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Stochastic modeling and generation of random fields of elasticity tensors: A unified information-theoretic approach

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In this Note, we present a unified approach to the information-theoretic modeling and simulation of a class of elasticity random fields, for all physical symmetry classes. The new stochastic representation builds upon a Walpole tensor decomposition, which allows the maximum entropy constraints to be decoupled in accordance with the tensor (sub)algebras associated with the class under consideration. In contrast to previous works where the construction was carried out on the scalar-valued Walpole coordinates, the proposed strategy involves both matrix-valued and scalar-valued random fields. This enables, in particular, the construction of a generation algorithm based on a memoryless transformation, hence improving the computational efficiency of the framework. Two applications involving weak symmetries and sampling over spherical and cylindrical geometries are subsequently provided. These numerical experiments are relevant to the modeling of elastic interphases in nanocomposites, as well as to the simulation of spatially dependent wood properties for instance.

1. Preliminaries

1.1. Introduction

The representation of spatially dependent uncertainties is a cornerstone of predictive simulations. Over the past three decades, this has been mostly achieved, in linear elasticity, by resorting to polynomial chaos expansions (see [1] and the references therein for a recent survey) and algebraic decompositions of random fields. The latter type of approaches includes the selection or construction of models in the class of all admissible second-order stochastic representations, where admissibility typically refers to the fulfillment (with probability one) of all the basic properties raised by the mathematical analysis of the stochastic boundary value problem [2,3]. In three-dimensional linear elasticity, such properties include, for instance, the positive-definiteness of the tensor-valued elasticity coefficient [4]. A contribution involving *a priori* model selection can be found, for instance, in [5] for isotropic materials, while construction methodologies building upon information theory [6,7] and the maximization of Shannon's entropy were proposed in [2,8–11], to list a few. Such models will be referred to as information-theoretic ones below, and define admissible subsets – with a minimal modeling bias – of the set of all second-order elasticity random fields. They enable, in particular, fast numerical simulations for physics-based uncertainty propagation and involve low-dimensional hyperparameters, which allows for an identification solving (underdetermined)

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statistical inverse problems. It should be noticed that a recent theoretical work addressing the modeling (through spectral expansions) of the complete set of elasticity tensors for all symmetry classes can be found in [12].

From a modeling standpoint, a key issue is the representation of anisotropy and the evolution of the latter as the elasticity tensor becomes random. Depending on the retained framework, the sought quantity of interest and computational resources, one may consider random fields of elasticity tensors with fluctuations in a given symmetry class (which may be inferred from microstructural information) or in the triclinic class (see [13] for a micromechanics-based discussion). The latter (triclinic) case was first addressed in [2], making use of earlier derivations proposed in [14] for structural dynamics. The model relies on a random matrix formulation that induces triclinic fluctuations and does not allow other symmetry classes to be considered, due the eigenvalue repulsion phenomenon [15]. Similar ideas were then pursued in [9,10], in which a decomposition onto an *ad hoc* tensor basis was used to circumvent this limitation. This approach involves an exponential map that allows one to relax the algebraic constraints generated by the positive-definiteness and symmetry properties of the tensor (in practice, these constraints can raise critical sampling issues for weak symmetries). Additionally, this construction enables efficient random field sampling through the integration of a family of stochastic differential equations.

In this Note, we show that these two constructions (namely, the one based on the random matrix approach and the one involving the tensorial decomposition) can indeed be unified in a rather simple form. This offers two benefits. First of all, the new random field model exhibits closed-form expressions (for some statistical properties) that are inherited from each stochastic representation and facilitate the calibration of the model hyperparameters. Secondly, the sampling algorithm turns out to be very robust and easy to implement. The model and generator are readily applicable, for instance, to the modeling of composite laminates and wood species (these materials being typically considered as orthotropic in an appropriate local or global coordinate system), and to the representation of bone properties (which may be modeled as a transversely isotropic material) in computational biomechanics.

This Note is organized as follows. The section 2 is concerned with the construction of the stochastic representation. The methodology is first outlined in Sec. 2.1. The definition of the probabilistic model is then addressed in the most general setting in Sec. 2.2. Numerical examples are finally provided in Sec. 3.

1.2. Notation

In this paper, deterministic scalars, vectors, second-order and fourth-order tensors are denoted by d, $\boldsymbol{d}$, $[D]$ and $[\![D]\!]$. Let $\langle \cdot, \cdot \rangle$ denote the Euclidean inner product in $\mathbb{R}^3$, with $\langle \boldsymbol{x}, \boldsymbol{y} \rangle := \sum_{i=1}^{3} x_i y_i$ for $(\boldsymbol{x}, \boldsymbol{y}) \in \mathbb{R}^3 \times \mathbb{R}^3$. Let $\mathbb{M}_6^S(\mathbb{R})$ be the set of symmetric real-valued (6×6) matrices. The inner product in $\mathbb{M}_6^S(\mathbb{R})$ is defined as $\ll [U], [V] \gg := \mathrm{Tr}([U][V])$ for any $[U]$ and $[V]$ in $\mathbb{M}_6^S(\mathbb{R})$, and the induced (Frobenius) norm reads as $\|[U]\|_F = \ll [U], [U] \gg^{1/2}$. In addition, let $\mathbb{M}_6^+(\mathbb{R}) \subset \mathbb{M}_6^S(\mathbb{R})$ be the set of symmetric positive-definite real-valued (6×6) matrices. The standard tensor product is denoted by $\otimes$, while the symmetric tensor product between second-order tensors is defined component-wise as: $([U] \boxtimes [V])_{ijkl} := (u_{ik} v_{jl} + u_{il} v_{jk})/2$. Let $[I_s]$ be the identity matrix of size s.

Stochastic scalars, vectors and second-order tensors are denoted by D, $\boldsymbol{D}$ and $[\boldsymbol{D}]$ respectively. The mathematical expectations $\mathbb{E}\{D\}$, $\mathbb{E}\{\boldsymbol{D}\}$ and $\mathbb{E}\{[\boldsymbol{D}]\}$ of random variables D, $\boldsymbol{D}$ and $[\boldsymbol{D}]$ are denoted by $\underline{d}$, $\underline{\boldsymbol{d}}$ and $[\underline{D}]$, respectively. The level of statistical fluctuations exhibited by a random matrix $[\boldsymbol{D}]$ is characterized by the parameter $\delta_{[\boldsymbol{D}]}$ defined as

$$\delta_{[\boldsymbol{D}]} := \left\{ \frac{\mathbb{E}\{\|[\boldsymbol{D}] - [\underline{D}]\|_F^2\}}{\|[\underline{D}]\|_F^2} \right\}^{1/2} \tag{1}$$

Note that when applied to a scalar random variable, the above equation coincides with the standard definition of the coefficient of variation. Finally, c_0 denotes the normalization constant involved in probability density functions. The value of c_0 may therefore change from line to line with no specific statement.

2. Construction of the random field model

2.1. Overview of the methodology

Let $\{[\boldsymbol{C}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ be the $\mathbb{M}$-valued random field of elasticity tensor, with $\mathbb{M} \subseteq \mathbb{M}_6^+(\mathbb{R})$ and $\Omega \subset \mathbb{R}^3$. The modified Voigt representation of fourth-order tensors is considered (see *e.g.*, [16]), and the elasticity field is expressed in a given Cartesian global coordinate system $\mathfrak{R}_g := (O, \boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ (with generic variables $\boldsymbol{x}$ and $\boldsymbol{y}$). Regarding the material symmetry exhibited by the material, two practical situations can be envisioned as follows:

- When the symmetry class under consideration is defined by crystallographic orientations that are independent of $\boldsymbol{x}$ in $\mathfrak{R}_g$ (in which case the symmetry properties hold in the global coordinate system), the state space $\mathbb{M}$ is equal to $\mathbb{M}_6^{\mathrm{sym}}(\mathbb{R})$, where $\mathbb{M}_6^{\mathrm{sym}}(\mathbb{R}) \subset \mathbb{M}_6^+(\mathbb{R})$ is the set of elasticity matrices belonging to the symmetry class parametrized by the aforementioned preferred directions (note that the dependence of $\mathbb{M}_6^{\mathrm{sym}}(\mathbb{R})$ on these directions is not made explicit in order to simplify notations).

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