



HAL
open science

Stochastic modeling of anisotropy in multiscale analysis of heterogeneous materials: A comprehensive overview on random matrix approaches

Johann Guilleminot, Christian Soize

► To cite this version:

Johann Guilleminot, Christian Soize. Stochastic modeling of anisotropy in multiscale analysis of heterogeneous materials: A comprehensive overview on random matrix approaches. *Mechanics of Materials*, 2012, 44 (SI), pp.35-46. 10.1016/j.mechmat.2011.06.003 . hal-00684288

HAL Id: hal-00684288

<https://hal.science/hal-00684288>

Submitted on 31 Mar 2012

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Stochastic modeling of anisotropy in multiscale analysis of heterogeneous materials: a comprehensive overview on random matrix approaches

Johann Guilleminot*, Christian Soize

*Université Paris-Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME
UMR8208 CNRS, 5 Bd Descartes, 77454 Marne la Vallée, France*

Abstract

The aim of this paper is to provide a general overview on random matrix ensembles for modeling stochastic elasticity tensors that exhibit uncertainties on material symmetries. Such an issue is of primal importance in many practical situations involving either a computational or experimental analysis on random heterogeneous materials (such as bones, reinforced composites, etc.). For this purpose, we first define a stochastic measure of anisotropy, the definition of which relies on the use of distances in the set of fourth-order elasticity tensors. We subsequently describe two random matrix ensembles that have been proposed within the framework of information theory and making use of a MaxEnt approach. In particular, we discuss the relevance of each of those with respect to constraints on the proposed anisotropy measure. It is shown that the capability of prescribing the mean distance to a given symmetry class depends, in view of the eigensystem-based characterization, on the behavior of the random eigenvalues. Finally, we propose a procedure allowing for the identification of the stochastic representation, should a set of experimental data be available. The approach, which is based on the use of the maximum likelihood principle, is exemplified in the case of experimental realizations that are almost transversely isotropic.

Key words: Anisotropy; Elasticity tensor; Material Symmetry; Maximum

[☆]J. Guilleminot and C. Soize, Stochastic modeling of anisotropy in multiscale analysis of heterogeneous materials: a comprehensive overview on random matrix approaches, *Mechanics of Materials*, **44** (Special Issue on Microstructures and Anisotropies), 35-46 (2012).

*Corresponding author

Email address: johann.guilleminot@univ-paris-est.fr (Johann Guilleminot)

Notations

The notations that will be used throughout the paper are presented in Table 1. Otherwise stated, the summation over repeated indices is assumed.

Symbol	Meaning
a	Scalar deterministic variable
α	Scalar random variable
$\mathbf{x}, \boldsymbol{\lambda}$	Deterministic vector
$\mathbf{X}, \boldsymbol{\Lambda}$	Random vector
$[A], [\Lambda]$	Deterministic matrix
$[\mathbf{A}], [\boldsymbol{\Lambda}]$	Random matrix
$[[A]], [[\Lambda]]$	Deterministic fourth-order tensor
$[[\mathbf{A}]], [[\boldsymbol{\Lambda}]]$	Random fourth-order tensor

Table 1: Nomenclature.

Hereafter, $[[A]]$ is a fourth-order tensor in three dimensions and the same notation will be used for both second-order tensors in n dimensions and $(n \times n)$ matrix representations.

Let $\mathbb{M}_n^S(\mathbb{R})$ and $\mathbb{M}_n^+(\mathbb{R})$ be the sets of all the $(n \times n)$ real symmetric matrices and the $(n \times n)$ real symmetric positive-definite matrices ($\mathbb{M}_n^+(\mathbb{R}) \subset \mathbb{M}_n^S(\mathbb{R})$), respectively. The determinant, trace and transpose of matrix $[A] \in \mathbb{M}_n(\mathbb{R})$ ($\mathbb{M}_n(\mathbb{R})$ being the set of all the square $(n \times n)$ real matrices) are denoted by $\det([A])$, $\text{tr}([A]) = [A]_{ii}$ and $[A]^T$, respectively. For $[A]$ and $[B]$ in $\mathbb{M}_n(\mathbb{R})$, the inner product $\langle \cdot, \cdot \rangle$ and the associated Frobenius (or Hilbert-Schmidt) norm $\|\cdot\|_F$ are defined as $\langle [A], [B] \rangle = \text{tr}([A]^T[B])$ and $\|[A]\|_F^2 = \langle [A], [A] \rangle$. All the random variables are defined on a probability space $(\Theta, \mathcal{F}, \mathcal{P})$ and \mathbb{E} denotes the mathematical expectation.

1. Introduction

In this paper, we consider the modeling of stochastic elasticity tensors, the parametrization of which has to be defined with respect to some anisotropy constraints. Such a situation arises in various applications, ranging from the modeling of complex heterogeneous materials (e.g. biological tissues or fiber-reinforced composite materials) for which no scale separation holds, to the experimental analysis of materials exhibiting uncertainties on

macroscale material symmetries. In the former, it is well known that the so-called *apparent* elasticity tensor exhibits aleatoric uncertainties (see [21] [19] [43] [38]), and a fundamental issue, beyond the one related to the probabilistic modeling, is to know whether the material symmetries that can be expected at the macroscale are preserved at the mesoscopic level. From a mechanical point of view, it can be clearly inferred that each realization of the apparent tensor does not belong to the set of tensors with the macroscopic material symmetries, but the “distance” between each realization and this class of symmetry may be bounded or at least, constrained. This simple observation can be schematically exemplified in the case of a two-phase composite material, made up with an isotropic matrix reinforced by isotropic or transversely isotropic fibers that are all aligned in a given direction, say \mathbf{e}_3 ; see Fig. 1. While such a material is transversely isotropic

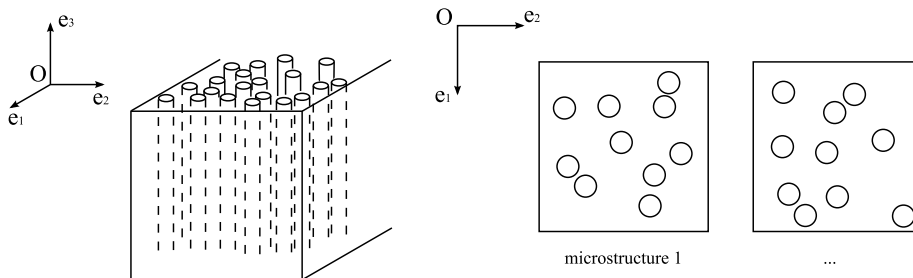


Figure 1: Schematic of an unidirectional composite: macroscale transversely isotropic representation (left) and 2D mesoscale representations in the transverse plane of macroscopic isotropy (right).

at the macroscale, it is very likely that the mesoscale realizations in the transverse plane ($\mathbf{e}_1, \mathbf{e}_2$) are not isotropic anymore, and that the distance to transverse isotropy is all the more small that the size of the mesoscopic domain tends to the size of the RVE. Even when the scale separation can be stated, experimental results often exhibit a large scattering (which may be due to either uncertainties induced by modeling errors on experimental setup or microstructure evolution while processing or testing the final material samples, for instance) that may not be ignored. Such anisotropic random fluctuations are seldom taken into account in practice and are, in many situations, either neglected or smoothed through an averaging procedure or having recourse to projection schemes (as will be discussed in Section 2.3). However, such choices do have important consequences for practical applications where the elastic anisotropy plays a key role in the physics of the modeled phenomenon (see [29], among others, for a brief discussion in

a deterministic context) and consequently, the modeling of such “random anisotropy” turns out to be of primal importance to ensure the consistency between the mathematical/mechanical model and the physical information carried by the realizations of the random microstructure, as well as to obtain more predictive and robust simulations. Three main issues can then be identified:

- (i) How can we model, in a way that is both mathematically and physically-sounded, such uncertainties on the elasticity tensor?
- (ii) Once such a model has been derived, how can we define model parameters so that the realizations of the elasticity tensor exhibit a certain level of material symmetry? Naturally, this question is closely related to the definition of an anisotropy measure that is suitable for stochastic analysis.
- (iii) Finally, assuming that some data are available, how can we identify the proposed stochastic representations, such that the probabilistic models are able to generate realizations that are consistent (in terms of anisotropy) with the experiments?

This work aims at addressing such issues by providing, in particular, a comprehensive overview on random matrix approaches. The paper is organized as follows. In Section 2, we then discuss the definition of anisotropy measures for elasticity tensors. The concept of distances in the set of fourth-order elasticity tensors is recalled and we make use of such derivations to define a stochastic measure of anisotropy (in connection with point (ii) mentioned above). In Section 3, we summarize an overall methodology for constructing probabilistic models in the context of information theory and present two random matrix ensembles, namely SE^+ and SE^{++} .

2. Characterization of anisotropy

2.1. Hooke’s law and second-order tensor representation of the elasticity tensor

Let $\mathbb{E}la$ be the set of fourth-order elasticity tensors. Therefore, $[[A]] \in \mathbb{E}la$ satisfy the usual positive-definiteness and symmetry properties:

- $[b] : [[A]] : [b] = [[A]]_{ijkl}[b]_{ij}[b]_{kl} > 0$, in which the symbol “:” denotes the twice contracted tensor product and $[b]$ is any nonzero symmetric second-order tensor.
- $[[A]]_{ijkl} = [[A]]_{jikl} = [[A]]_{ijlk} = [[A]]_{klij}$.

The inner product $\ll \cdot, \cdot \gg$ of $[[A]]$ and $[[B]]$ (both in $\mathbb{E}la$) and the associated norm $||| \cdot |||$ are defined as $\ll [[A]], [[B]] \gg = [[A]]_{ijkl} [[B]]_{ijkl}$ and $||| [[A]] |||^2 = \ll [[A]], [[A]] \gg$.

In this paper, we denote by $\mathcal{C}^{sym} \subset \mathbb{E}la$ the set of elasticity tensors with *sym* material symmetry, e.g. \mathcal{C}^{Iso} is the subset of all the fourth-order isotropic elasticity tensors.

In linear elasticity, the strain and stress (second-order symmetric) tensors $[\sigma]$ and $[\varepsilon]$ are related through the generalized Hooke's law:

$$[\sigma] = [[L]] : [\varepsilon], \quad (1)$$

in which $[[L]] \in \mathbb{E}la$. Alternative matrix forms of Eq. (1) have been proposed in the literature. One of the most commonly used notation in mechanics of anisotropic materials is the one introduced by Voigt [53], in which the components $[L]_{IJ}$ of the matrix representation are related to the components $[[L]]_{ijkl}$ of $[[L]]$ by the following index mapping: 11 \rightarrow 1, 22 \rightarrow 2, 33 \rightarrow 3, 23 \rightarrow 4, 13 \rightarrow 5 and 12 \rightarrow 6. Vectorial representation of $[\sigma]$ and $[\varepsilon]$ are then accordingly considered.

In this paper, we adopt a slightly different notation and rewrite Eq. (1) as [54]:

$$\boldsymbol{\sigma} = [L]\boldsymbol{\varepsilon}, \quad (2)$$

in which,

$$\boldsymbol{\sigma} = ([\sigma]_{11}, [\sigma]_{22}, [\sigma]_{33}, \sqrt{2}[\sigma]_{23}, \sqrt{2}[\sigma]_{13}, \sqrt{2}[\sigma]_{12}), \quad (3)$$

$$\boldsymbol{\varepsilon} = ([\varepsilon]_{11}, [\varepsilon]_{22}, [\varepsilon]_{33}, \sqrt{2}[\varepsilon]_{23}, \sqrt{2}[\varepsilon]_{13}, \sqrt{2}[\varepsilon]_{12}), \quad (4)$$

and $[L]$ is defined as:

$$\begin{bmatrix} [[L]]_{11} & [[L]]_{12} & [[L]]_{13} & \sqrt{2}[[L]]_{14} & \sqrt{2}[[L]]_{15} & \sqrt{2}[[L]]_{16} \\ & [[L]]_{22} & [[L]]_{23} & \sqrt{2}[[L]]_{24} & \sqrt{2}[[L]]_{25} & \sqrt{2}[[L]]_{26} \\ & & [[L]]_{33} & \sqrt{2}[[L]]_{34} & \sqrt{2}[[L]]_{35} & \sqrt{2}[[L]]_{36} \\ & & & 2[[L]]_{44} & 2[[L]]_{45} & 2[[L]]_{46} \\ & & & & 2[[L]]_{55} & 2[[L]]_{56} \\ & & & & & 2[[L]]_{66} \end{bmatrix}. \quad (5)$$

in which $[[L]]_{ij}$ is the component (i, j) of the matrix representation of the elasticity tensor in Voigt's notation. It can be shown that the matrix form (5) represents the components of a second-order tensor (which is not the case for the Voigt notation; see [31] for a discussion) and ensures the preservation of the norm no matter the representation of the elasticity tensor (that is to say, $||| [[L]] ||| = ||[L]||_F$).

2.2. Definition of anisotropy index

The simplest characterization of anisotropy was historically based on the study of the anisotropy of single crystals and achieved through the definition of a scalar parameter, written as a function of some specific components of the elasticity matrix. One of the very first attempt was carried out by Zener [55], resulting in the definition of the so-called Zener anisotropy index for cubic crystals:

$$z^{Zener}([L]) = \frac{[L]_{44}}{[L]_{11} - [L]_{12}}. \quad (6)$$

Note that the definition (6) of the Zener index has been slightly modified in order to be consistent with Eq. (5). When $z^{Zener}([L]) = 1$, the crystal is perfectly isotropic. Although the information given by such an index may appear somewhat limited, it turns out to be very useful in interpreting scale effects in polycrystalline microstructures for instance (see [40] for numerical evidences). Definitions of other anisotropy measures have been proposed in [9] [29] and [41]. However, the first two characterizations undoubtedly lack universality, since they are generally valid for anisotropic crystals with a particular class of symmetry (as pointed out in [41]), and all these measures are defined with respect to the isotropy class. In other words, these indexes are either such that they do not allow characterizing the “distance” between an elasticity tensor with *arbitrary symmetry* to the set of tensors exhibiting a material symmetry *different from isotropy*, or only provide a rough information about the anisotropy. Such limitations can be circumvented by introducing metrics in $\mathbb{E}la$, as discussed below.

2.3. Definition of distances and projections in $\mathbb{E}la$

The characterization of anisotropy can be put on a firm footing by introducing the concept of distances in $\mathbb{E}la$. Such distances have been introduced and widely used within the scope of seismology and geophysical applications, for which the accuracy in both forward simulations and inverse solving depends on whether or not anisotropic behavior can be accounted for by the retained model [20] [50]. The problem can then be stated as follows: how can we compute, from anisotropic experimental measurements, the associated closest approximations belonging to a given subset \mathcal{C}^{sym} ? Such an issue has been addressed by numerous authors. An Euclidean-projection-based strategy, taking advantage of the mathematical interpretation of the subsets of elasticity tensors exhibiting given symmetries, has been proposed in [15]. A more physically-sounded approach was alternately derived in [13], in which the author states the equivalence between the acoustic properties of

the anisotropic material and the ones of its closest isotropic approximation, making use of the slowness surfaces. These two treatments were later unified and shown to be equivalent in [36], hence providing a valuable and physical basis for the use of Euclidean projections. Note that the latter also benefit from their universality, since the projection procedure is not restricted to \mathcal{C}^{Iso} .

The first attempts for deriving closest approximations have been formalized making use of the Euclidean metric d_E , defined for two elasticity matrices $[C_1]$ and $[C_2]$ as:

$$d_E([C_1], [C_2]) = \|[C_1] - [C_2]\|_F. \quad (7)$$

However, the Euclidean distance is not invariant by inversion and therefore, does not provide a unique projection (which should be defined regardless of whether the stiffness or compliance tensor is considered). Consequently, alternative distances, which do not suffer from this deficiency, have been proposed in the literature. In particular, the Log-Euclidean [1] and Riemannian [34] metrics, denoted by d_{LE} and d_R respectively, were introduced and are defined as:

$$d_{LE}([C_1], [C_2]) = \|\log([C_2]) - \log([C_1])\|_F, \quad (8)$$

$$d_R([C_1], [C_2]) = \|\log\left([C_1]^{-1/2}[C_2][C_1]^{-1/2}\right)\|_F. \quad (9)$$

Assuming that the reference frame, defining the desired subset \mathcal{C}^{sym} on which the projection is sought, is known and upon using a tensorial basis of \mathcal{C}^{sym} , straightforward minimization procedures allows for the definition of the projected tensor (or equivalently, or its matrix representation). Due to the simple form of Eq. (7), closed-form expressions can be derived in the case of the Euclidean distance, while the use of either the Log-Euclidean or the Riemannian metric requires a numerical solving; see [35] for explicit derivations for all symmetry classes (see [37] for a specific discussion regarding the isotropic one), as well as [6] for results expressed in the form of vectorial representations. It is worthwhile to note that an overall closest approximation can be defined by minimizing the distance over all orthogonal transformations of the reference frame (see [30] for a parametrization of the orthogonal group $SO(6)$, for instance), thus providing the definition of what may be referred to as the effective closest approximation and reference frame; see [7] [26] [27] [28] (and the references therein) for reviews and applications to effective orthotropic and transversely isotropic tensors. However, such a consideration is not adapted to the present probabilistic

analysis, since the stochastic anisotropic fluctuations induced by the model intrinsically reflect the uncertainties on both the elasticity tensor and its reference frame.

2.4. Probabilistic analysis of distances in $\mathbb{E}la$

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. For any material symmetry class \mathcal{C}^{sym} , let \mathbf{P}_M^{sym} be the projection operator onto \mathcal{C}^{sym} , defined with respect to metric M (e.g. \mathbf{P}_E^{sym} is the projection operator defined with respect to the Euclidean distance; see section 2.3). Accordingly, $[\mathbf{C}_M^{sym}] = \mathbf{P}_M^{sym}\{[\mathbf{C}]\}$ is the $\mathbb{M}_n^+(\mathbb{R})$ -valued random variable corresponding to the associated projection of $[\mathbf{C}]$ onto \mathcal{C}^{sym} .

A natural stochastic measure of anisotropy can be obtained by considering the \mathbb{R}^+ -valued random variable μ_M^{sym} , defined as:

$$\mu_M^{sym} = d_M([\mathbf{C}], [\mathbf{C}_M^{sym}]). \quad (10)$$

Note that the term ‘‘anisotropy’’ has to be understood here in the sense of the distance to any given class of material symmetry, and that the usual (but more restricted) definition of anisotropy is recovered by considering μ_M^{Iso} . Consequently, the mean value $\underline{\mu}_M^{sym} = \mathbb{E}\{\mu_M^{sym}\}$ characterizes the mean distance of the random elasticity matrix to a given material symmetry class, while for a mean value close to zero, the variance of μ_M^{sym} reflects how ‘‘far’’ from \mathcal{C}^{sym} the realizations of the stochastic elasticity matrix can be. With reference to the issue of mesoscale modeling, briefly summarized in the introduction of this paper, these two statistical properties are worth characterizing and may be used as a basis for discussing the relevance of stochastic representations for the random elasticity tensor.

3. Probabilistic modeling

In this section, we introduce two ensembles of prior nonparametric probabilistic models, denoted respectively by SE^+ and SE^{++} , that are adapted to the representation of random elasticity matrices. Such an issue naturally involves the use of the random matrix theory, the presentation of which is far beyond the scope of the present paper, and the interested reader is referred to the synthesis provided by Mehta [32] for a general review. Furthermore, in order to avoid too many mathematical derivations and to preserve the overall readability of this paper, all the theoretical results which have been derived regarding these ensembles (as well as details about the random generators)

will not be recalled hereafter and can be found in the given references. For later convenience, let us introduce the (dispersion) parameter $\delta_{[\mathbf{A}]}$, allowing us to characterize the level of statistical fluctuations of an arbitrary random matrix $[\mathbf{A}]$ and defined as:

$$\delta_{[\mathbf{A}]} = \sqrt{\frac{\mathbb{E}\{\|[\mathbf{A}] - [\underline{\mathbf{A}}]\|_{\mathbb{F}}^2\}}{\|[\underline{\mathbf{A}}]\|_{\mathbb{F}}^2}}, \quad (11)$$

in which $[\underline{\mathbf{A}}] = \mathbb{E}\{[\mathbf{A}]\}$.

In this paper, we denote by $[C] \mapsto p_{[\mathbf{C}]}([C])$ the probability density function (p.d.f.), from $\mathbb{M}_n^+(\mathbb{R})$ into \mathbb{R}^+ , defining the probability distribution $P_{[\mathbf{C}]} = p_{[\mathbf{C}]}([C])d[C]$ of random matrix $[\mathbf{C}]$. The measure (volume element) $d[C]$ on $\mathbb{M}_n^S(\mathbb{R})$ is defined as [46]:

$$d[C] = 2^{n(n-1)/4} \prod_{1 \leq i < j \leq n} d[C]_{ij}. \quad (12)$$

A fundamental step (together with uncertainty propagation) of any probabilistic modeling is to infer about the form of p.d.f. $p_{[\mathbf{C}]}$, and this issue of constructing suitable stochastic representations will be the main topic addressed in the following.

The easiest approach consists in performing the analysis on a parametrization of a given class \mathcal{C}^{sym} , modeling all the elastic moduli as statistically independent random variables with assumed probability distributions (a log-normal probability distribution being often retained because it ensures the positiveness of the random moduli). However, such a procedure, which has been largely followed for the sake of simplicity in the literature, does have important consequences which are note worthy. First of all, the resulting model does not allow for the modeling of random elasticity tensors, the realizations of which exhibit weaker material symmetries (as it can be expected in mesoscale modeling of heterogeneous materials): in other words, this method basically requires the consideration of the largest class, namely the class of anisotropic elasticity tensors. Secondly, considering *a priori* choices for the probability distributions undoubtedly introduces some modeling bias and therefore, generates additional model uncertainties. Clearly, the assumption of statistical independence between the components is very strong and questionable from a physical standpoint. Finally, such assumptions have important consequences on the solution of the associated stochastic boundary problem (e.g. on the stochastic vector-valued displacement field) that are often ignored and clearly yield questionable results; see [2] among others.

As a consequence, it is highly desirable to derive the most “objective” probabilistic model, that is to say, a stochastic representation that does not introduce any modeling bias, while synthesizing as many physical and mathematical information as possible. The general framework of information theory (and more precisely, the Maximum Entropy principle) paves the way for such models to be derived, and is presented below.

3.1. An overall methodology for constructing probabilistic models: the Max-Ent principle

The Maximum Entropy (MaxEnt) principle is a general optimization procedure which has been derived within the framework of information theory, introduced by Shannon [45], and which allows the probability distribution to be explicitly constructed, taking into account a set of constraints that define the available information [45] [23] [24] [25] [10]. Before stating the MaxEnt principle, let us first clarify what is precisely meant by *available information*.

Since $p_{[\mathbf{C}]}$ is a probability density function, it has to satisfy the usual normalization condition:

$$\int_{\mathbb{M}_n^+(\mathbb{R})} p_{[\mathbf{C}]} ([C]) d[C] = 1. \quad (13)$$

Furthermore, we have to impose, in view of uncertainty propagation, that the inverse random matrix $[\mathbf{C}]^{-1}$ is a second-order random variable, that is:

$$\mathbb{E}\{\|[\mathbf{C}]^{-1}\|_{\mathbb{F}}^2\} < +\infty. \quad (14)$$

It can be proved that Eq. (14) holds if the following constraint is satisfied [46] [47]:

$$\int_{\mathbb{M}_n^+(\mathbb{R})} \ln(\det([C])) p_{[\mathbf{C}]} ([C]) d[C] = \beta, \quad |\beta| < +\infty, \quad (15)$$

wherein \ln is the Neperian logarithm. Clearly, any p.d.f. candidate has to satisfy Eqs. (13)-(15): these constraints define, therefore, the available (mathematical) information. Note that the positive-definiteness of the elasticity matrix can be readily ensured by using a particular algebraic construction. Additional constraints, synthesizing some physical information in particular (e.g. information related to the anisotropy), can be considered (as will be seen in sections 3.2 and 3.3), hence leading to the definition of different random matrix ensembles.

Let \mathcal{C}_{ad} be the set of all the probability density functions from $\mathbb{M}_n^+(\mathbb{R})$ into \mathbb{R}^+ such that all the constraints defining the available information are fulfilled. The MaxEnt principle then states that:

$$p_{[\mathbf{C}]} = \arg \max_{p \in \mathcal{C}_{ad}} S(p), \quad (16)$$

in which the measure of entropy $S(p)$ of p is defined as:

$$S(p) = - \int_{\mathbb{M}_n^+(\mathbb{R})} p([C]) \ln(p([C])) d[C]. \quad (17)$$

In other words, the probability density function, estimated by using the MaxEnt principle, is the function which maximizes the measure of entropy (that is to say, the uncertainties) over the admissible space \mathcal{C}_{ad} .

3.2. Ensemble SE^+ of symmetric positive-definite real random matrices

3.2.1. Probabilistic model

Let us now assume that the modeling is performed on an elasticity matrix, whose expected deterministic (nominal) value is denoted by $[\underline{C}]$. Such a value could correspond, within the context of mesoscale modeling, to the expected macroscopic (homogenized) value, for instance. Consequently, we may impose that the mean value of the stochastic model under construction be equal to this nominal value, namely:

$$\mathbb{E} \{[\mathbf{C}]\} = \int_{\mathbb{M}_n^+(\mathbb{R})} [C] p_{[\mathbf{C}]}([C]) d[C] = [\underline{C}]. \quad (18)$$

Eqs. (13), (15) and (18) thus define the admissible space \mathcal{C}_{ad} and the optimization problem (16) can easily be solved by introducing a set of Lagrange multipliers and making use of the Euler-Lagrange equation (calculus of variation). After some algebra, it can be proven that the p.d.f. $p_{[\mathbf{C}]}$, estimated by the MaxEnt procedure under the constraints (13), (15) and (18), takes the form [46] [47]:

$$p_{[\mathbf{C}]}([C]) = \mathbb{I}_{\mathbb{M}_n^+(\mathbb{R})}([C]) k \det([C])^{\ell-1} \exp\left\{-\frac{n-1+2\ell}{2} \text{tr}([\underline{C}]^{-1}[C])\right\}, \quad (19)$$

wherein $[C] \mapsto \mathbb{I}_{\mathbb{M}_n^+(\mathbb{R})}([C])$ is the indicator function of $\mathbb{M}_n^+(\mathbb{R})$, k is a normalization constant (whose expression can be found in [47]) and parameter ℓ is defined as:

$$\ell = \frac{(1 - \delta_{[\mathbf{G}]})^2}{2\delta_{[\mathbf{G}]}^2} n + \frac{1 + \delta_{[\mathbf{G}]}^2}{2\delta_{[\mathbf{G}]}^2}, \quad (20)$$

in which $\delta_{[\mathbf{G}]}$ is the dispersion parameter associated with the random matrix $[\mathbf{G}]$ such that $[\mathbf{C}] = [\underline{L}]^T[\mathbf{G}][\underline{L}]$ and $[\underline{C}] = [\underline{L}]^T[\underline{L}]$ (cholesky decomposition of the mean matrix $[\underline{C}]$); see [46] [47] for mathematical derivations. A closed-form expression relating parameters $\delta_{[\underline{C}]}$ and $\delta_{[\mathbf{G}]}$ can be found in [46] and it can be shown that Eq. (15) holds if parameter $\delta_{[\mathbf{G}]}$ is such that:

$$0 < \delta_{[\mathbf{G}]} < \sqrt{\frac{n+1}{n+5}}. \quad (21)$$

Such a boundedness property turns out to be very useful while addressing the identification of the model from experimental data, as will be seen in Section 4.1.

The *positive-definite ensemble* SE^+ , constructed in [46] [47], is the set of all $\mathbb{M}_n^+(\mathbb{R})$ -valued random matrices, defined on $(\Theta, \mathcal{F}, \mathcal{P})$, the probability density function of which (estimated by the MaxEnt principle under the information defined by Eqs. (13-15-18)) is given by Eq. (19). From a practical point of view, it should be emphasized that this ensemble is especially suitable for inverse (experimental) identification, since it benefits from a minimal parametrization through parameters $\delta_{[\underline{C}]}$ (or equivalently, $\delta_{[\mathbf{G}]}$) and $[\underline{C}]$. The objectivity regarding the methodology of construction is also note worthy, since the probability distribution is not assumed *a priori* and is subsequently estimated by considering available information only.

In the next section, we discuss the capability of SE^+ of taking into account constraints on the stochastic anisotropy measure.

3.2.2. Parametric study on stochastic anisotropy measure μ for $[\mathbf{C}] \in SE^+$

For illustration purpose, let the nominal value $[\underline{C}]$ be defined as:

$$[\underline{C}] = \begin{bmatrix} 10.1036 & 0.5391 & 2.9625 & -0.0040 & 0.0071 & -0.0165 \\ & 10.1061 & 2.9782 & -0.0041 & -0.0070 & -0.0036 \\ & & 182.690 & 0.0197 & 0.0016 & 0.0145 \\ & & & 14.0339 & 0.0068 & 0.0008 \\ & \text{Sym.} & & & 14.0121 & -0.0103 \\ & & & & & 9.5552 \end{bmatrix}. \quad (22)$$

Eq. (22) has been obtained from a random perturbation on the elasticity matrix (in GPa) of a carbon-epoxy unidirectional composite and can be interpreted as the mean value of a mesoscale representation for a heterogeneous material that is almost transversely isotropic from a macroscopic point of view. Consequently, let us consider the random variable μ_M^{TI} , corresponding to the stochastic measure of anisotropy (see Eq. (10)) defined

with respect to the set \mathcal{C}^{TI} of transversely isotropic elasticity tensors and metric M .

Figs. 2 and 3 display the graphs of the p.d.f. of μ^{TI} for several values of dispersion parameter $\delta_{[C]}$, considering the Euclidean and Riemannian distances respectively.

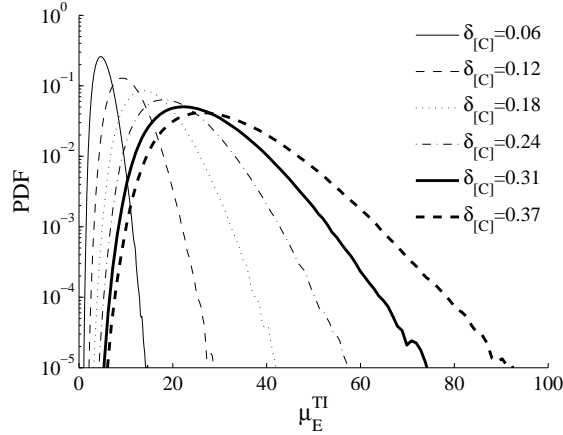


Figure 2: Plot (in semilog scale) of the p.d.f. of μ_E^{TI} for different values of $\delta_{[C]}$.

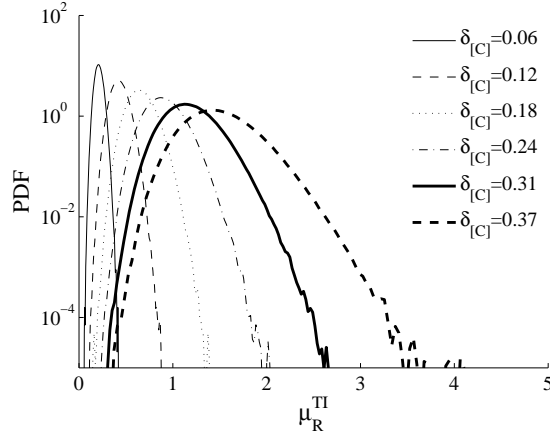


Figure 3: Plot (in semilog scale) of the p.d.f. of μ_R^{TI} for different values of $\delta_{[C]}$.

It is readily seen that both the mean distance to \mathcal{C}^{TI} and the level of statistical fluctuations increase together with dispersion parameter $\delta_{[C]}$, no matter the distance that is used. These characteristics can also be deduced

from Figs. 4 and 5, wherein the functions $\delta_{[C]} \mapsto E\{\mu^{TI}\}$ and $\delta_{[C]} \mapsto \text{Std}\{\mu^{TI}\}$ are plotted (Std denoting the standard deviation).

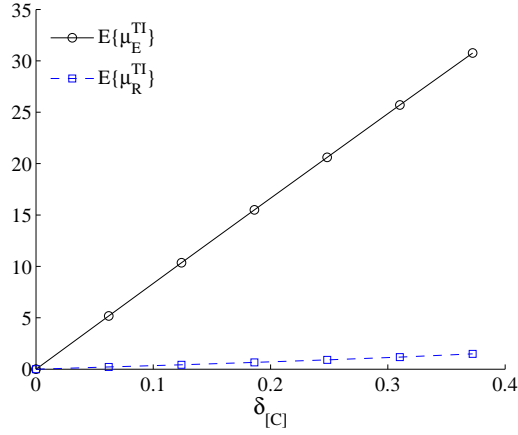


Figure 4: Evolution of the mean value of the stochastic measure of anisotropy, as a function of dispersion parameter $\delta_{[C]}$.

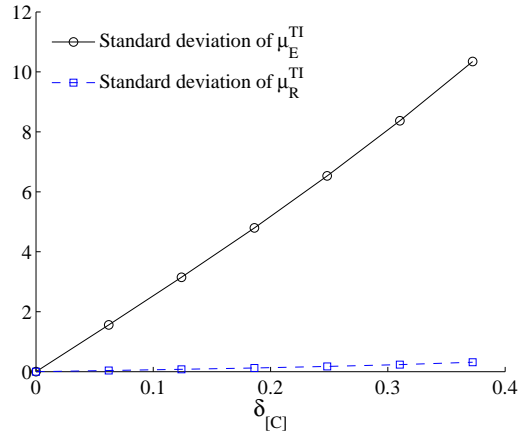


Figure 5: Evolution of the standard deviation of the stochastic measure of anisotropy, as a function of dispersion parameter $\delta_{[C]}$.

Consequently, as soon the level of statistical fluctuations of the random elasticity tensor (which is an intrinsic property resulting from the randomness in the local topology of the microstructure, as well as from local stochastic fluctuations in the mechanical properties of the constituents) is

fixed, there is no way, working in SE^+ , to specify either the mean value or the standard deviation of the stochastic anisotropy measure μ^{TI} . Before addressing such an issue further, let us briefly discuss an interpretation of the above phenomena.

A tremendous amount of work has been devoted to the classification [14] [8] [22] [51] and characterization (see [11] [3] [31] and the references therein, for instance) of material symmetries. Among the developed methodologies, the eigensystem-based characterization [42] [4] turns out to be especially suitable for the present work, since it allows for an interpretation of the above properties within the framework of random matrix theory. Such an approach states necessary and sufficient conditions for an elasticity tensor to belong to a given material symmetry class, in terms of properties for both the eigenvalues and the related eigenspaces. In particular, it was shown that the algebraic multiplicities of the eigenvalues provides relevant information, since any transversely isotropic tensor has two eigenvalues of multiplicity one and two eigenvalues of multiplicity two for instance. The nominal matrix $[\underline{C}]$, whose material symmetry is very close to transverse isotropy, clearly exemplifies this point, since it has two pairs of very closed eigenvalues ($\{9.5498, 9.5709\}$ and $\{14.0102, 14.0359\}$) and two eigenvalues that are separated from the others ($\{10.5417, 182.7925\}$). A necessary condition for a random matrix $[\mathbf{C}]$ with mean value $[\underline{C}]$ to stay close to \mathcal{C}^{TI} is, therefore, that its (ordered) random eigenvalues are such that $\lambda_1 \simeq \lambda_2$ and $\lambda_4 \simeq \lambda_5$ almost surely, regardless of whether high statistical fluctuations are considered. However, such a property is impossible, due to the phenomenon of level repulsion that is well-known from random matrix theory [32] (see also [46] for a numerical illustration in SE^+). This mathematical fact can be understood more intuitively by characterizing the p.d.f. of the random eigenvalues, as the overall level of fluctuations of $[\mathbf{C}]$ (i.e. $\delta_{[\mathbf{C}]}$) increases. Fig. 6 displays the graph of the p.d.f. of the five first random eigenvalues, for three different levels of fluctuations. As expected from the discussion above, the p.d.f. of random eigenvalues λ_1 and λ_2 (resp. λ_4 and λ_5) are pretty close from one another for small levels of fluctuations, but progressively split for increasing values of $\delta_{[\mathbf{C}]}$. This fundamental behavior of the random eigenvalues not only allows for an interpretation of the trends that are observed in Figs. 2 and 3, but also provides an insight about which information may be considered in the formulation of the MaxEnt principle while attempting to constraint the stochastic anisotropy measure μ^{TI} . More specifically, it can be deduced that the latter may be constrained, in a way to be defined, by tailoring the level of fluctuations of the stochastic eigenvalues that define, according to the eigensystem characterization of material

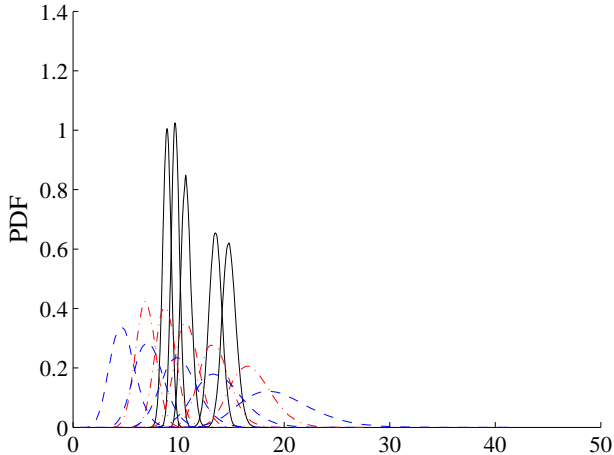


Figure 6: Plot of the p.d.f. of $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ and λ_5 . Black solid line: $\delta_{[\mathbf{C}]} = 0.06$; Red dash-dot line: $\delta_{[\mathbf{C}]} = 0.18$; Blue dashed line: $\delta_{[\mathbf{C}]} = 0.31$.

symmetries, the considered class of symmetry (here, \mathcal{C}^{TI}). Following Section 3.1, the construction of an associated probabilistic model necessitates the definition of an additional constraint (and hence, leads to the definition of a new random matrix ensemble), and is presented below in Section 3.3.

3.3. Ensemble SE^{++} of symmetric positive-definite real random matrices with constrained eigenvalues

3.3.1. Probabilistic model

Let $\mathcal{I}^{sym} = \{i_1, \dots, i_d\}$ be the index set of positive integers gathering the ranks of the random eigenvalues defining \mathcal{C}^{sym} . For the application retained in this paper (see Section 3.2.2), we consider $\mathcal{I}^{TI} = \{1, 2, 4, 5\}$ for instance. In addition to constraints (13), (15) and (18), let us consider, for the MaxEnt procedure, the d following constraints:

$$\mathbb{E} \left\{ \left(\underline{\varphi}^{i_k \top} [\mathbf{C}] \underline{\varphi}^{i_k} \right)^2 \right\} = s_k^2 \lambda_{i_k}^2, \quad k = 1, \dots, d, \quad (23)$$

wherein $\{(\lambda_{i_k}, \underline{\varphi}^{i_k})\}_{k=1}^d$ is the set of eigenpairs (eigenvalues and orthonormal eigenvectors) of the mean matrix $[\mathbf{C}]$ corresponding to the constrained eigenvalues and $\{s_k\}_{k=1}^d$ is a set of scalar parameters allowing, in view of Eq. (23), the variances of random eigenvalues $\{\lambda_{i_k}\}_{k=1}^d$ to be controlled. Introducing the Lagrange multipliers $m \in \mathbb{R}$, $(\ell - 1) \in \mathbb{R}$, $[\widetilde{M}] \in \mathbb{M}_d^S(\mathbb{R})$ and

$\{\tilde{t}_k \in \mathbb{R}^+\}_{k=1}^d$ associated with constraints (13), (15), (18) and (23), it can be deduced that the probability density function $[C] \mapsto p_{[\mathbf{C}]}([C])$ (estimated by the MaxEnt principle) writes:

$$p_{[\mathbf{C}]}([C]) = k_1 (\det([C]))^{\ell-1} \times \exp\left(-\text{tr}\left([\tilde{M}]^T [C]\right) - \sum_{k=1}^d \tilde{t}_k \left(\underline{\varphi}^{\text{ik}T} [C] \underline{\varphi}^{\text{ik}}\right)^2\right), \quad (24)$$

in which $k_1 = \exp\{-m\}$ is a normalization constant.

The ensemble SE^{++} is the set of all $\mathbb{M}_n^+(\mathbb{R})$ -valued random matrices, defined on $(\Theta, \mathcal{F}, \mathcal{P})$, the probability density function of which is given, taking into account the information synthesized by Eqs. (13), (15), (18) and (23), by Eq. (24). The construction of SE^{++} has been addressed in [33], while numerical investigations about the use of this ensemble in the framework of anisotropic linear elasticity have shown that [17]:

- Parameter $\ell \in \mathbb{R}^+$ mainly controls the overall level of statistical fluctuations of random elasticity matrix $[\mathbf{C}]$. More specifically, it can be shown that the level of statistical fluctuations for random elasticity matrix $[\mathbf{C}]$ (as measured by parameter $\delta_{[\mathbf{C}]}$) tends to 0 as ℓ goes to infinity, while non negligible fluctuations are typically observed for $\ell \leq 100$ (note that this value may change depending on the application though).
- Normalized parameters $t_k = \tilde{t}_k \lambda_{i_k}^2 \in \mathbb{R}^+$ allows for a reduction of the variances of the associated random eigenvalues (for sufficiently large values of t_i) and have a negligible effect on $\delta_{[\mathbf{C}]}$.
- Matrix $[\tilde{M}]$ can be expressed in terms of ℓ and $\{t_i\}_{i \in \mathcal{I}^{sym}}$ and consequently, may not be considered as a model parameter.

It should be noted that setting all parameters t_k to a null value allows us to recover ensemble $SE^+ \subset SE^{++}$. In the next section, we exemplify how the parametrization offered in SE^{++} provides some freedom in prescribing the behavior of the stochastic anisotropy measure introduced previously.

3.3.2. Parametric study on stochastic anisotropy measure μ for $[\mathbf{C}] \in SE^{++}$

Let us consider the mean model defined by Eq. (22) and let $\ell = 20$. Consequently, following Section 3.3, the level of statistical fluctuations of random elasticity matrix $[\mathbf{C}]$ is almost fixed. Since we are interested in prescribing, in some sense, stochastic anisotropy measure μ_R^{TI} , the variances of random eigenvalues 1, 2, 4 and 5 have to be constrained. In order to make

the interpretation of results easier, we set $t_k = t$ for all k in $\{1, \dots, d\}$. The p.d.f. of random variable μ_R^{TI} is displayed in Fig. 7, for several values of parameter t .

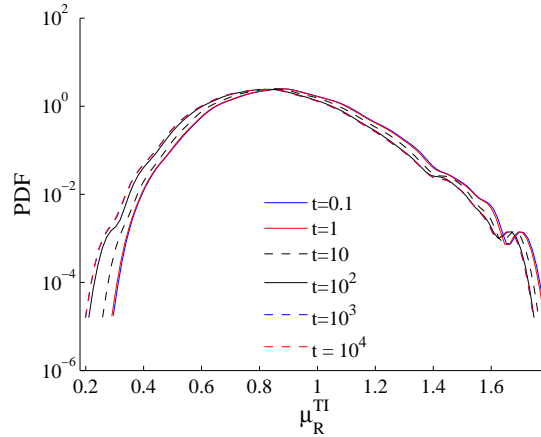


Figure 7: Plot (in semilog scale) of the p.d.f. of μ_R^{TI} for $\ell = 20$ and different values of parameter t .

Two conclusions can be drawn from this figure and are note worthy. First of all, it is readily seen that parameter t allows for the prescription of the behavior of the stochastic anisotropy measure. More precisely, setting a large value of t allows us to reduce the mean distance $E\{\mu_R^{TI}\}$, while the level of fluctuations is weakly affected. Secondly, it is seen that $t \rightarrow 0$ and $t \rightarrow +\infty$ correspond to two limit behaviors. The former allows us to recover SE^+ (as mentioned above), and the latter yields the smallest mean value of μ_R^{TI} that can be reached for given value of ℓ (or equivalently, of $\delta_{[C]}$). The limited range over which the behavior can be prescribed is a consequence of the repulsion phenomena and the fact that the eigenvalues of $[C]$ all remain stochastic (in other words, we can not prescribed a null variance for a given eigenvalue). All these facts are illustrated in Figs. 8 and 9, wherein the mean value and standard deviation of μ_R^{TI} are plotted as a function of parameter t , respectively.

3.4. Comments regarding other random matrix ensembles

Two other random matrix ensembles, defined having recourse to the same methodology (that is to say, within the framework of information theory and making use of the MaxEnt principle) have been introduced in the literature. A random matrix ensemble, derived considering a deterministic boundedness

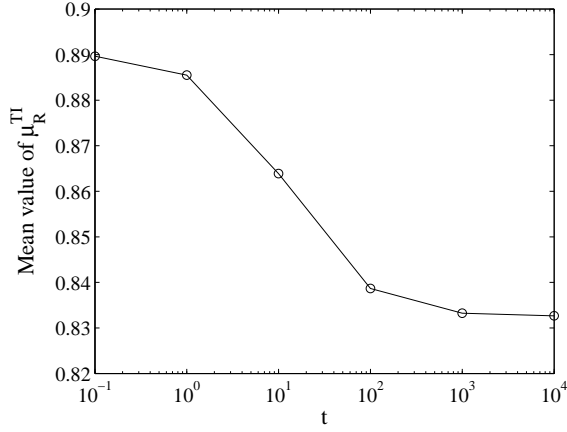


Figure 8: Plot (in semilog scale) of mapping $t \mapsto E\{\mu_R^{TI}\}$ for $\ell = 20$.

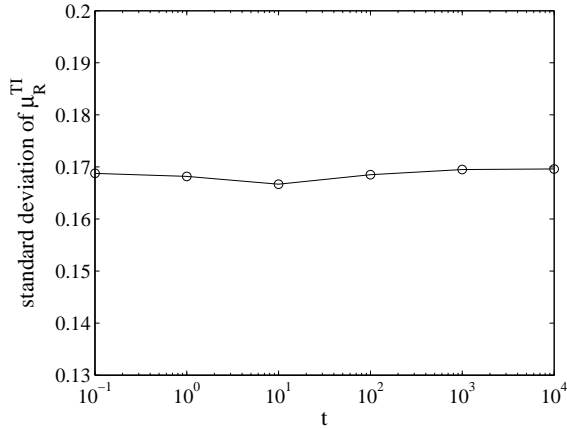


Figure 9: Plot (in semilog scale) of mapping $t \mapsto \text{Std}\{\mu_R^{TI}\}$ for $\ell = 20$.

constraint on $[\mathbf{C}]$ (defined using an approximation based on Huet's partition theorem [21]), has been proposed in [12] (see [16] for similar considerations in case of random fields). Since no specific constraint related to anisotropy is taken into account, random matrices in this ensemble exhibit the same behavior as the ones in SE^+ , so that there would not be any benefit to discuss this probabilistic model in the context of anisotropy modeling further. Ta and his coworkers proposed a refinement of the probabilistic model derived in [46] by introducing, through a modification of the algebraic definition of $[\mathbf{C}]$, a new parameter controlling the anisotropy index apart from the level

of fluctuations [49]. However, this flexibility is restricted, by construction, to the prescription of anisotropy with respect to \mathcal{C}^{Iso} .

4. Application: inverse identification based on stochastic anisotropy measure

In this final section, we assume that N^{exp} experimental realizations of $[\mathbf{C}]$ are available and address the identification of the probabilistic model for $[\mathbf{C}] \in SE^{++}$ (with $n = 6$). For this purpose, we first propose a possible methodology in Section 4.1 and exemplify the approach in Section 4.2.

4.1. Methodology

Without loss of generality, let us consider the Riemannian metric and let $\{\mu_j^{exp}\}_{j=1}^{N^{exp}}$ be the independent experimental realizations of μ_R^{TI} that are computed from the experimental realizations $\{[C_j^{exp}]\}_{j=1}^{N^{exp}}$ of $[\mathbf{C}]$ using Eq. (10):

$$\mu_j^{exp} = d_R \left([C_j^{exp}], [C_j^{sym}] \right), \quad j = 1, \dots, N^{exp}, \quad (25)$$

wherein the projection $[C_j^{sym}] = \mathbf{P}_E^{sym} \{[C_j^{exp}]\}$ (see Section 2.4) is computed using the Euclidean projection technique introduced in Section 2.3 (see [35] for details).

Let w be a structure gathering all the parameters of $[\mathbf{C}] \in SE^{++}$, such that $w(1) = [\mathcal{C}]$, $w(2) = \ell$ and $w(3) = \{t_1, t_2, t_3, t_4, t_5, t_6\}$. Let $\mu \mapsto p_{\mu_R^{TI}}(\mu; w)$ be the p.d.f. of μ_R^{TI} , defined by Eq. (10) and estimated using the kernel density estimation method [5] with N^{sim} independent realizations $\{[C_j^{sim}]\}_{j=1}^{N^{sim}}$ of $[\mathbf{C}]$ in SE^{++} (with parameters w) provided by the random generator:

$$p_{\mu_R^{TI}}(\mu; w) \simeq \frac{1}{hN^{sim}} \sum_{i=1}^{N^{sim}} K \left(\frac{\mu - \mu_j^{sim}(w)}{h} \right), \quad (26)$$

wherein h is the bandwidth, $u \mapsto K(u)$ is the kernel function (which is symmetric and whose integral over its support is equal to 1) and $\mu_j^{sim}(w)$ is the realization of μ_R^{TI} estimated (as mentioned above) from realization $[C_j^{sim}]$ and which depends, therefore, on structure w . In this study, a Gaussian kernel is used and smoothing parameter h is then chosen following the so-called Silverman's rule of thumb, $h \simeq 1.06 \text{ Std}(\mu_R^{TI}) N^{sim-1/5}$ ($\text{Std}(\mu_R^{TI})$ being the usual statistical estimator for the standard deviation of random variable μ_R^{TI}). Note that for notational convenience, we did not explicitly

distinguish the probability density function $p_{\mu_R^{TI}}$ from its kernel density estimate.

A natural and probabilistically sound method to estimate an optimal set w^{opt} of parameters for the stochastic model (constructed having recourse to the MaxEnt procedure) is the maximum likelihood method (see [39] for instance), according to which w^{opt} is defined as:

$$w^{opt} = \arg \max_{\mathcal{C}_{ad}^{likelihood}} \mathcal{L}(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; w), \quad (27)$$

in which the likelihood function is given by:

$$\mathcal{L}(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; w) = \prod_{j=1}^{N^{exp}} p_{\mu_R^{TI}}(\mu_j^{exp}; w), \quad (28)$$

and the admissible space $\mathcal{C}_{ad}^{likelihood}$ is written, by an abuse of notation, as:

$$\mathcal{C}_{ad}^{likelihood} = \mathbb{M}_6^+(\mathbb{R}) \times \mathbb{R}^+ \times \mathbb{R}^{+6}. \quad (29)$$

Note that for numerical stability, we may alternately consider maximizing the log-likelihood function $\mathcal{L}^* = \log_{10}(\mathcal{L})$. Clearly, solving such an optimization problem over $\mathcal{C}_{ad}^{likelihood}$ is a very challenging task and consequently, we propose tackling this difficulty in three steps.

In a first step, we may identify prior estimates for parameters $[\underline{C}]$ and ℓ , setting arbitrary small values for $\{t_i\}_{i=1}^6$. In others words, the identification may be initiated by working in SE^+ only, allowing for a prior calibration of the mean model and dispersion parameter. Two cases may then be distinguished. If the number of experimental realizations N^{exp} is large enough, a prior value $[\underline{C}^{prior}]$ of $[\underline{C}]$ can be obtained from the usual mathematical statistics [44], while ℓ^{prior} may be determined, either from the maximum likelihood principle (using, for instance, a random search over the range defined by Eq. (21)) or using a statistical estimate (see Eq. (20)). However, such a database is seldom available in practice, so that the convergence for the statistical estimate $[\widehat{C}]$ of $[\underline{C}]$ may not be reached. Subsequently, we may identify both $[\underline{C}^{prior}]$ and ℓ^{prior} solving Eq. (27). In this case, a random search strategy can still be retained, searching in the neighborhood of $[\widehat{C}]$ for $[\underline{C}^{prior}]$ and having recourse to the boundedness constraint (21) for ℓ^{prior} . It is worth pointing out at this stage that the positive-definiteness of $[\underline{C}^{prior}]$ must be preserved, which can be achieved at least in three ways. A first method consists in assuming that $[\underline{C}^{prior}]$ belongs to a given subset \mathcal{C}^{sym}

and performing the random search on the constants (e.g. engineering constants) parametrizing \mathcal{C}^{sym} , so that the algebraic definition of the elasticity tensor readily ensures that $[\underline{C}^{prior}] \in \mathbb{M}_6^+(\mathbb{R})$. Another strategy is to have recourse to specific semidefinite algorithms that are tailored to perform on $\mathbb{M}_6^+(\mathbb{R})$ [52]. Finally, we may proceed as follows. Let $[\underline{C}^{trial}]$ be a candidate for $[\underline{C}^{prior}]$, the definition of which is sought in $\mathbb{M}_6^+(\mathbb{R})$. Let $[\widehat{\underline{L}}]$ be the upper triangular matrix such that $[\widehat{\underline{C}}] = [\widehat{\underline{L}}]^T[\widehat{\underline{L}}]$ (Cholesky decomposition), and let $[\underline{L}^{trial}]$ be an upper triangular matrix defined for $i \leq j$ as:

$$[\underline{L}^{trial}]_{ij} = (1 + \nu(\epsilon_{ij}))[\widehat{\underline{L}}]_{ij}, \quad (30)$$

in which $\nu(\epsilon_{ij})$ is a scalar random variable that is uniformly distributed over $[-\epsilon_{ij}, \epsilon_{ij}]$. In practice, the value of parameter ϵ_{ij} (which controls the size of the hypercube over which the random search is performed) must be sufficiently (but not too) large for the solving algorithm to move from initial guess $[\widehat{\underline{C}}]$ (typical values may range from 0.1 to 0.3). The candidate $[\underline{C}^{trial}]$ for $[\underline{C}^{prior}]$ can then be defined as $[\underline{C}^{trial}] = [\underline{L}^{trial}]^T[\underline{L}^{trial}]$ and belongs to $\mathbb{M}_6^+(\mathbb{R})$ almost surely.

In the second step, we fix the values of $w(1)$ and $w(2)$ to the prior estimates identified in step one, and look for a prior estimate of $w(3)$ (searching hence a solution in SE^{++}). Although the identification problem can be solved in R^{+6} , it is likely that in most practical situations, some information about the material symmetries can be inferred from a (partial) knowledge of the microstructure. In this case, we may take advantage of the definition of \mathcal{C}^{sym} with respect to eigenvalue-based characterization, setting $t_i = t$ for $i \in \mathcal{I}^{sym}$ and $t_i = 0$ otherwise. Consequently, the dimension of the optimization problem may be significantly reduced and a prior value t^{prior} of parameter t may be obtained as:

$$t^{prior} = \arg \max_{\mathbb{R}^+} \mathcal{L}^*(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; [\underline{C}^{prior}], \ell^{prior}, t). \quad (31)$$

Eq. (31) can be solved in a trivial manner, characterizing the function $t \mapsto \mathcal{L}^*(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; [\underline{C}^{prior}], \ell^{prior}, t)$ on \mathbb{R}^+ .

In the last step, an optimal solution is finally identified by the trial method in the neighborhood of the prior estimates obtained in the previous steps.

4.2. Example

In order to exemplify the previous methodology, a database has been generated numerically, considering the mean model $[\underline{C}]$ defined by Eq. (22),

$\ell = 50$, $t_1 = t_2 = t_4 = t_5 = 100$ and $t_3 = t_6 = 0$. From these data, $N^{exp} = 20$ realizations have been arbitrarily extracted and are used for the calibration of the probabilistic model (in SE^{++}).

For this purpose, the trial method has been used to solve the maximum likelihood optimization problem, considering 1000 iterations for step 1 (setting $\epsilon_{ij} = 0.2$ for $i \leq j$; see Eq. (30)) and 100 iterations for the refinement around the prior estimates (step 3). Whenever required, the p.d.f. of μ_R^{TI} has been estimated using 10 000 realizations of $[\mathbf{C}]$. Step 2 has been performed considering a parametrization of \mathcal{C}^{TI} and Fig. 10 displays the graph of the log-likelihood function $t \mapsto \mathcal{L}^*(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; [\underline{\mathbf{C}}^{prior}], \ell^{prior}, t)$. It is seen that \mathcal{L}^* is almost constant for $t \geq 100$, which could have been expected in view of the (limit) behavior exhibited by the p.d.f. of μ_R^{TI} as $t \rightarrow +\infty$ (see Section 3.3.2).

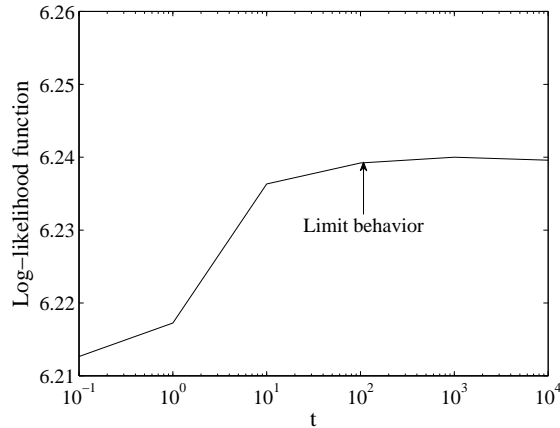


Figure 10: Plot (in semilog scale) of $t \mapsto \mathcal{L}^*(\mu_1^{exp}, \dots, \mu_{N^{exp}}^{exp}; [\underline{\mathbf{C}}^{prior}], \ell^{prior}, t)$.

Consequently, any value $t \geq 100$ can be selected as a prior estimate t^{prior} and we recommend retaining the smallest admissible value in order to ensure the numerical stability of the random generator. Finally, a comparison between the target (black thin line) p.d.f. of μ_R^{TI} and the one obtained from simulations (using the identified parameters; red thick line) is depicted, in semilog scale, in Fig. 11. It is readily seen that the two p.d.f. compare pretty well and therefore, the maximum likelihood principle, applied to the stochastic anisotropy measure, allows for an identification of the probabilistic model. The latter can then be used to generate independent realizations of the random elasticity matrix $[\mathbf{C}]$ that are consistent, in the mean sense, with a certain stochastic level of anisotropy. For the sake of completeness, it

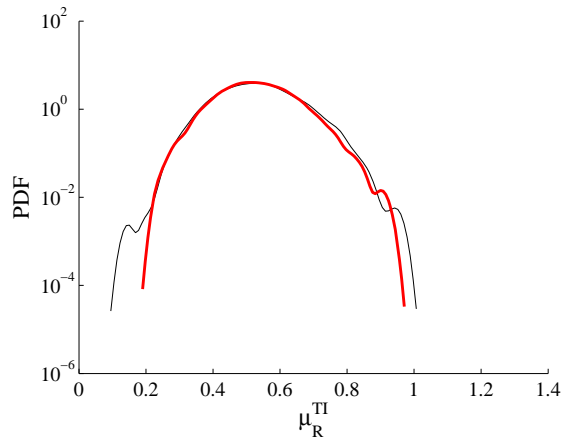


Figure 11: Plot (in semilog scale) of the target (black thin line) and simulated (red thick line) p.d.f. of μ_R^{TI} .

should be pointed out that random field approaches, the derivation of which is based on the use of ensembles SE^+ and SE^{++} , have been proposed in [48] and [18], respectively.

5. Conclusion

In this paper, we have investigated the use of random matrix ensembles for modeling stochastic elasticity tensors exhibiting uncertainties on material symmetries. Such an issue arises in many practical situations, in which the physics of the underlying phenomena that is either computationally or experimentally considered, strongly depends on the elastic anisotropy (e.g. mesoscale wave propagation in heterogeneous solids, such as bones).

For this purpose, we first recalled the concept of distances in the set of fourth-order elasticity tensors, and made use of such derivations to define a stochastic measure of anisotropy μ . The latter can be readily applied to any material symmetry class and allows for a complete probabilistic characterization of anisotropy.

Subsequently, we summarized a methodology that allows, working within the framework of information theory, to derive objective probabilistic models without assuming the probability distributions *a priori*. Two random matrix ensembles (namely SE^+ and SE^{++}), the definition of which has been performed having recourse to the MaxEnt principle, are presented and discussed from a mechanical, rather than mathematical, point of view. In particular,

numerical investigations based on the proposed stochastic anisotropy measure show that as soon as the overall level of statistical fluctuations $\delta_{[\mathbf{C}]}$ is fixed, ensemble SE^+ does not allow for the prescription of a distribution for μ and therefore, is well adapted to heterogeneous materials that exhibits fully anisotropic fluctuations. This fundamental property is consistent with the eigensystem-based characterization of material symmetries and turns out to be a consequence of the behavior of the random spectrum. The latter further provides a valuable basis for the use of ensemble SE^{++} in case the mean distance to a given material symmetry has to be prescribed.

Finally, we address the identification of the probabilistic model when a few experimental realizations of the elasticity tensor are available. The proposed procedure (which is by no means the only one that could be retained) relies on the use of the maximum likelihood principle, defined with respect to the stochastic anisotropy measure, and can be readily implemented, regardless of the symmetry class under consideration. A simple application of the methodology is provided and demonstrates the relevance of the approach.

Acknowledgements

This research was funded by the French Research Agency (Agence Nationale de la Recherche) under TYCHE contract ANR-2010-BLAN-0904.

References

- [1] V. Arsigny, P. Fillard, X. Pennec, and N. Ayache. Log-Euclidean Metrics for Fast and Simple Calculus on Diffusion Tensors. *Magnetic Resonance in Medicine*, 56:411–421, 2006.
- [2] I. Babuška, R. Tempone, and G. E. Zouraris. Solving elliptic boundary value problems with uncertain coefficients by the finite element method: the stochastic formulation. *Computer Methods in Applied Mechanics and Engineering*, 194(12-16):1251–1294, 2005.
- [3] A. Bóna, I. Bucataru, and M.A. Slawinski. Material symmetries of elasticity tensors. *The Quarterly Journal of Mechanics and Applied Mathematics*, 57(4):584–598, 2004.
- [4] A. Bóna, I. Bucataru, and M.A. Slawinski. Coordinate-free characterization of the symmetry classes of elasticity tensors. *Journal of Elasticity*, 87:109–132, 2007.

- [5] A. W. Bowman and A. Azzalini. *Applied Smoothing Techniques for Data Analysis*. Oxford University Press, 1997.
- [6] J.T. Browaeys and S. Chevrot. Decomposition of the elastic tensor and geophysical applications. *Geophys. J. Int.*, 159:667–678, 2004.
- [7] I. Bucataru and M. A. Slawinski. Invariant properties for finding distance in space of elasticity tensors. *Journal of Elasticity*, 94:97–114, 2009.
- [8] P. Chadwick, M. Vianello, and S.C. Cowin. A new proof that the number of linear elastic symmetries is eight. *Journal of the Mechanics and Physics of Solids*, 49:2471–2492, 2001.
- [9] D.H. Chung and W.R. Buessem. The elastic anisotropy of crystals. *Journal of Applied Physics*, 38(5):2010–2012, 1967.
- [10] T. M. Cover and J. A. Thomas. *Elements of Information Theory*. John Wiley & Sons, New-York, 2006.
- [11] S.C. Cowin and M.M. Mehrabadi. On the identification of material symmetry for anisotropic elastic materials. *The Quarterly Journal of Mechanics and Applied Mathematics*, 40:451–476, 1987.
- [12] S. Das and R. Ghanem. A Bounded Random Matrix Approach for Stochastic Upscaling. *Multiscale Modeling & Simulation*, 8(1):296–325, 2009.
- [13] F.I. Fedorov. *Theory of Elastic Waves in Crystals*. Plenum, New-York, 1968.
- [14] S. Forte and M. Vianello. Symmetry classes for elasticity tensors. *Journal of Elasticity*, 43:81–108, 1996.
- [15] D.C. Gazis, I. Tadjbakhsh, and R.A. Toupin. The elastic tensor of given symmetry nearest to an anisotropic elastic tensor. *Acta Crystallographica*, 16(9):917–922, 1963.
- [16] J. Guilleminot, A. Noshadravan, C. Soize, and R. G. Ghanem. A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures. *Computer Methods in Applied Mechanics and Engineering*, 200:1637–1648, 2011.

- [17] J. Guilleminot and C. Soize. A stochastic model for elasticity tensors with uncertain material symmetries. *International Journal of Solids and Structures*, 47:3121–3130, 2010.
- [18] J. Guilleminot and C. Soize. Non-gaussian positive-definite matrix-valued random fields with constrained eigenvalues: application to random elasticity tensors with uncertain material symmetries. *International Journal of Numerical Methods in Engineering*, 2011. in press (DOI: 10.1002/nme.3212).
- [19] S. Hazanov and C. Huet. Order relationships for boundary condition effect in heterogeneous bodies smaller than the representative volume. *Journal of the Mechanics and Physics of Solids*, 42(12):1995–2011, 1994.
- [20] K. Helbig. *Foundations of Anisotropy for Exploration Seismics*. Handbook of geophysical exploration. Pergamon, 1994.
- [21] C. Huet. Application of variational concepts to size effects in elastic heterogeneous bodies. *Journal of the Mechanics and Physics of Solids*, 38(6):813–841, 1990.
- [22] Y.Z. Huo and G. Del Piero. On the completeness of the crystallographic symmetries in the description of the symmetries of the elasticity tensor. *Journal of Elasticity*, 25:203–246, 1991.
- [23] E. T. Jaynes. Information theory and statistical mechanics. *Physical Review*, 106(4):620–630, 1957.
- [24] E. T. Jaynes. Information theory and statistical mechanics. *Physical Review*, 108(2):171–190, 1957.
- [25] H. K. Kapur, J. N. & Kesavan. *Entropy Optimization Principles with Applications*. Academic Press, San Diego, 1992.
- [26] M. Kochetov and M.A. Slawinski. Estimating effective elasticity tensors from Christoffel equations. *Geophysics*, 74(5):WB67–WB73, 2009.
- [27] M. Kochetov and M.A. Slawinski. On obtaining effective orthotropic elasticity tensors. *The Quarterly Journal of Mechanics and Applied Mathematics*, 62(2):149–166, 2009.
- [28] M. Kochetov and M.A. Slawinski. On obtaining effective transversely isotropic elasticity tensors. *Journal of Elasticity*, 94(1):1–13, 2009.

- [29] H. Ledbetter and A. Migliori. A general elastic-anisotropy measure. *Journal of Applied Physics*, 100:063516–1–5, 2006.
- [30] M. M. Mehrabadi, S. C. Cowin, and J. Jaric. Six-dimensional orthogonal tensor representation of the rotation about an axis in three dimensions. *International Journal of Solids and Structures*, 32:439–449, 1995.
- [31] M.M. Mehrabadi and S.C. Cowin. Eigentensors of linear anisotropic elastic materials. *The Quarterly Journal of Mechanics and Applied Mathematics*, 43(1):15–41, 1990.
- [32] M.L. Mehta. *Random Matrices*. Academic Press, New-York, third edition, 2004.
- [33] M. P. Mignolet and C. Soize. Nonparametric stochastic modeling of linear systems with prescribed variance of several natural frequencies. *Probabilistic Engineering Mechanics*, 23:267–278, 2008.
- [34] M. Moakher. On the averaging of symmetric positive-definite tensors. *Journal of Elasticity*, 82:273–296, 2006.
- [35] M. Moakher and A. N. Norris. The closest elastic tensor of arbitrary symmetry to an elasticity tensor of lower symmetry. *Journal of Elasticity*, 85:215–263, 2006.
- [36] A. N. Norris. Elastic moduli approximation of higher symmetry for the acoustical properties of an anisotropic material. *Journal of the Acoustical Society of America*, 119(4):2114–2121, 2006.
- [37] A. N. Norris. The isotropic material closest to a given anisotropic material. *J. Mech. Materials Structures*, 1(2):231–246, 2006.
- [38] M. Ostoja-Starzewski. *Microstructural Randomness and Scaling in Mechanics of Materials*. Chapman & Hall-CRC, 2008.
- [39] A. Papoulis and S. Unnikrishna Pillai. *Probability, Random Variables and Stochastic Processes (4th Ed.)*. McGraw-Hill Higher Education, New-York, 2002.
- [40] S.I. Ranganathan and M. Ostoja-Starzewski. Scaling function, anisotropy and the size of rve in elastic random polycrystals. *Journal of the Mechanics and Physics of Solids*, 56:2773–2791, 2008.

- [41] S.I. Ranganathan and M. Ostoja-Starzewski. Universal elastic anisotropy index. *Physical Review Letters*, 101(5):055504–1–4, 2008.
- [42] J. Rychlewski. On hooke’s law. *Prikl. Mat. Meh.*, 48(3):303–314, 1984.
- [43] K. Sab. On the homogenization and the simulation of random materials. *European Journal of Mechanics A/Solids*, 11(5):585–607, 1992.
- [44] R.J. Serfling. *Approximation Theorems of Mathematical Statistics*. John Wiley & Sons, 1980.
- [45] C. E. Shannon. A mathematical theory of communication. *Bell System Technical Journal*, 27:379–423/623–659, 1948.
- [46] C. Soize. A nonparametric model of random uncertainties on reduced matrix model in structural dynamics. *Probabilistic Engineering Mechanics*, 15(3):277–294, 2000.
- [47] C. Soize. Maximum entropy approach for modeling random uncertainties in transient elastodynamics. *Journal of the Acoustical Society of America*, 109(5):1979–1996, 2001.
- [48] C. Soize. Non-gaussian positive-definite matrix-valued random fields for elliptic stochastic partial differential operators. *Computer Methods in Applied Mechanics and Engineering*, 195:26–64, 2006.
- [49] Q.A. Ta, D. Clouteau, and R. Cottureau. Modeling of random anisotropic elastic media and impact on wave propagation. *European Journal of Computational Mechanics*, 19(1-2-3):241–253, 2010.
- [50] L. Thomsen. Weak elastic anisotropy. *Geophysics*, 51, 1986.
- [51] T. C. T. Ting. Generalized Cowin - Mehrabadi theorems and a direct proof that the number of linear elastic symmetries is eight. *International Journal of Solids and Structures*, 40:7129–7142, 2003.
- [52] L. Vandenberghe and S. Boyd. Semidefinite programming. *SIAM Review*, 38(1):49–95, 1996.
- [53] W. Voigt. *Lehrbuch der Kristallphysik*. B.G. Teubner, Leipzig and Berlin, 1910.
- [54] L.J. Walpole. Fourth-rank tensors of the thirty-two crystal classes: Multiplication tables. *Proceedings of the Royal Society of London A*, 391:149–179, 1984.

- [55] C. Zener. *Elasticity and Anelasticity of Metals*. The University of Chicago Press, Chicago, 1948.