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Probabilistic modeling of apparent tensors in elastostatics: A MaxEnt approach under material symmetry and stochastic boundedness constraints

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ABSTRACT

In this work, we address the stochastic modeling of apparent elasticity tensors, for which both material symmetry and stochastic boundedness constraints have to be taken into account, in addition to the classical constraint of invertibility. We first introduce a stochastic measure of anisotropy, which is defined using metrics in the set of elasticity tensors and used for quantitatively characterizing the fulfillment of material symmetry constraints. After having defined a numerical approximation for the stochastic boundedness constraint, we then propose a methodology allowing one to unify maximum entropy based models that have been previously derived by considering some of these constraints and which consists in constructing a probabilistic model for an auxiliary random variable. The latter can be interpreted as a stochastic compliance tensor, for which the available information to be used in the maximum entropy formulation can be readily deduced from the one considered for the elasticity tensor. A numerical illustration of the approach to an elastic microstructure is finally provided.

1. Introduction

Stochastic multiscale modeling has become a very fast growing discipline within the past decade and as such, it gave rise to an extensive literature in both mechanics and applied mathematics, ranging from the macroscale modeling of heterogeneous materials to very first attempts of stochastic atomistic-to-continuum simulations. As a matter of fact, most of the approaches have been derived within the general scopes of uncertainty propagation and hierarchical upscaling techniques (that is, characterizing the probabilistic behavior of a complex microstructure at some relevant scale, given some description of the underlying randomness occurring at finest scales), in conjunction with the tremendous amount of past and on-going works on functional (polynomial chaos) representations for random vector-valued quantities (see [1–4]). On the other hand, it is now widely recognized that the issue of stochastic representation is also very important, in the sense that the probabilistic model associated with any random variable of interest must ensure, not only some desired properties on the solution of the stochastic boundary value problem (such as the finiteness of some of its statistical moments, for instance, see [5,6] for discussions in the scalar and tensor-valued cases), but also the physical consistency of the modeling procedure. Clearly, the latter issue turns out to be fundamental in any multiscale approach where information exchange across the scales is arguably crucial.

The present work deals with the probabilistic modeling of the *apparent* elasticity tensor for heterogeneous microstructures, defined at a so-called mesoscale (i.e. for domains whose characteristic length is smaller or of the same order as the size of the representative volume element that is usually considered in stochastic homogenization theories). From a theoretical mechanics standpoint, properties exhibited by such tensors, together with their relationship to effective ones, have been studied in the nineties by Huet and his coworkers [7,8] (see the general review [9]). Specifically, the proposed methodology is derived within the general framework of information theory and having recourse to the Maximum Entropy (MaxEnt) principle. Such an approach, relying on random matrix theory, has been pioneered in [6] (making use of earlier derivations by the same author, obtained in the context of elastodynamics; see [10,11]) and later followed by numerous authors (see the non-exhaustive list below). In relation with some "philosophical" issues regarding which information should reasonably be taken into account, the formal derivations thus obtained differ by the use of additional constraints (combined to the classical constraints of normalization and invertibility; see Section 3), integrating information related to either boundedness (see [12,13] for applications in the random matrix and random field cases, respectively) or material symmetry (see [14,15]) properties for the random elasticity tensor. The aim of this study is therefore to unify these treatments and to propose a methodology allowing one to take into account all these constraints at the same time and within a nonparametric framework. For this purpose, we will have recourse to a change of variable which relaxes the boundedness constraint, thus introducing an auxiliary random variable which can be viewed as a stochastic compliance tensor and for which the probabilistic model will be

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finally constructed by a "translation" of the information available on the random elasticity matrix.

This paper is organized as follows. We first introduce and discuss, in Section 2, the definition of a stochastic measure of anisotropy which can be used for quantitatively characterizing, in some probabilistic sense (to be defined), the fulfillment of material symmetry constraints. Section 3 is devoted to the definition of the methodology and construction of the probabilistic model associated with the auxiliary random variable. In particular, we recall the MaxEnt principle and discuss a strategy regarding the definition of available information for this new variable. We finally provide, in Section 4, a numerical illustration of the approach.

2. Stochastic measure of anisotropy

2.1. Definition

The oldest and most widely used deterministic measure of anisotropy is based on the consideration of a scalar parameter, the definition of which depends on some given components of the elasticity tensor. Among others, the so-called Zener index, defined for crystals with cubic symmetry [16], is for instance written as $z = [C]_{44}/([C]_{11} - [C]_{12})$, where Kelvin's notation for the elasticity tensor is assumed. While such indexes benefit from their simplicity, they suffer from a lack of universality and can hardly be extended to other situations (e.g. when the crystal exhibits weaker material symmetries or when one is interested in measuring the distance to another class than the isotropic one); see the discussions in [17–19].

Indeed, the usual anisotropy measurement can be seen as the characterization of the *residual* distance between a given elasticity tensor with arbitrary symmetry and its projection onto the set of isotropic–elasticity tensors. Based on this observation, it follows that a more general definition of anisotropy, the latter being now understood as the distance to any material symmetry class (and not only the isotropic one), can be readily obtained by first defining a metric in the set $\mathbb{E}la$ of elasticity tensors and then, by defining a projection operator onto a given subset of $\mathbb{E}la$. A first natural distance is the Euclidean one, denoted as d_E and given for any elasticity matrices $[C]_1$ and $[C]_2$ by

$$d_E([C]_1, [C]_2) = \|[C]_1 - [C]_2\|_F, \tag{1}$$

wherein $\|\cdot\|_F$ denotes the Frobenius norm. Alternative metrics have been derived in the literature, among which the Log-Euclidean and Riemannian ones (see [20,21]), denoted respectively by d_{LE} and d_R and defined as

$$d_{LE}([C]_1, [C]_2) = \|\log[C]_1 - \log[C]_2\|_F, \tag{2}$$

$$d_R([C]_1, [C]_2) = \|\log([C]_1^{-\frac{1}{2}}[C]_2[C]_1^{-\frac{1}{2}})\|_F. \tag{3}$$

Let $\mathcal{C}^{sym} \subseteq \mathbb{E}la$ be the set of elasticity tensors with *sym* material symmetries (e.g. $\mathcal{C}^{Iso}$ – resp. $\mathcal{C}^{Trans\cdot\, Iso}$ – is the set of fourth-order isotropic – resp. transversely isotropic–elasticity tensors) and let P^{sym} be the projection operator onto $\mathcal{C}^{sym}$. We then denote by $[C]^{sym} = P^{sym}([C]) \in \mathcal{C}^{sym}$ the associated projection of any elasticity tensor $[C]$, defined as

$$[C]^{sym} = \arg\min_{[X]\in\mathcal{C}^{sym}} d([C] - [X]), \tag{4}$$

in which d is any of the metric defined above. Upon introducing a tensorial basis of $\mathcal{C}^{sym}$ (or equivalently, a parametric representation of the matrix form for an elasticity tensor in $\mathcal{C}^{sym}$), optimization problem (4) can be solved in a straightforward manner, yielding either closed-form expressions for the projected tensor (for the Euclidean distance) or equivalent optimization problems (formulated with respect to a finite set of parameters) when the Log-Euclidean or the Riemannian metric is used; see [22,23] for results expressed in matrix and vector forms, respectively. For instance, the closest isotropic approximation, in the Euclidean sense, of an arbitrary elasticity tensor $[C]$ written in Kelvin's notation is given by [24] (see also [22]):

$$[C]^{Iso} = \begin{bmatrix} \kappa + 4\upsilon/3 & \kappa - 2\upsilon/3 & \kappa - 2\upsilon/3 & 0 & 0 & 0 \\ & \kappa + 4\upsilon/3 & \kappa - 2\upsilon/3 & 0 & 0 & 0 \\ & & \kappa + 4\upsilon/3 & 0 & 0 & 0 \\ & & & 2\upsilon & 0 & 0 \\ & \text{Sym.} & & & 2\upsilon & 0 \\ & & & & & 2\upsilon \end{bmatrix}, \tag{5}$$

in which

$$\kappa = \frac{1}{9}\left([C]_{11} + [C]_{22} + [C]_{33} + 2([C]_{12} + [C]_{13} + [C]_{23})\right), \tag{6}$$

and

$$\upsilon = \frac{1}{30}(2([C]_{11} + [C]_{22} + [C]_{33} - [C]_{12} - [C]_{23} - [C]_{31}) + 3([C]_{44} + [C]_{55} + [C]_{66})). \tag{7}$$

Note that this result coincides with the one derived by Fedorov, having recourse to an apparently different and more physically-sounded approach [25], and that the two different treatments were later shown to be equivalent in [26]. It is worth while to note that within a deterministic framework and for material symmetry classes involving the definition of a reference frame (e.g. for transverse isotropy, orthotropy, etc.), the computation of the closest approximation exhibiting the required symmetries (which is often referred to as the *effective* approximation in the literature of elasticity) necessitates an additional minimization problem, defined over all orthogonal transformation of the reference frame, to be solved; see the discussions in [27–30], as well as the references therein. However, such a consideration is not relevant to this study, since the anisotropic statistical fluctuations induced by the probabilistic model can be seen as representing the randomness on both the mechanical properties and the reference frame.

Let us now consider the stochastic case, and let $[\mathbf{C}]$ be the $\mathbb{M}_n^+(\mathbb{R})$-valued random variable corresponding to the modeling of a random elasticity matrix with arbitrary symmetry. Following the previous discussions, we denote as $[\mathbf{C}^{sym}] = P^{sym}\{[\mathbf{C}]\}$ the $\mathbb{M}_n^+(\mathbb{R})$-valued random variable corresponding to the projection of $[\mathbf{C}]$ onto $\mathcal{C}^{sym}$, associated with projection operator P^{sym} (defined with respect to any suitable metric). Consequently, a stochastic measure of anisotropy can be defined by making use of the $\mathbb{R}^+$-valued random variable μ^{sym} defined as

$$\mu^{sym} = d([\mathbf{C}], [\mathbf{C}^{sym}]). \tag{8}$$

The statistical properties of μ^{sym} (and especially, its mean value) are worth characterizing and will be used in the sequel for discussing the relevance of stochastic representations for the random elasticity tensor.

2.2. Eigensystem-based characterization of symmetries

Having introduced the stochastic measure of anisotropy, a fundamental issue concerns the information that one may take into account in order some moments (e.g. the mean) of μ^{sym} to be specified. More specifically, one may answer the following question: how to characterize a given set $\mathcal{C}^{sym}$ of elasticity with *sym* material symmetries, so that the properties thus identified can be used in the construction of the probabilistic model? In fact, several approaches for elastic material symmetry classification and