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THE EFFECTIVE CHARACTERISTICS OF INHOMOGENEOUS MEDIA[†]

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The effective characteristics in inhomogeneous media, including composites, are determined. The fundamental boundary-value problem and its dual for determining the effective characteristics in an inhomogeneous medium of not necessarily regular structure is formulated. The example is a multilayered medium is given. © 1997 Elsevier Science Ltd. All rights reserved.

1. The idea of effective characteristics was introduced when constructing statistical theories for defining the properties of inhomogeneous materials [1]. Suppose a linear operator L is such that, for the equation

$$Lu = f \tag{1.1}$$

Green's operator G: LG = 1 (where *I* is the identity operator) is known. Then the solution of operator equation (1) has the form u = Gf. If the input data *f* are not random, for the input field $\langle u \rangle$ we have

$$\langle u \rangle = \langle G \rangle f \tag{1.2}$$

The effective operator L^* is defined as follows:

$$L^*\langle u \rangle = f \tag{1.3}$$

From (1.2) and (1.3) we obtain that

 $L^* = \langle G \rangle^{-1}$

i.e. the problem of averaging stochastically inhomogeneous materials reduces to constructing the averaged Green's function. It is usually not possible to obtain this function exactly, but there is a fair number of approximate approaches to this problem [2–5].

Below we present a deterministic approach to the problem of the effective characteristics of the thermal, electrical, magnetic and partially elastic properties of inhomogeneous materials, including composites.

2. Suppose that in a certain body, having a volume V and bounded by a closed surface Σ , we are given a specific form of the operator equation (1.1) for a certain quantity u in the form of an equation and a boundary condition

$$\left[C_{ij}(x)u_{,j}\right]_{,i} + f(x) = 0$$
(2.1)

$$u|_{\Sigma} = u^{0}(y), \ y \in \Sigma$$
(2.2)

We will assume always that $x = x_1, x_2, x_3$; $\xi = \xi_1, \xi_2, \xi_3 \in V$ and $y, \eta \in \Sigma$. Summation from 1 to 3 is carried out over the repeated index, denoted by a lower-case Latin letter, and from 1 to 2 over the index denoted by a capital Latin letter. For partial derivatives we will use the notation $\varphi_i \equiv \partial \varphi / \partial x_i$, $\varphi_i \equiv \partial \varphi / \partial \xi_i$. We will denote by angle brackets the mean value of a quantity over the volume, indicating if necessary the variable over which averaging is carried out

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$$\left\langle \varphi(x,\xi)\right\rangle_{x} \equiv \frac{1}{V} \int_{V} \varphi(x,\xi) dV_{x}$$

Problem (2.1), (2.2) will be called the first boundary-value problem (Problem 1). If, on the boundary of the body Σ , we are given the condition

$$C_{ij}u_{j}n_{i}|_{\Sigma} = S_{0}(y) \tag{2.3}$$

where n_i are the components of the unit vector of the outward normal to the surface Σ , problem (2.1), (2.3) will be called the second boundary-value problem.

For the dual formulation of the second boundary-value problem we will introduce the quantity

$$\varepsilon_i \equiv u_i \tag{2.4}$$

and the defining relations

$$\sigma_i = C_{ij}\varepsilon_j, \ \varepsilon_i = J_{ij}\sigma_j, \ C_{ij}J_{jk} = J_{ij}C_{jk} = \delta_{ik}$$
(2.5)

where C_{ij} and J_{ij} are the components of positive definite mutually inverse second-rank tensors [6]. If they depend on the coordinates ($C_{ij} = C_{ij}(x)$, $J_{ij} = J_{ij}(x)$), the medium is said to be inhomogeneous, while if these functions are discontinuous the inhomogeneous medium is said to be composite [5].

Using notation (2.4) and (2.5), Eq. (2.1) and boundary condition (2.3) can be rewritten in the form

$$\sigma_{ii}(x) + f(x) = 0 \tag{2.6}$$

$$\sigma_i n_i \Big|_{\Sigma} = S_0(y) \tag{2.7}$$

To Eq. (2.6) we must add the so-called compatibility equation, which, using (2.5) can be written in the form

$$\epsilon_{ilk} \left[J_{jl}(x)\sigma_l(x) \right]_k = 0$$
(2.8)

The second boundary-value problem in the dual formulation is specified by Eqs (2.6) and (2.8) and boundary condition (2.7) (Problem 2).

We will not dwell on the conditions for these boundary-value problems to be solvable and on whether a generalized solution exists in the case of a composite medium (see [7]). Note that if u(x) denotes a temperature field, $C_{ij}(x)$ will be the components of the thermal conductivity tensor, $\sigma_i(x)$ will be the components of the heat flux, $\varepsilon_i(x)$ will be the temperature gradient and f(x) will be the density of the mass heat source. If u(x) is the electrostatic potential, $C_{ij}(x)$ will be the components of the permittivity tensor, $\varepsilon_i(x)$ will be the components of the electric field vector and $\sigma_i(x)$ will be the electric induction. Using these quantities we can also discuss a magnetic field, and by increasing the rank of the tensors we can also include an elastic field (we deal with this topic in Section 6).

To determine the effective tensors, the components of which are denoted by C_{ij} and J_{ij} , respectively, we will formulate the first and second boundary-value problems with special boundary conditions and when there is no external field [8].

The first special boundary-value problem (Problem 1_0) consists of solving the homogeneous equation (2.1), when boundary conditions (2.2), in the form

$$u|_{\Sigma} = \gamma_i y_i, \ \gamma_i = \text{const}$$
(2.9)

are satisfied.

We will give the second special boundary-value problem (Problem 2_0) in dual formulation. It consists of solving the homogeneous equation (2.6) when the compatibility condition (2.8) and the boundary condition (2.7) are satisfied in the form

$$\sigma_i n_i |_{\Sigma} = \tau_i n_i(y), \ \tau_i = \text{const}$$
(2.10)

Identities are known [5] for Problems 1 and 1_0

$$\langle \varepsilon_i(x) \rangle = \frac{1}{V} \int_{\Sigma} u_0(y) n_i(y) d\Sigma_{y} = \gamma_i$$

and for Problems 2 and 2_0

$$\langle \sigma_i(x) \rangle = \frac{1}{V} \int_{\Sigma} S_0(y) y_i d\Sigma_y + \langle f(x) x_i \rangle = \tau_i$$

From the solution of Problem 1_0 we obtain the components of the effective tensor C_{ij}^*

$$\left\langle \sigma_{i}(x)\right\rangle = C_{ij}^{*}\gamma_{j} \tag{2.11}$$

and from the solution of Problem 2_0 we obtain the components of the effective tensor

$$\left\langle \varepsilon_{i}(x)\right\rangle = J_{ij}^{*}\tau_{j} \tag{2.12}$$

The main hypothesis, used in the mechanics of composites, asserts that for a statistically homogeneous medium tensors with components C_{ii}^* and J_{ii}^* are mutually inverse [2].

3. Exact values of the effective tensors can only be obtained for a small class of composites [2]. This is most often due to the difficulty in solving the Problems 1_0 and 2_0 .

The method of averaging, recently developed in a number of publications [5, 9, 10], enabled the range of accurately obtained effective characteristics to be extended somewhat, due to a more convenient formulation of the problems for determining them [5, 11-13]. This applies to so-called periodic structures [5, 9], since the averaging procedure can be applied to such structures. However, it should be noted that the effective moduli of elasticity obtained, for example, for multilayered composites with a periodic structure and even microstresses (stresses in each component of the composite), turn out to be justified for an arbitrary inhomogeneity along one coordinate [5].

The purpose of the present paper is to formulate special boundary-value problems for obtaining the effective characteristics of media with an arbitrary inhomogeneity convenient for investigation. The boundary conditions (if they exist) of such special boundary-value problems must be homogeneous, while the free term of the equations depends on $C_{ij}(x)$ or $J_{ij}(x)$, i.e. they must characterize the inhomogeneity of the structure of the material in question.

We will assume that Green's function of Problem 1 $G(x, \xi)$ and of Problem 2₀ $\tilde{G}(x, \xi)$ are known

$$\begin{bmatrix} C_{ij}(x)\tilde{G}_{,j}(x,\xi) \end{bmatrix}_{j} = -\delta(x-\xi)$$

$$C_{ij}(y)\tilde{G}_{,j}(y,\xi)n_{i}(y)|_{\Sigma} = 0$$
(3.1)

We will also introduce the following notation

$$E_{i}(x,\xi) \equiv G_{i}(x,\xi), \ \Gamma_{i}(x,\xi) \equiv C_{ij}(x)G_{j}(x,\xi)$$
(3.2)

$$\tilde{E}_{i}(x,\xi) \equiv \tilde{G}_{i}(x,\xi), \quad \tilde{\Gamma}_{i}(x,\xi) \equiv C_{ij}(x)\tilde{G}_{j}(x,\xi)$$
(3.3)

Note that it follows from (3.1) and (3.3) that

$$\left\langle \tilde{\Gamma}_{i}(x,\xi) \right\rangle_{x} = \frac{1}{V} \xi_{i}, \left\langle \tilde{\Gamma}_{ilj}(x,\xi) \right\rangle_{x} = \frac{1}{V} \delta_{ij}$$
(3.4)

The solution of Problem 1 can be expressed in terms of Green's function $G(x, \xi)$ using (3.2) as follows:

$$u(\xi) = -\int_{\Sigma} \Gamma_i(y,\xi) n_i(y) u_0(y) d\Sigma_y + \int_V G(x,\xi) f(x) dV_x$$
(3.5)

$$\varepsilon_{j}(\xi) = -\int_{\Sigma} \Gamma_{kj}(y,\xi) n_{i}(y) u_{0}(y) d\Sigma_{y} + \int_{V} E_{j}(x,\xi) f(x) dV_{x}$$
(3.6)

$$\sigma_j(\xi) = -C_{jk}(\xi) \int_{\Sigma} \Gamma_{ilk}(y,\xi) n_i(y) u_0(y) d\Sigma_y + \int_V \Gamma_j(x,\xi) f(x) dV_x$$
(3.7)

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while the solution of the second boundary-value problem (2.1), (2.3) (Problem 2) can be expressed in terms of Green's function $G^{-}(x, \xi)$ using (3.3) as follows:

$$u(\xi) = \int_{\Sigma} \tilde{G}(y,\xi) S_0(y) d\Sigma_y + \int_{V} \tilde{G}(x,\xi) f(x) dV_x$$
(3.8)

$$\varepsilon_i(\xi) = \int_{\Sigma} \tilde{G}_{\mathsf{l}i}(y,\xi) S_0(y) d\Sigma_y + \int_V \tilde{E}_i(x,\xi) f(x) dV_x$$
(3.9)

$$\sigma_i(\xi) = C_{ij}(\xi) \int_{\Sigma} \tilde{G}_{ij}(y,\xi) S_0(y) d\Sigma_y + \int_V \tilde{\Gamma}_i(x,\xi) f(x) dV_x$$
(3.10)

We will use (3.5)–(3.7) for Problem 1₀. Applying the Gauss–Ostrogradskii theorem we obtain

$$u(\xi) = \left[\xi_j - V \left\langle \Gamma_j(x,\xi) \right\rangle_x \right] \gamma_j$$

$$\varepsilon_i(\xi) = \gamma_i - V \left\langle \Gamma_{j|i}(x,\xi) \right\rangle_x \gamma_j$$
(3.11)

$$\sigma_{i}(\xi) = \left[C_{ij}(\xi) - VC_{ik}(\xi) \left\langle \Gamma_{j|k}(x,\xi) \right\rangle_{x} \right] \gamma_{j}$$
(3.12)

Comparing (2.11) and (3.12) we obtain

$$C_{ij}^{*} = \left\langle C_{ij}(\xi) - VC_{ik}(\xi) \left\langle \Gamma_{jik}(x,\xi) \right\rangle_{x} \right\rangle_{\xi}$$
(3.13)

We use (3.8)–(3.10) in exactly the same way for Problem 2₀. Using the Gauss–Ostrogradskii theorem we obtain

$$u(\xi) = \tau_j V \left\langle \tilde{E}_j(x,\xi) \right\rangle_x, \ \varepsilon_i(x) = \tau_j V \left\langle \tilde{E}_{j|i}(x,\xi) \right\rangle_x \tag{3.14}$$

$$\sigma_i(\xi) = \tau_j V C_{ik}(\xi) \left\langle \tilde{E}_{j|k}(x,\xi) \right\rangle_x \tag{3.15}$$

Comparing (2.12) and the second formula of (3.14) we obtain

$$J_{ij}^{*} = V \left\langle \left\langle \tilde{E}_{j|i}(x,\xi) \right\rangle_{x} \right\rangle_{\xi}$$
(3.16)

It can be seen that the tensors with components (3.13) and (3.16) are symmetrical. It can be shown that they are positive definite.

Note that, using Green's functions, one can construct integral operators on the boundary of the body which are a continual analogue of II'yushin's matrices [7]

$$u_0(\eta) = \int_{\Sigma} G(y,\eta) S_0(y) d\Sigma_y$$

$$S_0(\eta) = -n_j(\eta) C_{jk}(\eta) \int_{\Sigma} \Gamma_{ilk}(y,\eta) n_i(y) u_0(y) d\Sigma_y$$

4. We will now formulate the boundary-value problem for finding the components of the effective tensor C_{ii}^* of (3.13). We will put

$$N_i(\xi) \equiv -V \left\langle \Gamma_i(x,\xi) \right\rangle_x \tag{4.1}$$

It then follows from (3.13) that

$$C_{ij}^* = \left\langle C_{ij}(\xi) + C_{ik}(\xi) N_{j|k}(\xi) \right\rangle \tag{4.2}$$

We now uses notation (4.1) and substitute the expressions $u(\xi)$ and $\sigma_i(\xi)$ from (3.14) and (3.12) into the homogeneous equation (2.1) and condition (2.9). Taking into account the fact that the quantities γ_i are arbitrary, we obtain the required formulation of the boundary-value problem for the quantities N_i

$$\left[C_{ik}(\xi)N_{j|k}(\xi)\right]_{li} + C_{ij|i}(\xi) = 0$$
(4.3)

$$N_i(\eta)|_{\Sigma} = 0 \tag{4.4}$$

Indeed, the right-hand side of Eq. (4.3) depends on $C_{ij}(\xi)$, while boundary condition (4.4) is homogeneous. Consequently, the solution of problem (4.3), (4.4) is related to the structure of the material.

Suppose, for example, that C_{ij} depend on a single coordinate $\xi_3 = \zeta$. Then (4.3) can be converted into an ordinary differential equation

$$\left[C_{33}(\zeta)N'_{j}(\zeta)\right] + C'_{3j}(\zeta) = 0$$
(4.5)

where the prime denotes a derivative with respect to ζ . Boundary condition (4.4) takes the form

$$N_i(0) = N_i(l) = 0 (4.6)$$

The solution of problem (4.5), (4.6) is as follows:

$$N_{j}(\zeta) = \left\langle \frac{1}{C_{33}} \right\rangle^{-1} \left\langle \frac{C_{3j}}{C_{33}} \right\rangle_{0}^{\zeta} \frac{dz}{C_{33}(z)} - \int_{0}^{\zeta} \frac{C_{3j}(z)}{C_{33}(z)} dz$$
(4.7)

From (4.7) and (4.2) we obtain

$$C_{ij}^{*} = \left\langle C_{ij} \right\rangle - \left\langle \frac{C_{3i}C_{3j}}{C_{33}} \right\rangle + \left\langle \frac{C_{3i}}{C_{33}} \right\rangle \left\langle \frac{1}{C_{33}} \right\rangle^{-1} \left\langle \frac{C_{3j}}{C_{33}} \right\rangle$$
(4.8)

From an isotropic medium, i.e. for $C_{ij}(\zeta) = \lambda(\zeta)\delta_{ij}$, we have from (4.8)

$$C_{ij}^{*} = \langle \lambda \rangle \delta_{ij} + \left[\left\langle \frac{1}{\lambda} \right\rangle^{-1} - \langle \lambda \rangle \right] \delta_{3i} \delta_{3j}$$
(4.9)

5. We will consider Problem 20 to find the components of the effective tensor J_{ii}^* . We will put

$$M_i(\xi) \equiv V \left\langle \tilde{E}_i(x,\xi) \right\rangle_x \tag{5.1}$$

It follows from (3.16) that

$$J_{ij}^* = \left\langle M_{j|i} \right\rangle \tag{5.2}$$

We use the notation (5.1) and substitute (3.15) into homogeneous equation (2.6) and condition (2.10). We obtain

$$\tau_k \Big[C_{ij}(\xi) M_{klj}(\xi) \Big]_{li} = 0$$

$$\tau_j C_{ik}(\eta) M_{jlk}(\eta) n_i(\eta) \Big|_{\Sigma} = \tau_j n_j(\eta)$$

The compatibility equation is satisfied identically. Using the fact that the quantities τ_j are arbitrary, we obtain an equation and a boundary condition for $M_k(\xi)$ which, introducing the quantity

$$P_{ij}(\xi) \equiv C_{ik}(\xi) M_{j|k}(\xi)$$
(5.3)

we write in the form

$$P_{ikki}(\xi) = 0, \quad P_{ikki}(\eta)n_i(\eta) = n_k(\eta)$$
(5.4)

We write the compatibility equation (2.8) in the form

$$\epsilon_{ijk} \left[J_{jl}(\xi) P_{lm}(\xi) \right]_{lk} = 0$$
(5.5)

It follows from (3.4), (5.5) and (5.1) that

$$\left\langle P_{ij}(\xi) \right\rangle = \delta_{ij} \tag{5.6}$$

while from (5.2) and (5.3) we have

$$J_{ij}^* = \left\langle J_{ik}(\xi) P_{kj}(\xi) \right\rangle \tag{5.7}$$

However, boundary-value problem (5.4)–(5.6) also does not satisfy the requirements formulated in Section 3 for obtaining effective characteristics. Hence, we introduce the new quantities L_{ii}

$$P_{ij}(\xi) = \delta_{ij} + \epsilon_{ikl} L_{jkll}(\xi)$$
(5.8)

Equation (5.4), after substituting (5.8) into it, is satisfied identically. The compatibility equation (5.5) takes the form

$$\epsilon_{ijk} \epsilon_{pmn} \left[J_{jp}(\xi) L_{lmn}(\xi) \right]_{k} + \epsilon_{ijk} J_{jlk}(\xi) = 0$$
(5.9)

i.e. its right-hand side depends only on $J_{ij}(\xi)$. Boundary condition (5.4), after substituting (5.8) into it

$$n_i(\eta) \in_{ijk} L_{ijk}(\eta) \Big|_{\Sigma} = 0$$
(5.10)

becomes homogeneous. Consequently, boundary-value problem (5.9), (5.10) corresponds to the stated requirements. From (5.7) we determine the effective characteristics

$$J_{ij}^{*} = \left\langle J_{ij}(\xi) + \epsilon_{klm} J_{ik}(\xi) L_{jllm}(\xi) \right\rangle$$
(5.11)

and it follows from (5.6) that

$$\epsilon_{ikl} \left\langle K_{jkl}(\xi) \right\rangle = 0 \tag{5.12}$$

Consider the case when J_{ij} depends on one coordinate, for example, $\xi_3 = \zeta$. Equation (5.9) in this case becomes an ordinary differential equation

$$\epsilon_{IJ}\epsilon_{PM}\left[J_{JP}(\zeta)L'_{IM}\right] + \epsilon_{IJ}J'_{JI}(\zeta) = 0$$
(5.13)

while boundary condition (5.10)

$$n_I \varepsilon_{IJ} L_{IJ}'(\zeta) \Big|_{\Sigma} = 0$$

imposes no limitations on the relationship $L_{ij}(\zeta)$. However, we have limitations on these functions which arise from (5.12)

$$\epsilon_{IK} \left\langle L_{jK}(\zeta) \right\rangle = 0 \tag{5.14}$$

Solving Eq. (5.13) when conditions (5.14) are satisfied we obtain

$$\epsilon_{IK} L'_{JK}(\zeta) = J_{IJ}^{-1}(\zeta) \Big\langle J_{JK}^{-1} \Big\rangle^{-1} \Big\langle J_{KL}^{-1} J_{LJ} \Big\rangle - J_{IJ}^{-1}(\zeta) J_{JJ}(\zeta)$$

where J_{II}^{-1} are the elements of the 2 × 2 matrix which is inverse to the matrix with elements J_{II} . From (5.11) we obtain

$$J_{ij}^{*} = \left\langle J_{ij}(\zeta) + \epsilon_{KL} J_{iK}(\zeta) L_{jL}^{\prime} \right\rangle = \left\langle J_{ij} \right\rangle + \left\langle J_{il} J_{ll}^{-1} \right\rangle \left\langle J_{JK}^{-1} \right\rangle^{-1} \left\langle J_{KL}^{-1} J_{Lj} \right\rangle - \left\langle J_{il} J_{ll}^{-1} J_{lj} \right\rangle$$
(5.15)

For an isotropic medium, i.e. when

$$J_{ij}(\zeta) = \delta_{ij} / \lambda(\zeta)$$

we have from (5.15)

$$J_{ij}^{\star} = \frac{1}{\langle \lambda \rangle} \delta_{ij} + \left(\left\langle \frac{1}{\lambda} \right\rangle - \frac{1}{\langle \lambda \rangle} \right) \delta_{3i} \delta_{3j}$$

It can be established by a direct check that tensors (4.9) and (5.15) are mutually inverse, i.e. the fundamental hypothesis formulated in Section 2 for media with a one-dimensional inhomogeneity is satisfied.

6. To obtain the effective moduli of elasticity and the effective elastic compliances the equations are somewhat more complicated. We will only give the final formulation of the boundary-value problems (for details see [14]).

The components of the effective elasticity-modulus tensor is obtained by averaging the expression

$$C_{ijkl}^{*} = \left\langle C_{ijkl}(\xi) + C_{ijmn}(\xi) N_{mkl\ln}(\xi) \right\rangle$$

The quantities N_{ijk} are found from the system of differential equations with boundary conditions

$$\left[C_{ijkl}(\xi) + C_{ijmn}(\xi)N_{mkl|n}(\xi)\right]_{ij} = 0, \ N_{mkl|\Sigma} = 0$$

To obtain the components of the effective elastic-compliance tensor it is necessary to average the expression

$$J_{ijkl}^* = \left\langle J_{ijkl}(\xi) + \epsilon_{mpr} \epsilon_{nqs} J_{ijmn}(\xi) L_{pqklrs}(\xi) \right\rangle$$

The quantities L_{pakl} satisfy a system of differential equations with boundary conditions

$$\epsilon_{siw} \epsilon_{uvj} \left[J_{ijkl}(\xi) + \epsilon_{uvj} \epsilon_{nqs} J_{ijuus}(\xi) L_{pqkfirs}(\xi) \right]_{tvw} = 0$$

$$\epsilon_{ipr} \epsilon_{jqs} L_{pqtArs} n_j(\eta) \Big|_{\Sigma} = 0$$

Moreover, the quantities L_{pakl} must satisfy the conditions

$$\in_{ipr} \in_{jas} \langle L_{pathers}(\xi) \rangle \approx 0$$

For the case when the moduli C_{ijkl} depend only on one coordinate, the effective elasticity-modulus tensor and the elastic-compliance tensor are obtained in exactly the same way as for a multilayered medium, where they are mutually inverse.

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