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Modélisation et Simulation Multi Echelle **MSME UMR 8208**

Representations of non-Gaussian positive-definite matrix-valued random fields for elliptic BVP and statistical inverse identification in high dimension (HD) using partial and limited experimental data

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Statistical inverse problem to be solved (formulated in the framework of a 3D linear elastostatic problem)

Input

Elliptic BVP with random operator

$\mathbf{EllOp}(\mathbf{u}) = -[D_{\mathbf{x}}]^T[\mathbb{A}(\mathbf{x})][D_{\mathbf{x}}]\mathbf{u}$

Output

$\mathbf{u} = (u_1, ..., u_m)$

Parameter: Non-Gaussian random field in HD

$\mathbf{x} = (x_1, ..., x_d) \mapsto [\mathbb{A}(\mathbf{x})] : \mathbb{R}^d \supset \Omega \to L^2(\Theta, \mathbb{M}_n^+(\mathbb{R}))$

Partial observ. vector

$\mathbf{U}^{\text{obs}} \in L^2(\Theta, \mathbb{R}^{m_{\text{obs}}})$

Identification of $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ using the Maximum Likelihood and/or Bayesian methods

Exemple: 3D elasticity

$d = 3, m = 3, n = 6$

$[D_{\mathbf{x}}] = \sum_{i=1}^{3} [M^{(i)}] \frac{\partial}{\partial x_i}$

Limited exp. data

$\mathbf{u}^{\exp,\ell}, \ell = 1, \ldots, \nu_{\exp}$

corresponding to $\mathbf{U}^{\text{obs}}$

Difficulties of the statistical inverse problem in the framework of a general parametric representation of the random field $[\mathbb{A}]$ for the HD case

$\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ is a **second-order** random field in HD: a general parametric representation would be given by its **polynomial chaos expansion (PCE)**.

What would be the **difficulties**?

• Non-Gaussian **matrix-valued random field** should be identified, and **not a real valued** random field.

• **Algebraic properties** should be satisfied: deterministic or random bounds, random field with values in the positive-definite symmetric matrices with invariance properties (induced by material symmetries), constraints on the tensor-valued moments, etc.

$\Longrightarrow$ PCE coefficients would belong to a **manifold**, which could be very complicated to describe and to explore for computing the coefficients.

• **Convergence** of the PCE would require, a **very huge number of coefficients** (HD case).

• **Available experimental data sets** correspond to **partial data** for an observation vector requiring solving a stochastic boundary value problem $\Longrightarrow$ the **covariance matrix** of the discretized random field **could not be estimated** $\Longrightarrow$ the **statistical reduction** by principal component analysis **could not be used**.

CONSEQUENTLY: If no additional information is available, then it is an **ill-posed problem**: there are too many coefficients to be identified with respect to the available experimental data.

$\Longrightarrow$ A family of **prior algebraic stochastic models (PASM)**, containing additional information, and an **adapted identification methodology**, must be introduced.

Stochastic finite element approximation of the boundary value problem

- Let $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ be the matrix-valued random field.

- The **finite element approximation** of the BVP yields a finite family of N_p dependent random matrices $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \mathcal{I}\}$ in which $\mathcal{I} = \{\mathbf{x}^1, \ldots, \mathbf{x}^{N_p}\} \subset \Omega$ is the finite subset of Ω made up of all the integrations points of the finite elements used in the mesh of Ω. This set of random matrices is represented by a random vector $\mathbb{V} = (V_1, \ldots, V_{m_\mathbb{V}})$ that is then defined as:

$$\mathbb{V} \stackrel{\text{def}}{=} \textit{reshape}\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \mathcal{I}\} \quad , \quad m_\mathbb{V} = N_p \times (n \times n)$$

- The random vector $\mathbf{U} = (U_1, \ldots, U_{m_{\text{DOF}}})$ of the DOF (including observed and non-observed DOF) is such that

$$\mathbf{U} = \mathbf{h}(\mathbb{V}) \quad , \quad \mathbf{U} = (\mathbf{U}^{\text{obs}}, \mathbf{U}^{\text{nobs}}) \quad , \quad \mathbf{U}^{\text{obs}} = \mathbf{h}^{\text{obs}}(\mathbb{V}) \quad , \quad \mathbf{U}^{\text{nobs}} = \mathbf{h}^{\text{nobs}}(\mathbb{V})$$

in which $\mathbf{h} = (\mathbf{h}^{\text{obs}}, \mathbf{h}^{\text{nobs}})$ is a deterministic **nonlinear transformation from $\mathbb{R}^{m_\mathbb{V}}$ into $\mathbb{R}^{m_{\text{DOF}}} = \mathbb{R}^{m_{\text{obs}}} \times \mathbb{R}^{m_{\text{nobs}}}$**, constructed solving the BVP.

Introducing an adapted representation of the random field $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ in view of constructing its polynomial chaos expansion (PCE)

- **Why an adapted representation must be introduced?**

  $\forall \mathbf{x} \in \Omega\,,\; E\{\,\|[\mathbb{A}(\mathbf{x})]\|_F^2\,\} < +\infty \;\Rightarrow$ PCE is a general representation of $[\mathbb{A}(\mathbf{x})]$ (for its identification), which is written (in a finite approximation) as:

$$[\mathbb{A}^{(N_d,N_g)}(\mathbf{x})] = \sum_{j_1=0}^{N_d} \ldots \sum_{j_{N_g}=0}^{N_d} [\mathbb{a}_{j_1,\ldots,j_{N_g}}(\mathbf{x})]\, \phi_{j_1}(\Xi_1) \times \ldots \times \phi_{j_{N_g}}(\Xi_{N_g})$$

For representing properties (such as positiveness) of $[\mathbb{A}(\mathbf{x})]$, the **convergence** must be **accurate** $\Rightarrow N_d$ and N_g sufficiently large $\Rightarrow N = (N_g + N_d)!/(N_g!N_d!)$ of $\mathbb{M}_n^S(\mathbb{R})$-valued functions, $[\mathbb{a}_{j_1,\ldots,j_{N_g}}]$, **very large** (huge).

$\triangleright$ The objective is thus to introduce a representation that guaranties the lower bound and the positiveness.

• **Normalized representation with a shift to ensure ellipticity.**

$$\forall \mathbf{x} \in \Omega \quad , \quad [\mathbb{A}(\mathbf{x})] = [C_\ell(\mathbf{x})] + [L_{\underline{a}}(\mathbf{x})]^T [\mathbf{C}(\mathbf{x})]\, [L_{\underline{a}}(\mathbf{x})]$$

$[C_\ell(\mathbf{x})] \in \mathbb{M}_n^+(\mathbb{R})$ (lower bound) and $[\underline{\mathbb{a}}(\mathbf{x})] = E\{[\mathbb{A}(\mathbf{x})]\} \in \mathbb{M}_n^+(\mathbb{R})$.

$[L_{\underline{a}}(\mathbf{x})]^T\, [L_{\underline{a}}(\mathbf{x})] = [\underline{\mathbb{a}}(\mathbf{x})] - [C_\ell(\mathbf{x})] \in \mathbb{M}_n^+(\mathbb{R})$ (Cholesky factorization).

$[\mathbf{C}]$: normalized $\mathbb{M}_n^+(\mathbb{R})$-valued random field such that $E\{[\mathbf{C}(\mathbf{x})]\} = [I_n]$.

Particular choice: $[C_\ell(\mathbf{x})] = \frac{\varepsilon}{1+\varepsilon}[\underline{\mathbb{a}}(\mathbf{x})]\}$ with $0 < \varepsilon < 1$, then $[L_{\underline{a}}(\mathbf{x})] = \frac{1}{\sqrt{1+\varepsilon}}\, [L_{\underline{\mathbb{a}}}(\mathbf{x})]$ with $[L_{\underline{\mathbb{a}}}(\mathbf{x})]^T\, [L_{\underline{\mathbb{a}}}(\mathbf{x})] = [\underline{\mathbb{a}}(\mathbf{x})]$, and consequently,

$$\forall \mathbf{x} \in \Omega \quad , \quad [\mathbb{A}(\mathbf{x})] = \frac{1}{1+\varepsilon}[L_{\underline{\mathbb{a}}}(\mathbf{x})]^T \,\{\varepsilon[I_n] + [\mathbf{C}(\mathbf{x})]\}\, [L_{\underline{\mathbb{a}}}(\mathbf{x})]$$

• **Choosing a representation to ensure the positiveness of $[\mathbf{C}(\mathbf{x})]$.**

Non-Gaussian second-order $\mathbb{M}_n^+(\mathbb{R})$-valued random field $\{[\mathbf{C}(\mathbf{x})], \mathbf{x} \in \Omega\}$ is expressed as a given **invertible local transformation** T of a second-order $\mathbb{M}_n^S(\mathbb{R})$-valued random field $\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \Omega\}$ (*a priori* not Gaussian):

$$\forall \mathbf{x} \in \Omega \quad , \quad [\mathbf{C}(\mathbf{x})] = T([\mathbf{G}(\mathbf{x})]) \quad \Leftrightarrow \quad [\mathbf{G}(\mathbf{x})] = T^{-1}([\mathbf{C}(\mathbf{x})])$$

▷ **Exponential-type representation** and its inversion:

$$[\mathbf{C}(\mathbf{x})] = \mathrm{expm}([\mathbf{G}(\mathbf{x})]) \quad \Leftrightarrow \quad [\mathbf{G}(\mathbf{x})] = \mathrm{logm}([\mathbf{C}(\mathbf{x})])$$

If $[\mathbf{G}(\mathbf{x})]$ was Gaussian, then $[\mathbf{C}(\mathbf{x})]$ would be log-normal.

▷ **Square-type representation** and its inversion:

$$[\mathbf{C}(\mathbf{x})] = [\mathbf{L}(\mathbf{x})]^T\,[\mathbf{L}(\mathbf{x})] \ , \ [\mathbf{L}(\mathbf{x})] = \mathcal{L}([\mathbf{G}(\mathbf{x})]) \quad \Leftrightarrow \quad [\mathbf{G}(\mathbf{x})] = \mathcal{L}^{-1}([\mathbf{L}(\mathbf{x})])$$

Nonlinear transformation $\mathcal{L}$ is constructed with the MaxEnt principle (Soize CMAME 2006)

- **Expressing the invertible transformations for the discretized random fields**.

▷ Using the introduced representations, an invertible local transformation $\mathcal{A}$ and its inverse can be constructed explicitly:

$$\forall \mathbf{x} \in \Omega \quad , \quad [\mathbb{A}(\mathbf{x})] = \mathcal{A}([\mathbf{G}(\mathbf{x})]) \quad \Leftrightarrow \quad [\mathbf{G}(\mathbf{x})] = \mathcal{A}^{-1}([\mathbb{A}(\mathbf{x})])$$

▷ Similarly, introducing the $\mathbb{R}^{m_{\mathbb{V}}}$-valued random variables:

$$\mathbb{V} \stackrel{\text{def}}{=} \textit{reshape}\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \mathcal{I}\} \quad , \quad \mathbb{W} \stackrel{\text{def}}{=} \textit{reshape}\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \mathcal{I}\}$$

an invertible nonlinear transformation $\mathcal{A}_r$ and its inverse can be constructed explicitly:

$$\mathbb{V} = \mathcal{A}_r(\mathbb{W}) \quad , \quad \mathbb{W} = \mathcal{A}_r^{-1}(\mathbb{V})$$

Methodology proposed for the identification in HD

We propose the methodology introduced in **[1]**, with new improvements concerning the choices of the:

- family of prior algebraic stochastic models for $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ (from **[2]**)
- representations adapted to the polynomial chaos expansion (PCE) (from **[3]**)
- algorithm for computing realizations of PCE in high dimension (from **[4]** **[5]**)

[1] **C. Soize** , Identification of high-dimension polynomial chaos expansions with random coefficients for non-Gaussian tensor-valued random fields using partial and limited experimental data, *Computer Methods in Applied Mechanics and Engineering*, 199(33-36), 2150-2164 (2010).

[2] **J. Guilleminot, C. Soize**, Stochastic model and generator for random fields with symmetry properties: application to the mesoscopic modeling of elastic random media, *Multiscale Modeling and Simulation (A SIAM Interdisciplinary Journal)*, 11(3), 840-870 (2013).

[3] **A. Nouy, C. Soize**, Random fields representations for stochastic elliptic boundary value problems and statistical inverse problems, *European Journal of Applied Mathematics*, in press, (2014).

[4] **C. Soize, C. Desceliers**], Computational aspects for constructing realizations of polynomial chaos in high dimension, *SIAM Journal On Scientific Computing*, 32(5), 2820-2831 (2010).

[5] **G. Perrin, C. Soize, D. Duhamel, C. Funfschilling**, Identification of polynomial chaos representations in high dimension from a set of realizations, *SIAM Journal on Scientific Computing*, 34(6), A2917-A2945 (2012).

Step 1: Family of prior algebraic stochastic models (PASM)

- Introducing $\{[\mathbb{A}^{\text{PASM}}(\mathbf{x};\mathbf{s})]\,,\mathbf{x}\in\Omega\}$ on $(\Theta,\mathcal{T},\mathcal{P})$, depending on a vector-valued hyperparameter $\mathbf{s}\in\mathcal{C}_{\text{ad}}$ in **low** dimension (mean values, dispersion parameters, spatial correlation lengths, etc).
- Deducing a family $\{\mathbb{V}^{\text{PASM}}(\mathbf{s}),\mathbf{s}\in\mathcal{C}_{\text{ad}}\}$ of random vectors with values in $\mathbb{R}^{m_{\mathbb{V}}}$, $\mathbb{V}^{\text{PASM}}(\mathbf{s})\overset{\text{def}}{=}\textit{reshape}\{[\mathbb{A}^{\text{PASM}}(\mathbf{x};\mathbf{s})],\mathbf{x}\in\mathcal{I}\}$.
- A **generator** of independent realizations $\mathbb{V}^{\text{PASM}}(\theta_1;\mathbf{s}),\ldots,\mathbb{V}^{\text{PASM}}(\theta_\nu;\mathbf{s})$ is then available.

Comment: In HD, the real possibility to correctly **identify a general representation** (such as the PCE) of random field $\{[\mathbb{A}(\mathbf{x})],\mathbf{x}\in\Omega\}$, through a stochastic BVP, is directly related to the **capability** of the constructed PASM for **representing fundamental properties** such as lower bound, positiveness, invariance related to material symmetry, mean value, support of the spectrum, spatial correlation lengths, level of statistical fluctuations, etc.

Step 2: Identification of an optimal PASM in the constructed family using partial and limited experimental data sets

Identifying the optimal value $\mathbf{s}^{\text{opt}}$ in $\mathcal{C}_{\text{ad}}$ of hyperparameter $\mathbf{s}$ using partial and limited experimental data $\{\mathbf{u}^{\text{exp},1}, \ldots, \mathbf{u}^{\text{exp},\nu_{\text{exp}}}\}$ relative to $\mathbf{U}^{\text{obs}}$:

- Using the family, $\mathbf{U}^{\text{obs,PASM}}(\mathbf{s}) = \mathbf{h}^{\text{obs}}(\mathbb{V}^{\text{PASM}}(\mathbf{s}))$ for $\mathbf{s} \in \mathcal{C}_{\text{ad}}$, of random observation vectors, constructed with the PASM and the computational model.

- Using the *moment method*, the *least-square method* or the *maximum likelihood method*, for calculating $\mathbf{s}^{\text{opt}}$ in $\mathcal{C}_{\text{ad}}$, and then, deducing the **optimal PASM**:

$$\mathbb{V}^{\text{PASM,opt}} = \mathbb{V}^{\text{PASM}}(\mathbf{s}^{\text{opt}})$$

- A **generator** of independent realizations $\mathbb{V}^{\text{PASM,opt}}(\theta_1), \ldots, \mathbb{V}^{\text{PASM,opt}}(\theta_\nu)$ is then available allowing the calculation of independent realizations $\mathbb{W}^{\text{PASM,opt}}(\theta_1), \ldots, \mathbb{W}^{\text{PASM,opt}}(\theta_\nu)$ of $\mathbb{W}^{\text{PASM,opt}}$ such that

$$\mathbb{W}^{\text{PASM,opt}}(\theta_\ell) = \mathcal{A}_r^{-1}(\mathbb{V}^{\text{PASM,opt}}(\theta_\ell))$$

• **Why steps 1 and 2 are necessary to guaranty a possible and realistic identification of a general representation of the unknown random vector $\mathbb{W} = \mathcal{A}_r^{-1}(\mathbb{V})$ in high dimension**.

$E\{\,\|\mathbb{W}\|^2\,\} < +\infty \;\Rightarrow$ PCE is a general representation of $\mathbb{W}$ (for its identification), which is written (in a finite approximation) as:

$$\mathbb{W}^{(N_d,N_g)} = \sum_{j_1=0}^{N_d} \ldots \sum_{j_{N_g}=0}^{N_d} \mathbb{w}_{j_1,\ldots,j_{N_g}} \, \phi_{j_1}(\Xi_1) \times \ldots \times \phi_{j_{N_g}}(\Xi_{N_g})$$

At convergence (in N_d,N_g), the number of vectors, $\mathbb{w}_{j_1,\ldots,j_{N_g}}$ to be identified is $N = (N_g + N_d)!/(N_g!N_d!)$: **very large number**.

In the framework of a non convex optimization problem, trying to perform an identification in a high-dimension hypercube **without specifying a small region** (defined by the knowledge of a prior information) of the hypercube that has to be explored, is an ill-posed problem. Consequently, **Steps 1-2 is a very fundamental steps in the identification procedure**.

Step 3: Construction of a statistical reduced-order (RO) optimal PASM in the representation $\mathbb{W}$ using a principal component analysis

- Estimation of the mean value $\underline{\mathbb{W}}$ and the covariance matrix $[C_{\mathbb{W}}]$ of $\mathbb{W}^{\text{PASM,opt}}$ using the independent realizations: $\{\mathbb{W}^{\text{PASM,opt}}(\theta_\ell), \ell = 1, \ldots, \nu\}$.

- Solving $[C_{\mathbb{W}}]\mathbb{w}^j = \lambda_j \mathbb{w}^j$ and deducing the **RO optimal PASM**:

$$\mathbb{W}^{\text{PASM,opt}} \simeq \underline{\mathbb{W}} + \sum_{j=1}^{n} \sqrt{\lambda_j}\, \eta_j^{\text{PASM,opt}}\, \mathbb{w}^j$$

$$E\{\boldsymbol{\eta}^{\text{PASM,opt}}\} = 0 \quad , \quad E\{\boldsymbol{\eta}^{\text{PASM,opt}}\, (\boldsymbol{\eta}^{\text{PASM,opt}})^T\} = [I_n]$$

- Mean-square convergence $n \mapsto \text{err}(n) = 1 - (\sum_{j=1}^{n} \lambda_j)/(\text{tr}[C_{\mathbb{W}^{\text{PASM,opt}}}])$. At convergence n is **large** (several hundred or even a thousand or more).

- The **independent realizations**, $\boldsymbol{\eta}^{\text{PASM,opt}}(\theta_1), \ldots, \boldsymbol{\eta}^{\text{PASM,opt}}(\theta_\nu)$, are calculated by

$$\eta_j^{\text{PASM,opt}}(\theta_\ell) = \frac{1}{\sqrt{\lambda_j}}\, (\mathbb{W}^{\text{PASM,opt}}(\theta_\ell) - \underline{\mathbb{W}})^T\, \mathbb{w}^j$$

Step 4: Construction of the polynomial chaos expansion (PCE) with deterministic coefficients of random vector $\boldsymbol{\eta}^{\text{PASM,opt}}$

- Gaussian polynomial chaos expansion of random vector $\boldsymbol{\eta}^{\text{PASM,opt}}$:

$$\boldsymbol{\eta}^{\text{PASM,opt}} \simeq \boldsymbol{\eta}^{\text{chaos}}(N) \quad , \quad \boldsymbol{\eta}^{\text{chaos}}(N) = \sum_{\alpha=1}^{N} \mathbf{y}^{\alpha}\, \Psi_{\alpha}(\boldsymbol{\Xi})$$

$$\boldsymbol{\Xi} = (\Xi_1, \ldots, \Xi_{N_g}) \quad , \quad N = (N_d + N_g)!\,/(N_d!\, N_g!)$$

$$E\{\Psi_{\alpha}(\boldsymbol{\Xi})\} = 0 \quad , \quad E\{\Psi_{\alpha}(\boldsymbol{\Xi})\, \Psi_{\beta}(\boldsymbol{\Xi})\} = \delta_{\alpha\beta}$$

- **Constraint**: $\sum_{\alpha=1}^{N} \mathbf{y}^{\alpha}\, \mathbf{y}^{\alpha\, T} = [I_n]$
- **Analyzing the convergence** with respect to N_g and N_d:

$$\text{err}_j(N_g, N_d) = \int_{\text{BI}_j} |\log_{10} p_{\eta_j^{\text{PASM}}}(e) - \log_{10} p_{\eta_j^{\text{chaos}}(N)}(e\,;\mathbf{y}^1, \ldots, \mathbf{y}^N)|\, de$$

BI_j = adapted bounded interval.

- **Optimal values** $[\,\underline{y}\,] = [\underline{\mathbf{y}}^1 \ldots \underline{\mathbf{y}}^N]^T$ of $[y] = [\mathbf{y}^1 \ldots \mathbf{y}^N]^T$ calculated with the **maximum likelihood method**, and the independent realizations: $\boldsymbol{\eta}^{\text{PASM,opt}}(\theta_1), \ldots, \boldsymbol{\eta}^{\text{PASM,opt}}(\theta_\nu)$

For the **high-dimension case** (n large and $N \gg n$ very large), this optimization (challenging) problem can be solved in using the efficient random search algorithm proposed in **[1]**,

- ▷ which is adapted to the high dimension,
- ▷ which explores the constraint $\sum_{\alpha=1}^N \mathbf{y}^\alpha\, \mathbf{y}^{\alpha\, T} = [I_n]$,
- ▷ and for which good results have been obtained for $n = 550$ and $N = 10,625$ yielding $5,843,750$ real coefficients, $[y]_{j\alpha}\ ,\ 1 \leq j \leq n\ ,\ 1 \leq \alpha \leq N$.

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[1] **C. Soize** , Identification of high-dimension polynomial chaos expansions with random coefficients for non-Gaussian tensor-valued random fields using partial and limited experimental data, *Computer Methods in Applied Mechanics and Engineering*, 199(33-36), 2150-2164 (2010).

Step 5: Construction of a posterior model in the region localized by the optimal value, $[\,\underline{y}\,] = [\underline{\mathbf{y}}^1 \ldots \underline{\mathbf{y}}^N]^T$ of $[y] = [\mathbf{y}^1 \ldots \mathbf{y}^N]^T$

Construction of a posterior model of random vector $\mathbb{V}$ (discretization of random field $[\mathbb{A}]$), obtained using the Bayes method with the following procedure proposed in **[3]** and made up of 7 stages:

[3] **A. Nouy, C. Soize**, Random fields representations for stochastic elliptic boundary value problems and statistical inverse problems, *European Journal of Applied Mathematics*, in press (2014).

• **(i) Introduction of a minimal parameterization of the constraint:**
$\sum_{\alpha=1}^{N} \mathbf{y}^\alpha\, \mathbf{y}^{\alpha\, T} = [I_n]$

▷ $[y] = [\mathbf{y}^1 \ldots \mathbf{y}^N]^T \in \mathbb{M}_{N,n}(\mathbb{R}) \Rightarrow$ the constraint is rewritten as $[y]^T\,[y] = [I_n]$.

▷ Introduction of the compact Stiefel manifold:

$$\mathcal{V}_n(\mathbb{R}^N) = \{\, [y] \in \mathbb{M}_{N,n}(\mathbb{R}) \;;\; [y]^T\,[y] = [I_n]\,\}$$

with $\nu_s = \dim\{\mathcal{V}_n(\mathbb{R}^N)\} = nN - n(n+1)/2$.

▷ For the case $N \geq n$ and possibly, for $N \gg n$, introduction of the minimal parameterization of $\mathcal{V}_n(\mathbb{R}^N)$, with complexity $O(Nn^2)$ (instead of $O(N^3)$), proposed in **[3]**, consisting in constructing, for any $[y_0]$ fixed in $\mathcal{V}_n(\mathbb{R}^N)$, a surjective mapping $\mathcal{M}_{[y_0]}$ from $\mathbb{R}^{\nu_s}$ onto $\mathcal{V}_n(\mathbb{R}^N)$:

$$\mathbf{z} \mapsto [y] = \mathcal{M}_{[y_0]}(\mathbf{z})$$

• **(ii) Introducing a parameterization** $\mathcal{B}_{[\underline{y}]}(\mathbf{z})$ of $\mathbb{V}$ (discretizing random field $[\mathbb{A}]$**), in the region localized by the optimal value,** $[\,\underline{y}\,] = [\underline{\mathbf{y}}^1 \ldots \underline{\mathbf{y}}^N]^T$

Defining the parameterized random mapping $\mathcal{B}_{[\underline{y}]}$:

$$\mathbf{z} \mapsto \mathbb{V} = \mathcal{B}_{[\underline{y}]}(\mathbf{z}) \;:\; \mathbb{R}^{\nu_s} \rightarrow L^2(\Theta, \mathbb{R}^{m_{\mathbb{V}}})$$

using the following mappings (previously defined):

$[y] = \mathcal{M}_{[\underline{y}]}(\mathbf{z})$ ($[\underline{y}]$ optimal value computed in Step 4 with the opt PASM)

$\boldsymbol{\eta} = \sum_{\alpha=1}^{N} \mathbf{y}^\alpha\, \Psi_\alpha(\boldsymbol{\Xi}) = [\,y\,]^T\, \boldsymbol{\Psi}(\boldsymbol{\Xi})$

$\mathbb{W} \simeq \underline{\mathbb{W}} + \sum_{j=1}^{n} \sqrt{\lambda_j}\,\eta_j\, \mathbb{w}^j \quad , \quad \boldsymbol{\eta} = (\eta_1, \ldots, \eta_n)$

$\mathbb{V} = \mathcal{A}_r(\mathbb{W})$

- **(iii) Estimating the optimal value**, $\mathbf{z}^{\rm opt}$ of parameter $\mathbf{z}$ in $\mathbb{R}^{n_s}$, using the maximum likelihood method,

  ▷ for observation $\mathbf{U}^{\rm obs} = \mathbf{h}^{\rm obs}(\mathbb{V})$ with $\mathbb{V} = \mathcal{B}_{[\underline{y}]}(\mathbf{z})$
  ▷ with the partial experimental data $\{\mathbf{u}^{{\rm exp},1}, \ldots, \mathbf{u}^{{\rm exp},\nu_{\rm exp}}\}$ relative to $\mathbf{U}^{\rm obs}$

- **(iv) Computing** $[y^{\rm opt}]$ **associated with** $\mathbf{z}^{\rm opt}$: $[y^{\rm opt}] = \mathcal{M}_{[\underline{y}]}(\mathbf{z}^{\rm opt})$

- **(v) Introducing random coefficients** $[\mathbf{Y}] = [\mathbf{Y}^1 \ldots \mathbf{Y}^N]^T$ in the PCE for a stochastic modeling of $[y] = [\mathbf{y}^1 \ldots \mathbf{y}^N]^T$, in the region defined by $[y^{\rm opt}]$, and thus, $\mathbf{Z}$ is a random vector such that: $[\mathbf{Y}] = \mathcal{M}_{[y^{\rm opt}]}(\mathbf{Z})$.

- **(vi) Computing a posterior estimation** $\mathbf{Z}^{\rm post}$ using the Bayes method with a prior centered Gaussian vector $\mathbf{Z}^{\rm prior}$.

  ▷ for observation $\mathbf{U}^{\rm obs} = \mathbf{h}^{\rm obs}(\mathbb{V})$ with $\mathbb{V} = \mathcal{B}_{[y^{\rm opt}]}(\mathbf{Z})$
  ▷ with the partial experimental data $\{\mathbf{u}^{{\rm exp},1}, \ldots, \mathbf{u}^{{\rm exp},\nu_{\rm exp}}\}$ relative to $\mathbf{U}^{\rm obs}$

- **(vii) Iterating the identification procedure** in restarting from Step 3 with $\mathbb{W}^{\rm PASM,opt}$ replaced by $\mathbb{W}^{\rm post}$

A few details on important ingredients required for such an identification procedure

A family of prior algebraic stochastic models (PASM) for non-Gaussian matrix-valued random field $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$ and its generator

• **Framework**: 3D linear elasticity of microstructures;
$\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$: **apparent elasticity field** of microstructure Ω at mesoscale.

For all $\mathbf{x}$ fixed in Ω, random elasticity matrix $[\mathbb{A}(\mathbf{x})]$:

(i) is, **in mean**, close to a **given symmetry class** (independent of $\mathbf{x}$), induced by a material symmetry;

(ii) exhibits more or less **anisotropic fluctuations** around this symmetry class;

(iii) exhibits a level of statistical fluctuations in the symmetry class, which must be **controlled independently** of the level of statistical anisotropic fluctuations.

• Notation and properties for positive matrices with symmetry classes

$\mathbb{M}_n^+(\mathbb{R}) \subset \mathbb{M}_n^S(\mathbb{R}) \subset \mathbb{M}_n(\mathbb{R})$ (positive-definite, symmetric, all).

A given symmetry class is defined by the subset $\mathbb{M}_n^{\text{sym}}(\mathbb{R}) \subset \mathbb{M}_n^+(\mathbb{R})$ such that,

$$[M] = \sum_{i=1}^{n_s} m_i [E_i^{\text{sym}}] \quad , \quad \mathbf{m} = (m_1, \ldots, m_{n_s}) \in \mathcal{C} \quad , \quad [E_i^{\text{sym}}] \in \mathbb{M}_n^S(\mathbb{R})$$

$$\mathcal{C} = \{\mathbf{m} \in \mathbb{R}^{n_s} \mid \sum_{i=1}^{n_s} m_i [E_i^{\text{sym}}] \in \mathbb{M}_n^+(\mathbb{R})\}$$

$\{[E_i^{\text{sym}}], i = 1, \ldots, n_s\}$ is a matrix basis (Walpole's tensor basis).

Examples of usual symmetry classes for $n = 6$ (3D elasticity),

$n_s = 2$: isotropic symmetry

$n_s = 5$: transverse isotropic symmetry

$n_s = 9$: orthotropic symmetry

etc... and, $n_s = 21$: anisotropy

Property: if $[M] \in \mathbb{M}_n^{\text{sym}}(\mathbb{R})$, then $[M]^{1/2} \in \mathbb{M}_n^{\text{sym}}(\mathbb{R})$

if $[M]$ and $[M'] \in \mathbb{M}_n^{\text{sym}}(\mathbb{R})$, then $[M]\,[M'] \in \mathbb{M}_n^{\text{sym}}(\mathbb{R})$

• An advanced prior stochastic model $\{[\mathbb{A}^{\text{PASM}}(\mathbf{x})], \mathbf{x} \in \Omega\}$ for $\{[\mathbb{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$

[**C. Soize**], Non Gaussian positive-definite matrix-valued random fields for elliptic stochastic partial differential operators, *Computer Methods in Applied Mechanics and Engineering*, 195(1-3), 26-64 (2006).

[**J. Guilleminot, C. Soize**], Stochastic model and generator for random fields with symmetry properties: application to the mesoscopic modeling of elastic random media, *Multiscale Modeling and Simulation (A SIAM Interdisciplinary Journal)*, 11(3), 840-870 (2013).

Prior algebraic representation (*Guilleminot & Soize SIAM MMS 2013*):

$$\forall \mathbf{x} \in \Omega \quad , \quad [\mathbb{A}^{\text{PASM}}(\mathbf{x})] = [C_\ell(\mathbf{x})] + [\mathbf{A}(\mathbf{x})]$$

$\{[C_\ell(\mathbf{x})], \mathbf{x} \in \Omega\}$: $\mathbb{M}_n^+(\mathbb{R})$-valued deterministic field (lower-bound)

$\{[\mathbf{A}(\mathbf{x})], \mathbf{x} \in \Omega\}$: $\mathbb{M}_n^+(\mathbb{R})$-valued random field

$$[\mathbf{A}(\mathbf{x})] = [\underline{S}(\mathbf{x})]^T \, [\mathbf{M}(\mathbf{x})]^{1/2} [\mathbf{G}(\mathbf{x})] \, [\mathbf{M}(\mathbf{x})]^{1/2} \, [\underline{S}(\mathbf{x})]$$

$\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \Omega\}$: $\mathbb{M}_n^+(\mathbb{R})$-valued random field.

$\{[\mathbf{M}(\mathbf{x})], \mathbf{x} \in \Omega\}$: $\mathbb{M}^{\text{sym}}(\mathbb{R})$-valued random field independent of $\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \Omega\}$.

$\{[\underline{S}(\mathbf{x})], \mathbf{x} \in \Omega\}$: $\mathbb{M}_n(\mathbb{R})$-valued deterministic field.

Anisotropic statistical fluctuations: $\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \Omega\}$ which is a non-Gaussian $\mathbb{M}_n^+(\mathbb{R})$-valued random field (*MaxEnt construction and generator are given in Soize, CMAME 2006*), for which $E\{[\mathbf{G}(\mathbf{x})]\} = [I_n]$.
The hyperparameters of $\{[\mathbf{G}(\mathbf{x})], \mathbf{x} \in \Omega\}$ are: $d \times n(n+1)/2$ spatial correlation lengths and a scalar dispersion parameter δ_G controlling the anisotropic statistical fluctuations.

Statistical fluctuations in the given symmetry class: $\{[\mathbf{M}(\mathbf{x})], \mathbf{x} \in \Omega\}$ (independent of $[\mathbf{G}]$), which is a non-Gaussian $\mathbb{M}_n^{\rm sym}(\mathbb{R})$-valued random field (*algebraic representation, MaxEnt construction and generator using an ISDE are given in Guilleminot & Soize, SIAM MMS 2013*), for which

$$E\{[\mathbf{M}(\mathbf{x})]\} = [\underline{M}(\mathbf{x})] = \mathcal{P}^{\rm sym}([\underline{a}(\mathbf{x})]),$$

with $\mathcal{P}^{\rm sym}$ the projection operator from $\mathbb{M}_n^+(\mathbb{R})$ on $\mathbb{M}_n^{\rm sym}(\mathbb{R})$, and

$$[\underline{a}(\mathbf{x})] = E\{[\mathbf{A}(\mathbf{x})]\} = E\{[\mathbb{A}(\mathbf{x})]\} - [C_\ell(\mathbf{x})] \in \mathbb{M}_n^+(\mathbb{R}),$$

$$[\mathbf{M}(\mathbf{x})] = [\underline{M}(\mathbf{x})]^{1/2}[\mathbf{N}(\mathbf{x})]\,[\underline{M}(\mathbf{x})]^{1/2} \quad \text{with} \quad E\{[\mathbf{N}(\mathbf{x})]\} = [I_n].$$

$\{[\mathbf{N}(\mathbf{x})], \mathbf{x} \in \Omega\}$ is a non-Gaussian $\mathbb{M}_n^{\rm sym}(\mathbb{R})$-valued random field written as $[\mathbf{N}(\mathbf{x})] = {\rm expm}([\boldsymbol{\mathcal{N}}(\mathbf{x})])$ in which $[\boldsymbol{\mathcal{N}}(\mathbf{x})] = \sum_{i=1}^{n_s} \nu_i(\mathbf{x})[E_i^{\rm sym}]$ with $\{\boldsymbol{\nu}(\mathbf{x}), \mathbf{x} \in \Omega\}$ is a $\mathbb{R}^{n_s}$-valued random process.

The hyperparameters of $\{[\mathbf{M}(\mathbf{x})], \mathbf{x} \in \Omega\}$ are: $d \times n_s$ spatial correlation lengths and a scalar dispersion parameter δ_M controlling the statistical fluctuations in the symmetry class.

Construction of the $\mathbb{M}_n(\mathbb{R})$-valued deterministic field $\{[\underline{S}(\mathbf{x})], \mathbf{x} \in \Omega\}$:

The Cholesky factorizations of $[\underline{a}(\mathbf{x})] = E\{[\mathbb{A}(\mathbf{x})]\} - [C_\ell(\mathbf{x})] \in \mathbb{M}_n^+(\mathbb{R})$ yields the upper matrix $[L_{\underline{a}}(\mathbf{x})]$, and $[\underline{M}(\mathbf{x})] = \mathcal{P}^{\rm sym}([\underline{a}(\mathbf{x})]) \in \mathbb{M}_n^{\rm sym}(\mathbb{R})$ yields the upper matrix $[L_{\underline{M}}(\mathbf{x})]$. Since $[\underline{a}(\mathbf{x})] = [\underline{S}(\mathbf{x})]^T\, [\underline{M}(\mathbf{x})]\, [\underline{S}(\mathbf{x})]$, it can be deduced that

$$[\underline{S}(\mathbf{x})] = [L_{\underline{M}}(\mathbf{x})]^{-1}\, [L_{\underline{a}}(\mathbf{x})]$$

Fully anisotropic case: the "sym class" is chosen as the "anisotropic class" with $n_s = 21$ and δ_M is taken as 0; then $[\mathbf{A}(\mathbf{x})] = [\underline{a}(\mathbf{x})]^{1/2}[\mathbf{G}(\mathbf{x})]\, [\underline{a}(\mathbf{x})]^{1/2}$.

Computational aspects for constructing realizations of polynomial chaos in high dimension and for an arbitrary measure

• The **objective** is to compute the $(N \times \nu)$ real matrix $[\Psi]$ of the ν independent realizations (**in preserving the orthogonality properties**) of the PCE in **high dimension** and for an **arbitrary probability measure** $p_{\boldsymbol{\Xi}}(\boldsymbol{\xi})\, d\boldsymbol{\xi}$ on $\mathbb{R}^{N_g}$:

$$[\Psi] = \begin{bmatrix} \psi_1(\boldsymbol{\Xi}(\theta_1)) & \dots & \psi_1(\boldsymbol{\Xi}(\theta_\nu)) \\ \cdot & \dots & \cdot \\ \psi_N(\boldsymbol{\Xi}(\theta_1)) & \dots & \psi_N(\boldsymbol{\Xi}(\theta_\nu)) \end{bmatrix}$$

Orthogonality property: $\lim_{\nu \to +\infty} \frac{1}{\nu} [\Psi] [\Psi]^T = [I_N]$.

• **Difficulties**: Problem not trivial at all: the use of the **explicit algebraic formula** (constructed with a symbolic Toolbox) or the use of the **computational recurrence relation** with respect to the degree, induces important numerical noise and the orthogonality property is lost.

If a global orthogonalization was done to correct this problem, then the independence of the realizations would be lost.

• **A new method is proposed to preserve the orthogonality properties and the independence of the realizations**:

[**C. Soize, C. Desceliers**], Computational aspects for constructing realizations of polynomial chaos in high dimension, *SIAM Journal On Scientific Computing*, 32(5), 2820-2831 (2010).

[**G. Perrin, C. Soize, D. Duhamel, C. Funfschilling**], Identification of polynomial chaos representations in high dimension from a set of realizations, *SIAM Journal on Scientific Computing*, 34(6), A2917-A2945 (2012).

(1) Constructing the realizations of the multivariate monomials using a generator of independent realizations of the germs whose probability distribution is the given arbitrary measure.

(2) Performing an orthogonalization of the realizations of the multivariate monomials with an algorithm different from the Gram-Schmidt orthogonalization algorithm which is not stable in high dimension.

• Method proposed for the high dimension and an arbitrary measure

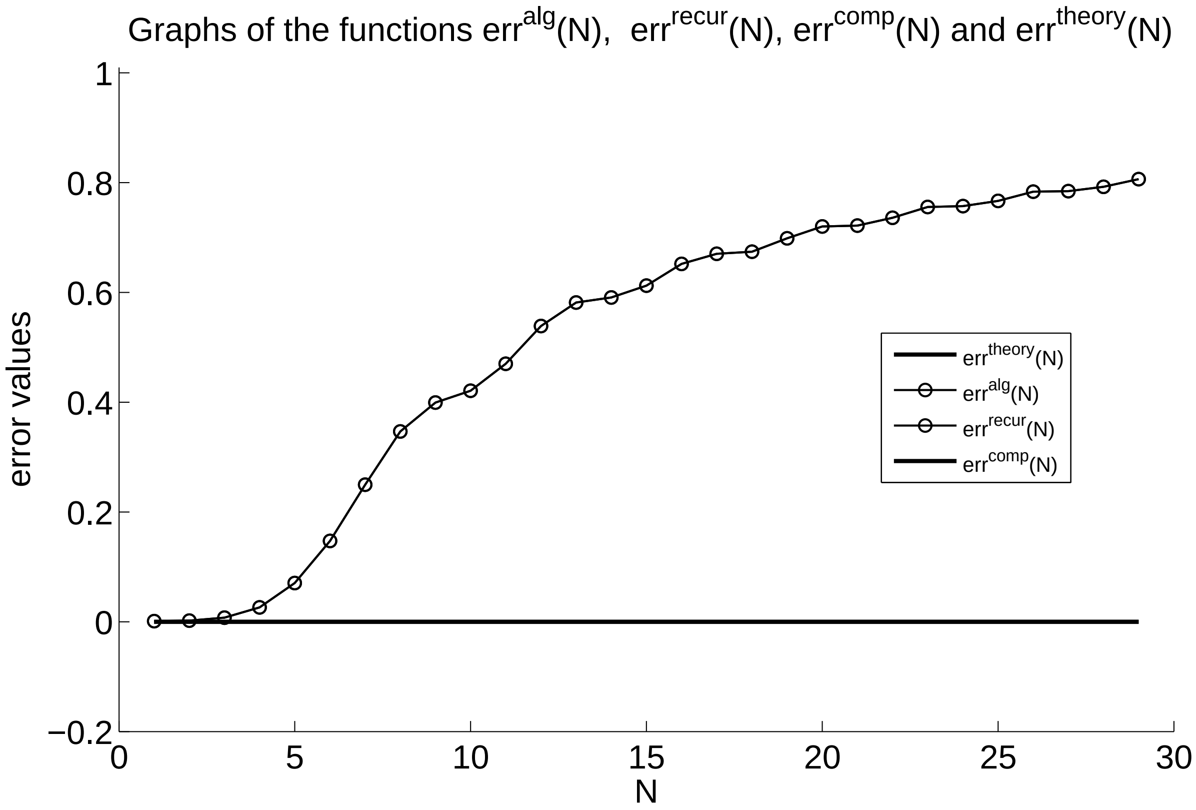
. Multivariate monomials $\mathcal{M}_\alpha(\boldsymbol{\xi}) = \xi_1^{j_1} \times \ldots \times \xi_{N_g}^{j_{N_g}}, \quad \alpha = 1, \ldots, N$.
. Computing the $(N \times \nu)$ real matrix of the ν independent realizations:

$$[M] = [\boldsymbol{\mathcal{M}}(\boldsymbol{\Xi}(\theta_1)) \ldots \boldsymbol{\mathcal{M}}(\boldsymbol{\Xi}(\theta_\nu))] = \begin{bmatrix} \mathcal{M}_1(\boldsymbol{\Xi}(\theta_1)) & \ldots & \mathcal{M}_1(\boldsymbol{\Xi}(\theta_\nu)) \\ \cdot & \ldots & \cdot \\ \mathcal{M}_N(\boldsymbol{\Xi}(\theta_1)) & \ldots & \mathcal{M}_N(\boldsymbol{\Xi}(\theta_\nu)) \end{bmatrix}$$

. Matrix $[\Psi]$ can be written as $[\Psi] = [A]\,[M]$.
. Thus $[\,R\,] = E\{\boldsymbol{\mathcal{M}}(\boldsymbol{\Xi})\,\boldsymbol{\mathcal{M}}(\boldsymbol{\Xi})^T\} = \lim_{\nu \rightarrow +\infty} \frac{1}{\nu}\,[M]\,[M]^T = [A]^{-1}[A]^{-T}$.

The algorithm is then the following:

. Computing matrix $[M]$ and then $[\,R\,] \simeq \frac{1}{\nu}\,[M]\,[M]^T$ for ν sufficiently high.
. Computing $[A]^{-T}$ that corresponds to the Cholesky decomposition of $[\,R\,]$.
. Computing the lower triangular matrix $[A]$.
. Computing $[\Psi] = [A]\,[M]$.



For $N_g = 1$ graphs of the relative error as a function of $N = N_d = 1, \ldots, 30$ with $\nu = 10^6$: Explicit algebraic formula and recurrence equations (thin line with circles); proposed computational method and theory (thick line).

Conclusion

• A new methodology were introduced in 2010-2011 to identify (in high dimension) polynomial chaos expansion of non-Gaussian tensor-valued random fields, with partial experimental data, through a stochastic boundary value problem. Some numerical experiments were performed in high dimension with success (about 6 millions of coefficients were identified for the elasticity random field in 3D).).

• We have presented important improvements of such a methodology for which some recent results obtained in different domains have been included. The numerical validation of such methodology is in progress.