A MAXIMUM ENTROPY APPROACH TO WAVE PROPAGATION IN STOCHASTIC HETEROGENEOUS MATERIALS

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Abstract

The effective response of stochastic heterogeneous media is affected by the randomness of phase geometry as well as by the randomness of phase material constants and volume concentrations. The paper presents a theoretical framework, which accounts for both of the above effects with the help of the stochastic Hashin-Shtrikman bounds and associated bounds for wave velocity, without any appeal to a correlation function of the microstructure. For evaluation of relevant probability density functions, the paper makes use of the principle of maximum entropy, which allows for account of inherent uncertainties.

Key words: random media, Hashin-Shtrikman bounds, maximum entropy, wave velocity.

1. Introduction

The response of a heterogeneous medium with random phase geometry but the deterministic phase constants and volume concentration has been a subject of intensive investigations. Because of the uncertain phase configuration only the bounds on effective moduli can be specified. For details concerning the effective static response of such materials, the reader is referred to [1-3]. A probability density function which governs a wave velocity within the bounds has been recently found [4].

The physical constants of the phases and their volume concentrations (the phase constants) are also subjected to significant dispersion as a manifestation of material statistical inhomogeneity. Thus, the effective response of a stochastic heterogeneous medium is affected by both the randomness of phase geometry as well as by the randomness of phase material constants and volume concentration. A general theoretical framework is therefore desirable, which would address the above factors in their totality. Such a framework is given herein with the help of the stochastic Hashin-Shtrikman (*H-S*) bounds and the related low-frequency limit of phase velocity, without any appeal to a correlation function of the microstructure. For evaluation of these values, the paper makes use of the principle of maximum entropy (*PME*), which allows for account of uncertainties typical of many applications and the control of order of approximation. For a comprehensive exposition of the *PME* the reader is referred, for example, to [5].

It should be noted that homogenisation techniques make use of the concept of representative volume element (*RVE*), which is large as compared to dimensions of a typical phase region but is small compared to the entire composite structure [1-3]. This concept usually assumes a statistically homogeneous medium, in a sense that the *RVE* may be moved within a heterogeneous medium without any change of the phase constants, and is therefore not directly applicable to this case. Nevertheless, if variability of the phase constants is smooth enough to allow for formation of the *RVE*, one may think of a large collection (ensemble) of the representative volume elements as associated with realizations of a random process governing the above constants. Then, the *H-S* bounds hold for each of these realizations. Under the ergodicity assumption, the average over this ensemble equals the spatial average, which means that it may apply to statistically inhomogeneous media as a homogenisation technique. Given these bounds, the analyses may be so extended as to include the low-frequency limit of the phase velocity.

2. Basic equations

Consider a linearly elastic medium, which consists of m isotropic phases with the elastic bulk and shear moduli K_i, G_i, respectively, the mass densities ρ_i, i=1,2, …, m, and the volume concentrations ϕ_i, $\sum_{i=1}^{m}\phi_i = 1$, which will be referred as the phase constants in what follows. It is assumed that: i) the medium's phase geometry is not completely known and is specified in terms of the volume concentration only; ii) the random phase geometry and random phase constants, including the volume concentrations, are statistically independent and may be treated separately; iii) the medium's microstructure allows for a formation of the representative volume element (*RVE*), which may be considered as effectively isotropic and macroscopically homogeneous.

Denote by J the set of the random phase constants. The *H-S* bounds, $K_+(J)$, $K_-(J)$, for the effective bulk modulus, $K(J)$, and $G_+(J)$, $G_-(J)$, for the effective shear modulus, $G(J)$, which hold for such a medium can be found elsewhere [2]. Without any loss of generality, we present below their explicit form for a two-phase medium, which will be of use in what follows:

$$K_- = K_1 + \frac{\phi_2}{\dfrac{1}{K_2 - K_1} + \dfrac{3\phi_1}{3K_1 + 4G_1}}, \tag{1a}$$

$$K_+ = K_2 + \frac{\phi_1}{\dfrac{1}{K_1 - K_2} + \dfrac{3\phi_2}{3K_2 + 4G_2}}, \tag{1b}$$

$$G_- = G_1 + \frac{\phi_2}{\dfrac{1}{G_2 - G_1} + \dfrac{6\phi_1(K_1 + 2G_1)}{5G_1(3K_1 + 4G_1)}}, \tag{1c}$$

$$G_+ = G_2 + \frac{\phi_1}{\dfrac{1}{G_1 - G_2} + \dfrac{6\phi_2(K_2 + 2G_2)}{5G_2(3K_2 + 4G_2)}}, \tag{1d}$$

with $K_1 < K_2$, $G_1 < G_2$. The above *H-S* bounds enable one to estimate the stochastic low-frequency limit of the wave velocity.

$$\lim_{\omega\to 0} c(\omega) = \sqrt{\frac{Z}{\rho}} = c_0 \tag{2}$$

where Z is the relevant elastic constant, ρ the effective density given by

$$\rho = \sum_{i=1}^{m}\phi_i\rho_i \tag{3}$$

and $Z = K + 4G/3$ for the compression wave and $Z = G$ for the shear wave. Incorporating in (2) the proper upper and lower *H-S* bounds and extreme values of the density ρ, one gets the bounds for c_0, C_+ and C_-, respectively.

3. Maximum entropy solution

For a probability density function $p_Y(y)$ of a generic bound $Y \in \{K_+, K_-, G_+, G_-, C_+, C_-\}$ the entropy functional takes the form

$$H[p_Y(y)] = -\int_{-\infty}^{\infty} p_Y(y)\ln\frac{p_Y(y)}{m(Y)}dy \tag{4}$$

It can be shown (see [4] for details) that under the present conditions the reference measure m(Y)=1. The functional (4) is subject to constraints in the form of various moments of Y, $\langle Y^n \rangle$, n = 1, 2, …, N, which are assumed to be known form Monte-Carlo simulations for the bound Y as given by (1)-(3). The probability density function follows as

$$p_Y(y) = \begin{cases} \exp\left(\lambda_0 + \sum_{n=1}^{N} \lambda_n y^n\right), & Y_{min} \le y \le Y_{max} \\ 0, & \text{otherwise} \end{cases} \qquad (5)$$

where the Lagrange multipliers λ_n, n = 0, 1, …, N stem from the above moments and Y_{min}, Y_{max} are the extreme values of Y.

Consider a two-phase solid with $K_2 = 418.5$, $G_2 = 288.2$, $\phi_2 = 0.63$ and the random elastic constant K_1, which is uniformly distributed over the following interval:

$$0 \le K_1 \le 172.0 \qquad (6)$$

thereby allowing, for illustration purposes, for a particularly large dispersion of the elastic modulus of one of the phases (here and in what follows the elastic constants are given in GPa). Substituting the extreme values of K_1 into (1a), one gets the maximum and minimum values of the bound, K_+, as follows:

$$K_+^{min} = 187.9\,, \quad K_+^{max} = 305.4 \qquad (7)$$

which provides the zero-order probability density function (GPa^{-1})

$$p_{K_+,0}(k_+) = s_{K_+}(k_+) = \begin{cases} 0.851 \cdot 10^{-2}, & 187.9 \le k_+ \le 305.4 \\ 0, & \text{otherwise} \end{cases} \qquad (8)$$

In order to obtain a more accurate first-order density, the Monte-Carlo simulations have been performed, based on generation of random values for K_1 according to the uniform distribution over the interval (6) and computation of random values of K_+. The number of realization varied from 100 to 2500, indicating convergence to the following mean and standard deviation of K_+:

$$Y_1 = \langle K_+ \rangle = 251. \qquad \qquad (9)$$
$$\mathrm{STD}[K_+] = 33.5\,,$$

Solving the constrained maximum problem as given by (5) with N = 1, one gets the first-order density (GPa^{-1}).

$$p_{K_+,1}(k_+) = \begin{cases} \exp(\lambda_0 + \lambda_1 k_+), & 187.9 \le k_+ \le 305.4 \\ 0, & \text{otherwise} \end{cases} \qquad (10)$$

with $\lambda_0 = -5.7515$ GPa^{-1} and $\lambda_1 = 0.39574 \cdot 10^{-2}$ GPa^{-2}.

By finding higher moments from the Monte-Carlo simulations one may specify higher–order density functions, arriving thus at the hierarchy of approximations. The same techniques applies to the upper and lower bounds for the wave velocity, C_+ and C_-, respectively.

5. Conclusions

The effective response of a stochastic heterogeneous medium is affected by the randomness of phase geometry and by that of the phase constants. The first of these factors comes into play in the disparity between the *H-S* bounds, while the second in the randomness of the bounds themselves. The random bounds for the low-frequency limit of the wave velocity may be computed in terms of the *H-S* bounds and density.

By invoking the *RVE*-concept, one may think of an ensemble of these volumes as a large collection of realizations of a random process governing the values of phase material constants and volume concentrations. The *H-S* bounds and the expression for the effective density hold for each of the realizations and thus become random quantities. If variability of the microstructure is smooth enough to allow for formation of the *RVE* and the ergodicity assumption holds, the average over this ensemble equals the spatial average, which implies its applicability to statistically inhomogeneous media.

For a multivariate case, the straightforward computation of the probability density functions, which govern the bounds may be tedious at best and a resort to the maximal entropy approach provides a useful alternative. It also allows one to take into account the uncertainties inherent in the very definition of the problem.

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