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Prior representations of random fields for stochastic multiscale modeling*

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Abstract

In this presentation, we will present and discuss some of the most recent contributions to the construction of Prior Algebraic Stochastic Models (PASM) for non-Gaussian tensor-valued random fields. We will first motivate the need of such prior models accounting, not only for mathematical constraints, but also for physically sounded constraints such as local anisotropy. In a second step, we will expose a methodology that aims at constructing such probabilistic models. Computational issues related to random generation will be addressed as well. Finally, we will exemplify both the approach and the algorithms by considering the modeling of mesoscopic elasticity tensor random fields, for which information associated with a stochastic anisotropy measure must be taken into account.

Keywords: random field; MaxEnt principle; Itô stochastic differential equation; probabilistic model

1. Introduction

Multiscale descriptions of physical problems generally involves the representation of the underlying randomness at a given, arbitrary scale. Whereas the theoretical framework of homogenization theories usually refers to the so-called micro-scale and macro-scale, a complete (probabilistic) description of the random elastic microstructure at the former scale is seldom (if ever) achievable in practice. One may then be interested in proceeding alternatively, by considering an intermediate, mesoscopic scale at which the remaining statistical fluctuations of the overall locally-averaged properties reflect the smoothing of the randomness occurring at finest scales. In addition, it is worthwhile to notice that such mesoscale modelling also turns out to be genuinely necessary whenever the classical assumption of scale separation cannot be invoked (which may be the case for some concretes or for some reinforced composite materials). From that point of view, such models can also be used for computing (and for characterizing the convergence towards) the effective deterministic properties associated with the random microstructure, should they be defined; such a convergence analysis can be found in [1] for instance. The stochastic modelling of the aforementioned apparent properties has been quite extensively addressed in the literature of Stochastic Mechanics and Uncertainty Quantification. In particular, it has often been performed, either by assuming the related probability distributions or by having recourse to functional (chaos) representations. Whereas the latter benefit from a well-established mathematical framework and have motivated numerous developments around efficient stochastic solvers (e.g. stochastic spectral methods), their identifications typically require a large amount of experimental data, hence justifying the development of alternative probabilistic representations, such as Prior Algebraic Stochastic Models (PASM). In essence, such representations ensure all the mathematical properties (such as positive-definiteness or some boundedness properties) that must be satisfied by the considered quantities and are constructed in a way that intrinsically

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reduces the modelling bias (see the discussion below). Further, their parameterization is generally restricted to a few parameters (controlling the spatial correlation lengths and the overall level of statistical fluctuations, for instance), hence allowing for an inverse identification with limited data. A methodology of construction for such prior models has been proposed and investigated in [2]. The strategy turns out to be very flexible and can accommodate, in addition to the usual mathematical properties, physically sound constraints (such as those related to stochastic anisotropy, which may be critical in inverse measurements or for a wave propagation analysis; see [3] [4] and the references therein). In this paper, we present some of the latest developments related to these Prior Algebraic Stochastic Models and exemplify the approach by considering the case of mesoscopic elasticity tensor random fields. The paper is organized as follows. First of all, we present, in Section 2, some of the key aspects of the overall methodology. In particular, we introduce the so-called generalized stochastic prior representation and briefly address the issue of random generation. More specifically, we propose a novel algorithm which is based on solving a family of Itô stochastic differential equations (ISDE) and which turns out to be very efficient, regardless of the probabilistic dimension under consideration. We finally exemplify the efficiency of the algorithm in Section 3.

2. Construction of PASM

Let Ω be an open bounded domain in \mathbb{R}^d , $1 \leq d \leq 3$. We denote by $\mathcal{M}^+(\mathbb{R})$ the set of all the $(n \times n)$ symmetric positive-definite real matrices. Let $\{[\mathbf{C}(\mathbf{x})], \mathbf{x} \text{ in } \Omega\}$ be the mesoscopic $\mathcal{M}^+(\mathbb{R})$ -valued random field, the probabilistic model of which has to be constructed. Let $\{\boldsymbol{\Xi}(\mathbf{x}), \mathbf{x} \text{ in } \mathbb{R}^d\}$ and $\{\boldsymbol{\xi}(\mathbf{x}), \mathbf{x} \text{ in } \mathbb{R}^d\}$ be two normalized homogeneous Gaussian random fields with values in \mathbb{R}^N and \mathbb{R}^p respectively, with $p = n(n+1)/2$.

2.1. Methodology of construction

The construction of a PASM is achieved following the methodology detailed in [2]. Therefore, we proceed in two steps:

- We first define a set of homogeneous Gaussian normalized random fields, which are referred to as the stochastic germs. These random fields are specifically used within the random generation procedure (see below) and allows for spatial dependencies to be introduced.
- Secondly, we prescribe, through a particular algebraic decomposition of $[\mathbf{C}(\mathbf{x})]$ at any point \mathbf{x} of Ω , the family of first order marginal distributions for the random field $\{[\mathbf{C}(\mathbf{x})], \mathbf{x} \text{ in } \Omega\}$. Specifically, such a prior decomposition involves measurable deterministic mappings acting on the aforementioned stochastic germs, hence inducing spatial correlations in the probabilistic model.

It should be noticed at this stage that the prior decomposition is not designed in order to prescribe a given correlation structure on random field $\{[\mathbf{C}(\mathbf{x})], \mathbf{x} \text{ in } \Omega\}$, and that the correlation functions induced by such a construction, while not known a priori, can be set up having recourse to an inverse analysis.

2.2. Generalized probabilistic representation

For all \mathbf{x} in Ω , we decompose the random matrix $[\mathbf{C}(\mathbf{x})]$ as follows:

$$[\mathbf{C}(\mathbf{x})] = [\mathbf{L}(\mathbf{x})] [\mathbf{G}(\mathbf{x})] [\mathbf{L}(\mathbf{x})], \tag{1}$$

where $\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \text{ in } \Omega\}$ is assumed to belong to the class SFG+ of non-Gaussian positive-definite matrix-valued random fields defined in [2] and basically acts as an anisotropic germ in the representation of the mesoscale random field. It follows from [2] that $[\mathbf{G}(\mathbf{x})]$ can be written as

$$[\mathbf{G}(\mathbf{x})] = [\mathbf{K}(\mathbf{x})]^T [\mathbf{K}(\mathbf{x})], \quad (2)$$

for all \mathbf{x} in Ω , where $[\mathbf{K}(\mathbf{x})]$ is a upper-triangular random matrix such that:

$$[\mathbf{K}(\mathbf{x})] = T(\{\boldsymbol{\xi}(\mathbf{x})\}), \quad (3)$$

with T a non-linear measurable deterministic mapping (see [2] for details about its construction and its explicit form, as well as for the derivations of the associated probability laws). In Eq. (1), the random field $\{[\mathbf{L}(\mathbf{x})], \mathbf{x}$ in $\Omega\}$ is defined as the unique positive-definite square root of a random field, denoted by $\{[\mathbf{M}(\mathbf{x})], \mathbf{x}$ in $\Omega\}$, which takes its values in the subset $\mathcal{M}^{inv}(\mathbb{R}) \subset \mathcal{M}^+(\mathbb{R})$ of matrices exhibiting some $SO(n)$ -invariance properties:

$$[\mathbf{L}(\mathbf{x})] = [\mathbf{M}(\mathbf{x})]^{1/2} \text{ for all } \mathbf{x} \text{ in } \Omega. \quad (4)$$

Within the context of linear elasticity, the set $\mathcal{M}^{inv}(\mathbb{R})$ can readily be identified with a set of elasticity matrices exhibiting some given material symmetries (e.g. isotropy or transverse isotropy). From a practical perspective, the generalized probabilistic representation defined by Eq. (1) allows the level of stochastic anisotropy to be controlled apart from the overall level of statistical fluctuations (see [5] for an illustration in the isotropic case; see [3] [4] for the generalization to all symmetry classes and algorithmic details).

In order to construct the probabilistic model for random matrix $[\mathbf{M}(\mathbf{x})]$, we further introduce the tensor decomposition

$$[\mathbf{M}(\mathbf{x})] = \sum_{i=1..N} M_i(\mathbf{x}) [E_i], \quad (5)$$

in which the set of deterministic matrices $[E_1], \dots, [E_N]$ is a basis of $\mathcal{M}^{inv}(\mathbb{R})$. We then construct the explicit form of the probability density function (p.d.f.) for the vector-valued random variable $\mathbf{M}(\mathbf{x}) = (M_1(\mathbf{x}), \dots, M_N(\mathbf{x}))$ by invoking the information theory and more specifically, by having recourse to the maximum entropy principle (MaxEnt) [6]. Note that $\mathbf{M}(\mathbf{x})$ takes its values in a given subset S of \mathbb{R}^N , the definition of which ensures that the random matrix $[\mathbf{M}(\mathbf{x})]$ defined by Eq. (5) is positive-definite almost surely and yields some specific constraints in the generation procedure. The constraints that are integrated (in addition to the normalization condition) within the maximum entropy formulation are given by:

$$E\{\mathbf{M}(\mathbf{x})\} = \underline{\mathbf{M}}, \quad (6)$$

$$E\{\log(\det(\sum_{i=1..N} M_i(\mathbf{x}) [E_i]))\} = \nu, \quad |\nu| < +\infty, \quad (7)$$

wherein E denotes the mathematical expectation. The MaxEnt-induced p.d.f. for random vector $\mathbf{M}(\mathbf{x})$ then involves a set of Lagrange multipliers whose numerical values can be determined by solving an optimization problem (see [3] for the case of transverse isotropy). Unlike the anisotropic germ $\{[\mathbf{G}(\mathbf{x})], \mathbf{x}$ in $\Omega\}$, the random field $\{[\mathbf{M}(\mathbf{x})], \mathbf{x}$ in $\Omega\}$ cannot be expressed in terms of a vector-valued Gaussian random field, at least in a way that turns out to be efficient from a computational standpoint. In order to tackle this issue, a new random generation procedure is then proposed and defined below.

The numerical strategy essentially builds on [7] and is based upon solving a family of Itô Stochastic Differential Equations that is indexed by Ω . A cornerstone of the method thus consists in introducing a family $\{W_{\mathbf{x}}(r), r \geq 0\}_{\mathbf{x}}$ of normalized Wiener processes indexed by Ω , such that for all $0 \leq s < r$ and for all \mathbf{x} in Ω ,

$$\int_s^r dW_{\mathbf{x}} = \sqrt{r-s} \Xi^{(rs)}(\mathbf{x}) \quad (8)$$

where $\mathbf{x} \mapsto \mathbf{\Xi}^{(rs)}(\mathbf{x})$ is an independent realization of the Gaussian random field $\{\mathbf{\Xi}(\mathbf{x}), \mathbf{x} \text{ in } \mathbb{R}^d\}$. Owing to the convergence towards the stationary solution at all points of domain Ω (which has to be thoroughly characterized), such a strategy does generate spatial dependencies that are worth taking into account and which cannot be determined beforehand. Note that such a random generator can be readily applied to any vector-valued random field whose family of first-order marginal probability distributions is induced by the maximum entropy approach. In this work, the conservative part of each ISDE is discretized by using a symplectic Störmer-Verlet scheme, which is found to converge much faster than an explicit Euler scheme for the investigated cases. The reader is referred to [4] for the mathematical background and for further details about this algorithm. In the next section, we illustrate the efficiency of the proposed numerical strategy.

3. Application

3.1. Description

In this application, we consider the case where $\mathcal{M}^{inv}(\mathbb{R})$ corresponds to the set of elasticity matrices exhibiting isotropy. Consequently, one has $\mathbf{M}(\mathbf{x}) = (k(\mathbf{x}), \mu(\mathbf{x}))$, where $\{k(\mathbf{x}), \mathbf{x} \text{ in } \Omega\}$ and $\{\mu(\mathbf{x}), \mathbf{x} \text{ in } \Omega\}$ are the bulk modulus and shear modulus random fields, respectively. It can then be shown, through the MaxEnt principle under the constraints stated by Eqs. (6-7), that these random fields are mutually independent and exhibit Gamma first-order marginal p.d.f. [4] [5]. Although this case is of limited interest in terms of random generation algorithms, since the mapping between $\{\mathbf{M}(\mathbf{x}), \mathbf{x} \text{ in } \Omega\}$ and $\{\mathbf{\Xi}(\mathbf{x}), \mathbf{x} \text{ in } \mathbb{R}^d\}$ can be straightforwardly defined through a isoprobabilistic transformation, it exhibits a reference solution and is therefore used below to demonstrate the efficiency of the approach.

3.2. Results

Figs. (1) and (2) show the comparison, for the two random moduli, between the first-order marginal p.d.f. estimated using the proposed approach (dashed line) and the reference solution (solid line).

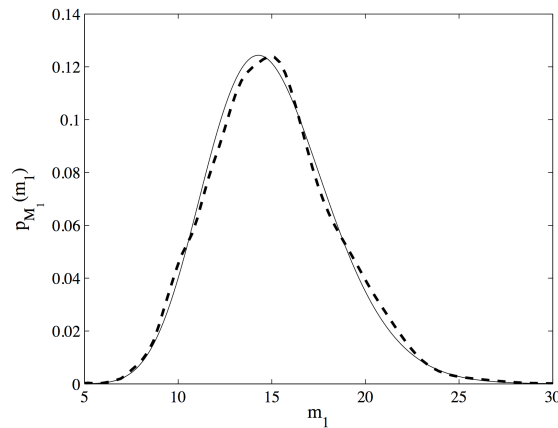


Fig. (1) comparison between the reference solution (solid line) and the ISDE-based estimation (dashed line) for the random bulk modulus.

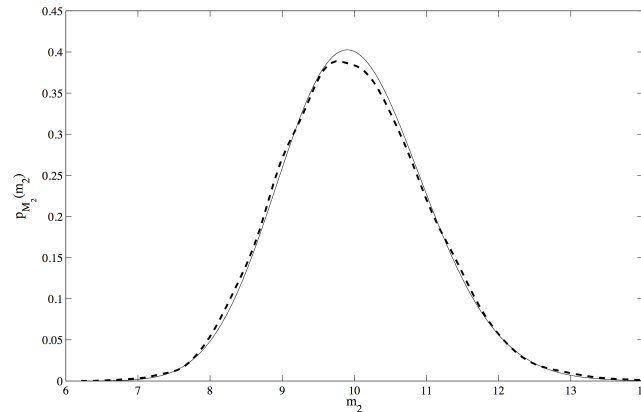


Fig. (2) comparison between the reference solution (solid line) and the ISDE-based estimation (dashed line) for the random shear modulus.

In both cases, it is seen that the two p.d.f. match very well, hence demonstrating the relevance of the random generation procedure (see [4] for similar results in the case of random transversely isotropic elasticity matrices).

4. Conclusion

This paper is devoted to the construction of a generalized Prior Algebraic Stochastic Models (PASM) for non-Gaussian tensor-valued random fields. In a first step, we have recalled the MaxEnt-based methodology of construction and have presented the generalized prior representation. Some computational issues related to the construction of a random generator have been discussed as well. Finally, the algorithm is exemplified by considering the modelling of a.s. isotropic elasticity tensor random fields.

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