Méthodes spectrales stochastiques et réduction de modèle pour la quantification et la propagation d'incertitudes

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Uncertainty quantification and propagation

Uncertainty quantification has become an essential path in prediction science

- More realistic predictions
  confidence on predictions, robust design
- Analyze the impact of input uncertainty
  variance, sensitivity, hierarchization, reliability and risk
- Comprehension and selection of models

When considering a physical model $\mathcal{M}$ with output u

1. Quantification of input uncertainty. Modeling step using available information.
   Define a probability space $(\Theta, \mathcal{B}, P)$ and consider the model as random:

$$\theta \in \Theta \mapsto \boxed{\mathcal{M}(\theta)}$$

2. Propagation of uncertainty. Characterization of random output $u(\theta)$

$$\boxed{\mathcal{M}(\theta)} \longrightarrow u(\theta)$$

Spectral stochastic methods for uncertainty quantification I

Spectral stochastic methods, initiated by the works of Ghanem and Spanos (1991), can be seen as a functional approach to probability for prediction of the solution of stochastic models. Closely related to Wiener's Polynomial Chaos and its generalizations (Fourier-type representations of random variables)

Main ideas:

- Uncertainties represented by a finite number of "simple" random variables $\boldsymbol{\xi}$ defined on a probability space $(\Theta, \mathcal{B}, P)$.
- Functional representation of any $\sigma(\boldsymbol{\xi})$-measurable random variable $\eta(\theta)$

$$\eta(\theta) = \tilde{\eta}(\boldsymbol{\xi}(\theta))$$

  Random parameters $\boldsymbol{\xi} : \Theta \to \boldsymbol{\Xi}$ are new coordinates of the model defining the stochastic dimensions.

- Classical approximation theory for approximation of functionals

$$\tilde{\eta}(\mathbf{y}) \approx \sum_{\alpha} \eta_\alpha \psi_\alpha(\mathbf{y}), \quad \mathbf{y} \in \boldsymbol{\Xi}$$

Spectral stochastic methods for uncertainty quantification II

Quantification/Discretization of input uncertainty

$$\theta \in \Theta \longrightarrow \boldsymbol{\xi}(\theta) \in \boldsymbol{\Xi}$$

Propagation of uncertainty through a model

$$\boldsymbol{\xi} \longrightarrow \boxed{\mathcal{M}(\boldsymbol{\xi})} \longrightarrow u(\boldsymbol{\xi})$$

Interests

- A general framework for both quantification and propagation of uncertainty
- Information is preserved (not only samples or statistics...)
- Explicit expression of random quantities in terms of random variables $\boldsymbol{\xi}$ with "simple measure" $P_{\boldsymbol{\xi}}$. Cheap post-processing via classical integration

$$\mathbb{E}(f(\eta(\theta))) = \mathbb{E}(f(\tilde{\eta}(\boldsymbol{\xi}(\theta)))) = \int_{\boldsymbol{\Xi}} f(\tilde{\eta}(\mathbf{y}))dP_{\boldsymbol{\xi}}(\mathbf{y})$$

- Other parametric analyses: sensitivity, optimization, inverse problems

Some questions

1. Discretization of uncertainties ?
2. Choice of expansion basis ?
3. Definition and computation of an approximation ?
4. Introduction of extra dimensions dramatically increases the computational complexity. Can we circumvent the curse of dimensionality ?

Outline

Outline

An important question in stochastic analysis: how to represent square integrable functionals of a Brownian motion

- Expansion with multiple Wiener integrals
- Stochastic Itô integrals
- Polynomial Chaos expansions

A Cameron-Martin Theorem I

Let $W_t(\theta)$, $t \in (0, T)$, be a brownian motion defined on probability space $(\Theta, \mathcal{B}, P)$, and let $\{\alpha_k(t)\}_{k\in\mathbb{N}^*}$ be a complete orthonormal system in $L^2(0, T)$. Let

$$\boxed{\xi_k(\theta) = \int_0^T \alpha_k(t) dW_t(\theta), \quad k = 1, ..., \infty}$$

$\boldsymbol{\xi} = \{\xi_k\}_{k\in\mathbb{N}^*}$ forms a countable set of independent Gaussian random variables.

Let $\{h_i\}_{i\in\mathbb{N}} \subset L^2(\mathbb{R})$ be the set of normalized Hermite polynomials and let introduce

$$\boxed{H_\alpha(\boldsymbol{\xi}) = \prod_{k=1}^{\infty} h_{\alpha_k}(\xi_k)}$$

with α a multi-index in

$$\mathcal{I} = \{\alpha = (\alpha_k)_{k\in\mathbb{N}^*}; \alpha_k \in \mathbb{N}, |\alpha| = \sum_{k=1}^{\infty} \alpha_k < \infty\}$$

The H_α are multidimensional Hermite polynomials in Gaussian random variables $\boldsymbol{\xi}$.

A Cameron-Martin Theorem II

Theorem (Cameron-Martin (1947))

The set $\{H_\alpha(\boldsymbol{\xi})\}_{\alpha\in\mathcal{I}}$ *forms a complete orthogonal system in* $L^2(\Theta, \mathcal{B}_T^W, P)$, *with* $\mathcal{B}_T^W = \sigma(W_t; 0 \le t \le T)$. *In other terms, any random variable* $\eta \in L^2(\Theta, \mathcal{B}_T^W, P)$ *can be expressed*

$$\eta = \sum_{\alpha\in\mathcal{I}} \eta_\alpha H_\alpha(\boldsymbol{\xi}), \qquad (\star)$$

with $\eta_\alpha = \mathbb{E}(\eta H_\alpha(\boldsymbol{\xi}))$ *and where the series expansion* $(\star)$ *converges in* $L^2(\Theta, \mathcal{B}_T^W, P)$.

$(\star)$ is a polynomial chaos expansion (Wiener Chaos expansion) of a second order functional of the brownian motion.

▸ Wiener Chaos

Summary

1. Discretization of the Brownian motion, “replaced” by a countable set of random variables $\boldsymbol{\xi}$.
2. Second order functionals of the Brownian motion expressed in terms of $\boldsymbol{\xi}$.

Outline

Polynomial Chaos and Generalizations I

Given a set of random variable $\boldsymbol{\xi}$ on $(\Theta, \mathcal{B}, P)$, with arbitrary measure $P_{\boldsymbol{\xi}}$, we define a Hilbertian basis $\{\psi(\boldsymbol{\xi})\}_{\alpha\in\mathcal{I}}$ of $L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$. For $\eta \in L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$,

$$\boxed{\eta = \sum_{\alpha\in\mathcal{I}} \eta_\alpha \psi_\alpha(\boldsymbol{\xi})}$$

is called a generalized chaos decomposition of η.

Polynomial Chaos and Generalizations II

Generalizations of chaos expansions

- Infinite dimensional case
  - Gaussian measure [Wiener 38]
  - Poisson, Levy processes [Ito 56]
  - Tensor algebras over Hilbert spaces [Segal 56]
  - Polynomial spaces in random variables with arbitrary measure [Ernst 10]
- Finite dimensional case (more classical approximation theory)

$$L^2(\Theta, \sigma(\boldsymbol{\xi}), P) \simeq L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})$$

  - Orthogonal polynomials in independent random variables [Ghanem 91, Xiu 02]
  - "Modified polynomials" for dependent variables with arbitrary measure [Soize 04]
  - Piecewise polynomials [Deb 01, Wan 05], wavelets [Le Maitre 04]
  - Enriched approximation (discontinuities, ...) [Ghosh 08, AN 09]

Polynomials | Non Smooth | Tensorization

Outline

Probabilistic modeling using chaos representations I

Two types of uncertainties can be distinguished

- aleatory uncertainty: random and not reducible.
- epistemic uncertainty: lack of knowledge (information), modeling error

Chaos expansions provide a general framework for uncertainty representation and identification.

Probabilistic modeling using chaos representations II

In practice, uncertainty are characterized by random parameters $X(\theta)$, which have to be expressed in terms of basic random variables

$$X(\theta) = \tilde{X}(\boldsymbol{\xi}(\theta))$$

Uncertainty quantification from data using chaos expansions

▸ Details

Chaos expansion of X in terms of a set of random variables $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_m)$

$$X \approx \sum_{\alpha \in \mathcal{I}_P} a_\alpha \psi_\alpha(\boldsymbol{\xi})$$

- Inference techniques to identify the set of parameters $A = \{a_\alpha\}_{\alpha \in \mathcal{I}_P}$ from data set $\mathcal{X} = \{X^{(i)}\}_{i=1}^{Q}$ [Desceliers 2006, Soize 2010]
- Epistemic uncertainty modeling with further chaos expansion of coefficients $a_\alpha(\theta) \approx \sum_{\alpha'} a_{\alpha,\alpha'} \psi_{\alpha'}(\boldsymbol{\xi}'(\theta))$ [Arnst 2010, Soize 2010]

Outline

Spectral stochastic methods for uncertainty propagation I

After uncertainty modeling and discretization, the model $\mathcal{M}$ is considered as a random parameterized model $\mathcal{M}(\boldsymbol{\xi})$. Random output is seen as a functional

$$\boxed{u : \mathbf{y} \in \boldsymbol{\Xi} \to u(\mathbf{y}) \in \mathcal{V}}$$

and for most models

$$u \in L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}}; \mathcal{V}) = \left\{ u : \boldsymbol{\Xi} \to \mathcal{V} \; ; \; \mathbb{E}(\|u(\boldsymbol{\xi})\|_{\mathcal{V}}^2) \right\} \simeq \mathcal{V} \otimes L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})$$

Propagation of uncertainty

- Construction of an approximation space

$$\boxed{\mathcal{S}_P = span\{\psi_\alpha\}_{\alpha=1}^{P} \subset \mathcal{S} := L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})}$$

Polynomial basis [Ghanem 91, Xiu 02], piecewise polynomials [Deb 01, Le Maitre 04, Wan 05], enriched spectral basis [Ghosh 08, AN 09], generalized chaos basis [Soize 04], ...

Spectral stochastic methods for uncertainty propagation II

- Definition and computation of an approximate functional representation

$$u = \sum_\alpha u_\alpha \otimes \psi_\alpha \in \mathcal{V}_N \otimes \mathcal{S}_P$$

Direct simulations(L^2 *Projection, Interpolation, Regression*) ▸ Link

$$u_\alpha = \sum_k \omega_k^\alpha u(\mathbf{y}_k)$$

where $(\omega_k^\alpha, \mathbf{y}_k) \in \mathbb{R} \times \mathbf{\Xi}$ and the $u(\mathbf{y}_k)$ are solution of deterministic problems:

$$\mathcal{M}(\mathbf{y}_k) \longrightarrow u(\mathbf{y}_k) \in \mathcal{V}_N$$

Galerkin projections

Approximation based on stochastic-weak formulations. In general, equivalent to the solution of a set of P coupled deterministic problems:

$$\boldsymbol{\mathcal{M}}(u_{\alpha_1}, \ldots, u_{\alpha_P}) \longrightarrow \{u_{\alpha_1}, \ldots, u_{\alpha_P}\} \in \mathcal{V}_N \times \ldots \times \mathcal{V}_N$$

Galerkin projections I

Most models in computational science can be synthetized into an operator equation

$$u(\boldsymbol{\xi}) \in \mathcal{V}, \quad A(u(\boldsymbol{\xi}); \boldsymbol{\xi}) = b(\boldsymbol{\xi})$$

which admits a weak solution

$$u \in L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}}; \mathcal{V}) := \mathcal{V} \otimes \mathcal{S}$$

A stochastic-weak solution can be defined by

$$\boxed{< \psi, A(u) >=< \psi, b > \quad \forall \psi \in \mathcal{S}}$$

where for $\psi, \varphi \in \mathcal{S}$, $< \psi, \varphi >= \mathbb{E}(\psi(\boldsymbol{\xi})\varphi(\boldsymbol{\xi}))$.

Galerkin projections II

Galerkin approximation

Approximate solution $u = \sum_{\alpha \in \mathcal{I}_P} u_\alpha \otimes \psi_\alpha \in \mathcal{V} \otimes \mathcal{S}_P$ is defined by

$$\boxed{<\psi, A(u)> = <\psi, b> \quad \forall \psi \in \mathcal{S}_P} \qquad (*)$$

System of coupled deterministic equations defining the coefficients $\{u_\alpha\}_{\alpha \in \mathcal{I}_P} \in (\mathcal{V})^P$

Pros:

Nice mathematical framework, a priori and a posteriori error estimates, stability, efficiency

Cons:

Requires a (sometimes minor) modification of existing deterministic solution techniques. Complexity of system $(*)$.

Galerkin projections III

Galerkin system of equations

After deterministic approximation (finite elements, finite differences, ...), the Galerkin system of equations is

$$\boxed{\mathbf{u} \in \mathbb{R}^N \otimes \mathcal{S}_P, \quad < \psi, \mathbf{A}(\mathbf{u}) >=< \psi, \mathbf{b} > \quad \forall \psi \in \mathcal{S}_P} \tag{1}$$

For linear problems (or linearized nonlinear problems), Galerkin approximation $\mathbf{u}(\boldsymbol{\xi}) = \sum_{\alpha \in \mathcal{I}_P} \mathbf{u}_\alpha \psi_\alpha(\boldsymbol{\xi}) \in \mathbb{R}^N \otimes \mathcal{S}_P$ has its coefficients determined by the system of equations:

$$\sum_{\beta \in \mathcal{I}_P} \mathbb{E}(\mathbf{A}\psi_\alpha \psi_\beta)\mathbf{u}_\beta = \mathbb{E}(\mathbf{b}\psi_\alpha), \quad \forall \alpha \in \mathcal{I}_P$$

System of size $N \times P$

$$\begin{pmatrix} \mathbf{A}_{\alpha_1\alpha_1} & \mathbf{A}_{\alpha_1\alpha_2} & \dots & \mathbf{A}_{\alpha_1\alpha_P} \\ \mathbf{A}_{\alpha_2\alpha_1} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathbf{A}_{\alpha_P\alpha_1} & \dots & \dots & \mathbf{A}_{\alpha_P\alpha_P} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{\alpha_1} \\ \mathbf{u}_{\alpha_2} \\ \vdots \\ \mathbf{u}_{\alpha_P} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_{\alpha_1} \\ \mathbf{b}_{\alpha_2} \\ \vdots \\ \mathbf{b}_{\alpha_P} \end{pmatrix}$$

Galerkin projections IV

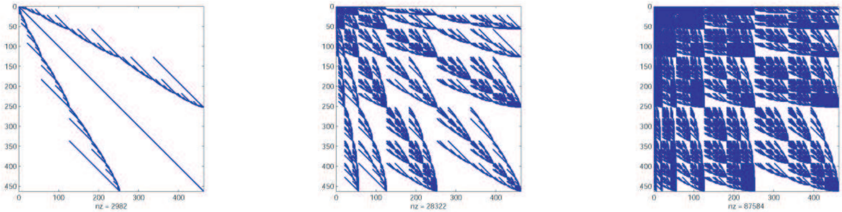
Two levels of sparsity

- Eventual sparsity of each block (inherited from sparsity of $\mathbf{A}(\boldsymbol{\xi})$)
- Block-sparsity (inherited from properties of functions ψ_α)

Illustration of block sparsity: approximation of a Hermite Polynomial Chaos with degree $p = 6$ in dimension $m = 5$

$$\textit{block}\ (\alpha, \beta):\ \mathbf{A}_{\alpha\beta} = \mathbb{E}(\mathbf{A}\psi_\alpha\psi_\beta), \quad \text{with} \quad \mathbf{A}(\boldsymbol{\xi}) = \sum_{|\gamma| \leqslant p_A} \mathbf{A}_\gamma \psi_\gamma(\boldsymbol{\xi})$$

$p_A = 1$ $\qquad$ $p_A = 3$ $\qquad$ $p_A = 5$



If $\mathbf{A}(\boldsymbol{\xi})$ is highly nonlinear in $\boldsymbol{\xi}$, not so sparse !!!

Stochastic Partial Differential Equation I

Model problem: stationary diffusion equation

$$-\nabla \cdot (\kappa(x)\nabla u(x)) = f(x) \quad \textit{for } x \in \Omega, \quad u(x) = 0 \quad \textit{for } x \in \partial\Omega$$

with conductivity κ and source f.

Model stochastic problem

$$-\nabla \cdot (\kappa(x,\theta)\nabla u(x,\theta)) = f(x,\theta) \quad \textit{for } x \in \Omega, \quad u(x) = 0 \quad \textit{for } x \in \partial\Omega$$

where κ and f are stochastic fields defined on a probability space $(\Theta, \mathcal{B}, P)$.

Stochastic Partial Differential Equation II

Space Weak formulation. A space-weak solution u is considered as a random variable with values in $\mathcal{V} \subset H^1(\Omega)$, and should verify

$$\boxed{u(\theta) \in \mathcal{V}, \quad a(u(\theta), v; \theta) = b(v; \theta), \quad \forall v \in \mathcal{V}}$$

with

$$a(u, v; \theta) = \int_\Omega \kappa(x, \theta) \nabla u \cdot \nabla v \, dx, \quad b(v; \theta) = \int_\Omega f(x, \theta) v \, dx$$

Space-Stochastic Weak formulation. A weak solution u is searched in

$$L^2(\Theta, \mathcal{B}, P; \mathcal{V}) \simeq \mathcal{V} \otimes L^2(\Theta, \mathcal{B}, P)$$

such that

$$\boxed{u \in \mathcal{V} \otimes \mathcal{S}, \quad \mathcal{A}(u, v) = \mathcal{L}(v), \quad \forall v \in \mathcal{V} \otimes \mathcal{S}}$$

with

$$\mathcal{A}(u, v) = \mathbb{E}(a(u(\theta), v(\theta); \theta)), \quad \mathcal{L}(v) = \mathbb{E}(b(v(\theta); \theta))$$

Mathematical and numerical analysis I

- Classical functional analysis applies [Babuska 2005, Matthies 2005, Frauenfelder 2005]. Well-posedness in the sense of Hadamard (existence, uniqueness, continuous dependence on data) if $f \in L^2_P(\Theta; L^2(\Omega))$ and

$$0 < \kappa_0 \leq \kappa(x, \theta) \leq \kappa_1 < \infty$$

  See [Soize 2006] for weaker ellipticity conditions. See [Holden 1996] for functional analysis in generalized random variables spaces (distribution) for "non-smooth" data.

- Approximations may be achieved by Galerkin methods

$$\boxed{u_{N,P} \in \mathcal{V}_N \otimes \mathcal{S}_P, \quad \mathcal{A}(u_{N_P}, v_{N,P}) = \mathcal{L}(v_{N,P}), \quad \forall v_{N,P} \in \mathcal{V}_N \otimes \mathcal{S}_P}$$

  Convergence is ensured by Cea's lemma. If $\mathcal{A}$ is a symmetric continuous and coercive bilinear form, it defines a norm $\|\cdot\|_{\mathcal{A}}$ and $u_{N,P}$ is the best approximation of the exact solution u with respect to this norm

$$u_{N,P} = \arg \min_{v \in \mathcal{V}_N \otimes \mathcal{S}_P} \|u - v\|_{\mathcal{A}}$$

- $\mathcal{S}_P$ should represent functions of a finite number of random variables (for computational purpose). Requires a discretization of stochastic fields,

$$\kappa(x,\theta) \approx \kappa^{(m)}(x,\theta) = \kappa(x, \xi_1(\theta), \dots, \xi_m(\theta))$$

e.g. using

  - Finite dimensional Polynomial Chaos expansion
  - Karhunen-Loeve expansion Go

$$\kappa(x,\theta) = \mu_\kappa(x) + \sum_{i=1}^{m} w_i(x)\eta_i(\theta)$$

and eventual further chaos expansion

$$\eta_i(\theta) = \sum_{\alpha \in \mathcal{I}_p^m} \eta_{i,\alpha}\psi_\alpha(\{\xi_k\}_{k=1}^m)$$

- Galerkin methods are stable if no variational crime is committed

The exact random field $\kappa(x,\theta)$ can be expanded in terms of independent random variables $\{\xi_i\}_{i=1}^{\infty}$

$$\kappa(x,\theta) = \sum_{\gamma\in\mathcal{I}} \kappa_\gamma(x)\psi_\gamma(\{\xi_i(\theta)\}_{i=1}^{\infty})$$

where $span\{\psi_\gamma\}_{\gamma\in\mathcal{I}} = L^2(\Theta,\sigma(\{\xi_i\}_{i=1}^{\infty}),P) := \mathcal{S}^\infty$. Initial bilinear form A

$$u,v\in\mathcal{V}\otimes\mathcal{S}^\infty,\quad \mathcal{A}(u,v) = \mathbb{E}(a(u,v;\theta)) = \mathbb{E}(\int_\Omega \kappa(x,\theta)\nabla u\cdot\nabla v\,dx)$$

We introduce a finite dimensional space $span\{\psi_\alpha(\boldsymbol{\xi})\}_{\alpha\in\mathcal{I}_p^m} = \mathcal{S}_p^m \subset \mathcal{S}^\infty$, with $\boldsymbol{\xi} = \{\xi_i\}_{i=1}^m$ (m-dimensional chaos with degree p).

$$u,v\in\mathcal{V}\otimes\mathcal{S}_p^m,\quad \mathcal{A}(u,v) = \sum_{\alpha,\beta\in\mathcal{I}_p^m}\sum_{\gamma\in\mathcal{I}_{2p}^m} \mathbb{E}(\psi_\gamma\psi_\alpha\psi_\beta)\int_\Omega \kappa_\gamma(x)\nabla u_\alpha\cdot\nabla v_\alpha\,dx$$

since $(\psi_\alpha\psi_\beta)\in\mathcal{S}_{2p}^m \perp span\{\psi_\alpha;\alpha\in\mathcal{I}\backslash\mathcal{I}_{2p}^m\}$.

- No variational crime if we replace $\kappa(x,\theta)$ by $\kappa^{(m,2p)}(x,\theta) = \sum_{\gamma\in\mathcal{I}_{2p}^m}\kappa_\gamma\psi_\gamma(\boldsymbol{\xi}(\theta))$
- Galerkin problem is well-posed, while direct methods are not necessarily

Complementary topics

- Improvement of solvers (preconditioners, parallelization, ...)
  [Ghanem 1999, Pellissetti 2000, Matthies 2005, Keese 2005, Powell 2007]
- Random Geometry

$$-\nabla \cdot (\kappa(x)\nabla u(x)) = f(x) \quad \text{for } x \in \Omega(\theta), \quad u(x) = 0 \quad \text{for } x \in \partial\Omega(\theta)$$

  - Fictitious domain [Canuto 2007]
  - Random Mapping [Tartakovsky 2006, Xiu 2006]
  - Level-set and Extended Finite Element [AN 07, AN 08]
- Error estimation, Adaptive approximation
  [Wan 2005, Frauenfelder 2005, Ladevèze 2006, Mathelin 2007]
- Model reduction
  - Stochastic Reduced Basis [Nair 2001, Sachdeva 2006] $\approx$ Krylov iterative solvers.
  - Approximate spectral decompositions [Matthies 2005, Doostan 2007]
  - Generalized Spectral Decomposition [AN 07, AN 08]
  - High dimensional separated representations [Doostan 09, AN 10]

Outline

Tensor product structure of stochastic problems

Stochastic (parameterized) PDEs

$$-\nabla_x(\kappa(x,\boldsymbol{\xi})\nabla_x u(x,\boldsymbol{\xi})) = f(x,\boldsymbol{\xi}), \quad x \in \Omega, \quad \boldsymbol{\xi} = (\xi_1,\ldots,\xi_s) \in \boldsymbol{\Xi}$$

$$u \in H^1(\Omega) \otimes L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}}) := \mathcal{V} \otimes \mathcal{S}$$

Tensor product structure of stochastic function space $\mathcal{S} = L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})$

For independent random variables $(\xi_1,\ldots,\xi_s)$

$$\mathcal{S} = L^2(\Xi_1, \mathcal{B}_{\Xi_1}, P_{\xi_1}) \otimes \ldots \otimes L^2(\Xi_s, \mathcal{B}_{\Xi_s}, P_{\xi_s})$$

Possibly high stochastic (parametric) dimensionality $s \approx 10, 100, 1000, \ldots$

- Many input (random) parameters (source terms, operator's parameters, bc's, ...)
- Random fields or processes with high spectral (multiscale) content:

$$\kappa(x,\theta) = \sum_{i=1}^{s} \kappa_i(x)\xi_i(\theta) \equiv \kappa(x, \xi_1(\theta), \ldots, \xi_s(\theta))$$

Limitation of spectral approaches: the curse of dimensionality

Classical construction of approximation spaces $\mathcal{S}_P \subset \mathcal{S} := \mathcal{S}^1 \otimes \ldots \otimes \mathcal{S}^s$

- Full tensor product approximation

  $\mathcal{S}_P = \mathcal{S}_n^1 \otimes \ldots \otimes \mathcal{S}_n^s$ $\boxed{dim(\mathcal{S}_P) = n^s}$ (exponential increase with s)

- Sparse tensor product approximation

  $\mathcal{S}_P = \sum_{|i| \leqslant n} \mathcal{S}_{i_1}^1 \otimes \ldots \otimes \mathcal{S}_{i_s}^s$ $\boxed{dim(\mathcal{S}_P) = \frac{(n+s)!}{n!s!}}$ (factorial increase with s)

$dim(\mathcal{S}_P) \approx 10, 10^{10}, 10^{100}, 10^{1000}, \ldots$

Simply unreachable with usual representations !!!

Do we need to come back to Monte-Carlo simulations ?

Dimensionality reduction based on separated representations

Separated representation of $v \in \mathcal{S}_n^1 \otimes \ldots \otimes \mathcal{S}_n^s$

$$v(\boldsymbol{\xi}) \approx v_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \alpha_k \phi_k^1(\xi_1) \ldots \phi_k^s(\xi_s)$$

Optimal approximation space for the representation of random variable v

$$v_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \alpha_k \Psi_k(\boldsymbol{\xi}), \quad \Psi_k(\boldsymbol{\xi}) = \phi_k^1(\xi_1) \ldots \phi_k^s(\xi_s) \quad \boxed{span\{\Psi_k\}_{k=1}^{Z} = \mathcal{S}_Z \subset \mathcal{S}_P}$$

$$\boxed{dim(\mathcal{S}_Z) = Z \times n \times s} \quad \text{(linear increase with the dimension } s\text{)}$$

Observation in many applications: for a given precision, the optimal decomposition order Z may be of several orders of magnitude lower than P

$$\boxed{Z \ll P} \quad (\text{typically } Z \approx 10,\ P \approx 10^{100})$$

How to construct these representations ?

Tensor product spaces and Separated representations I

Tensor product of Banach spaces

- Algebraic tensor product space of Banach spaces

$$ {}^{a}\otimes_{k=1}^{d} V_k = span\{w^1 \otimes \ldots \otimes w^d ; w^k \in V_k\} $$

- Tensor product of Banach spaces, endowed with norm $\|\cdot\|$:

$$ V = {}^{\|\cdot\|}\otimes_{k=1}^{d} V_k = \overline{{}^{a}\otimes_{k=1}^{d} V_k}^{\|\cdot\|} $$

Example: SPDEs

$$ L^2(\boldsymbol{\Xi}; \mathcal{V}) = \mathcal{V} \overset{\|\cdot\|}{\otimes} L^2_{P_{\boldsymbol{\xi}}}(\boldsymbol{\Xi}), \quad \|v\|^2 = \int_{\boldsymbol{\Xi}} \|v(\mathbf{y})\|^2_{\mathcal{V}} dP_{\boldsymbol{\xi}}(\mathbf{y}) $$

$$ L^2_{P_{\boldsymbol{\xi}}}(\boldsymbol{\Xi}) = {}^{\|\cdot\|}\otimes_{k=1}^{s} L^2_{P_{\xi_k}}(\Xi_k), \quad \|v\|^2 = \int_{\Xi_1} \ldots \int_{\Xi_s} v(y_1, \ldots, y_s)^2 dP_{\xi_1}(y_1) \ldots dP_{\xi_s}(y_s) $$

Tensor product spaces and Separated representations II

Sets of finite rank tensors

- Rank-1 tensors $\boxed{\mathcal{R}_1 = \{w^1 \otimes \ldots \otimes w^d \ : \ w^k \in V_k\}}$
- Rank-m tensors $\boxed{\mathcal{R}_m = \{\sum_{i=1}^m z_i \ ; \ z_i \in \mathcal{R}_1\} = \mathcal{R}_{m-1} + \mathcal{R}_1}$

Separated representation (tensor product approximation)

$$\boxed{u \approx u_m = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes w_i^d \in \mathcal{R}_m} \qquad \boxed{\|u - u_m\| \underset{m \to \infty}{\longrightarrow} 0}$$

Construction of separated representations

A posteriori construction: knowing u

V is equipped with a crossnorm $\|\cdot\|$

$d = 2$ SVD (Proper Orthogonal Decomposition, Karhunen-Loeve decomposition, ...)

$$\|u - u_m\| = \min_{v_m \in \mathcal{R}_m} \|u - v_m\|$$

$d > 2$ Multidimensional versions of SVD

$$\|u - u_m\| = \min_{v_m \in \mathcal{S}_m \subset \mathcal{R}_m} \|u - v_m\|$$

with $\mathcal{S}_m$ a subset of $\mathcal{R}_m$ with suitable constraints (orthogonality, boundedness, ...)

[Chen 2008, de Silva 2008, Kolda 2009, Uschmajew 2010]

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[Chen 2008, de Silva 2008, Kolda 2009, Uschmajew 2010]

A priori construction: without knowing u but only the problem it solves

Proper Generalized Decomposition

Proper Generalized Decomposition

Weak form of the problem

$$u \in V, \quad \mathcal{A}(u, v) = \mathcal{L}(v) \quad \forall v \in V$$

Aim:

- Define a separated representation u_m of u which is computable without knowing u but only $\mathcal{A}$ and $\mathcal{L}$.

Criteria for the definition of separated representations and associated algorithms:

- Convergence
- Robustness
- Ability to capture a low rank approximation if it exists
- Low computational costs

Variational problems associated with convex optimization I

We consider the case where

$$\mathcal{A}(u,v) - \mathcal{L}(v) = \langle \mathcal{J}'(u), v\rangle$$

where $\mathcal{J}' : V \to V'$ is the differential of a convex and Fréchet differentiable functional $\mathcal{J} : V \to \mathbb{R}$. Equivalent minimization problem:

$$\mathcal{J}(u) = \min_{v\in V} \mathcal{J}(v)$$

Natural definition of PGD

$$\boxed{\mathcal{J}(u_m) = \min_{v_m\in\mathcal{S}_m\subset\mathcal{R}_m} \mathcal{J}(v_m)}$$

- Progressive: knowing $u_{m-1} \in \mathcal{R}_{m-1}$,

$$\mathcal{S}_m = u_{m-1} + \mathcal{R}_1, \quad \mathcal{J}(u_m) = \min_{z\in\mathcal{R}_1} \mathcal{J}(u_{m-1} + z)$$

- Direct, with a suitable choice of $\mathcal{S}_m \subset \mathcal{R}_m$ (for well-posedness)
- Progressive with updates

Variational problems associated with convex optimization II

Well-posedness and convergence results for progressive constructions
[Le Bris & al 2009, Cances & al 2010, Falco & AN 2010]

- Well posedness of this optimization problem is ensured by properties of J (convexity and coercivity) and $\mathcal{R}_1$ (weakly closed in V).
- Under quite general assumptions on $\mathcal{J}$ (ellipticity, uniform continuity of $\mathcal{J}'$ on bounded sets), strong convergence of the sequence u_m can be proved .

Remark *:*

- For $\boxed{d = 2}$, generalized spectral decomposition. Dedicated algorithms [AN 2008].
- For $\boxed{d > 2}$, same (and more) difficulties as for multidimensional SVDs.

Particular case of linear elliptic problems

If $\mathcal{A}$ is a symmetric continuous coercive bilinear form on a Hilbert space $(V, \|\cdot\|)$,

$$\mathcal{J}(v) = \frac{1}{2}\mathcal{A}(v,v) - \mathcal{L}(v)$$

$\mathcal{A}$ defines a norm $\|\cdot\|_{\mathcal{A}} : v \mapsto \mathcal{A}(v,v)^{1/2}$, which is equivalent to $\|\cdot\|$.

Progressive PGD

$$\mathcal{J}(u_m + z_{m+1}) = \min_{z \in \mathcal{R}_1} \mathcal{J}(u_m + z) \quad \Leftrightarrow \quad \boxed{\|u - u_m - z_{m+1}\|_{\mathcal{A}}^2 = \min_{z \in \mathcal{R}_1} \|u - u_m - z\|_{\mathcal{A}}^2}$$

Interpretation as a generalized multidimensional SVD [AN 2007, Falco & AN 2010]

$$\boxed{\|u - u_m\|_{\mathcal{A}}^2 = \|u\|_{\mathcal{A}}^2 - \sum_{i=1}^m \sigma_i^2 \underset{m\to\infty}{\longrightarrow} 0} \qquad \boxed{\sigma_m = \max_{w \in \mathcal{R}_1; \|w\|_{\mathcal{A}}=1} (u - u_{m-1}, w)_{\mathcal{A}}}$$

where $\sigma_m = \|z_m\|_{\mathcal{A}}$ is interpreted as the dominant singular value of $(u - u_m)$.

Possible construction with alternated direction algorithm

In order to compute $z_{m+1} \in \mathcal{R}_1$,

$$\min_{w^1 \in V_1} \mathcal{J}(u_m + w^1 \otimes w^2 \otimes \ldots) \quad \ldots \quad \ldots \quad \min_{w^d \in V_d} \mathcal{J}(u_m + \ldots \otimes w^{d-1} \otimes w^d)$$

For a given $z = \otimes_{k=1}^{d} w^k$, we introduce the linear subspace $\mathcal{R}_1^l(z) \subset \mathcal{R}_1 \subset V$ defined by

$$\mathcal{R}_1^l(z) = w^1 \otimes \ldots \otimes V_l \otimes \ldots \otimes w^d$$

Alternated direction algorithm

Starting from an initial guess $z^{(0)} \in \mathcal{R}_1$, we construct a sequence $\{z^{(n)}\}_{n\in\mathbb{N}}$ defined by

$$\boxed{z^{(n+1)} = f_m^d \circ \ldots \circ f_m^1(z^{(n)})} \qquad f_m^l(z) = \arg \min_{\hat{z} \in \mathcal{R}_1^l(z)} \mathcal{J}(u_m + \hat{z})$$

corresponding to successive Galerkin projections on linear subspaces

$$\boxed{z^\diamond = f_m^l(z) \quad \Leftrightarrow \quad z^\diamond \in \mathcal{R}_1^l(z), \quad \mathcal{A}(u_m + z^\diamond, z^*) = \mathcal{L}(z^*) \quad \forall z^* \in \mathcal{R}_1^l(z)}$$

The important case $d = 2$: Generalized Spectral Decomposition

$$\min_{w^1 \in V_1, w^2 \in V_2} \mathcal{J}(u_m + w^1 \otimes w^2)$$

$$w^1 = f_m^1(w^2) \quad \Leftrightarrow \quad w^1 = \arg\min_{w^1 \in V_1} \mathcal{J}(u_m + w^1 \otimes w^2)$$

$$w^2 = f_m^2(w^1) \quad \Leftrightarrow \quad w^2 = \arg\min_{w^2 \in V_2} \mathcal{J}(u_m + w^1 \otimes w^2)$$

Equivalent pseudo eigenproblem formulated on $w^1 \in V_1$

Find the dominant eigenvector w^1 of the following pseudo-eigenproblem

$$\boxed{w^1 = f_m^1 \circ f_m^2(w^1) := \sigma_m(w^1)^{-1} T(w^1)}$$ T $\equiv$ pseudo correlation operator

with $$\boxed{w^1 \in \arg\min_{w^1 \in V_1} \mathcal{J}(u_m + w^1 \otimes f_m^2(w^1))}$$ $\sigma_m(w^1) \equiv$ dominant singular value

Efficient algorithms inspired from classical eigenproblems [AN CMAME 2007, 2008]

Alternative definitions for Proper Generalized Decompositions

Alternative formulations for general nonsymmetric problems

- Minimal Residual PGD [AN & Ladeveze 2004, **Doostan 2009**, Ammar 2010, AN & Falco 2010]
- Galerkin PGD [Ladeveze 1980, **AN 2007, AN 2008, AN & Le Maitre 2009**, Chinesta 2007]
- Petrov-Galerkin (MiniMax) PGD [AN 2010]
- Norm induced by the operator [Lozinski 2010]

Progressive or Direct construction of rank-m approximations

- Purely progressive
- Progressive with updates
- Direct

A. Nouy (2010). PGD for time dependent PDEs.
Computer Methods in Applied Mechanics and Engineering.

Solution strategy for high dimensional stochastic problems

A 2-level tensor product approximation $u \in \mathcal{V} \otimes \underbrace{\mathcal{S}^1 \otimes \ldots \otimes \mathcal{S}^s}_{\mathcal{S}}$

1. 2D PGD for a quasi optimal deterministic/stochastic separation

$$\boxed{u \approx u_M(\boldsymbol{\xi}) = \sum_{i=1}^{M} w_i \lambda_i(\boldsymbol{\xi})} \quad W = (w_i)_{i=1}^{M} \in (\mathcal{V})^M, \quad \Lambda = (\lambda_i)_{i=1}^{M} \in (\mathcal{S})^M$$

Requires the solution of a few deterministic problems ($\approx M$) and stochastic algebraic equations (reduced order model at the deterministic level).

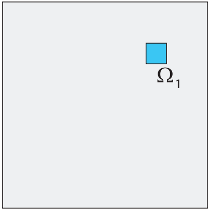
2. Multidimensional PGD for solving stochastic algebraic equations

$$\boxed{\Lambda(\boldsymbol{\xi}) \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \phi_k^1(\xi_1) \ldots \phi_k^s(\xi_s)}, \quad \phi_k^0 \in \mathbb{R}^M, \quad \phi_k^j \in \mathcal{S}_n^j$$

Nouy, A. (2010, In press).
PGD and separated representations for the numerical solution of high dimensional stochastic problems.
Archives of Computational Methods in Engineering

Illustration : stationary advection-diffusion-reaction equation

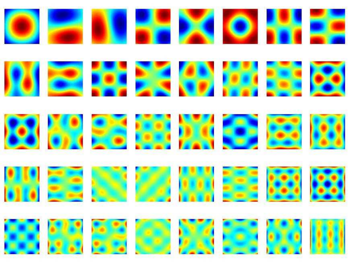
$$-\nabla \cdot (\kappa \nabla u) + c \cdot \nabla u + \gamma u = \delta I_{\Omega_1}(x) \quad on \quad \Omega$$



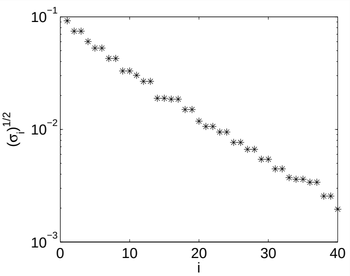
Random field

$$\kappa(x, \boldsymbol{\xi}) = \mu_\kappa + \sum_{i=1}^{40} \sqrt{\sigma_i} \kappa_i(x) \xi_i, \quad \xi_i \in U(-1, 1)$$

Spatial modes $\kappa_i(x)$



Amplitudes σ_i



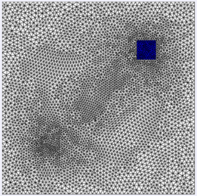
Stochastic approximation

$$\boldsymbol{\xi} = (\xi_1, \dots, \xi_{40}), \quad \boldsymbol{\Xi} = (-1,1)^{40} = \Xi_1 \times \dots \times \Xi_{40}$$

$$\mathcal{S}_P = \mathbb{P}_4(\Xi_1) \otimes \dots \otimes \mathbb{P}_4(\Xi_{40})$$

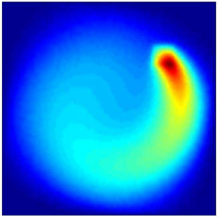
$$dim(\mathcal{S}_P) = 5^{40} \approx 10^{28}$$

Finite element mesh



$$dim(\mathcal{V}_N) = 4435$$

Solution $u(\cdot, \boldsymbol{\mu}_{\boldsymbol{\xi}})$ for mean parameters



Results... in brief

Deterministic/stochastic separation

$$u(\boldsymbol{\xi}) \approx u_M(\boldsymbol{\xi}) = \sum_{i=1}^{M} w_i \lambda_i(\boldsymbol{\xi})$$

$\hookrightarrow$ $\boxed{\mathcal{V}_M = span\{w_i\}_{i=1}^{M}}$

Random variables separation

$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^{M} \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

$\hookrightarrow$ $\boxed{\mathcal{S}_Z = span\{\prod_{j=1}^{s} \phi_k^j(\xi_j)\}_{k=1}^{Z}}$

For a precision $\|u - u_{M,Z}\|_{L^2} \leqslant 10^{-2}$

- $\boxed{dim(\mathcal{V}_M) \approx 15} \ll 4435 = dim(\mathcal{V}_N)$
- $\boxed{dim(\mathcal{S}_Z) \approx 10} \ll 10^{28} = dim(\mathcal{S}_P)$
- 15 classical deterministic problems in order to build $\mathcal{V}_M \subset \mathcal{V}_N$
- about 1 minute computation on a laptop with matlab

▸ Results

Conclusions

PGD methods for stochastic problems

- Separation of difficulties: deterministic/stochastic separation
  partly non intrusive Galerkin stochastic method
- Reduced order model construction
  a priori construction of quasi-optimal reduced basis
- Separation in high-dimensional tensor product spaces :
  a way to circumvent the curse of dimensionality

Special Issue on Recent advances in PGD.
Chinesta, Cueto, Ladevèze & Nouy (Eds).
Archives Computational Methods in Engineering, 2010 (In press).

Open questions and perspectives

Open questions for PGD

- Mathematical analysis of the pseudo eigenproblem ?
- Optimality for non-symmetric problems ?
- Error estimation and Goal-oriented approximations

Open questions for separated representations in stochastic analysis

- How to separate dimensions ? Depends on the "separability" of the solution
- Adaptive stochastic dimension: hierarchical tensor product, ...

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SIAM J. Sci. Comput., 28(3):1167–1185.

Karhunen-Loève expansion

Return

We consider a random field $\kappa(x,\theta)$, $(x,\theta) \in \Omega \times \Theta$, such that

$$\kappa \in L^2(\Omega) \otimes L^2(\Theta, \mathcal{B}, P)$$

with mean and covariance functions

$$\mu_\kappa(x) = \mathbb{E}(\kappa(x,\theta)), \quad C_\kappa(x,y) = \mathbb{E}\left((\kappa(x,\theta) - \mu_\kappa(x))(\kappa(y,\theta) - \mu_\kappa(y))\right)$$

- We introduce the covariance operator

  $$T : w \in L^2(\Omega) \mapsto \int_\Omega C_\kappa(x,y) w(y)\, dy \in L^2(\Omega)$$

  and consider the eigenproblem

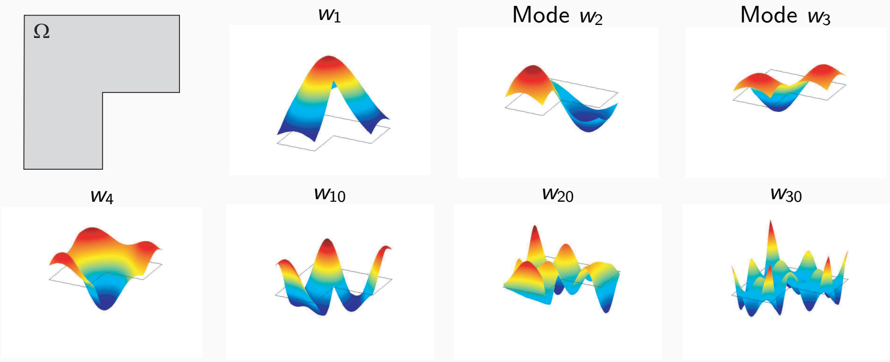
  $$T(w) = \sigma w$$

- Operator T is compact and classical spectral theory applies
  - Countable set of eigenvalues $\{\sigma_i\}_{i=1}^\infty$, positive, bounded and with only accumulation point 0.
  - The set of eigenfunctions $\{w_i(x)\}_{i=1}^\infty$ forms a hilbertian basis of $L^2(\Omega)$

Illustration

L-shaped domain $\Omega \subset (0,2) \times (0,2)$. Exponential square covariance function

$$C_\kappa(x,y) = exp(-\frac{|x-y|^2}{2l^2}), \quad l = 1/2.$$



Karhunen-Loève expansion

Karhunen-Loeve expansion

Random field κ admits the following series expansion

$$\kappa(x,\theta) = \mu_\kappa(x) + \sum_{i=1}^{\infty} w_i(x)\eta_i(\theta), \qquad \eta_i = < \kappa - \mu_\kappa, w_i >_{L^2(\Omega)}$$

where convergence is in $L^2(\Omega) \otimes L^2(\Theta, \mathcal{B}, P)$.

Truncation (Discretization)

$$\kappa(x,\theta) \approx \kappa^{(m)}(x,\theta) = \mu_\kappa(x) + \sum_{i=1}^{m} w_i(x)\eta_i(\theta)$$

$\kappa^{(m)}$ is the best approximation of this form in $L^2(\Omega) \otimes L^2_P(\Theta)$, i.e.

$$\|\kappa - \kappa^{(m)}\|^2 = \min_{w_i \in L^2(\Omega), \eta_i \in L^2(\Theta)} \|\kappa - \mu_\kappa - \sum_{i=1}^{m} w_i \otimes \eta_i\|^2$$

Karhunen-Loeve $\Leftrightarrow$ Singular Value Decompositon

Let $\kappa \in L^2(\Omega) \otimes L^2_P(\Theta)$ and let $u = \kappa - \mu_\kappa \in L^2(\Omega) \otimes L^2_P(\Theta)$. We introduce the operator

$$\begin{array}{cccccl} U & : & L^2(\Omega) & \longrightarrow & L^2_P(\Theta) \\ & & w & \longmapsto & \eta(\theta) =< u(\cdot,\theta), w >_{L^2(\Omega)} = \int_\Omega u(y,\theta)w(y)dy \end{array}$$

Karhunen-Loeve expansion of u is equivalent to a Singular Value Decomposition of operator U.

For $w \in L^2(\Omega)$ and $\eta \in L^2_P(\theta)$

$$< \eta, U(v) >_{L^2_P(\Theta)} =< U^*(\eta), v >_{L^2(\Omega)}$$

with U^* the adjoint operator of U defined by

$$\begin{array}{cccccl} U^* & : & L^2_P(\Theta) & \longrightarrow & L^2(\Omega) \\ & & \eta & \longmapsto & w(x) =< u(x,\cdot), \eta >_{L^2_P(\Theta)} = \mathbb{E}(u(x,\theta)\eta(\theta)) \end{array}$$

and U^*U is the covariance operator of κ:

$$U^*U(w) =< u, < u, w >_{L^2(\Omega)} >_{L^2_P(\Theta)} = \int_\Omega \mathbb{E}(u(\cdot,\theta)u(y,\theta))w(y)dy = T(w)$$

Let $(\Theta, \mathcal{B}, P)$ be a probability space. Let $\boldsymbol{\xi} = (\xi_k)_{k\in\mathbb{N}^*}$ be a set of centered Gaussian random variables called basic random variables. $\sigma(\boldsymbol{\xi}) \subset \mathcal{B}$ denotes the corresponding σ-algebra.

We consider the set of second order random variables $L^2(\Theta, \mathcal{B}, P)$ which is a Hilbert space for the inner product

$$< f, g >_{L^2(\Theta,\mathcal{B},P)} = \mathbb{E}(f(\theta)g(\theta)) = \int_\Theta f(\theta)g(\theta)dP(\theta)$$

Let $\mathbb{P}_n(\mathbb{R}^m)$ be the set of m-variate polynomial of degree n and let $\mathcal{P}_n(\boldsymbol{\xi})$ be the set of polynomials of degree n in a finite subset of random variables $\boldsymbol{\xi}$

$$\mathcal{P}_n(\boldsymbol{\xi}) = \{p(\xi_{i_1}, \ldots, \xi_{i_m}); p \in \mathbb{P}_n(\mathbb{R}^m), i_1, \ldots, i_m \in \mathbb{N}^*, m \in \mathbb{N}\}$$

$$\mathcal{P}_n(\boldsymbol{\xi}) \subset L^2(\Theta, \sigma(\boldsymbol{\xi}), P) \subset L^2(\Theta, \mathcal{B}, P)$$

$\mathcal{P}_n(\boldsymbol{\xi})$ is called the polynomial chaos of degree n.

We then define

$$\mathcal{H}_n(\boldsymbol{\xi}) = \mathcal{P}_n(\boldsymbol{\xi}) \ominus \mathcal{P}_{n-1}(\boldsymbol{\xi})$$

$\mathcal{H}_n(\boldsymbol{\xi})$ is called the homogeneous chaos of degree n.

Wiener (1938)

$L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$ admits the following orthogonal decomposition

$$L^2(\Theta, \sigma(\boldsymbol{\xi}), P) = \overline{\bigoplus_{n=0}^{\infty} \mathcal{H}_n}$$

If we denote Π_n the orthogonal projector from $L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$ onto $\mathcal{H}_n(\boldsymbol{\xi})$, any $\eta \in L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$ admits the mean square convergent orthogonal series expansion

$$\eta = \sum_{n=0}^{\infty} \Pi_n \eta$$

For a practical construction of chaos expansion, we introduce the set of normalized Hermite polynomials $\{h_i\}_{i\in\mathbb{N}}$ and

$$H_\alpha(\boldsymbol{\xi}) := \prod_{k=1}^{\infty} h_{\alpha_k}(\xi_k)$$

with α a multi-index in $\mathcal{I} = \{\alpha = (\alpha_k)_{k\in\mathbb{N}^*}; \alpha_k \in \mathbb{N}, |\alpha| = \sum_{k=1}^{\infty} \alpha_k < \infty\}$. Therefore,

$$\boxed{\mathcal{P}_n(\boldsymbol{\xi}) = span\{H_\alpha(\boldsymbol{\xi}); \alpha \in \mathcal{I}_n\}, \quad \mathcal{I}_n = \{\alpha \in \mathcal{I}, |\alpha| \leq n\}}$$

and

$$\boxed{\mathcal{H}_n(\boldsymbol{\xi}) = span\{H_\alpha(\boldsymbol{\xi}); \alpha \in \mathcal{J}_n\}, \quad \mathcal{J}_n = \{\alpha \in \mathcal{I}, |\alpha| = n\}}$$

Any second order random variable $\eta \in L^2(\Theta, \sigma(\boldsymbol{\xi}), P)$ admits the following mean square convergent expansion

$$\boxed{\eta = \sum_{\alpha \in \mathcal{I}} \eta_\alpha H_\alpha(\boldsymbol{\xi}) = \sum_{n=0}^{\infty} \sum_{\alpha \in \mathcal{J}_n} \eta_\alpha H_\alpha(\boldsymbol{\xi})}$$

For computational purpose, approximations may be achieved by

- using finite order Polynomial Chaos expansions

$$\eta = \sum_{\alpha \in \mathcal{I}_p} \eta_\alpha H_\alpha(\boldsymbol{\xi}) = \sum_{n=0}^{p} \sum_{\alpha \in \mathcal{J}_n} \eta_\alpha H_\alpha(\boldsymbol{\xi})$$

- retaining a finite number of random variables $\boldsymbol{\xi} = \{\xi_i\}_{i=1}^m$ and using a finite dimensional polynomial chaos

$$\mathcal{P}_n(\boldsymbol{\xi}) = span\{H_\alpha(\boldsymbol{\xi}); \alpha \in \mathcal{I}_n^m\} \quad \mathcal{I}_n^m = \{\alpha \in \mathbb{N}^m; |\alpha| \leq n\}$$

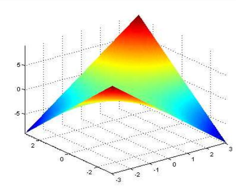
Wiener Chaos

Return V

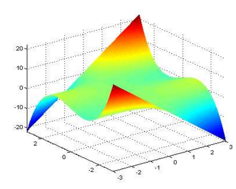
First Polynomials of the Chaos expansion

$$
\begin{array}{llll}
\text{Order } 0: & H_{(0,0,0,\dots)}(\boldsymbol{\xi}) = 1 & & \\
\text{Order } 1: & H_{(1,0,0,\dots)}(\boldsymbol{\xi}) = \xi_1, & H_{(0,1,0,\dots)}(\boldsymbol{\xi}) = \xi_2, & \dots \\
\text{Order } 2: & H_{(1,1,0,\dots)}(\boldsymbol{\xi}) = \xi_1\xi_2, & H_{(2,0,0,\dots)}(\boldsymbol{\xi}) = \frac{1}{\sqrt{2}}(\xi_1^2 - 1), & \dots \\
\dots & & &
\end{array}
$$

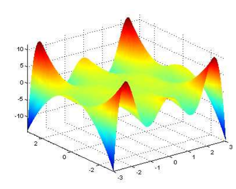
$H_{(1,1)}(x_1, x_2)$



$H_{(1,3)}(x_1, x_2)$



$H_{(8,2)}(x_1, x_2)$



Outline

L^2 projection

Return

Letting $\{\psi_\alpha\}_{\alpha=1}^{P}$ be an orthonormal basis of $\mathcal{S}_P \subset L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})$, we define

$$u(\boldsymbol{\xi}) \approx \sum_{\alpha=1}^{P} u_\alpha \psi_\alpha(\boldsymbol{\xi}), \quad u_\alpha \in \mathcal{V}_N$$

with

$$u_\alpha = < u, \psi_\alpha >_{L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})} = \mathbb{E}(u(\boldsymbol{\xi})\psi_\alpha(\boldsymbol{\xi})) = \int_{\boldsymbol{\Xi}} u(\mathbf{y})\psi_\alpha(\mathbf{y}) dP_{\boldsymbol{\xi}}(\mathbf{y})$$

Numerical quadrature

$$u_\alpha \approx \sum_{k=1}^{Q} u(\mathbf{y}_k)\psi_\alpha(\mathbf{y}_k)\omega_k$$

with $\{\mathbf{y}_k, \omega_k\}_{k=1}^{Q}$ a quadrature rule on $\boldsymbol{\Xi}$ adapted to measure $P_{\boldsymbol{\xi}}$:

- Monte-Carlo or Quasi Monte-Carlo
- Gauss quadrature [Le Maitre 01, Reagan 03, ...]
- Sparse quadrature [Smolyak 1963, Keese & Matthies 2005]

Interpolation - Collocation

Return

Letting $\{\psi_\alpha\}_{\alpha=1}^P$ be an interpolation basis associated with interpolation points $\{\mathbf{y}_\alpha\}_{\alpha=1}^P$.

$$u(\boldsymbol{\xi}) \approx \sum_{\alpha=1}^{P} u_\alpha \psi_\alpha(\boldsymbol{\xi}),$$

with

$$u_\alpha = u(\mathbf{y}_k) \in \mathcal{V}_N$$

Construction of interpolation grids

- Tensorized grids [Babuska 2007]
- Sparse Grids [Webster 2007, Nobile 2008]
- Anisotropic Sparse Grids [Nobile 2008], based on a priori error estimates

Regression

Let $J(\boldsymbol{\xi}) = f(u(\boldsymbol{\xi}))$ be a quantity of interest, with $J : \boldsymbol{\Xi} \to \mathbb{R}$. We seek for an approximation

$$J(\boldsymbol{\xi}) \approx \sum_{\alpha \in \mathcal{I}_P} J_\alpha \psi_\alpha(\boldsymbol{\xi})$$

We define a set of regression points $\{\mathbf{y}_k\}_{k=1}^{Q}$ and associated weights ω_k. Then, we solve

$$\min_{\{J_\alpha\}_{\alpha \in \mathcal{I}_P}} \sum_{k=1}^{Q} \omega_k \Big(J(\mathbf{y}_k) - \sum_{\alpha \in \mathcal{I}_P} J_\alpha \psi_\alpha(\mathbf{y}_k)\Big)^2$$

or equivalently a system of equations

$$\sum_{\alpha \in \mathcal{I}_P} \left(\sum_{k=1}^{Q} \omega_k \psi_\beta(\mathbf{y}_k) \psi_\alpha(\mathbf{y}_k) \right) J_\alpha = \sum_{k=1}^{Q} \omega_k \psi_\beta(\mathbf{y}_k) J(\mathbf{y}_k), \quad \beta \in \mathcal{I}_P$$

Choice of regression points and weights: Pseudorandom samplings, Quasi-random samplings, Gauss-Quadrature points (full or sparse) [Berveiller 2006].

Regression

Experimental design must be sufficiently rich in order to obtain a well-conditioned system for the P coefficients

$$\boxed{Q \gg P}$$

Some ways to reduce P, and therefore Q

- Choice of hyperbolic sets of polynomials $\mathcal{I}_P$ [Blatman 10]
- Adaptive chaos representations based on adaptive regression techniques [Blatman & Sudret 08,09] (adaptive construction of $\mathcal{I}_P$)

Remark

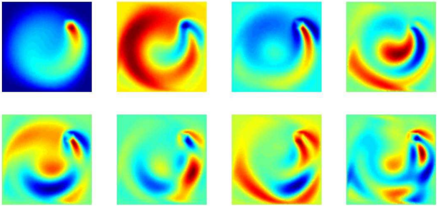
If $\{\mathbf{y}_k, \omega_k\}_{k=1}^{Q}$ constitutes an integration rule on $\boldsymbol{\Xi}$ associated with measure $P_{\boldsymbol{\xi}}$, then

$$\sum_{k=1}^{Q} \omega_k (J(\mathbf{y}_k) - \sum_{\alpha \in \mathcal{I}_P} J_\alpha \psi_\alpha(\mathbf{y}_k))^2 \approx \mathbb{E}((J(\boldsymbol{\xi}) - \sum_{\alpha \in \mathcal{I}_P} J_\alpha \psi_\alpha(\boldsymbol{\xi}))^2) = \| J - \sum_{\alpha \in \mathcal{I}_P} J_\alpha \psi_\alpha \|^2_{L^2(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})}$$

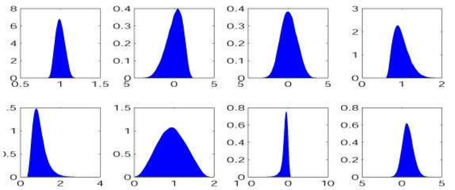
and regression is equivalent to a projection with a “numerical pseudo-norm”.

Example: Illustration of the decomposition $u_8 = \sum_{i=1}^{8} w_i(x)\lambda_i(\xi)$

Spatial modes $W = \{w_1(x)...w_8(x)\}$



Random variables $\Lambda = \{\lambda_1(\boldsymbol{\xi})...\lambda_8(\boldsymbol{\xi})\}$



To compute these modes
$\Rightarrow$ only 8 deterministic problems

$$-\nabla \cdot (\kappa_i \nabla w_i) + c \cdot \nabla w_i + \gamma w_i = f_i$$

Separated representation of random variables

$$\Lambda(\boldsymbol{\xi}) \approx \sum_{k=1}^{Z} \phi_k^0 \phi_k^1(\xi_1)...\phi_k^{40}(\xi_{40}) \in \mathcal{S}_P$$

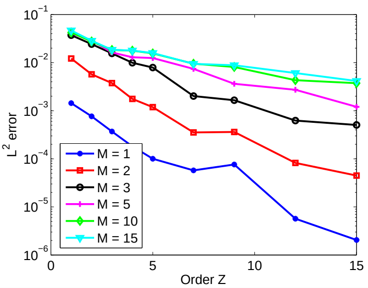
Convergence of multidimensional separated representations

Stochastic algebraic equation: problem defined on the reduced space $\mathcal{V}_M \otimes \mathcal{S} \simeq \mathbb{R}^M \otimes \mathcal{S}$

$$\mathbb{E}_{\boldsymbol{\xi}}(\Lambda(\boldsymbol{\xi})^{*T}\mathbf{A}(\boldsymbol{\xi})\Lambda(\boldsymbol{\xi})) = \mathbb{E}_{\boldsymbol{\xi}}(\Lambda(\boldsymbol{\xi})^{*T}\mathbf{b}(\boldsymbol{\xi})) \quad \forall \Lambda^* \in \mathbb{R}^M \otimes \mathcal{S}$$

$$\Lambda(\boldsymbol{\xi}) \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \Psi_k(\boldsymbol{\xi}), \quad \phi_k^0 \in \mathbb{R}^M, \quad \Psi_k(\boldsymbol{\xi}) = \phi_k^1(\boldsymbol{\xi}_1)\ldots\phi_k^{40}(\boldsymbol{\xi}_{40}) \in \mathcal{S}_P$$

Convergence with Z for different M
$\|\Lambda - \Lambda_Z\|_{L^2}^2$



$$u_M(\boldsymbol{\xi}) \approx \sum_{k=1}^{Z} \left(W \cdot \phi_k^0\right) \Psi_k(\boldsymbol{\xi})$$

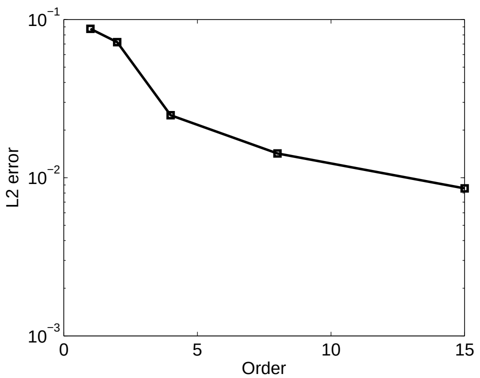
For a precision of 10^{-2}: $\boxed{Z \approx 10}$
to be compared with $\boxed{P = 10^{28}}$

Convergence of generalized spectral decomposition

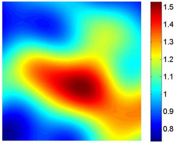
Mean square convergence

$$\|u_M - u\|^2_{L^2(\Xi;L^2(\Omega))} = \mathbb{E}_\xi(\|u_M - u\|^2_{L^2(\Omega)}) \approx \frac{1}{N_s}\sum_{n=1}^{N_s} \|u_M(\xi^n) - u(\xi^n)\|^2_{L^2(\Omega)}$$

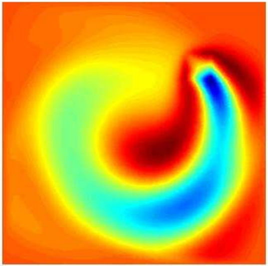
$\|u_M - u\|^2_{L^2}$ $(N_s = 500)$



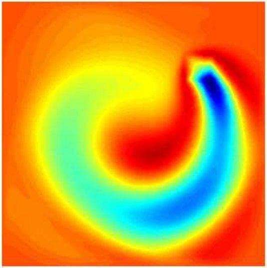
Sample of $\kappa(x, \boldsymbol{\xi})$



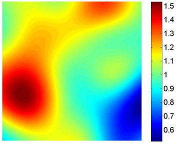
$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu_\xi})$



$u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu_\xi})$

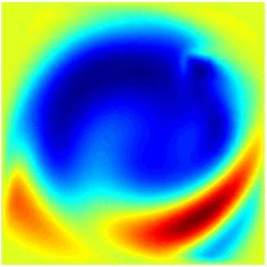


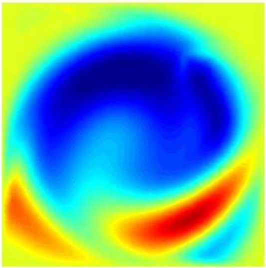
Sample of $\kappa(x, \boldsymbol{\xi})$



$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$

$u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$

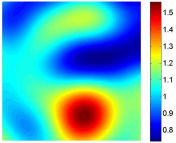




Convergence properties of generalized spectral decomposition

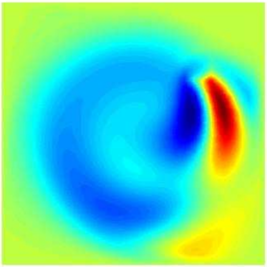
Samples

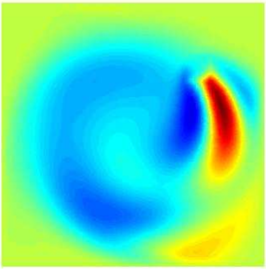
Sample of $\kappa(x, \boldsymbol{\xi})$



$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$

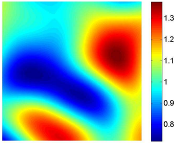
$u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$



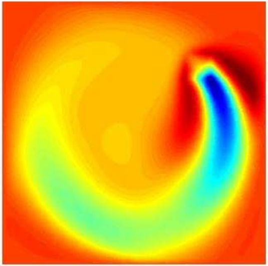


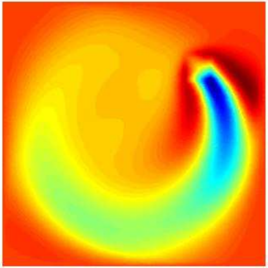
Samples

Sample of $\kappa(x, \boldsymbol{\xi})$



$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$ $u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$



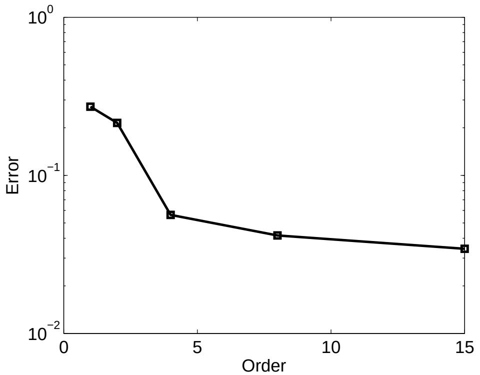


Convergence properties of generalized spectral decomposition

Uniform convergence

$$\|u_M - u\|_{L^\infty(\Xi;L^2(\Omega))} = \sup_{\xi\in\Xi}\|u_M(\xi) - u(\xi)\|_{L^2(\Omega)} \approx \sup_{n\in\{1\dots N_s\}}\|u_M(\xi^n) - u(\xi^n)\|_{L^2(\Omega)}$$

$\|u_M - u\|^2_{L^\infty}$ $(N_s = 500)$

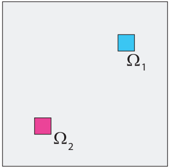


Convergence properties of quantities of interest

Probability density function

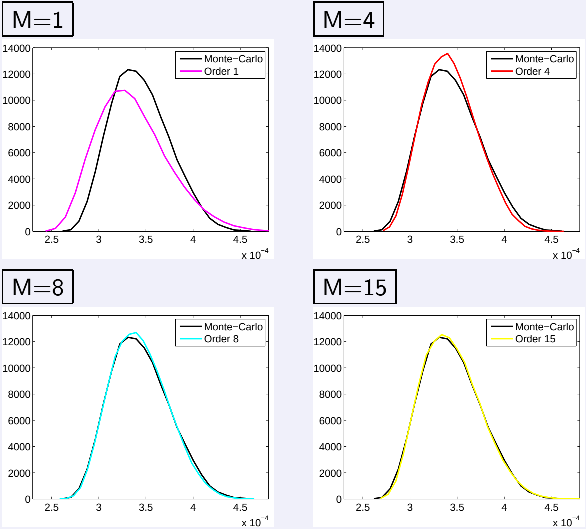
Quantity of interest

$$Q(\xi) = \int_{\Omega_2} u(x,\xi)\, dx$$



$$Q_M(\xi) = \int_{\Omega_2} u_M(x,\xi)\, dx$$

Probability density function of $Q(\xi)$

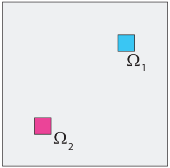


Convergence properties of quantities of interest

Probability of events

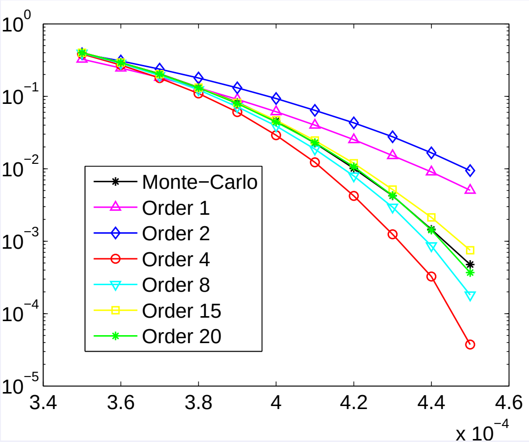
Quantity of interest

$$Q(\boldsymbol{\xi}) = \int_{\Omega_2} u(x, \boldsymbol{\xi})\, dx$$



$$Q_M(\boldsymbol{\xi}) = \int_{\Omega_2} u_M(x, \boldsymbol{\xi})\, dx$$

$P(Q > q), \quad q \in (3.5, 5.4)$



Sensitivity analysis

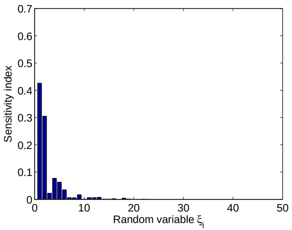
$$Q(\boldsymbol{\xi}) \approx Q_M(\boldsymbol{\xi}) \approx Q_{M,Z}(\boldsymbol{\xi}) = \sum_{k=1}^{Z} q_k \Psi_k(\boldsymbol{\xi}), \quad \Psi_k(\boldsymbol{\xi}) = \prod_{i=1}^{40} \phi_k^i(\xi_i)$$

First order Sobol sensitivity index with respect to parameter ξ_i

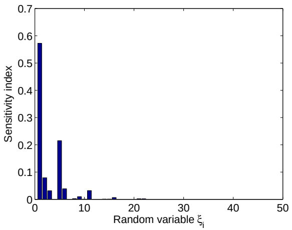
$$\boxed{S_i = \frac{Var(E(Q|\xi_i))}{Var(Q)}} \quad E(Q|\xi_i) = \sum_{k=1}^{Z} \alpha_k^i \phi_k^i(\xi_i), \quad \alpha_k^i = q_k \prod_{\substack{j=1 \\ j \neq i}}^{40} E(\phi_k^i(\xi_i))$$

First order sobol sensivity indices S_i

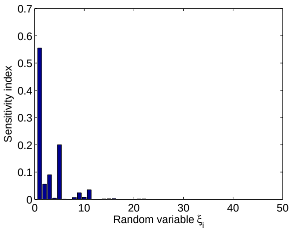
M=1



M=5



M=15



Results... in brief

Deterministic/stochastic separation

$$u(\boldsymbol{\xi}) \approx u_M(\boldsymbol{\xi}) = \sum_{i=1}^{M} w_i \lambda_i(\boldsymbol{\xi})$$

$$\hookrightarrow \quad \mathcal{V}_M = span\{w_i\}_{i=1}^M$$

Random variables separation

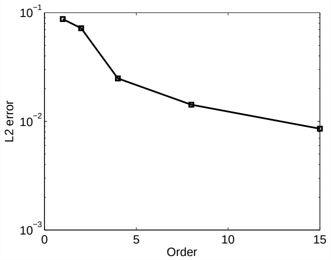
$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^M \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

$$\hookrightarrow \quad \mathcal{S}_Z = span\{\textstyle\prod_{j=1}^s \phi_k^j(\xi_j)\}_{k=1}^Z$$

For a precision $\|u - u_{M,Z}\|_{L^2} \leqslant 10^{-2}$

- $dim(\mathcal{V}_M) \approx 15$ $\ll 4435 = dim(\mathcal{V}_N)$

$\|u_M - u\|_{L^2}^2$



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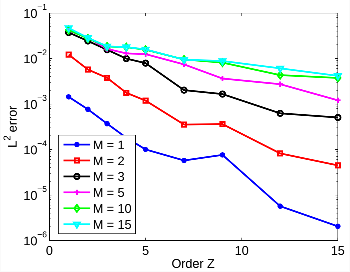
- $dim(\mathcal{S}_Z) \approx 10$ $\ll 10^{28} = dim(\mathcal{S}_P)$

$\|\Lambda - \Lambda_Z\|_{L^2}^2$ for different M



Results... in brief

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Random variables separation

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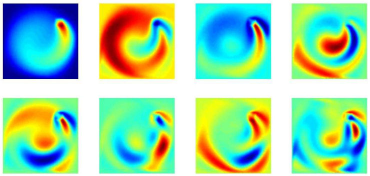
For a precision $\|u - u_{M,Z}\|_{L^2} \leqslant 10^{-2}$

- $dim(\mathcal{V}_M) \approx 15$ $\ll 4435 = dim(\mathcal{V}_N)$
- $dim(\mathcal{S}_Z) \approx 10$ $\ll 10^{28} = dim(\mathcal{S}_P)$
- 15 classical deterministic problems in order to build $\mathcal{V}_M \subset \mathcal{V}_N$

First spatial modes $\{w_1(x) \dots w_8(x)\}$



Return

Results... in brief

Deterministic/stochastic separation

$$u(\boldsymbol{\xi}) \approx u_M(\boldsymbol{\xi}) = \sum_{i=1}^{M} w_i \lambda_i(\boldsymbol{\xi})$$

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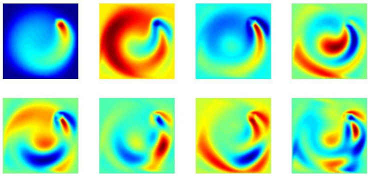
For a precision $\|u - u_{M,Z}\|_{L^2} \leqslant 10^{-2}$

- $dim(\mathcal{V}_M) \approx 15$ $\ll 4435 = dim(\mathcal{V}_N)$
- $dim(\mathcal{S}_Z) \approx 10$ $\ll 10^{28} = dim(\mathcal{S}_P)$
- 15 classical deterministic problems in order to build $\mathcal{V}_M \subset \mathcal{V}_N$
- about 1 minute computation on a laptop with matlab

First spatial modes $\{w_1(x) \ldots w_8(x)\}$



Return