Une nouvelle approche probabiliste non paramétrique des incertitudes de modélisation dans les modèles d'ordre réduit non linéaires

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Outline

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II. Construction of the stochastic model of the SROB on a subset of a compact Stiefel manifold

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I. Problem to be solved and novel approach proposed

I.1- Types of uncertainties and usual terminologies

- **Aleatory uncertainties** concern physical phenomena, which are random by nature

  Examples:

  ▷ The pressure field in a fully developed turbulent boundary layer.

  ▷ The geometrical distribution of the inclusions inside the matrix of a biphasic microstructures.

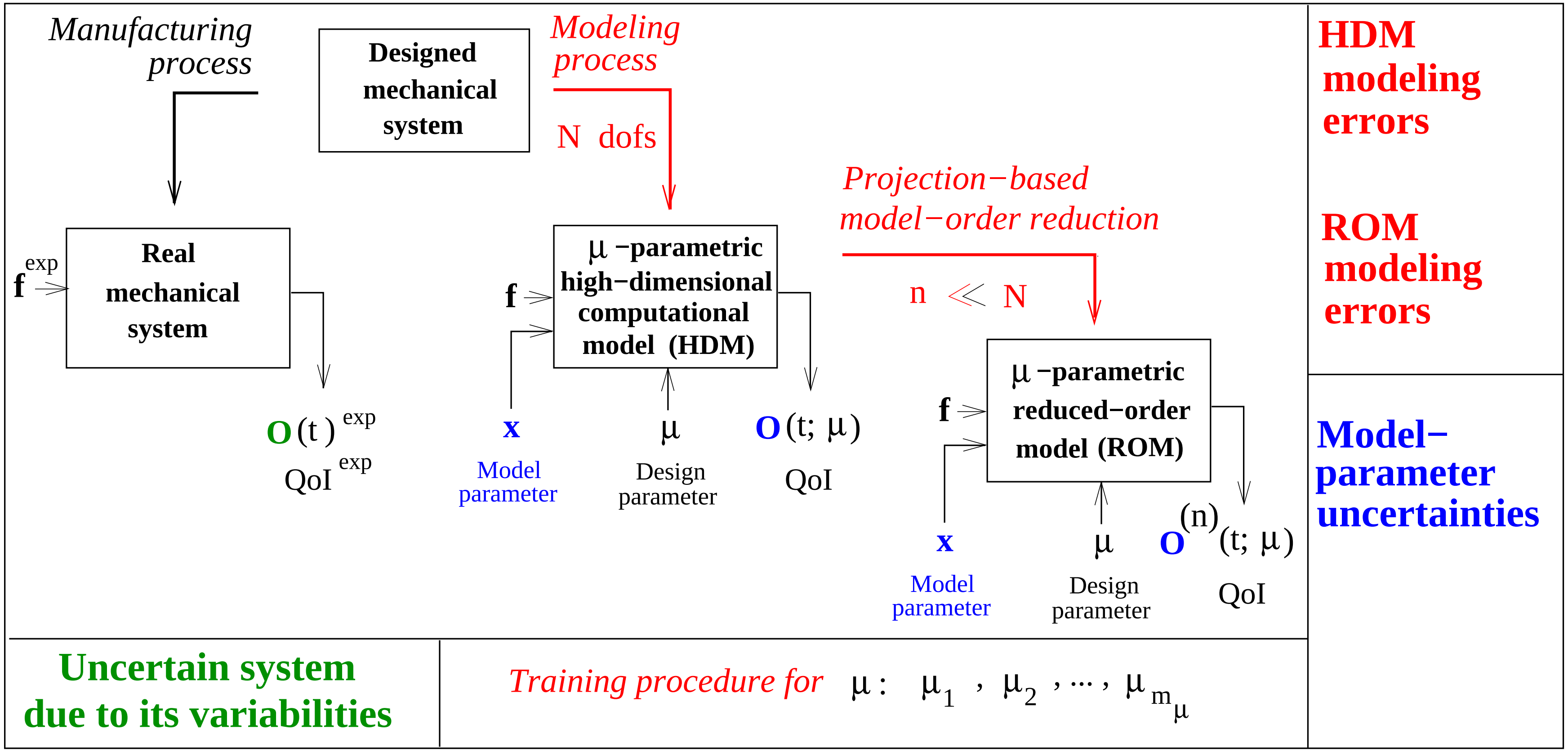
- **Epistemic uncertainties** concern the **model parameters** of a computational model, for which there is a lack of knowledge, and also the **modeling errors**, **which can not be described in terms of uncertainties on the model parameters** of the computational model:

Examples of modeling errors:

▷ No modeling of existing hidden degrees of freedom:
  . Use of some reduced kinematics in a computational model (beam theory instead of the 3D elasticity).
  . Secondary dynamical subsytems that are not modeled.

▷ Modeling errors introduced in the μ-**parametric nonlinear reduced-order model** (**ROM**) constructed from a μ-**parametric nonlinear high-dimensional computational model** (**HDM**).

I.2- Sources of uncertainties and variabilities for a μ-parametric nonlinear ROM constructed from a μ-parametric nonlinear HDM



- Two types of uncertainties: **Model-parameter uncertainties** and **Model uncertainties** induced by **Modeling errors** in the **HDM** and in the **ROM**.
- There are **Variabilities** in the real system, due to the **manufacturing process** and due to **small differences in the configurations** that differ from the designed mechanical system, and is never perfectly known.

I.3- Brief background on the nonlinear time-dependent HDMs and on the projection-based ROMs

- **Usefulness of introducing a nonlinear ROM**

  ▷ Time-dependent numerical simulations based on a μ-**parametric nonlinear HDM** remain so cost-prohibitive that it cannot be used as often as needed.

  ▷ For this reason, μ-**parametric nonlinear ROM** has emerged as a promising numerical tool for **parametric applications** such as design optimization and simulation-based decision making.

  ▷ Among numerous works devoted to the construction of a μ-parametric nonlinear ROM from a μ-parametric nonlinear HDM:

  Grepl, Maday, Nguyen, Patera, Peraire: 2007, 2010
  Chaturantabut, Sorensen: 2010
  Degroote, Virendeels, Willcox: 2010
  Amsallem, Bou-Mosleh, Carlberg, Choi, Cortial, Farhat, Zahr: 2011-2015

• A few words on the construction of a μ-parametric nonlinear ROM

▷ The **projection** of the μ-parametric nonlinear HDM of dimension N onto a subspace dimension $n << N$ is done by using a $(N \times n)$ **reduced-order basis** (**ROB**) $[V]$ **independent of μ**, which yields the μ-parametric nonlinear ROM.

▷ The knowledge about the HDM response is obtained during a **training** procedure: the design parameter vector μ is sampled at **a few points** using an effective sampling strategy

Paul-Dubois-Taine, Amsallem, Farhat: 2015

▷ A set of problems related to the HDM are solved to obtain a set of parametric solution **snapshots** that are **compressed** using, for example, the Singular Value Decomposition (SVD) to construct the ROB $[V]$ independent of μ.

• Computational feasibility and modeling errors

▷ Despite its low dimension, the resulting μ-parametric nonlinear ROM does not necessarily guarantee **computational feasibility** (the construction of the nonlinear ROM does not scale only with its size n, but also with that of the underlying μ-parametric nonlinear HDM, $N >> n$).

A remedy consists in equipping the nonlinear ROM with a procedure for approximating the resulting reduced operators whose computational complexity scales only with the small size n of the ROM (**hyper-reduction method**)

Ryckelynck: 2005
Grepl, Maday, Nguyen, Patera: 2007
Chaturantabut, Sorensen: 2010
Farhat, Avery, Chapman, Cortial: 2014, 2015

▷ It follows that a μ-parametric nonlinear ROM inherits the **modeling errors** induced by the construction of the ROM and also of the modeling errors introduced during the construction of the μ-parametric nonlinear HDM.

I.4- Brief background on how to take into account modeling errors in computational models in the framework of probability theory

▷ Output-predictive error method
▷ Parametric probabilistic methods
▷ Nonparametric probabilistic approach

- **Output-predictive error method**

  ▷ This is an efficient method that consists in introducing a **noise on the output** (or on the QoI) of the computational model (this noise must be identified).

  ▷ Not well-suited for design optimization problems where ROMs are needed, because the μ-parametric HDM and its associated μ-parametric ROM do not learn from data.

  ▷ In the HDM, the modeling errors cannot be taken into account with such a method if there are no available experimental data.

- **Parametric probabilistic methods for modeling uncertainties**

  ▷ Highly developed for model-parameter uncertainties and very efficient for both the μ-parametric HDM and its associated ROM.

  ▷ Among numerous works devoted to methodologies:

  Ghanem, Spanos: 1991, 2003
  Karniadakis, Lucor, Su, Wan, Xiu, Zabaras: 2002, 2004-2015
  Debusschere, Ghanem, Le Maitre, Knio, Najm, Pebay: 2004-2015
  Desceliers, Ghanem, Guilleminot, Nouy, Noshadravan, Perrin, Soize: 2004-2015
  Deodatis, Mace, Pradlwarter, Schueller, Sudret: 2005-2011, 2015
  Arnst, Das, Doostan, Finette, Ghanem, Ghosh, Spall, Tipireddy: 2007-2015
  Cui, Bui-Thanh, Fidkowski, Galbally, Ghattas, Lieberman, Marzouk, Najm, Willcox: 2007-2015

  ▷ However, it **does not allow for taking into account** the model uncertainties induced by **modeling errors introduced** during the construction of the μ-parametric HDM and of the μ-parametric ROM.

• Nonparametric probabilistic approach for modeling uncertainties

▷ Model uncertainties induced by **modeling errors** was initially introduced in the context of *linear* structural dynamics (Soize: 1999, 2000).

Among numerous works devoted to methods and experimental validations:

Arnst, Avalos, Batou, Capiez-Lernout, Chebli, Chen, Clouteau, Cottereau, Desceliers, Duchereau, Durand, Fernandez, Kassem, Mbaye, Mignolet, Murthy, Ohayon, Pellissetti, Poloskov, Ritto, Wang: 2003-2015

▷ Consist in modeling the reduced matrices of the **linear ROM** by **random matrices** whose probability distribution are constructed using the Maximum Entropy Principle (can be used even if there are no available experimental data and can learn from available experimental data).

▷ Although this nonparametric approach was extended to the *nonlinear* geometrical effects in 3D elasticity (Mignolet, Capiez-Lernout: 2008, 2014), this extension **does not hold** for arbitrarily **nonlinear** dynamical systems.

I.5- A novel nonparametric probabilistic approach proposed for taking into account the modeling errors in the nonlinear reduced-order computational models [1]

Independently of the type of nonlinearities, the objective is to take into account the modeling errors that are responsible for the distance between the predictions given by the μ-parametric nonlinear ROM and the available data.

- ◦ Modeling errors associated with the construction of the ROM from the HDM (training for μ, global basis, reduction order).

- ◦ Modeling errors introduced in the construction of the HDM (with respect to the real dynamical system and its variabilities). If experimental data are available, then these uncertainties can be quantified.

[1] Soize C, Farhat C, A nonparametric probabilistic approach for quantifying uncertainties in low- and high-dimensional nonlinear models, *International Journal for Numerical Methods in Engineering*, doi:10.1016/j.jmbbm.2016.06.011, on line, 2016.

- **The nonparametric probabilistic approach proposed consists in:**

  ▷ substituting the deterministic reduced-order basis (ROB) with a **stochastic reduced-order basis** (SROB).

  ▷ constructing the **probability measure** of the SROB on a subset of a **compact Stiefel manifold** in order to preserve some important properties of a ROB.

  ▷ obtaining a SROB that depends on a **small** number of **hyperparameters** that can be identified by solving a reduced-order statistical **inverse problem**.

• Example of a μ-parametric nonlinear HDM

▷ For $\mu \in \mathcal{C}_\mu \subset \mathbb{R}^{m_\mu}$, the μ-parametric nonlinear HDM on $\mathbb{R}^N$ is written as:

$$[M]\,\ddot{\mathbf{y}}(t) + \mathbf{g}(\mathbf{y}(t), \dot{\mathbf{y}}(t); \mu) = \mathbf{f}(t; \mu) \quad , \quad t > t_0$$

$$\mathbf{y}(t_0) = \mathbf{y}_0 \quad , \quad \dot{\mathbf{y}}(t_0) = \mathbf{y}_1$$

with and with $N_{\text{CD}} < N$ constraint equations

$$[B]^T \mathbf{y}(t) = \mathbf{0}_{N_{\text{CD}}} \quad \text{with} \quad [B]^T [B] = [I_{N_{\text{CD}}}]$$

▷ At time t, the quantity of interest (QoI) is a vector in $\mathbb{R}^{m_o}$,

$$\mathbf{o}(t; \mu) = \mathbf{h}(\mathbf{y}(t; \mu), \dot{\mathbf{y}}(t; \mu), \mathbf{f}(t; \mu), t; \mu)$$

• Construction of the associated μ-parametric nonlinear ROM

▷ The **ROB** $[V] \in \mathbb{M}_{N,n}$ (with $n \ll N$) is independent of μ and satisfies

$$[V]^T [M]\, [V] = [I_n] \quad , \quad [B]^T [V] = [0_{N_{\mathrm{CD}},n}]$$

▷ For $\mu \in \mathcal{C}_\mu \subset \mathbb{R}^{m_\mu}$, the μ-parametric nonlinear **ROM** on $\mathbb{R}^n$ is written as:

$$\mathbf{y}^{(n)}(t) = [V]\, \mathbf{q}(t)$$

$$\ddot{\mathbf{q}}(t) + [V]^T \mathbf{g}([V]\, \mathbf{q}(t), [V]\, \dot{\mathbf{q}}(t); \mu) = [V]^T \mathbf{f}(t; \mu) \quad , \quad t > t_0$$

$$\mathbf{q}(t_0) = [V]^T [M]\, \mathbf{y}_0 \quad , \quad \dot{\mathbf{q}}(t_0) = [V]^T [M]\, \mathbf{y}_1$$

$$\mathbf{o}^{(n)}(t; \mu) = \mathbf{h}(\mathbf{y}^{(n)}(t; \mu), \dot{\mathbf{y}}^{(n)}(t; \mu), \mathbf{f}(t; \mu), t; \mu)$$

- **Construction of the associated μ-parametric nonlinear SROM**

  ▷ The **SROB** is the $\mathbb{M}_{N,n}$-valued random matrix $[\mathbf{W}]$, independent of μ, which must satisfy (subset of a compact Stiefel manifold)

$$[\mathbf{W}][M]\,[\mathbf{W}] = [I_n] \quad , \quad [B]^T[\mathbf{W}] = [0_{N_{\mathrm{CD}},n}] \quad , \quad a.s.$$

  ▷ For $\mu \in \mathcal{C}_\mu \subset \mathbb{R}^{m_\mu}$, the μ-parametric nonlinear **ROM** on $\mathbb{R}^n$ is written as:

$$\mathbf{Y}^{(n)}(t) = [\mathbf{W}]\,\mathbf{Q}(t)$$

$$\ddot{\mathbf{Q}}(t) + [\mathbf{W}]^T\mathbf{g}([\mathbf{W}]\,\mathbf{Q}(t), [\mathbf{W}]\,\dot{\mathbf{Q}}(t);\mu) = [\mathbf{W}]^T\mathbf{f}(t;\mu) \quad , \quad t > t_0$$

$$\mathbf{Q}(t_0) = [\mathbf{W}]^T[M]\,\mathbf{y}_0 \quad , \quad \dot{\mathbf{Q}}(t_0) = [\mathbf{W}]^T[M]\,\mathbf{y}_1$$

$$\mathbf{O}^{(n)}(t;\mu) = \mathbf{h}(\mathbf{Y}^{(n)}(t;\mu), \dot{\mathbf{Y}}^{(n)}(t;\mu), \mathbf{f}(t;\mu), t;\mu)$$

• Identification of the hyperparameters of the probability distribution of $[\mathbf{W}]$

▷ The probability distribution of $[\mathbf{W}]$ depends on a hyperparameter $\boldsymbol{\alpha} \in \mathcal{C}_{\boldsymbol{\alpha}} \subset \mathbb{R}^{m_{\boldsymbol{\alpha}}}$, constructed with $m_{\boldsymbol{\alpha}}$ small in order that the identification of $\boldsymbol{\alpha}$ be feasible.

▷ Identification of hyperparameter $\boldsymbol{\alpha}$:

$$\boldsymbol{\alpha}^{\text{opt}} = \min_{\boldsymbol{\alpha} \in \mathcal{C}_{\boldsymbol{\alpha}}} J(\boldsymbol{\alpha})$$

▷ $J(\boldsymbol{\alpha})$ measures a distance between the stochastic QoI $\mathbf{O}^{(n)}$ constructed with the SROM and a corresponding target $\mathbf{o}^{\text{targ}}$:

◇ For modeling errors induced by the use of the ROM instead of the HDM, then $\mathbf{o}^{\text{targ}} = \mathbf{o}$.

◇ For the two types of modeling errors, the one induced by the use of the ROM instead of the HDM and the other one introduced during the construction of the HDM, then $\mathbf{o}^{\text{targ}} = \mathbf{o}^{\text{exp}}$ (experimental data).

II. Construction of the stochastic model of the SROB on a subset of a compact Stiefel manifold

II.1- Compact Stiefel manifold $\mathbb{S}_{N,n}$ and its subspace $\mathcal{S}_{N,n}$

▷ Definition of the compact **Stiefel manifold** $\mathbb{S}_{N,n}$:

$$\mathbb{S}_{N,n} = \{ \ [W] \in \mathbb{M}_{N,n} \ , \ [W]^T [M] \, [W] = [I_n] \ \} \subset \mathbb{M}_{N,n}$$

▷ Definition of the **subspace** $\mathcal{S}_{N,n} \subset \mathbb{S}_{N,n}$ associated with the constraint $[B]^T [W] = [0_{N_{\text{CD}},n}]$ with $[B]^T \, [B] = [I_{N_{\text{CD}}}]$:

$$\mathcal{S}_{N,n} = \{ \ [W] \in \mathbb{M}_{N,n} \ , \ [W]^T [M] \, [W] = [I_n] \ , \ [B]^T [W] = [0_{N_{\text{CD}},n}] \ \}$$

II.2- Parameterization of $\mathbb{S}_{N,n}$ adapted to the high-dimension

For $[V]$ given in $\mathbb{S}_{N,n}$, a non classical parameterization has been constructed:

$$\mathbb{M}_{N,n} \to \mathbb{S}_{N,n}$$
$$[U] \;\mapsto\; [W] \;=\; \mathcal{R}_{s,V}([U])$$

▷ that depends on a parameter s that controls the distance of $[W]$ to $[V]$.

▷ that satisfies the desired property $[V] = \mathcal{R}_{s,V}([0_{N,n}]) \in \mathbb{S}_{N,n}$.

▷ that avoids the usual construction of a big matrix in $\mathbb{M}_{N,N-n}$.

▷ that is based on the use of the polar decomposition of the mapping that maps the tangent vector space $T_V\mathbb{S}_{N,n}$ of $\mathbb{S}_{N,n}$ at the given point $[V]$, into $\mathbb{S}_{N,n}$.

II.3- Construction of a stochastic reduced-order basis (SROB)

- **Stochastic construction that must be done**

▷ The ROB $[V]$ in given in $\mathcal{S}_{N,n} \subset \mathbb{S}_{N,n}$

$$[V][M]\,[V] = [I_n] \quad , \quad [B]^T[V] = [0_{N_{\rm CD},n}]\,.$$

▷ The associated SROB is the random matrix $[\mathbf{W}]$ with values in $\mathcal{S}_{N,n} \subset \mathbb{S}_{N,n}$

$$[\mathbf{W}][M]\,[\mathbf{W}] = [I_n] \quad , \quad [B]^T[\mathbf{W}] = [0_{N_{\rm CD},n}] \qquad a.s.$$

▷ We then have to construct the probability measure $P_{[\mathbf{W}]}$ on $\mathbb{M}_{N,n}$ of random matrix $[\mathbf{W}]$ for which its support is the manifold $\mathcal{S}_{N,n}$,

$$\text{supp}\,P_{[\mathbf{W}]} = \mathcal{S}_{N,n} \subset \mathbb{S}_{N,n} \subset \mathbb{M}_{N,n}$$

and such that, if the statistical fluctuations of $[\mathbf{W}]$ goes to zero, then $[\mathbf{W}]$ goes to $[V]$ in probability distribution.

• Stochastic representation that has been constructed

$[\mathbf{W}]$ is a second-order non-Gaussian and not centered random matrix with values in the manifold $\mathcal{S}_{N,n} \subset \mathbb{S}_{N,n} \subset \mathbb{M}_{N,n}$, which is written as

$$
\begin{aligned}
[\mathbf{W}] &= R_{s,V}([\mathbf{Z}]) = ([V] + s\,[\mathbf{Z}])\,[H_s(\mathbf{Z})]\,,\\
[H_s(\mathbf{Z})] &= ([I_n] + s^2\,[\mathbf{Z}]^T[M]\,[\mathbf{Z}])^{-1/2}\,,\\
[\mathbf{Z}] &= [\mathbf{A}] - [V]\,[\mathbf{D}]\,,\\
[\mathbf{D}] &= ([V]^T[M]\,[\mathbf{A}] + [\mathbf{A}]^T[M]\,[V])/2\,,\\
[\mathbf{A}] &= [\mathbf{U}] - [B]\,\{[B]^T\,[\mathbf{U}]\}\,,\\
[\mathbf{U}] &= [\mathbf{G}(\beta)]\,[\sigma]\,.
\end{aligned}
$$

$[\mathbf{G}(\beta)]$ is a non-Gaussian centered $\mathbb{M}_{N,n}$-valued random matrix detailed in [1].

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[1] Soize C, Farhat C, A nonparametric probabilistic approach for quantifying uncertainties in low- and high-dimensional nonlinear models, *International Journal for Numerical Methods in Engineering*, doi:10.1016/j.jmbbm.2016.06.011, on line, 2016.

• Hyperparameters of the stochastic model

For $[V]$ given in $\mathcal{S}_{N,n}$, the $2 + n(n+1)/2$ hyperparameters of the stochastic model of random matrix $[\mathbf{W}]$ with values in $\mathcal{S}_{N,n}$ are:

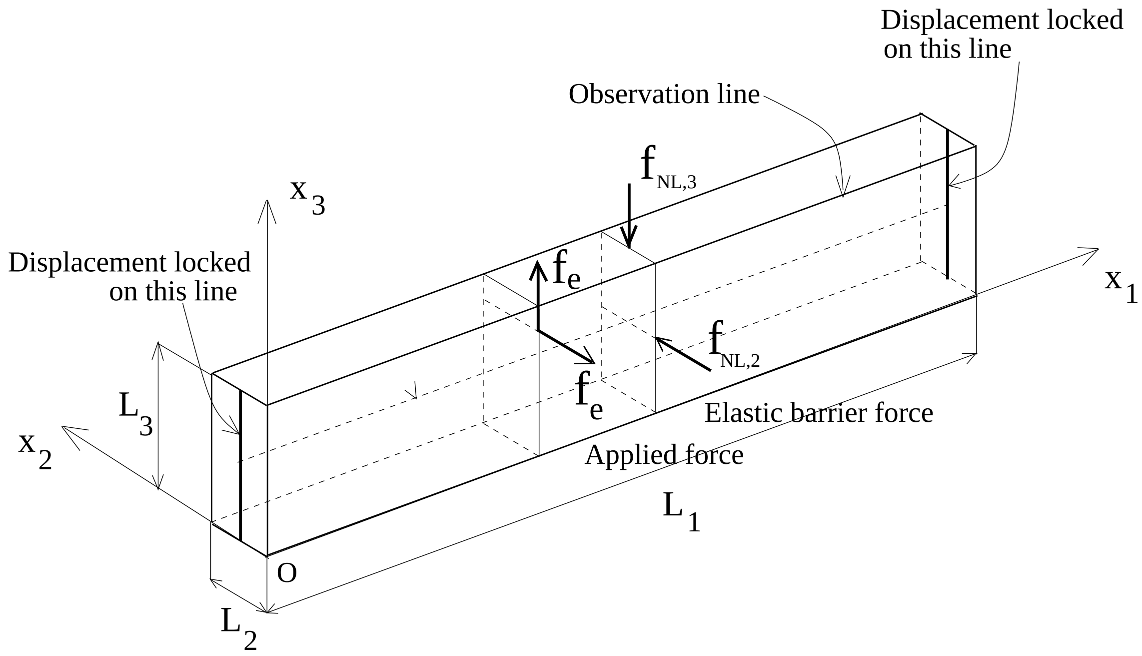
- ▷ $s \geq 0$: control of the level of the statistical fluctuations of $[\mathbf{W}]$ around $[V] \in \mathcal{S}_{N,n}$ (if $s = 0$, then $[\mathbf{W}] = [V]$ a.s.).
- ▷ $\beta > 0$: control of the correlation of the random components of each column of $[\mathbf{W}]$.
- ▷ $[\sigma]$: $(n \times n)$ upper triangular matrix with positive diagonal entries for controlling the correlation between the columns of $[\mathbf{W}]$.

The hyperparameter is thus $\boldsymbol{\alpha} = (s, \beta, \{[\sigma]_{kk'}, 1 \leq k \leq k' \leq n\})$ with length $m_{\boldsymbol{\alpha}} = 2 + n(n+1)/2$, which belongs to the admissible set $\mathcal{C}_{\boldsymbol{\alpha}}$

III. An application in nonlinear structural dynamics

• Description of the mechanical system

▷ 3D slender damped linear elastic bounded medium with two nonlinear elastic barriers that induce **impact non-linearities** in the dynamical system.



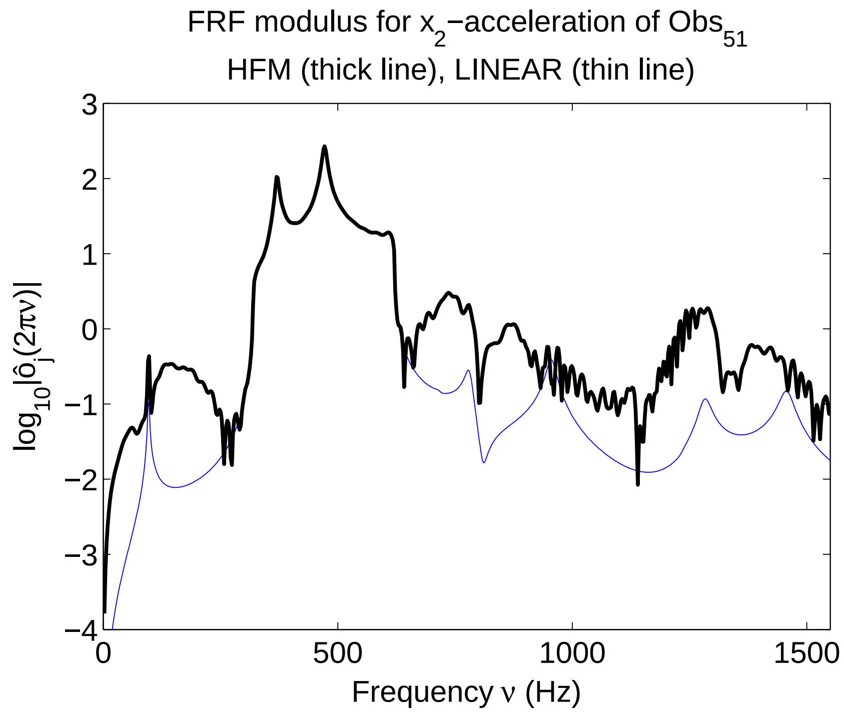
▷ The excitation has an **energy located in a narrow frequency band** $B_e = [320\,,620]$ Hz within a broad frequency band of analysis $B_a = [0\,,1500]$ Hz.

- **HDM, numerical solver, quantification of the effects of the nonlinearities**

  ▷ *HDM*: FEM with $N = 16,653$ dofs and $N_{\rm CD} = 78$.

  ▷ *Numerical solver*: Implicit Newmark time-integration scheme, fixed point method at each sampling time, local adaptive time step (for the shocks).

  ▷ *Quantification of the effects of the nonlinearities*:

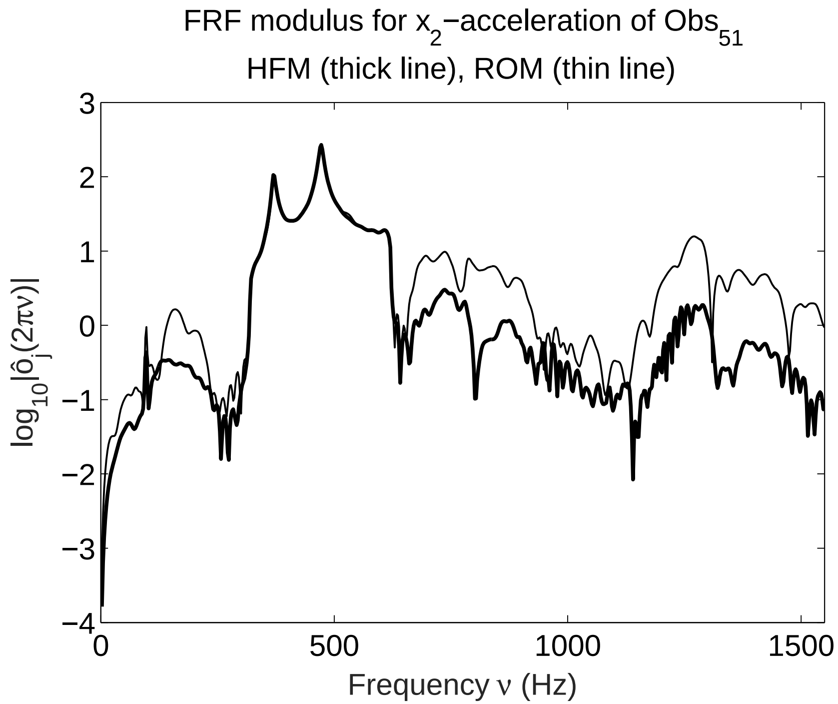


- **ROM, quantification of the errors due to the use of ROM instead of HDM**

▷ *ROM*: $n = 20$ elastic modes (11 in $[0\,,1550]$ Hz and 9 in $[1550\,,3100]$ Hz).

▷ *Numerical solver*: The same as for the HDM.

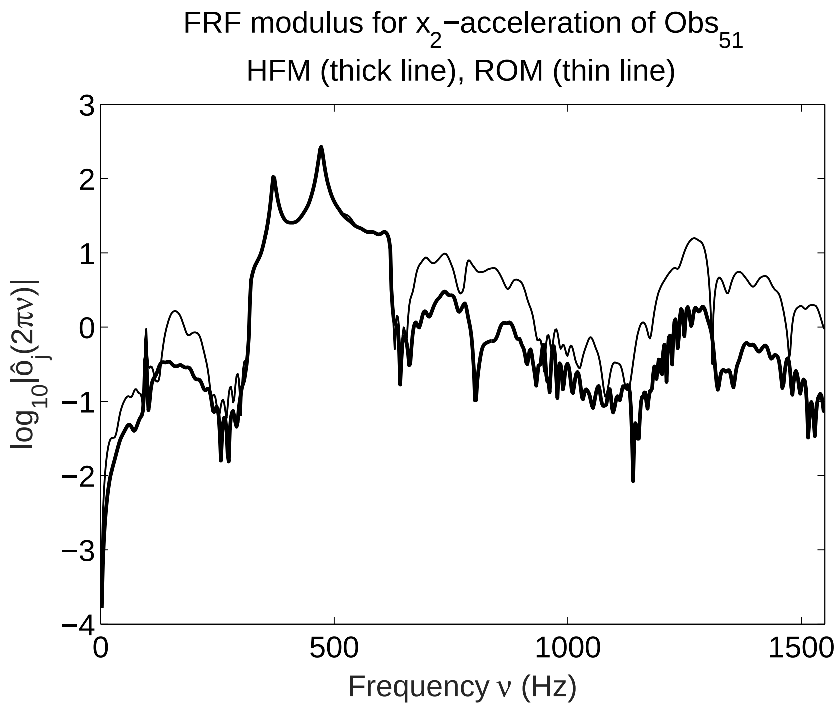
▷ *Quantification of the errors induced by the use of the ROM instead of the HDM*:



▷ Differences between HDM and ROM: small uncertainties in B_e, but large uncertainties outside B_e.

▷ Large uncertainties outside B_e (due to the energy transfer outside B_e) are associated with second-order contributions.

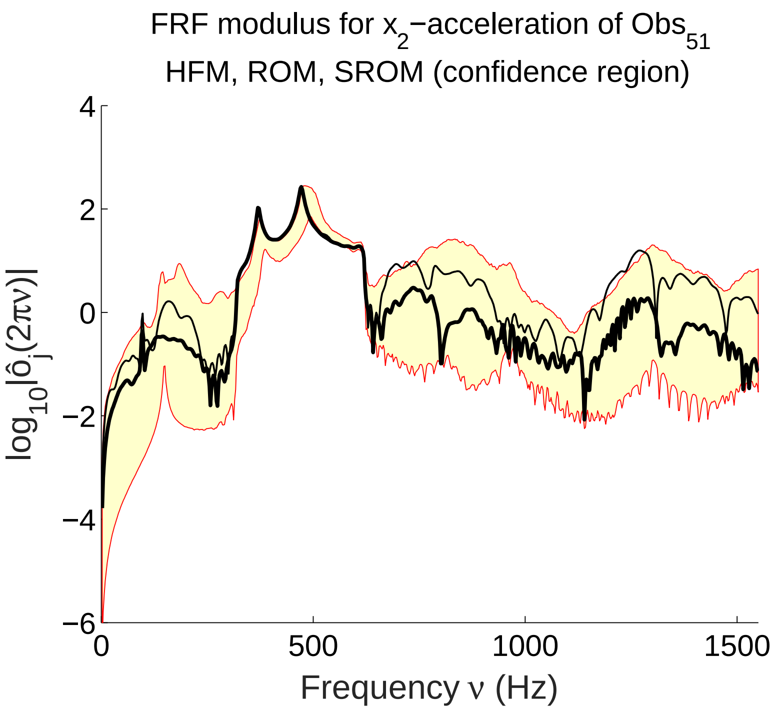
▷ Predicting uncertainties for such a situation is a challenging problem in UQ.



• SROM, stochastic solver, and result

▷ *Identification of the hyperparameter*: $\boldsymbol{\alpha} = (s, \beta, \sigma)$ with length 212, interior-point algorithm with constraints, Monte Carlo with $1\,000$ realizations.

▷ *Prediction of the confidence region (*$p_c = 0.98$*) with the SROM*



IV. Conclusions

- **Novel nonparametric probabilistic approach** for taking into account **modeling errors** in any **nonlinear** high-fidelity model (**HDM**) for which a nonlinear ROM can be constructed.

- The nonparametric probabilistic model is controlled by small number of **hyperparameters** that can be

  - either used as parameters for performing a **sensitivity analysis** with respect to the level of uncertainties

  - or **identified** by solving a statistical inverse problem.

- For the **identification**, the given **target** can be chosen

  - as the level of uncertainties corresponding to the **errors induced by the use of the ROM instead of the HDM**,

  - and/or by the modeling errors (model form uncertainties) introduced in the **HDM with respect to experimental data**.

- This novel **nonparametric** probabilistic approach of **modeling errors** in computational sciences and engineering

  ▷ can simultaneously be **used with** the **parametric** probabilistic approach of the uncertain parameters of the computational models.

  ▷ can also be used for the case of a HDM for which the level of **modeling errors is not the same in the different parts** of the system.

  ▷ can be extended to **CFD**, to **coupled system**, and to any computational model for which a ROM can be constructed.

THANK YOU FOR YOUR ATTENTION