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.

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. Subsequently, one may be interested in considering an intermediate, mesoscopic scale at which the remaining statistical fluctuations reflect the smoothing of the randomness occurring at finest scales. In addition, one should note 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; see [1] for an illustration. 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 type of probability distributions or by having recourse to functional (chaos) representations. The latter benefit from a well-established mathematical framework and have motivated numerous developments around efficient stochastic solvers (e.g. stochastic spectral methods). However, their identifications typically

*Preprint version (to appear in Procedia IUTAM: IUTAM Symposium on Multiscale Problems in Stochastic Mechanics 2012).

require a large amount of experimental data, hence justifying the development of alternative probabilistic representations, such as Prior Algebraic Stochastic Models (PASM). 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 intended to reduce the modeling bias. 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 investigated in [2]. Besides some important theoretical issues (related for instance to the ellipticity condition) and a few technicalities, the strategy is essentially similar to the approach which is commonly pursued in the analysis and generation of non-Gaussian stochastic processes. It 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] [5] [6] [7] 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 [8]. 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 the PASM

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

2.1 Methodology of construction

The construction of a PASM is achieved following a methodology similar to that pursued in [2]. In essence, we proceed in two steps:

- We first define a set of homogeneous Gaussian normalized random fields, which are referred to as the stochastic germs and which are used for the random generation procedure.
- Secondly, we prescribe, through a particular algebraic decomposition of $[\boldsymbol{C}(\boldsymbol{x})]$ at any point $\boldsymbol{x}$ of Ω, the family of first order marginal distributions for the random field $\{[\boldsymbol{C}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$. Such a prior decomposition involves a deterministic mapping as well as a measurable operator 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 $\{[\boldsymbol{C}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$, and that the correlation functions induced by such a construction, while unknown *a priori*, can be set up having recourse to an inverse analysis.

2.2 Generalized probabilistic representation

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

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

where $\{[\boldsymbol{G}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ and $\{[\boldsymbol{L}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ are two auxiliary second-order random fields defined below.

The random field $\{[\boldsymbol{G}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ is introduced as an anisotropic germ in the representation of the mesoscale random field. It exhibits fully anisotropic stochastic fluctuations, and is then assumed to belong to the class SFG^+ of non-Gaussian positive-definite matrix-valued random fields defined in [2] (and for which the family of first-order marginal probability distributions is constructed within the maximum entropy - MaxEnt - paradigm [9]). Consequently, the random matrix $[\boldsymbol{G}(\boldsymbol{x})]$ is written as

$$[\boldsymbol{G}(\boldsymbol{x})] = [\boldsymbol{K}(\boldsymbol{x})]^{\mathrm{T}}\ [\boldsymbol{K}(\boldsymbol{x})], \tag{2}$$

for all $\boldsymbol{x}$ in Ω, with $[\boldsymbol{K}(\boldsymbol{x})]$ an upper-triangular random matrix. From Eq. (2) and the p.d.f. of $[\boldsymbol{G}(\boldsymbol{x})]$ (which is not recalled below for the sake of simplicity), it can be deduced that $[\boldsymbol{K}(\boldsymbol{x})]$ reads as

$$[\boldsymbol{K}(\boldsymbol{x})] = \mathcal{T}\left(\boldsymbol{\xi}(\boldsymbol{x})\right), \tag{3}$$

where $\mathcal{T}$ is a nonlinear measurable (deterministic mapping) (see [2] for a closed-form expression).

The random field $[\boldsymbol{L}(\boldsymbol{x})], \boldsymbol{x} \in \Omega$ is defined as the unique positive-definite square root of a random field, denoted by $\{[\boldsymbol{M}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$, which takes its values in the subset $\mathbb{M}_n^{\mathrm{inv}}(\mathbb{R}) \subset \mathbb{M}_n^+(\mathbb{R})$ of matrices exhibiting some $SO(n)$-invariance properties:

$$[\boldsymbol{L}(\boldsymbol{x})] = [\boldsymbol{M}(\boldsymbol{x})]^{1/2}, \quad \forall \boldsymbol{x} \in \Omega. \tag{4}$$

In the framework of linear elasticity (to which the derivations are restricted from now on), the set $\mathbb{M}_n^{\mathrm{inv}}(\mathbb{R})$ 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 [7] for an illustration in the isotropic case; see [5] [8] for the generalization to all symmetry classes and algorithmic details). Note that a fully anisotropic stochastic elasticity matrix can be recovered by setting the level of fluctuations of $[\boldsymbol{L}(\boldsymbol{x})]$ to 0. In order to construct the probabilistic model for random matrix $[\boldsymbol{M}(\boldsymbol{x})]$, we first decompose $[\boldsymbol{M}(\boldsymbol{x})]$ as

$$[\boldsymbol{M}(\boldsymbol{x})] = [\underline{C}(\boldsymbol{x})]^{1/2}\ \mathrm{expm}\left([\boldsymbol{A}(\boldsymbol{x})]\right)\ [\underline{C}(\boldsymbol{x})]^{1/2}, \tag{5}$$

where expm denotes the matrix exponential. In Eq. (5), $[\boldsymbol{A}(\boldsymbol{x})]$ is a random matrix exhibiting the same topological structure as $[\boldsymbol{M}(\boldsymbol{x})]$ and such that

$$\mathbb{E}\{\mathrm{expm}\left([\boldsymbol{A}(\boldsymbol{x})]\right)\} = [I_n], \tag{6}$$

with $[I_n]$ the $(n \times n)$ identity matrix. It can be shown [8] that $[\boldsymbol{A}(\boldsymbol{x})]$ can be expanded as

$$[\boldsymbol{A}(\boldsymbol{x})] = \sum_{i=1}^{i=N} a_i(\boldsymbol{x})\ [E^i], \tag{7}$$

in which the set of deterministic matrices $[E^1]$, ..., $[E^N]$ is a basis of $\mathbb{M}_n^{\mathrm{inv}}(\mathbb{R})$ and $\boldsymbol{a}(\boldsymbol{x}) = (a_1(\boldsymbol{x}), \ldots, a_N(\boldsymbol{x})) \in \mathbb{R}^N$. Note that $[\boldsymbol{A}(\boldsymbol{x})]$ is not positive-definite and consequently, $[\boldsymbol{A}(\boldsymbol{x})]$ does not belong to $\mathbb{M}_n^{\mathrm{inv}}(\mathbb{R})$. As for the anisotropic germ, the p.d.f. of the random vector $\boldsymbol{a}(\boldsymbol{x})$ is inferred through the MaxEnt principle, for which the following constraints (in addition to the normalization condition) are used:

$$\mathbb{E}\left\{\sum_{i=1}^{i=N} a_i(\boldsymbol{x})\ [E^i]\right\} = [I_n], \tag{8}$$

$$\sum_{i=1}^{i=N} \mathbb{E}\{a_i(\boldsymbol{x})\}\mathrm{tr}\left([E^i]\right) = \nu(\boldsymbol{x}). \tag{9}$$

The induced p.d.f. for random vector $\boldsymbol{a}(\boldsymbol{x})$ then involves a set of Lagrange multipliers whose numerical values can be determined by solving an optimization problem (see [8]). Unlike the anisotropic germ $\{[\boldsymbol{G}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$, the random field $\{\boldsymbol{a}(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$ 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 in the next section.

2.3 Random generator for random field $\{\boldsymbol{a}(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$

We propose a novel generation procedure which is based upon solving a family of Itô Stochastic Differential Equations indexed by Ω. This family if ISDE is such that the family of p.d.f. associated with the family of invariant measures exactly matches the family of MaxEnt first-order marginal distributions introduced above (see [10] for the construction of each ISDE). A cornerstone of the method thus consists in introducing a family $\{\boldsymbol{W}_{\boldsymbol{x}}(r), r \geqslant 0\}_{\boldsymbol{x}\in\Omega}$ of normalized $\mathbb{R}^N$-valued Wiener processes, indexed by Ω, such that the Gaussian increment of the Wiener process at point $\boldsymbol{x}$ between times r and s (with $r < s$) reads as

$$\forall 0 \leqslant r < s, \quad \boldsymbol{W}_{\boldsymbol{x}}(s) - \boldsymbol{W}_{\boldsymbol{x}}(r) = \sqrt{s-r}\ \boldsymbol{\Xi}^{rs}(\boldsymbol{x}), \tag{10}$$

where $\boldsymbol{x} \mapsto \boldsymbol{\Xi}^{rs}(\boldsymbol{x})$ is an independent realization of the Gaussian random field $\{\boldsymbol{\Xi}(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d\}$. Owing to the convergence towards the stationary solution at all points of domain Ω (which has to be characterized beforehand), such a strategy does generate spatial dependencies for random field $\{\boldsymbol{a}(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$ (and then, for random field $\{[\boldsymbol{C}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ in view of Eq. (1)). From a conceptual point of view, this algorithm amounts to define the random field $\{[\boldsymbol{L}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ as

$$[\boldsymbol{L}(\boldsymbol{x})] = \mathcal{H}\left(\boldsymbol{\Xi}(\boldsymbol{x})\right), \tag{11}$$

in which $\mathcal{H}$ is a nonlinear operator. It is worth noticing 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 a MaxEnt 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 [8] for the mathematical background and further details about this algorithm. In the next section, we illustrate the approach by considering the case of tensors that are almost isotropic.

3 Application

3.1 Problem description

Let $\Omega =]0, 100[$ (in [mm]). Below, all the spatial correlation lengths associated with the stochastic germs are set to the same value, namely $\mathcal{L} = 20$ [mm]. We assume that $\{[\boldsymbol{L}(x)], x \in \Omega\}$ takes its values in the set of isotropic elasticity tensors, spanned by the two projectors $[E^1]$ and $[E^2]$. The mean function $x \mapsto [\underline{C}(x)]$ is then written as $[\underline{C}(x)] = 3\underline{c}_1\ [E^1] + 2\underline{c}_2\ [E^2]$, where $\underline{c}_1$ and $\underline{c}_2$ are set to 1.5 and 1 (both in [GPa]) respectively. Those parameters can be interpreted as the mean bulk and shear moduli, respectively. Furthermore, we take $\nu = -0.2$ (see Eq. (9)) and the level of statistical fluctuations associated with the anisotropic term $\{[\boldsymbol{G}(x)], x \in \Omega\}$ is set to 0.2.

3.2 Numerical results

It follows that

$$[\boldsymbol{A}(x)] = a_1(x)\ [E^1] + a_2(x)\ [E^2], \tag{12}$$

where the $\mathbb{R}$-valued random fields $\{a_1(x), x \in \Omega\}$ and $\{a_2(x), x \in \Omega\}$ exhibit first-order marginal p.d.f. that do not depend on x (since ν is constant over Ω). Those p.d.f., denoted by p_{a_1} and p_{a_2} respectively, are defined through Lagrange multipliers, the values of which are calibrated within an optimization algorithm. The graphs of p_{a_1} and p_{a_2} are shown in Figure 1. A few samples of the random fields $\{C_{11}(x), x \in \Omega\}$ and $\{C_{12}(x), x \in \Omega\}$, defined through the generalized representation and generated by the proposed algorithm, are finally shown in Figure 2.

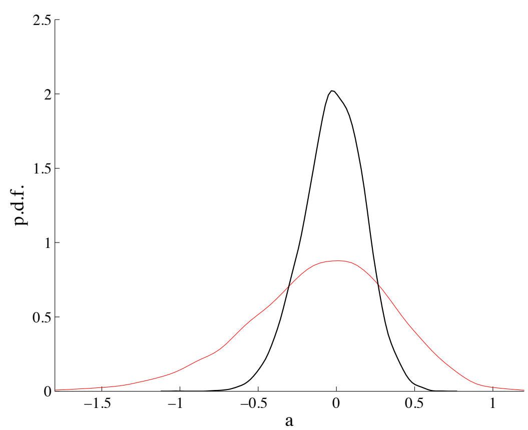

Figure 1: Graphs of the p.d.f. $a \mapsto p_{a_1}(a)$ and $a \mapsto p_{a_2}(a)$.

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 a generalized prior algebraic representation. Some computational issues related to the construction of a random generator are briefly reviewed and a new algorithm, allowing for the generation of vector-valued non-Gaussian random fields, is designed. Finally, the algorithm is exemplified by considering the modeling of almost isotropic elasticity tensor random fields.

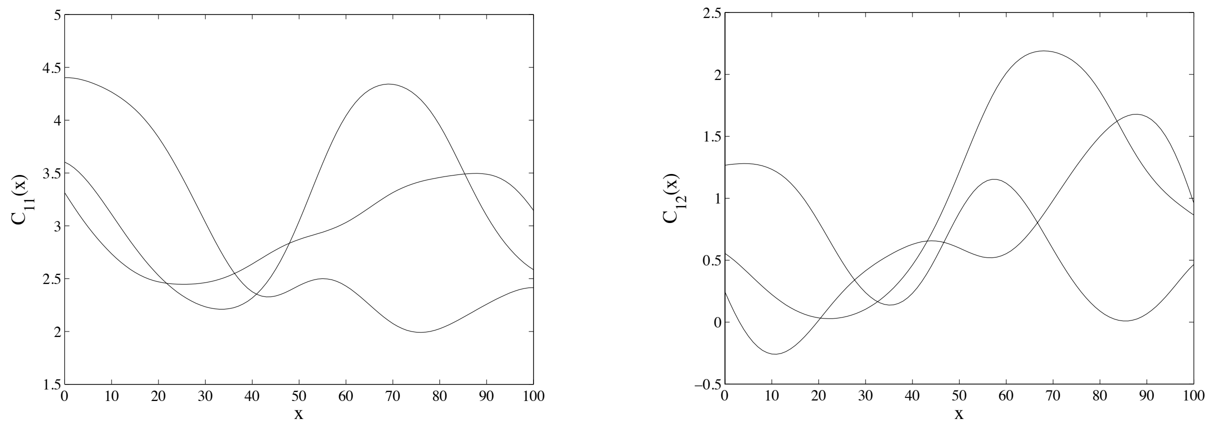

Figure 2: A few samples of random fields $\{C_{11}(x), x \in \Omega\}$ and $\{C_{12}(x), x \in \Omega\}$.

Acknowledgements

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

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