\rangle$$
$$\equiv \int_{\Omega} C_{ijkl}(x,\omega)\,dP(\omega) \tag{5}$$

at any x in the domain of $\boldsymbol{B}_\delta$, where $\overline{\underline{C}}$ and $\langle\underline{C}\rangle$ denote the volume and ensemble averages of $\underline{C}$, respectively. In fact $\langle\underline{C}\rangle$ is a so-called Voigt (or upper) bound $\underline{C}^{V}$ on the effective stiffness $\underline{C}^{\text{eff}}$ of a very large body. Similarly, we also have

$$\overline{S}_{ijkl} = \langle S_{ijkl}\rangle \tag{6}$$

for the compliance tensor field. This is a so-called Reuss (or lower) bound $\underline{S}^{R}$ on $\underline{S} = (\underline{C}^{\text{eff}})^{-1}$.

We note here that:

(i) the above formulation is sufficiently general to deal with other linear transport problems, such as, for example, conductivity;
(ii) there are many kinds of random microstructures, other than of Voronoi geometry, described by random fields with piecewise-constant realizations, such as, for example, matrix-inclusion composites with randomly located inclusions that have random diameters, Fig. 1(b);
(iii) 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.

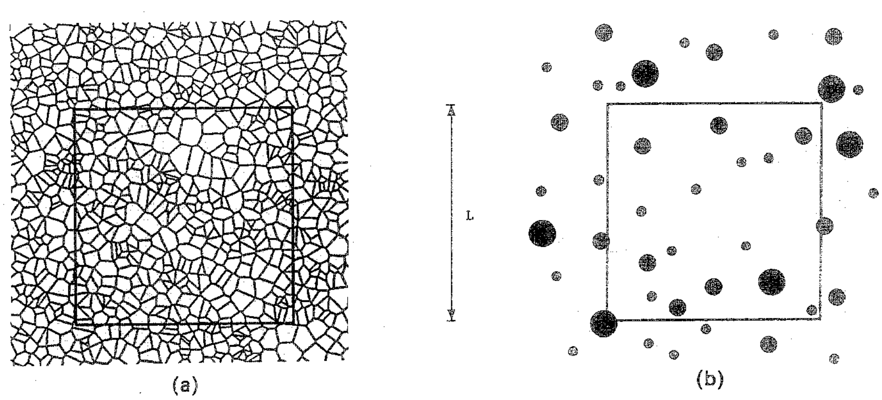

Fig. 1. (a) A Voronoi tessellation with an average cell size d; (b) a matrix-inclusion composite with inclusions of average diameter d; in both cases a window of size L is indicated.

3 TWO SCALE-DEPENDENT INHOMOGENEOUS CONTINUUM APPROXIMATIONS

First, with the help of Fig. 1, we introduce a square-shaped window of scale

$$\delta = \frac{L}{d} \tag{7}$$

Equation (7) defines a nondimensional parameter $\delta \geq 1$ specifying the scale L of observation (and/or measurement) relative to a typical microscale d (i.e. grain size) of the material structure. $\delta = 1$ is the smallest scale we consider: scale of a crystal. In view of the fact that the Voronoi tessellation is a random medium, the window bounds a random structure $B_\delta = \{B_\delta(\omega); \omega \in \Omega\}$, where $B_\delta(\omega)$ is a single realization from a given specimen $\mathbf{B}(\omega)$.

A continuum-type constitutive law is obtained by postulating the existence of an effective homogeneous continuum $B_\delta^{\mathrm{cont}}(\omega)$ of the same volume V_δ (i.e. area in 2-D), whose potential energy U, or complementary energy U^*, under given uniform boundary conditions equals that of a microstructure $B_\delta(\omega)$ under the same boundary conditions

$$U(B_\delta^{\mathrm{cont}}(\omega)) = U(B_\delta(\omega))$$

or

$$U^*(B_\delta^{\mathrm{cont}}(\omega)) = U^*(B_\delta(\omega)) \tag{8}$$

Clearly, we are now looking at a random medium $B_\delta^{\mathrm{cont}} = \{B_\delta^{\mathrm{cont}}(\omega); \omega \in \Omega\}$.

If we choose displacement-controlled (essential) boundary conditions on ∂B_δ

$$u_i = \bar{\epsilon}_{ij} x_j \tag{9}$$

we note that they generate a uniform strain field $\bar{\underset{\sim}{\epsilon}}$ in the homogeneous continuum. On the other hand, (9) results in some fluctuating field $\bar{\underset{\sim}{\epsilon}}$ in the heterogeneous microstructure $B_\delta(\omega)$, whose volume average equals $\bar{\underset{\sim}{\epsilon}}$. Now, from $(8)_1$ and (9) we obtain an effective random stiffness tensor $\underset{\sim}{C}_\delta^{\mathrm{e}}$ (superscript e stands for essential boundary conditions)

$$V_\delta \bar{\underset{\sim}{\epsilon}} \underset{\sim}{C}_\delta^{\mathrm{e}}(\omega) \bar{\underset{\sim}{\epsilon}} = \int_{V_\delta} \underset{\sim}{\epsilon}(x) \underset{\sim}{C}(\omega, x) \underset{\sim}{\epsilon}(x)\, \mathrm{d}V \tag{10}$$

On the other hand, if we choose stress-controlled (natural) boundary conditions on ∂B_δ

$$t_i = \bar{\sigma}_{ij} n_j \tag{11}$$

we note that they generate a uniform stress field $\bar{\underset{\sim}{\sigma}}$ in the homogeneous continuum B_δ^{cont}, and a fluctuating stress field in $B_\delta(\omega)$, whose volume average equals $\bar{\underset{\sim}{\sigma}}$. $(8)_2$ and (11) result now in an effective random compliance tensor $\underset{\sim}{S}_\delta^{\mathrm{n}}$ (superscript n stands for natural boundary conditions)

$$V_\delta \bar{\underset{\sim}{\sigma}} S_\delta^{n}(\omega) \bar{\underset{\sim}{\sigma}} = \int_{V_d} \underset{\sim}{\sigma}(x) \underset{\sim}{S}(\omega, x) \underset{\sim}{\sigma}(x)\, \mathrm{d}V \tag{12}$$

We make here the following observations:

(i) Due to the heterogeneity of the microstructure $B_\delta(\omega)$, the inverse

$$\underset{\sim}{C}_\delta^{\mathrm{n}}(\omega) = [\underset{\sim}{S}_\delta^{\mathrm{n}}(\omega)]^{-1} \tag{13}$$

is for any finite δ, in general, different from $\underset{\sim}{C}_\delta^{\mathrm{e}}$ of (10), see also Ref. 4.

(ii) In view of the spatial homogeneity of microstructure's statistics, $\underset{\sim}{C}_\delta^{\mathrm{n}}(\omega)$ and $\underset{\sim}{C}_\delta^{\mathrm{e}}(\omega)$ converge as δ tends to infinity; this defines a deterministic continuum $\mathbf{B}_{\mathrm{det}}$ for a single specimen $\mathbf{B}(\omega)$

$$\underset{\sim}{C}^{\mathrm{det}}(\omega) = \underset{\sim}{C}_\infty^{\mathrm{n}}(\omega) = \underset{\sim}{C}_\infty^{\mathrm{e}}(\omega) \tag{14}$$

whereby the window of infinite extent plays the role of an RVE of deterministic elasticity theory; in other words, it is at $\delta \to \infty$ that the invertibility of the constitutive law is obtained.

(iii) Ergodicity of the microstructure implies that

$$\underset{\sim}{C}^{\mathrm{det}}(\omega) = \underset{\sim}{C}^{\mathrm{eff}} \qquad \forall(\omega \in \Omega) \tag{15}$$

where $\underset{\sim}{C}^{\mathrm{eff}}$ is the effective response tensor (independent of ω) of a homogeneous medium.

(iv) At any finite δ both response tensors are, in general, anisotropic, with the nature of the anisotropy dependent on any specific $B_\delta(\omega)$. This indicates that the model (3) is invalid. On the other hand, (14) is isotropic due to the spatial homogeneity of the Poisson point process underlying the Voronoi tessellation and the spatial homogeneity of $P(\underset{\sim}{C})$.

(v) Since the window may move in the domain of $\mathbf{B}(\omega)$, the essential and natural boundary conditions (9) and (11) define two different inhomogeneous tensor fields at the scale δ with continuous realizations, which lead to two basic *random continuum approximations*: $\boldsymbol{B}_\delta^{\mathrm{e}} = \{\mathbf{B}_\delta^{\mathrm{e}}(\omega); \omega \in \Omega\}$ and $\boldsymbol{B}_\delta^{\mathrm{n}} = \{\mathbf{B}_\delta^{\mathrm{n}}(\omega), \omega \in \Omega\}$, respectively; accordingly, a window of size δ may be considered as an RVE of these two continuum models; the fact that there are two different response laws at any finite δ, calls into question the unique constitutive law (1)–(2), and, indeed, the existence of such a unique law remains a moot issue.[5]

(vi) This definition of two inhomogeneous tensor fields is conceptually similar, but not the same(!), as the procedure of local averaging in the theory of random fields applied to a single realization $\underset{\sim}{C}(\omega)$; $\omega \in \Omega$;[6] it becomes the same in case of a 1-D model only. In 2-D and 3-D computational mechanics methods have to be implemented to find the energies $U(B_\delta(\omega))$ and $U^*(B_\delta(\omega))$ in (8).

4 SCALE-DEPENDENT BOUNDS ON CONSTITUTIVE RESPONSE

Observe that the principle of minimum potential energy implies that the energy $U(\omega)$ stored in the body $B_\delta(\omega)$ under boundary conditions (9) does not exceed the energy $\bar{U}(\omega)$ in the same body subjected to a uniform strain field $\bar{\epsilon}$

$$\tfrac{1}{2}V_\delta\bar{\epsilon}\underset{\sim}{C}^{\mathrm{e}}_\delta(\omega)\bar{\underset{\sim}{\epsilon}} = U(\omega) \le \bar{U}(\omega) = \tfrac{1}{2}V_\delta\bar{\underset{\sim}{\epsilon}}\bar{\underset{\sim}{C}}_\delta(\omega)\bar{\underset{\sim}{\epsilon}} \qquad (16)$$

Tensor $\bar{\underset{\sim}{C}}_\delta(\omega)$ in (16) is the volume average of the tensor field $\underset{\sim}{C}_\delta(\omega)$ in $B_\delta(\omega)$. We write (16) as†

$$\underset{\sim}{C}^{\mathrm{e}}_\delta(\omega) \le \bar{\underset{\sim}{C}}_\delta(\omega) \qquad (17)$$

By carrying out ensemble averaging and noting its commutativity with volume averaging, as well as the ergodic property, we find

$$\langle \underset{\sim}{C}^{\mathrm{e}}_\delta \rangle \le \langle \underset{\sim}{C}_1 \rangle \equiv \underset{\sim}{C}^{\mathrm{V}} \qquad (18)$$

where with $\underset{\sim}{C}_1$ we denoted the stiffness of a single crystal (i.e. at scale $\delta = 1$). Since the ensemble average over all the crystal stiffnesses is just the Voigt bound, (18) explains why $\underset{\sim}{C}^{\mathrm{V}}$ is the upper bound on the average stiffness tensor at any scale δ.

Dually to the above, we observe that the principle of minimum complementary energy implies that the energy $U^*(\omega)$ stored in the body $B_\delta(\omega)$ under boundary conditions (11) does not exceed the energy $\bar{U}^*(\omega)$ in the same body subjected to a uniform stress field $\bar{\underset{\sim}{\sigma}}$

$$\tfrac{1}{2}V\bar{\underset{\sim}{\sigma}}S^{\mathrm{n}}_\delta(\omega)\bar{\underset{\sim}{\sigma}} = U^*(\omega) \le \bar{U}^*(\omega) = \tfrac{1}{2}V_\delta\bar{\underset{\sim}{\sigma}}\bar{\underset{\sim}{S}}_\delta(\omega)\bar{\underset{\sim}{\sigma}} \qquad (19)$$

In (19) $\bar{\underset{\sim}{S}}_\delta$ is the volume average of the compliance $\underset{\sim}{S}_\delta$ in B_δ. Again, carrying out the ensemble averaging and using the ergodic assumption we arrive at

$$\langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle \le \langle \underset{\sim}{S}_1 \rangle \equiv \underset{\sim}{S}^{\mathrm{R}} \qquad (20)$$

which explains why $\underset{\sim}{S}^{\mathrm{R}}$ is the upper bound on the ensemble average compliance at any scale δ, and, hence, the lower bound on the stiffness $\langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle^{-1}$.

Result (18) suggests a conjecture

$$\langle \underset{\sim}{C}^{\mathrm{e}}_{\delta'} \rangle \ge \langle \underset{\sim}{C}^{\mathrm{e}}_\delta \rangle \qquad \text{for} \qquad \delta' < \delta \qquad (21)$$

We prove it following Huet[7] by considering a partition of the window of scale δ (i.e. $L \times L$) into four smaller square-shaped sub-windows B^s_δ, $s = 1, 2, \ldots, 4$, of sizes $\delta' = \delta/2$ (i.e. $L/2 \times L/2$). Now, we define two types of boundary conditions, in terms of the strain field $\bar{\epsilon}$, over the larger window with any given microstructure $B_\delta(\omega) = \cup_{s=1}^4 B_{\delta'}(\omega)$: unrestricted

$$u_i = \bar{\epsilon}_{ij}x_j \qquad x \in \partial B_\delta \qquad (22)$$

and: restricted

$$u^{\mathrm{r}}_i = \bar{\epsilon}_{ij}x_j \qquad x \in \partial B^s_{\delta'}, s = 1, 2, \ldots 4 \qquad (23)$$

Superscript r in (23) indicates a 'restriction'. In view of the principle of minimum potential energy, the potential energies $U(\omega)$ and $U^{\mathrm{r}}(\omega)$ (i.e. unrestricted versus restricted conditions) stored in $B_\delta(\omega)$ under conditions (22) and (23), respectively, satisfy the inequality

$$\tfrac{1}{2}V_\delta\bar{\underset{\sim}{\epsilon}}\underset{\sim}{C}^{\mathrm{e}}_\delta(\omega)\bar{\underset{\sim}{\epsilon}} = U(\omega) \le U^{\mathrm{r}}(\omega) = \sum_{s=1}^{4}\tfrac{1}{2}V_{\delta'}\bar{\underset{\sim}{\epsilon}}\underset{\sim}{C}^{\mathrm{es}}_{\delta'}(\omega)\bar{\underset{\sim}{\epsilon}} \qquad (24)$$

in which $\underset{\sim}{C}^{\mathrm{es}}_{\delta'}$ and $V_{\delta'}$ are the effective stiffness and volume of $B^s_{\delta'}(\omega)$, respectively. After carrying out ensemble averaging we obtain (21) from (24) for $\delta' = \delta/2$. This can now be used to prove (21) by iteration for arbitrary δ and δ'. A particular consequence of the above result combined with (15) is that

$$\underset{\sim}{C}^{\mathrm{det}} \le \langle \underset{\sim}{C}^{\mathrm{e}}_\delta \rangle \qquad \text{for} \qquad \delta < \infty \qquad (25)$$

Guided by the results (20) and (21) we can conjecture

$$\langle \underset{\sim}{S}^{\mathrm{n}}_{\delta'} \rangle \ge \langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle \qquad \text{for} \qquad \delta' < \delta \qquad (26)$$

In order to prove it we introduce two natural boundary conditions on $B_\delta(\omega)$: unrestricted

$$t_i = \bar{\sigma}_{ij}x_j \qquad x \in \partial B_\delta \qquad (27)$$

and: restricted

$$t^r_i = \bar{\sigma}_{ij}x_j \qquad x \in \partial B^s_{\delta'},\ s = 1, 2, \ldots, 4 \qquad (28)$$

The principle of minimum complementary energy implies that, the complementary energies $U^*(\omega)$ and $U^{*r}(\omega)$ stored in $B_\delta(\omega)$ under conditions (27) and (28), respectively, satisfy the inequality

$$\tfrac{1}{2}V_1\bar{\underset{\sim}{\sigma}}\underset{\sim}{S}^{\mathrm{n}}_{\delta'}(\omega)\underset{\sim}{\sigma} = U^*(\omega) \le U^{*\mathrm{r}}(\omega) = \sum_{s=1}^{4}\tfrac{1}{2}V_{\delta'}\bar{\underset{\sim}{\sigma}}\underset{\sim}{S}^{\mathrm{ns}}_{\delta'}(\omega)\bar{\underset{\sim}{\sigma}} \qquad (29)$$

in which $\underset{\sim}{S}^{\mathrm{ns}}_{\delta'}$ and $V_{\delta'}$ are the effective compliance and volume of $B_{\delta'}(\omega)$, respectively. After carrying out ensemble averaging we prove (26) for $\delta' = \delta/2$. A proof for arbitrary $\delta' < \delta$ results by iteration.

A consequence of (26) combined with (15) is that

$$\underset{\sim}{S}^{\mathrm{det}} \le \langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle \qquad \text{for} \qquad \delta < \infty \qquad (30)$$

At this stage we can combine the inequalities (18), (20), (21), (25), (26) and (30) to obtain a hierarchy of bounds on the effective stiffness tensor $\underset{\sim}{C}^{\mathrm{eff}}$

$$(\underset{\sim}{S}^{\mathrm{R}})^{-1} \equiv \langle \underset{\sim}{S}^{\mathrm{n}}_1 \rangle^{-1} \le \langle \underset{\sim}{S}^{\mathrm{n}}_{\delta'} \rangle^{-1} \le \langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle^{-1} \le \underset{\sim}{C}^{\mathrm{eff}} \le \langle \underset{\sim}{C}^{\mathrm{e}}_\delta \rangle$$
$$\le \langle \underset{\sim}{C}^{\mathrm{e}}_{\delta'} \rangle \le \langle \underset{\sim}{C}^{\mathrm{e}}_1 \rangle \equiv \underset{\sim}{C}^{\mathrm{V}} \qquad \forall \delta' < \delta \qquad (31)$$

This is equivalent, by inversion, to a hierarchy of bounds on the effective compliance tensor $\underset{\sim}{S}^{\mathrm{eff}} = (\underset{\sim}{C}^{\mathrm{eff}})^{-1}$

$$S^{\mathrm{R}} \equiv \langle \underset{\sim}{S}^{\mathrm{n}}_1 \rangle \ge \langle \underset{\sim}{S}^{\mathrm{n}}_{\delta'} \rangle \ge \langle \underset{\sim}{S}^{\mathrm{n}}_\delta \rangle \ge \underset{\sim}{S}^{\mathrm{eff}} \ge \langle \underset{\sim}{C}^{\mathrm{e}}_\delta \rangle^{-1} \ge \langle \underset{\sim}{C}^{\mathrm{e}}_{\delta'} \rangle^{-1}$$
$$\ge \langle \underset{\sim}{C}^{\mathrm{e}}_1 \rangle^{-1} \equiv (\underset{\sim}{C}^{\mathrm{V}})^{-1} \qquad \forall \delta' < \delta \qquad (32)$$

† Hererinafter, for two fourth-rank tensors $\underset{\sim}{A}$ and $\underset{\sim}{B}$, an order relation $\underset{\sim}{B} \le \underset{\sim}{A}$ means $t_{ij}B_{ijkl}t_{kl} \le t_{ij}A_{ijkl}t_{kl} \forall \underset{\sim}{t} \ne \underset{\sim}{0}$.

Hierarchies of that type were first derived by Huet.[7,8] In Refs 9–11 we obtained numerically such hierarchies on $\underline{C}^{e}_{\delta}$ for co-called Delaunay networks, which, by virtue of duality to Voronoi tessellations, are generic models of granular and fibrous media. While the computational complexity increases significantly with growing δ for polycrystalline media due to the necessity of resolution of local stress fields in all the crystal cells of any given realization $B_{\delta}(\omega)$, computations for all graph-representable microstructures will have a basic common feature. Namely, the sequence of ever larger windows resulting in hierarchies convergent to the $\underline{C}^{\text{eff}} = (\underline{S}^{\text{eff}})^{-1}$ represents, at every step δ' to δ, the inclusion of a 'strip' of neighborhood adjacent to $\boldsymbol{B}_{\delta'}$ that results in $\boldsymbol{B}_{\delta}$. This procedure was called the *method of neighborhoods*.[12]

5 BOUNDS ON HIGHER-ORDER MOMENTS, AND TWO-POINT CORRELATION FUNCTIONS

It is clear from the preceding section that at any $\delta < \infty$ we deal with two random continuum fields—$\underline{C}^{e}_{\delta}$ of the approximation $\boldsymbol{B}^{e}_{\delta}$ and $\underline{S}^{n}_{\delta}$ of the approximation $\boldsymbol{B}^{n}_{\delta}$—bounding the response of an actual heterogeneous material. It is seen from (14) that the fluctuations (i.e. scatter) in these two tensor fields are zero at $\delta \to \infty$. On the other hand, they must be strongest at $\delta = 1$. Thus, some monotonic properties resembling (31) and (32) are expected for higher-order moments. In fact, by using the same partition procedure as before, it can be shown that the following inequalities hold between second-order moments of successively smaller windows (also in the sense of eigenvalues)

$$(\underline{C}^{\text{eff}})^2 = \langle(\underline{C}^{e}_{\infty})^2\rangle \leq \langle(\underline{C}^{e}_{\delta})^2\rangle \leq \langle(\underline{C}^{e}_{\delta'})^2\rangle \leq \langle(\underline{C}^{e}_{1})^2\rangle \quad \text{for} \quad \forall\delta' < \delta \tag{33}$$

where the equality on the left-hand side expresses the fact that there is no scatter at the infinite scale. Similarly, we have for the second-order moments of compliances

$$(\underline{S}^{\text{eff}})^2 = \langle(\underline{S}^{n}_{\infty})^2\rangle \geq \langle(\underline{S}^{n}_{\delta})^2\rangle \geq \langle(\underline{S}^{n}_{\delta'})^2\rangle \geq \langle(\underline{S}^{n}_{1})^2\rangle \quad \text{for} \quad \forall\delta' < \delta \tag{34}$$

In fact, the proof of (33) and (34) indicates that strong inequalities are more likely to hold. These results may be generalized to higher powers of $n > 2$.

With the help of the above we immediately confirm the heuristic result that the scatter is strongest at the microscale $\delta = 1$, while zero at infinity, which is the deterministic continuum limit.

As noted in point (vi) of Section 3, definitions (10) and (12) 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 to be obtained from micromechanics too. This has to be done in the Monte Carlo sense by conducting computations of effective constitutive moduli at two different spatial positions for a sufficient number of samples $B(\omega)$ from the Ω space. Since there are basically two possible definitions of effective moduli, two different autocorrelation functions will result.

Analyses carried out so far in this vein by Ostoja-Starzewski & Wang[9–11] for Delaunay networks lead to the following principal conclusions, which may be argued to hold for a number of other graph-representable microstructures (e.g. granular media[13]):

(i) The autocorrelation functions of shear moduli are isotropic, while those of other moduli are anisotropic.

(ii) The uniform strain approximation results in autocorrelation functions practically identical to those obtained by the exact method; this suggests a very inexpensive computational method for finding the second moments.

(iii) The isotropy of the material is approached only asymptotically as $\delta \to \infty$, and simultaneously with the coefficient of variation tending to zero (recall obser vation (iv) of Section 3); thus, the usage of random locally isotropic media models with noise-to-signal ratios of up to 30%, employed in some recent stochastic finite element studies, is physically unrealistic. In fact, even the assumption of a Gaussian character of, say, Young's modulus, is unjustified there. Rather, the micromechanics approach should be used in a Monte Carlo sense to determine probability densities of the stiffness and compliance tensors as a function of scale δ; such a characterization of the microstructures of Fig. 1(a) and (b) is presently in progress.

6 METHODOLOGY OF SOLUTION OF STOCHASTIC BOUNDARY VALUE PROBLEMS

6.1 Basic considerations

Three measuring levels may be introduced: microscale $\delta = 1$, mesoscale δ_{meso}, and macroscale δ_{M}, where $\delta_{\text{M}} =$ macroscopic dimension of the random body $\boldsymbol{B}$. At this point we note that the scatter in both tensors $\underline{S}^{n}_{\bar{\delta}}$ and $\underline{C}^{e}_{\bar{\delta}}$ becomes eventually negligible at some large, or very large, $\bar{\delta}$, so that we arrive at an invertible constitutive law with very small scatter (vide (14) and (15))

$$\underline{C}^{\text{eff}} \cong \underline{C}^{n}_{\bar{\delta}} \cong \underline{C}^{e}_{\bar{\delta}} \tag{35}$$

$\bar{\delta}$ may then be taken as the scale of an RVE of a deterministic medium $\mathbf{B}_{\text{det}}$. However, in case $\bar{\delta}$ of eqn (35) is of the order of, or even greater than, the macroscale δ_{M}, one is forced to deal with spatial random fluctuations on the macroscale. Analytical solutions of stochastic boundary value problems may only be obtained in those special cases where solutions of a corresponding deterministic (i.e. for each ω) inhomogeneous anisotropic medium problem are possible. Thus, in general, a recourse to numerical methods will be necessary.

Since two different random anisotropic continua result, a given boundary value problem must then be solved to find the upper and lower bounds on response according as random fields $\underline{C}_\delta^e$ and $\underline{C}_\delta^n$ with $\delta = \delta_{meso}$ are used. While the choice of δ_{meso} is up to the analyst, we point out that:

(i) smaller δ_{meso} resolves more details in the microstructure and hence more scatter, but the difference between both average moduli is larger and, hence, the difference between the upper and lower bounds on the ensemble-averaged response of an actual medium $\boldsymbol{B}$ is larger too;
(ii) larger δ_{meso} resolves less detail, gives less scatter and closer upper and lower bounds on this response;
(iii) adopting effective moduli $\underline{C}^{eff} = \underline{C}_\infty$ with noise corresponding to some finite scale is inconsistent; moreover, in that case it would not be clear whether the noise corresponding to $\underline{C}^e_{\delta_{meso}}$ or $\underline{C}^n_{\delta_{meso}}$ should be adopted; finally, we have observation (iv) of Section 3 regarding the anisotropy at $\delta < \infty$.

In case of a finite-difference solution of a stochastic boundary value problem of a random continuum, δ_{meso} should play the role of the resolution of a mesh, which typically is constant for the entire mesh. This is illustrated in Section 6.2 below.

In case of a finite element solution, the resolution of the mesh may vary spatially in order to resolve the particular details of sought-for fields in the body domain. Hence, δ_{meso} corresponds to the size of a particular finite element.

6.2 An example problem

In keeping with the notes (i) and (ii) at the end of Section 2, we consider here the elastostatics of a membrane having the microstructure of a matrix-inclusion composite (vide Fig. 1(b)) with both phases being locally isotropic. Specifically, we want to study the (out-of-plane) displacements $u(x_1, x_2)$ governed by the partial differential equation

$$\frac{\partial}{\partial x_i}\left(C_{ij}(x,\omega)\frac{\partial u}{\partial x_j}\right) = f(x) \qquad (36)$$

corresponding to a random continuum approximation $\boldsymbol{B}_\delta^e$ or $\boldsymbol{B}_\delta^n$ at some scale δ. Thus, C_{ij} in (36) are components, and realizations, of the random tensor fields $\underline{C}_\delta^e$ or $\underline{C}_\delta^n$. It is clear that the fluctuations in these two fields are directly related to the local fluctuations of the volume fraction of the inclusions, see Ref. 14.

The microstructure is modeled under the following assumptions:

— inclusions are round disks, of diameter $d = 5\Delta l$, where Δl is the unit length, and occupy 10% of the (aerial) volume fraction of the system;
— both phases are locally isotropic homogeneous continua described by

$$C_{ij}^\alpha = C^\alpha \delta_{ij} \qquad (37)$$

where α stands for the matrix (m) or the inclusion (i);
— the distribution of centers of inclusions corresponds to a planar Poisson process with a restriction that the distance between any two centers is no less than a minimal spacing, taken here at 110% of the diameter.

The membrane problem is being set up at the Poisson equation (36) under Dirichlet boundary conditions

$$u = 0 \quad \text{on} \quad \partial\boldsymbol{B} \qquad (38)$$

on a square-shaped body domain of the size $100\Delta l \times 100\Delta l$, and the force distribution $f = 10^{-4}/(\Delta l)^2$. This boundary value problem is then solved by treating the continuum equations with the help of a finite-difference method using a 10×10 mesh (see Fig. 2). We see immediately from (7) that $\delta = 2$. Let us consider a Monte Carlo type approach to this stochastic finite-difference problem. Then, as the input for solving the problem, each and every cell of the mesh (i.e. a $10\Delta l \times 10\Delta l$ window) needs to be assigned its upper and lower moduli, both being calculated at $\delta = 2$. There are, in principle, two ways of doing it:

(a) by generating, in a Monte Carlo sense, each realization $\mathbf{B}(\omega)$ in a matrix-inclusion composite and calculating $\underline{C}_2^e(\omega)$ under (9), and $\underline{C}_2^n(\omega)$ under (11), for every one of one hundred windows;
(b) by sampling, also in a Monte Carlo sense, $\underline{C}_2^e$ and $\underline{C}_2^n$ from the appropriate statistics, in accordance with the autocorrelation functions, describing this class of composites.

Since we have not yet fully developed the continuum random field characterizations needed in (b), we find it expedient to use the method of (a). To that end, 40 different samples of $\mathbf{B}(\omega)$ are generated and in each case, following the calculations of the upper and lower moduli of every one of 100 windows, two responses—random fields $u^{(e)}(x,\omega)$ and $u^{(n)}(x,\omega)$—of a given sample are obtained by a finite-difference method; here (e) and (n) correspond to the input of essential and natural moduli, respectively. Calculation of these moduli is conducted using a finite-difference type mesh representing the continuous phases of matrix and inclusions, in the same manner as used in computational physics to determine the effective moduli, see, for example, Ref. 15.

As a measure of the global response of $\mathbf{B}(\omega)$ we chose the volume contained under the membrane, so that we obtain a set of 40 'upper' estimates $V^{(e)}(\omega)$ and a set of

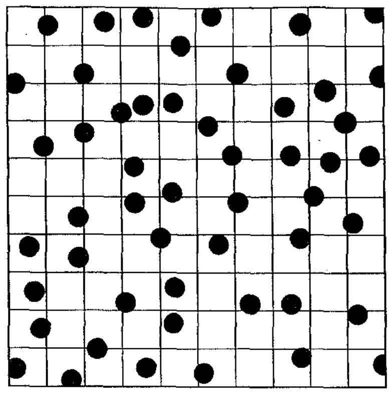

Fig. 2. A finite-difference mesh of $\delta = 2$ superposed on a random medium having a matrix-inclusion microstructure.

40 'lower' estimates $V^{(n)}(\omega)$. Figure 3 shows the ensemble averages $\langle V^{(e)}\rangle$ and $\langle V^{(n)}\rangle$ plotted as functions of the increasing stiffness C^i of the inclusions with C^m kept constant; here C^m is taken as unity for the sake of simplicity so that C^i is a so-called contrast, and both 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 deformation of a membrane according to the essential estimates of moduli is smaller than that according to the natural estimates, since the latter ones, that is $\underset{\sim}{C}_{\delta}^{n}$, are always (i.e. for any ω) softer than $\underset{\sim}{C}_{\delta}^{e}$. On the other hand, an increase in the stiffness of the inclusions leads to a stiffening of the membrane and hence to the reduction of deformation and, consequently, of volumes $V^{(e)}$ and $V^{(n)}$. Thus, we see two curves which decrease monotonically and diverge away from $C^i = C^m = 1$, becoming ever more widely spread with increasing C^i. Also, the coefficient of variation and the skewness of both volume measures of response have been found to increase with increasing C^i, but the family of 40 samples is too small to reduce their uneven variability and hence they are not plotted here.

6.3 Closure

The membrane example problem presented here is a very simple one, but illustrates the role of both random field estimates in describing the microstructure and bounding the response of a random heterogeneous medium. Let us discuss several possible refinements.

(i) A coarser finite-difference mesh could be used to solve the membrane problem and this would lead to closer upper and lower bounds on the response.

(ii) A finite element method could be used here, and would very likely result in better results than the finite differences for the same δ. Also, in place of a Monte Carlo approach, the existing analytical methods for random fields and stochastic finite elements developed in Refs 2 and 3 may be adapted to incorporate the micromechanical input; see also refs 16 and 17.

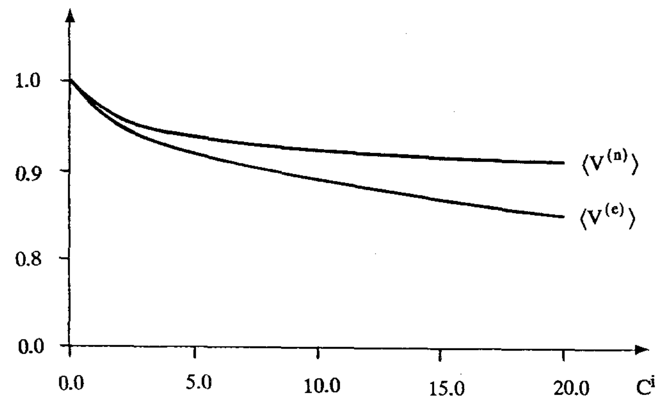

Fig. 3. Graph of ensemble average 'upper' and 'lower' responses $\langle V^{(e)}\rangle$ and $\langle V^{(n)}\rangle$ as function of contrast C^i, normalized over the response in the deterministic case $C^i = C^m = 1$

(iii) A finer net could be used for determination of the effective moduli of windows. However, as pointed out earlier, the computational expense in the micromechanical characterization of two continuum random fields of material properties increases with the window size. On the other hand, the computational expense in the finite difference (or element) solution decreases with the coarseness of the mesh. Thus, it appears that in the micromechanically-based stochastic boundary value problems there will be an optimum δ_{meso} leading to the lowest total computational costs.

ACKNOWLEDGEMENTS

This research was supported in part by the AFOSR under Contract No. AFOSR-89-0423 (Dr W. Jones is the program manager) and in part by the NSF under Grant No. MSS 9202772.

REFERENCES

1. Baecher, G.B. & Ingra, T.S., Stochastic FEM in settlement prediction. *J. Geotech. Engng Div., ASCE,* **107** (GT4) (1981) 449.
2. Spanos, P.D., *Stochastic Finite Elements: a Spectral Approach.* Springer-Verlag, Berlin, 1991.
3. Shinozuka, M. & Yamazaki, F., Stochastic finite element analysis: an introduction. In *Stochastic Structural Dynamics: Progress in Theory and Applications,* ed. S.T. Ariaratnam, G.I. Schueller & I. Elishakoff. Elsevier Applied Science, London, 1988, pp. 241–91.
4. Willis, J.R., Variational and related methods for the overall properties of composites. *Adv. Appl. Mech.* **21** (1981) 2.
5. Milton, G.W., Private communication, Courant Institute of Mathematical Sciences, 1991.
6. Vanmarcke, E., *Random Fields: Analysis and Synthesis.* The MIT Press, Cambridge, MA, 1983.
7. Huet, C., Application of variational concepts to size effects in elastic heterogeneous bodies. *J. Mech Phys. Solids,* **38**(6) (1990) 813.

8. Huet, C., Hierarchies and bounds for size effects in heterogeneous bodies. In *Continuum Models and Discrete Systems, Vol. 2*, ed. G.A. Maugin. Longman Scientific and Technical, London, 1991, pp. 203–10.
9. Ostoja-Starzewski, M. & Wang, C., Effective moduli of planar random elastic Delaunay networks. In *Continuum Mechanics and Its Applications*, ed. G.A.C. Graham & S.K. Malik. Hemisphere Publishers, New York, 1989, pp. 121–30.
10. Ostoja-Starzewski, M. & Wang, C., Linear elasticity of planar Delaunay networks: random field characterization of effective moduli. *Acta Mech.*, **80** (1989) 61.
11. Ostoja-Starzewski, M. & Wang, C., Linear elasticity of planar Delaunay networks—II: Voigt and Reuss bonds, and modification for centroids. *Acta Mech.*, **84** (1990) 47.
12. Ostoja-Starzewski, M., Bounds on constitutive response for a class of random material microstructures. *Comp. & Struct.*, **37** (1990) 163.
13. Ostoja-Starzewski, M., Random fields and processes in mechanics of granular materials. 2nd US–Japan Seminar on Micromechanics of Granular Materials, 1991; *Studies Appl. Mech.* (in press), Elsevier, 1992; extended version in *Mech Mater.* (*Special Issue*) (in press).
14. Lu, B. & Torquato, S., Local volume fraction fluctuations in heterogeneous media. *J. Chem. Phys.*, **93**(5) (1990) 3452.
15. Day, A.R., Snyder, K.A., Garboczi, E.J. & Thorpe, M.F., The elastic moduli of a sheet containing circular holes. *J. Mech. Phys. Solids*, **40**(5) (1992) 1031.
16. Ostoja-Starzewski, M., Micromechanics as a basis of continuum random fields. *Appl. Mech. Rev.* (*Special Issue: Micromechanics of Random Media*), **46** (1993) in press.
17. Ostoja-Starzewski, M., Micromechanics as a basis of stochastic finite elements and differences—an overview. *Appl. Mech. Rev.* (*Special Issue: Mechanics Pan-America 1993*), **46** (1993) in press.