



Homogenization in probabilistic terms: The variational principle and some approximate solutions



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ABSTRACT

Studying of materials with evolving random microstructures requires the knowledge of probabilistic characteristics of local fields because the path of the microstructure evolution is controlled by the local fields. The probabilistic characteristics of local fields are determined by the probabilistic characteristics of material properties. In this paper it is considered the problem of finding the probabilistic characteristic of local fields, if the probabilistic characteristics of material properties are given. The probabilistic characteristics of local fields are sought from the variational principle for probabilistic measure. Minimizers of this variational problem provide all statistical information of local fields as well as the effective coefficients. Approximate solutions are obtained for electric current in composites for two cases: multi-phase isotropic composites with lognormal distribution of conductivities and two-phase isotropic composites. The solutions contain a lot of statistical information that has not been available previously by analytical treatments.

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1. Introduction

Numerical studies reveal the enormous complexity of local fields in composites with random microstructures (see, e.g., Escola et al., 2011; Willot et al., 2013; Kalidindi et al., 2011). There is no doubt that the local fields can be described adequately only in probabilistic terms. Such description is needed not only for characterization of the state of a composite, but also for prediction of the evolution of microstructures due to plasticity, fatigue, or fracture, where the path of evolution is controlled by the local fields. At the moment, the probabilistic characteristics of local fields are sought by statistical analysis of a huge number of numerical simulations conducted for different realizations of microstructures. Apparently, a more practical way is desirable. In this paper we explore the possibility of using for such purposes the variational principle for probabilistic measure (Berdichevsky, 1987).

The variational principle is based on a simple idea. Consider conductivity of composites. Conductivity may have different physical meaning (electric, heat, filtration, etc.), and for definiteness we will use the terminology of electrical conductivity of composites. Let the composite occupy some three-dimensional region V . Denote by $a_{ij}(x)$ electrical conductivities, with x being points of three-dimensional space referred to a Cartesian frame x_i ; small Latin indices run through values 1,2,3. The electric potential $\varphi(x)$ is prescribed at the boundary ∂V of region V as a linear function of coordinates,

$$\varphi(x) = v_i x_i \quad \text{on } \partial V, \quad (1)$$

constants v_i are the components of the external homogeneous electric field, summation over repeated indices is always implied. Denote by $\psi(x)$ the electric potential caused by micro-inhomogeneities:

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$$\varphi(x) = v_i x_i + \psi(x) \text{ in } V, \quad \psi(x) = 0 \text{ on } \partial V.$$

The corresponding electric field is denoted by u_i , $u_i = \partial\psi/x_i$. In homogeneous conductors $\psi = u_i = 0$. As is known, the true electric potential minimizes the functional,

$$\frac{1}{|V|} \int_V \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) dV, \tag{2}$$

on the set of all functions $\psi(x)$ vanishing on ∂V . In (2) $a_{ij}(x)$ are prescribed conductivities, and $|V|$ is volume of region V . In theory of composites, the functional to be minimized has the meaning of either energy or dissipation. For electric conductors, (2) is dissipation per unit volume (up to the factor 1/2). In general considerations we take liberty to call the functional to be minimized energy functional keeping in mind that in a particular physical problem its actual physical meaning could be dissipation.

Due to linearity of the problem, the minimum value of the functional (2) is a quadratic function of parameters v_i . The coefficients of this quadratic form a_{ij}^{eff} have the meaning of effective coefficients of the composite,

$$\frac{1}{2} a_{ij}^{\text{eff}} v_i v_j = \min_{\psi} \frac{1}{|V|} \int_V \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) dV. \tag{3}$$

If the characteristic length of micro-inhomogeneities, ε , is much smaller than the size of region V , then a_{ij}^{eff} are fluctuating slightly when the microstructure changes. The following key observation giving rise to modern homogenization theory of random structures was made by Kozlov (1978): under some physically non-constraining assumptions, a_{ij}^{eff} take certain deterministic values as $\varepsilon \rightarrow 0$. In the limit problem the boundary condition $\psi = 0$ can be replaced by an integral condition,

$$\frac{1}{|V|} \int_V u_i dV = 0.$$

Another observation was that the problem is scale invariant (asymptotically), and, instead of tending ε to zero, one can fix ε and tend V to infinity. Denote by $\langle \varphi \rangle$ the space average of function $\varphi(x)$ defined in entire space,

$$\langle \varphi \rangle = \lim_{|V| \rightarrow \infty} \frac{1}{|V|} \int_V \varphi(x) dV.$$

Then the statement formulated can be written as

$$\frac{1}{2} a_{ij}^{\text{eff}} v_i v_j = \min_{\psi} \left\langle \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) \right\rangle \tag{4}$$

where minimum is sought over all ψ , such that

$$\langle u_i \rangle = 0. \tag{5}$$

This is the so-called Kozlov's cell problem for random structures. Kozlov justified (4) considering the two-scale expansion of the solution of the original problem (Kozlov, 1977, 1978; see also Jikov et al., 1994). Numerous works on the subject have been reviewed by Milton (2002), Cherkaev (2000), Torquato (2001), and Berdichevsky (2009).

Euler equations of variational problem (4) are partial differential equations with random coefficients. Our goal is to find the probabilistic characteristics of the solution. To this end, note that the functional to be minimized has the meaning of space average of some random fields. If these fields are stationary and ergodic, then space average can be replaced by mathematical expectation. Let $f(a, u)$ be the joint one-point probability density of conductivities a_{ij} and electric field u_i . Then the space average of dissipation is equal to its mathematical expectation

$$\left\langle \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) \right\rangle = \int \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) f(a, u) da du.$$

In the right hand side a denotes points in six-dimensional space of conductivities, $a = \{a_{11}, a_{12}, a_{13}, a_{22}, a_{23}, a_{33}\}$, $u = \{u_1, u_2, u_3\}$, da and du are volume elements in a -space and u -space, respectively. So, one can expect that the effective characteristics and the statistics of local fields can be determined from the variational principle

$$\frac{1}{2} a_{ij}^{\text{eff}} v_i v_j = \min_{f(a,u)} \int \frac{1}{2} a_{ij}(x)(v_i + u_i)(v_j + u_j) f(a, u) da du \tag{6}$$

where minimization is conducted over probabilistic measure $f(a, u)$. Function $f(a, u)$ must obey some constraints. First of all,

$$f(a, u) \geq 0, \quad \int f(a, u) da du = 1.$$

For stationary ergodic fields, vanishing of space average of u_i (5) is written in terms of probability density as

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