Tensor based numerical methods for high dimensional stochastic and parametric problems

Anthony Nouy

In collaboration with M. Billaud, G. Bonithon, P. Cartraud, M. Chevreuil, A. Falco, L. Giraldi, G. Legrain, O. Le Maitre, P. Rai, O.Zahm

GeM
Ecole Centrale Nantes / Université de Nantes / CNRS

Supported by the ANR (projects SIM-DREAM and TYCHE) and GNR MOMAS.

Uncertainty quantification

Uncertainty quantification has become an essential path in science and engineering

- Comprehension and selection of models (exploration of model predictions over a range of uncertainty)
- Assess confidence in numerical predictions
- Robust optimization and design
- Validation of models using (noisy) data
- Data assimilation and model construction

Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Uncertainty quantification using functional approaches

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

$$\eta(\theta) \equiv \eta(\xi(\theta))$$

- Approximation theory for the approximation of functionals

$$\eta(\xi) \approx \sum \eta_\alpha \psi_\alpha(\xi), \quad \xi \in \Xi$$

Uncertainty quantification using functional approaches

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

$$\eta(\theta) \equiv \eta(\xi(\theta))$$

- Approximation theory for the approximation of functionals

$$\eta(\xi) \approx \sum \eta_\alpha \psi_\alpha(\xi), \quad \xi \in \Xi$$

Stochastic/parametric models

$$u : \xi \in \Xi \mapsto u(\xi) \in \mathcal{V} \quad \text{such that} \quad \mathcal{A}(u(\xi); \xi) = f(\xi)$$

Uncertainty quantification using functional approaches

Stochastic/parametric analyses: a unified framework

$$u : \Xi \to \mathcal{V}, \quad \mathcal{A}(u(\xi); \xi) = f(\xi), \quad \xi \in \Xi$$

- Forward problem (propagation): $P_\xi \longrightarrow \mathcal{O}(u)$
- Optimization or identification: $\mathcal{O}(u) \longrightarrow \xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow \xi_2$
- Probabilistic inverse problem: $\mathcal{O}(u) \longrightarrow P_\xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow P_{\xi_2}$

Uncertainty quantification using functional approaches

Stochastic/parametric analyses: a unified framework

$$u : \Xi \to \mathcal{V}, \quad \mathcal{A}(u(\xi);\xi) = f(\xi), \quad \xi \in \Xi$$

- Forward problem (propagation): $P_\xi \longrightarrow \mathcal{O}(u)$
- Optimization or identification: $\mathcal{O}(u) \longrightarrow \xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow \xi_2$
- Probabilistic inverse problem: $\mathcal{O}(u) \longrightarrow P_\xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow P_{\xi_2}$

Ideal approach

Compute an accurate and explicit representation of $u(\xi)$ (a metamodel) that allows fast evaluations of output quantities of interest, observables, or objective function.

Uncertainty quantification using functional approaches

Stochastic/parametric analyses: a unified framework

$$u : \Xi \rightarrow \mathcal{V}, \quad \mathcal{A}(u(\xi);\xi) = f(\xi), \quad \xi \in \Xi$$

- Forward problem (propagation): $P_\xi \longrightarrow \mathcal{O}(u)$
- Optimization or identification: $\mathcal{O}(u) \longrightarrow \xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow \xi_2$
- Probabilistic inverse problem: $\mathcal{O}(u) \longrightarrow P_\xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow P_{\xi_2}$

Ideal approach

Compute an accurate and explicit representation of $u(\xi)$ (a metamodel) that allows fast evaluations of output quantities of interest, observables, or objective function.

Issue

Approximation of a high dimensional function $u(\xi)$, $\xi \in \Xi \subset \mathbb{R}^d$.

Construction of approximation spaces

$$u \in L^p_\mu(\Xi;\mathcal{V}) = \mathcal{V} \otimes \mathcal{S}$$

Tensorization of predefined bases

$$u \approx \sum_{i=1}^{N} \sum_{\alpha \in \mathcal{I}_P} u_{i,\alpha} \varphi_i \psi_\alpha(\xi) \in \mathcal{V}_N \otimes \mathcal{S}_P$$

with given approximation spaces

$$\mathcal{V}_N = span\{\varphi_i\}_{i=1}^N$$

$$\mathcal{S}_P = span\{\psi_\alpha(\xi) = \psi^1_{\alpha_1}(\xi_1)\ldots\psi^d_{\alpha_d}(\xi_d); \alpha \in \mathcal{I}_P\}$$

- Pre-defined index set $\mathcal{I}_P$

$$\left\{\alpha \in \mathbb{N}^d; |\alpha|_\infty \leq r\right\} \supset \left\{\alpha \in \mathbb{N}^d; |\alpha|_1 \leq r\right\} \supset \left\{\alpha \in \mathbb{N}^d; |\alpha|_q \leq r\right\},\ 0 < q < 1$$

- Choice of $\mathcal{I}_P$ based on a priori analysis

Definition of approximate functional expansions

Direct simulation methods (L^2 projection, regression, interpolation)

$$u(\xi) \approx \sum_{\alpha \in \mathcal{I}_P} u_\alpha \psi_\alpha(\xi) \quad u_\alpha \in \mathcal{V}_N$$

with coefficients

$$u_\alpha = \sum_{k=1}^{Q} \omega_k^\alpha u_N(y_k), \quad \alpha \in \mathcal{I}_P$$

where $\{y_k\}_{k=1}^Q$ is a collection of sample points and the $u(y_k)$ are approximate solutions of deterministic problems

$$\mathcal{A}(u(y_k); y_k) = f(y_k)$$

- Use of classical deterministic solvers (black box)
- Numerous solutions of deterministic problems: $Q = O(\#\mathcal{I}_P)$

Definition of approximate functional expansions

Weak solution

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad \langle \mathcal{A}(u), v \rangle = \langle f, v \rangle \quad \forall v \in \mathcal{V} \otimes \mathcal{S}$$

Galerkin-type projections

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

where coefficients $\{u_\alpha\}_{\alpha \in \mathcal{I}_P}$ are solutions of a coupled system of deterministic problems:

$$\left\langle \mathcal{A}(\sum_\alpha u_\alpha \psi_\alpha), v_\beta \psi_\beta \right\rangle = \langle f, v_\beta \psi_\beta \rangle \quad \forall v_\beta \in \mathcal{V}_N, \quad \beta \in \mathcal{I}_P \qquad (\star)$$

- Nice mathematical framework: error estimates, stability, possible efficiency
- Generally require modifications of (or strong interaction with) existing solvers.
- Complexity of systems of equations $(\star)$

Complexity issue

Possibly fine deterministic models

$$\boxed{dim(\mathcal{V}_N) \approx 10^6, 10^9, 10^{12} \ldots}$$

Make inacceptable numerous evaluations of the model and the solution of coupled systems of deterministic problems

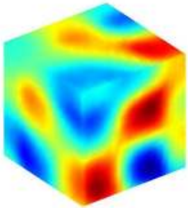
$\rightarrow$ Need model reduction

Possibly high parametric dimensionality

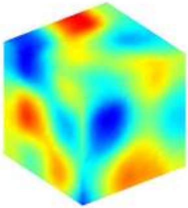
Many input parameters or stochastic processes with high spectral content

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

$\rightarrow$ Need adapted representations for high dimensional functions



$$\kappa(x,\theta) = \sum_{i=1}^{m} \kappa_i(x)\xi_i(\theta)$$



Outline

1 Uncertainty quantification with functional approaches

2 Strategies for complexity reduction

3 Tensor-based methods

4 Optimal model order reduction

5 Tensor formats for stochastic problems

6 Non intrusive tensor methods

7 References

Optimal model reduction

Optimal approximation spaces for $u \in \mathcal{V} \otimes \mathcal{S}$

$$\sigma_m(u) = \inf_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \inf_{u_m \in \mathcal{V}_m \otimes \mathcal{S}} \|u - u_m\| = \inf_{\substack{\mathcal{S}_m \subset \mathcal{S} \\ dim(\mathcal{S}_m)=m}} \inf_{u_m \in \mathcal{V} \otimes \mathcal{S}_m} \|u - u_m\|$$

- m-dimensional approximation spaces $\mathcal{V}_m$ and $\mathcal{S}_m$ are optimal w.r.t. the norm $\|\cdot\|$.
- For $\mathcal{S} = L^2_\mu(\Xi)$ and for the natural norm in $L^2_\mu(\Xi;\mathcal{V})$, the best approximation u_m is the rank-m singular value decomposition

A fact

In many applications and for reasonable precisions ϵ,

$$\boxed{\sigma_m(u) \leq \epsilon \text{ for } m \text{ small}}$$

Optimal model reduction

Optimal approximation spaces for $u \in \mathcal{V} \otimes \mathcal{S}$

$$\sigma_m(u) = \inf_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \inf_{u_m \in \mathcal{V}_m \otimes \mathcal{S}} \|u - u_m\| = \inf_{\substack{\mathcal{S}_m \subset \mathcal{S} \\ dim(\mathcal{S}_m)=m}} \inf_{u_m \in \mathcal{V} \otimes \mathcal{S}_m} \|u - u_m\|$$

- m-dimensional approximation spaces $\mathcal{V}_m$ and $\mathcal{S}_m$ are optimal w.r.t. the norm $\|\cdot\|$.
- For $\mathcal{S} = L^2_\mu(\Xi)$ and for the natural norm in $L^2_\mu(\Xi; \mathcal{V})$, the best approximation u_m is the rank-m singular value decomposition

A fact

In many applications and for reasonable precisions ϵ,

$$\boxed{\sigma_m(u) \leq \epsilon \text{ for } m \text{ small}}$$

Question

Can we compute these low dimensional approximation spaces a priori ?

Strategies for high dimensional approximation

Optimal sparse approximation in $\mathcal{S}_P = span\{\psi_\alpha\}_{\alpha \in \mathcal{I}_P}$

For $\boxed{K \subset \mathcal{I}_P}$, we define $\boxed{\mathcal{S}_K = span\{\psi_k\}_{k \in K}} \subset \mathcal{S}_P$. For the approximation of $u \in \mathcal{S}$, we want the smallest subspace $\mathcal{S}_K$ yielding a precision at least ϵ:

$$\boxed{\min_K \#K \quad \text{subject to} \quad \inf_{v \in \mathcal{S}_K} \|u - v\| \leq \epsilon}$$

Computational aspects

- Adaptive construction of the index set [Cohen2010, Crestaux2011,...]
- Non adaptive construction by approximation of the ideal formulation [Blatman2011, Doostan2011, Mathelin2012, Najm2012]

Strategies for high dimensional approximation

Optimal sparse approximation in $\mathcal{S}_P = span\{\psi_\alpha\}_{\alpha \in \mathcal{I}_P}$

For $\boxed{K \subset \mathcal{I}_P}$, we define $\boxed{\mathcal{S}_K = span\{\psi_k\}_{k \in K}} \subset \mathcal{S}_P$. For the approximation of $u \in \mathcal{S}$, we want the smallest subspace $\mathcal{S}_K$ yielding a precision at least ϵ:

$$\boxed{\min_K \#K \quad \text{subject to} \quad \inf_{v \in \mathcal{S}_K} \|u - v\| \leq \epsilon}$$

Computational aspects

- Adaptive construction of the index set [Cohen2010, Crestaux2011,...]
- Non adaptive construction by approximation of the ideal formulation [Blatman2011, Doostan2011, Mathelin2012, Najm2012]

Issues

- K may be small for reasonable ϵ (strongly depends on the chosen basis).
- Strategies of exploration for adaptive constructions ?
- Computability of non adaptive constructions for high dimensional spaces $\mathcal{S}_P$?
- Approximation of function $u \in \mathcal{V}_N \otimes \mathcal{S}_P$?

Strategies for high dimensional approximation

Nonlinear approximation in a subset $\mathcal{M} \subset \mathcal{V}_N \otimes \mathcal{S}_P$

- $\mathcal{M}$ should have nice approximation properties: for a class of functions u and for a reasonable precision ϵ,

$$\inf_{v \in \mathcal{M}} \|u - v\| \leq \epsilon$$

- $\mathcal{M}$ is not a linear space (nor a convex set): nonlinear approximation problem
- $\mathcal{M}$ has a small dimension (i.e. can be parameterized with a small number of parameters)
- An approximation can be computed with suitable algorithms (e.g. alternating minimization on the parameters)

Strategies for high dimensional approximation

Nonlinear approximation using tensor approximation methods

- Exploit the tensor structure of function space

$$\mathcal{V}_N \otimes \mathcal{S}_P = \mathcal{V}_N \otimes \mathcal{S}^1_{P_1} \otimes \ldots \otimes \mathcal{S}^d_{P_d}$$

- Choose suitable tensor subsets $\mathcal{M}$, e.g.

$$\mathcal{M} = \left\{ \sum_{i=1}^{m} v_i \otimes \phi_i^1 \otimes \ldots \otimes \phi_i^d ; v_i \in \mathcal{V}_N, \phi_i^k \in \mathcal{S}^k_{P_k} \right\},$$

  with $\boxed{dim(\mathcal{M}) = O(d)}$.

- Best approximation problems in tensor subsets are related to singular value decompositions and their generalizations

[Nouy2010, Doostan2010, Khoromskij2010, Ballani2010...]

Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Tensor spaces

Tensor Banach space

We consider Banach spaces V_k equipped with norms $\|\cdot\|_k$. A tensor Banach space equipped with norm $\|\cdot\|$ is defined by

$$V = \overline{{}_a \otimes_{k=1}^d V_k}^{\|\cdot\|} \quad \text{with} \quad {}_a \otimes_{k=1}^d V_k = span\{v^1 \otimes \ldots \otimes v^d \ : \ v^k \in V_k\}$$

Examples

$$L^2_\mu(\Xi; \mathcal{V}) = \overline{\mathcal{V} \otimes_a L^2_\mu(\Xi)}^{\|\cdot\|}, \quad \|v\|^2 = \int_\Xi \|v(y)\|^2_{\mathcal{V}} d\mu(y)$$

$$L^2_\mu(\Xi) = \overline{{}_a \otimes_{k=1}^s L^2_{\mu_k}(\Xi_k)}^{\|\cdot\|}, \quad \|v\|^2 = \int_{\Xi_1} \ldots \int_{\Xi_s} v(y_1, \ldots, y_s)^2 d\mu_1(y_1) \ldots d\mu_s(y_s)$$

Tensor spaces

Tensor Banach space

We consider Banach spaces V_k equipped with norms $\|\cdot\|_k$. A tensor Banach space equipped with norm $\|\cdot\|$ is defined by

$$V = \overline{{}_a \otimes_{k=1}^{d} V_k}^{\|\cdot\|} \quad \text{with} \quad {}_a \otimes_{k=1}^{d} V_k = span\{v^1 \otimes \ldots \otimes v^d \ : \ v^k \in V_k\}$$

Examples

$$L^2_\mu(\Xi;\mathcal{V}) = \overline{\mathcal{V} \otimes_a L^2_\mu(\Xi)}^{\|\cdot\|}, \quad \|v\|^2 = \int_\Xi \|v(y)\|^2_{\mathcal{V}} d\mu(y)$$

$$L^2_\mu(\Xi) = \overline{{}_a \otimes_{k=1}^{s} L^2_{\mu_k}(\Xi_k)}^{\|\cdot\|}, \quad \|v\|^2 = \int_{\Xi_1} \ldots \int_{\Xi_s} v(y_1,\ldots,y_s)^2 d\mu_1(y_1)\ldots d\mu_s(y_s)$$

Finite dimensional spaces

$V = {}_a \otimes_{k=1}^{d} V_k$. Denoting $\{\psi_i^k\}_{i=1}^{n_k}$ a basis of V_k,

$$V = \left\{ v = \sum_{i_1=1}^{n_1} \ldots \sum_{i_d=1}^{n_d} \alpha_{(i_1,\ldots,i_d)} \psi^1_{i_1} \otimes \ldots \otimes \psi^d_{i_d} ; \alpha_{(i_1,\ldots,i_d)} \in \mathbb{R} \right\} \qquad \boxed{dim(V) = n_1 n_2 \ldots n_d}$$

Tensor subsets

Tensor subsets $\mathcal{M}$

- Rank one tensors
$$\mathcal{R}_1 = \left\{ \otimes_{k=1}^d v^k \ : \ v^k \in V_k \right\}$$
- Rank-m (canonical) tensors
$$\mathcal{R}_m = \left\{ \sum_{i=1}^m \otimes_{k=1}^d v_i^k \ : \ v_i^k \in V_k \right\}$$
- Tucker tensors with rank $\mathbf{r} = (r_1, \ldots, r_d)$
$$\mathcal{T}_{\mathbf{r}} = \left\{ \sum_{i_1=1}^{r_1} \ldots \sum_{i_d=1}^{r_d} \alpha_{(i_1,\ldots,i_d)} \otimes_{k=1}^d v_{i_k}^k ; \alpha_{(i_1,\ldots,i_d)} \in \mathbb{R}, v_i^k \in V_k \right\}$$
$$= \left\{ v \in V : \begin{array}{l} \text{there exist subspaces } U_k \subset V_k \text{ such that} \\ dim(U_k) = r_k \text{ and } v \in U_1 \otimes \ldots \otimes U_d \end{array} \right\}$$
- Hierarchical tensors $\mathcal{H}_{\mathbf{r}}$
- ...

Tensor based methods

Tensor approximation methods for solving problems of type

$$A(u) = f \quad \text{with} \quad u \in V = V_1 \otimes \ldots \otimes V_d$$

(1) Iterative or direct solvers ?

(2) How to define an approximation of u in a tensor subset without information on u ?

(3) Construction of a tensor decomposition with a prescribed accuracy:
directly (in increasing tensor subsets) or progressively (with successive corrections in small tensor subsets) ?

(4) Optimal model reduction for stochastic/parametric analyses ?

(5) How to define suitable tensor subsets for stochastic analyses ?

(6) Can we build tensor approximations using samples of u (black-box approach) ?

Iterative or direct solvers ?

Approximation of the solution of $A(u) = f$ in a tensor subset $\mathcal{M}$

- Iterative methods and classical tensor approximation methods (SVD) .
  Construction of a sequence of tensor approximations $u_n \in \mathcal{M}$, perturbations of ideal iterations.

$$u_n \approx B(u_{n-1}) \quad \text{with} \quad \|u_n - B(u_{n-1})\| \approx \inf_{v \in \mathcal{M}} \|v - B(u_{n-1})\|$$

Iterative or direct solvers ?

Approximation of the solution of $A(u) = f$ in a tensor subset $\mathcal{M}$

- Iterative methods and classical tensor approximation methods (SVD) .
  Construction of a sequence of tensor approximations $u_n \in \mathcal{M}$, perturbations of ideal iterations.

$$u_n \approx B(u_{n-1}) \quad \text{with} \quad \|u_n - B(u_{n-1})\| \approx \inf_{v \in \mathcal{M}} \|v - B(u_{n-1})\|$$

- Direct (a priori) construction of a tensor approximation (PGD/GSVD)
  Requires new definitions of "best approximations" and associated algorithms.

$$\inf_{v \in \mathcal{M}} \|A(v) - f\|_*$$

Iterative or direct solvers ?

Approximation of the solution of $A(u) = f$ in a tensor subset $\mathcal{M}$

- Iterative methods and classical tensor approximation methods (SVD) .
  Construction of a sequence of tensor approximations $u_n \in \mathcal{M}$, perturbations of ideal iterations.

$$u_n \approx B(u_{n-1}) \quad \text{with} \quad \|u_n - B(u_{n-1})\| \approx \inf_{v \in \mathcal{M}} \|v - B(u_{n-1})\|$$

- Direct (a priori) construction of a tensor approximation (PGD/GSVD)
  Requires new definitions of "best approximations" and associated algorithms.

$$\inf_{v \in \mathcal{M}} \|A(v) - f\|_*$$

- Coupling iterative methods and PGD.
  A larger class of iterative methods can be used.

$$C(u_n) \approx B(u_{n-1}) \quad \text{with} \quad \|C(u_n) - B(u_{n-1})\|_* \approx \inf_{v \in \mathcal{M}} \|C(v) - B(u_{n-1})\|_*$$

Best approximation in a tensor subset $\mathcal{M}$ without information on u

Approximation of the solution of $Au = f$ in a tensor subset $\mathcal{M}$.
Definition of a set of "good approximations" $\boxed{\Pi_{\mathcal{M}}(u) \subset \mathcal{M}}$?

- Optimization problems: if $A(u) - f = \mathcal{J}'(u)$ with $\mathcal{J}$ a convex functional

$$\Pi_{\mathcal{M}}(u) = \arg\min_{w \in \mathcal{M}} \mathcal{J}(w)$$

- Galerkin projection:

$$\Pi_{\mathcal{M}}(u) \subset \{w \in \mathcal{M} \ : \ \langle A(w) - f, \delta w \rangle = 0 \quad \forall \delta w \in T_w(\mathcal{M})\}$$

- Minimal residual:

$$\Pi_{\mathcal{M}}(u) = \arg\min_{w \in \mathcal{M}} \|A(w) - f\|_* \quad \text{(Good residual norms)}$$

- Minimax (Petrov-Galerkin):

$$\Pi_{\mathcal{M}}(u) \subset \left\{ w \in \mathcal{M} \ : \ \begin{array}{ll} \langle A(w) - f, \delta z \rangle = 0 & \forall \delta z \in T_z(\mathcal{M}) \\ \langle \delta w, A^* z \rangle = \langle \delta w, w \rangle & \forall \delta w \in T_w(\mathcal{M}) \end{array} \right\}$$

Direct constructions (PGDs)

Tensor subsets

Define a sequence of tensor subsets $\{\mathcal{M}_m\}_{m\geq 1}$ such that

- $\mathcal{M}_m \subset \mathcal{M}_{m+1}$
- $\cup_{m\geq 1}\mathcal{M}_m$ is dense in V

Typical choices: $\mathcal{M}_m = \mathcal{R}_m$, $\mathcal{M}_m = \mathcal{M}_{m-1} + \mathcal{M}_1$ with $\mathcal{R}_1 \subset \mathcal{M}_1$, $\mathcal{M}_m = \mathcal{T}_{(m,\ldots,m)}$.

Definition (Direct PGD of u)

For a given sequence of tensor subsets $\{\mathcal{M}_m\}_{m\geq 1}$, define a sequence $\{u_m\}_{m\geq 1}$ by

$$\boxed{u_m \in \Pi_{\mathcal{M}_m}(u)}$$

- Generalization of the concept of spectral decomposition: Proper Generalized Decomposition (to be clarified...)
- Useful when we want an optimal decomposition for a given precision
- Computational complexity increases with m.

Progressive constructions (PGDs)

Tensor subsets

Define a (small) tensor subset $\mathcal{M}$ satisfying

- $\mathcal{M}$ is weakly closed in V,
- $span(\mathcal{M})$ is dense in V,
- $\lambda \mathcal{M} \subset \mathcal{M}$ for all $\lambda \in \mathbb{R}$

Typical choices: $\mathcal{M} = \mathcal{R}_1$ (elementary tensors), $\mathcal{M} = \mathcal{T}_r$ (tucker set) or $\mathcal{M} = \mathcal{H}_r$ (hierarchical tensors) with small r.

Definition (Progressive PGD of u)

Let $u_0 = 0$. For $m \geq 1$,

1. Compute a correction $w_m \in \mathcal{M}$ of u_{m-1}:

$$\boxed{w_m \in \Pi_{\mathcal{M}}(u - u_{m-1})}$$

2. Set $\boxed{u_m = u_{m-1} + w_m}$

Progressive constructions with updates

Definition (Updated progressive PGD)

Let $u_0 = 0$. For $m \geq 1$,

1. Compute a correction $w_m \in \mathcal{M}$ of $u - u_{m-1}$:

$$\boxed{w_m \in \Pi_{\mathcal{M}}(u - u_{m-1})}$$

2. Set $\boxed{v_m = u_{m-1} + w_m}$ and $\boxed{\text{construct a linear subspace } U_m \text{ such that } v_m \in U_m}$.
   Then, define u_m as the best approximation of u in U_m

$$\boxed{u_m \in \Pi_{U_m}(u)}$$

Progressive constructions with updates

Definition (Updated progressive PGD)

Let $u_0 = 0$. For $m \geq 1$,

1. Compute a correction $w_m \in \mathcal{M}$ of $u - u_{m-1}$:

$$\boxed{w_m \in \Pi_{\mathcal{M}}(u - u_{m-1})}$$

2. Set $\boxed{v_m = u_{m-1} + w_m}$ and $\boxed{\text{construct a linear subspace } U_m \text{ such that } v_m \in U_m}$.
   Then, define u_m as the best approximation of u in U_m

$$\boxed{u_m \in \Pi_{U_m}(u)}$$

Link to model reduction

Progressive construction of a low dimensional approximation space U_m which defines a reduced order model.

- Nonlinear approximation for the construction of U_m
- Linear approximation in U_m.

Strategies of updates: construction of linear spaces
with G. Bonithon, L. Giraldi, G. Legrain

For v_m given, strategies for constructing a linear space U_m such that $v_m \in U_m$:

- Suppose $v_m = \sum_{i=1}^m w_i$, with $w_i \in \mathcal{M}$.

$$U_m = span\{w_i\}_{i=1}^m = \left\{ \sum_{i=1}^m \alpha_i w_i : \alpha_i \in \mathbb{R} \right\} \quad \boxed{dim(U_m) = m}$$

- Suppose $v_m = \sum_{i=1}^m \otimes_{k=1}^d w_i^k \in \mathcal{R}_m$.

$$U_m = \left\{ \sum_{i=1}^m \delta w_i^k \otimes \left(\bigotimes_{\substack{k'=1 \\ k' \neq k}}^d w_i^{k'} \right) \; : \; \delta w_i^k \in V_k \right\} \quad \boxed{dim(U_m) = m \times dim(V_k)}$$

- Suppose $v_m = u_{m-1} + \otimes_{k=1}^d w_m^k$, with $\mathcal{M} = \mathcal{R}_1$. Define

$$U_m \subset U_1^m \otimes \ldots \otimes U_d^m \quad \text{with} \quad U_k^m = U_k^{m-1} + span\{w_m^k\} \subset V_k \quad \boxed{dim(U_m) \leq m^d}$$

Convergence results for convex optimization problems

Best approximations for the optimization of a functional $\mathcal{J}$ with minimizer u

$$\Pi_{\mathcal{M}}(u) = \arg\min_{w \in \mathcal{M}} \mathcal{J}(w), \quad \Pi_{\mathcal{M}}(u - v) = \arg\min_{w \in \mathcal{M}} \mathcal{J}(v + w)$$

Theorem (Convex optimization in tensor Banach spaces)

Let $\mathcal{J} : V \to \mathbb{R}$ be a Fréchet differentiable functional such that

- *$\mathcal{J}$ is elliptic: $\langle \mathcal{J}'(v) - \mathcal{J}'(w), v - w \rangle \geq \alpha \|u - w\|^s$, with $s > 1$*
- *(H1) $\mathcal{J}'$ weakly continuous or (H2) $\mathcal{J}'$ Lipschitz continuous on bounded sets*

Then, the (updated) progressive PGD $\{u_m\}_{m \geq 1}$ converges towards the solution u if (H1). If (H2), it converges

- *for $s > 1$ if there exists a subsequence of updates*
- *for $1 < s \leq 2$ otherwise*

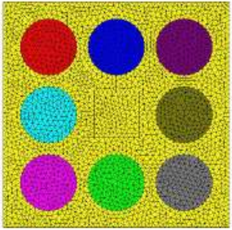
Falco & Nouy, Numerische Mathematik (2012).

A simple illustration on a diffusion equation

$$\begin{cases} -\nabla \cdot (\kappa \nabla u) = I_D(x) \quad on \quad \Omega = (0,1) \times (0,1) \\ u = 0 \quad on \quad \partial\Omega \end{cases}$$

$$\kappa(x,\xi) = \begin{cases} 1 & \text{if } x \in \Omega_0 \\ 1 + 0.1\xi_i & \text{if } x \in \Omega_i, \ i = 1...8 \end{cases}$$

with $\xi_i \in U(-1,1)$



$$\mathcal{J}(v) = \int_\Omega \kappa \nabla v \cdot \nabla v - 2 \int_\Omega I_D v = \|v - u\|_A^2 - \|u\|_A^2$$

Approximation spaces

$$u \in \mathcal{V}_N \otimes \mathcal{S}_P, \quad \mathcal{S}_P = \mathbb{P}_{10}(-1,1) \otimes \ldots \otimes \mathbb{P}_{10}(-1,1)$$

Underlying approximation space with dimension 5.10^{11}

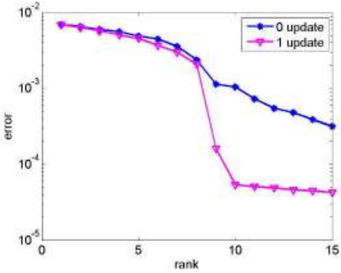
Progressive PGD

Progressive Galerkin PGD

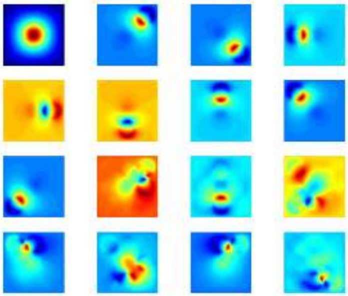
$$u \approx u_m = \sum_{k=1}^m w_k, \quad w_k = v_k \otimes \phi_k^1 \otimes \ldots \otimes \phi_k^s \in \mathcal{R}_1$$

$$\min_{w_m \in \mathcal{R}_1} \|u - u_{m-1} - w_m\|_A^2 \quad + \quad \text{updates of functions } \{\phi_k^1, \ldots, \phi_k^s\}_{k=1}^m$$

Convergence (in L^2 norm)



Spatial modes w_k



Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Optimal model reduction for stochastic parametric problems

$$u_m(\xi) = \sum_{i=1}^{m} v_i \phi_i(\xi) \in \mathcal{V}, \quad v_i \in \mathcal{V}, \quad \phi_i \in \mathcal{S}$$

Best approximation of $u \in \mathcal{V} \otimes \mathcal{S}$ by $u_m \in \mathcal{R}_m(\mathcal{V} \otimes \mathcal{S})$

$$\min_{u_m \in \mathcal{R}_m(\mathcal{V}\otimes\mathcal{S})} \left\| u - u_m \right\|_\star = \min_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \min_{\substack{\mathcal{S}_m \subset \mathcal{S} \\ dim(\mathcal{S}_m)=m}} \min_{u_m \in \mathcal{V}_m \otimes \mathcal{S}_m} \left\| u - u_m \right\|_\star$$

- m-dimensional approximation spaces $\mathcal{V}_m$ and $\mathcal{S}_m$ are optimal w.r.t. the norm $\| \cdot \|_\star$
- Define $\left\| \cdot \right\|_\star$ that makes u_m computable without information on u.
- More than a simple best approximation problem: generalized spectral decomposition (Karhunen-Loeve)

Optimal model reduction for stochastic parametric problems

$$u_m(\xi) = \sum_{i=1}^{m} v_i \phi_i(\xi) \in \mathcal{V}, \quad v_i \in \mathcal{V}, \quad \phi_i \in \mathcal{S}$$

Best approximation of $u \in \mathcal{V} \otimes \mathcal{S}$ by $u_m \in \mathcal{R}_m(\mathcal{V} \otimes \mathcal{S})$

$$\min_{u_m \in \mathcal{R}_m(\mathcal{V}\otimes\mathcal{S})} \|u - u_m\|_\star = \min_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \min_{\substack{\mathcal{S}_m \subset \mathcal{S} \\ dim(\mathcal{S}_m)=m}} \min_{u_m \in \mathcal{V}_m \otimes \mathcal{S}_m} \|u - u_m\|_\star$$

- m-dimensional approximation spaces $\mathcal{V}_m$ and $\mathcal{S}_m$ are optimal w.r.t. the norm $\|\cdot\|_\star$
- Define $\|\cdot\|_\star$ that makes u_m computable without information on u.
- More than a simple best approximation problem: generalized spectral decomposition (Karhunen-Loeve)

Different (computational) approaches

1. construct (an approximation of) $\mathcal{V}_m = span\{v_1, \ldots, v_m\}$ and project on $\mathcal{V}_m \otimes \mathcal{S}$
2. construct (an approximation of) $\mathcal{S}_m = span\{\phi_1, \ldots, \phi_m\}$ and project on $\mathcal{V} \otimes \mathcal{S}_m$
3. construct directly (an approximation of) $\mathcal{V}_m$ and $\mathcal{S}_m$ and the representation of u in $\mathcal{V}_m \otimes \mathcal{S}_m$

Optimal model reduction for stochastic parametric problems

Case of inner product norms $\|\cdot\|_\star$

$$\|u - u_m\|_\star^2 = \min_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \|u - P_{\mathcal{V}_m} u\|_\star^2 = \|u\|_\star^2 - \max_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \sigma(\mathcal{V}_m; u)^2$$

with $P_{\mathcal{V}_m}$ the $\|\cdot\|_\star$-orthogonal projector onto $\mathcal{V}_m \otimes \mathcal{S}$ and $\sigma(\mathcal{V}_m; u) = \|P_{\mathcal{V}_m} u\|_\star$.

Nonlinear eigenproblem

$$\max_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m)=m}} \sigma(\mathcal{V}_m; u) = \|P_{\mathcal{V}_m} u\|_\star$$

with $\sigma(\mathcal{V}_m; u)$ interpreted as a Rayleigh quotient

- Dedicated algorithms for the construction of optimal reduced bases (subspace iterations) or approximations of optimal reduced bases (Arnoldi algorithm, updated progressive construction) [Nouy 2008, Nouy & Le Maitre 2009, Chevreuil 2011]
- For $\|v \otimes \phi\|_\star = \|v\|_{\mathcal{V}} \|\phi\|_{L^2_\mu}$, classical Karhunen-Loeve decomposition. The maximum of $\sigma(\mathcal{V}_m; u)$ is reached for the dominant left singular subspace of u.

Dedicated algorithms

Direct PGD (Subspace iterations)

For a given m, alternate minimization on $\mathcal{V}_m$ and $\mathcal{S}_m$.

$$\min_{\substack{\mathcal{V}_m \subset \mathcal{V} \\ dim(\mathcal{V}_m) = m}} \min_{u_m \in \mathcal{V}_m \otimes \mathcal{S}_m} \|u - u_m\|_\star \circlearrowleft \min_{\substack{\mathcal{S}_m \subset \mathcal{S} \\ dim(\mathcal{S}_m) = m}} \min_{u_m \in \mathcal{V}_m \otimes \mathcal{S}_m} \|u - u_m\|_\star$$

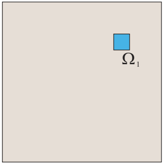
Updated progressive PGD (Power method with deflation)

Let $u_0 = 0$. For $m \geq 1$,

1. Compute a rank-one correction
$$w_m = v_m \otimes \phi_m \in \arg \min_{w \in \mathcal{R}_1(\mathcal{V} \otimes \mathcal{S})} \|u - u_m - w\|_\star$$
2. Set
$$\mathcal{V}_m = \mathcal{V}_{m-1} + span\{v_m\} = span\{v_i\}_{i=1}^m \quad \text{and} \quad U_m = \mathcal{V}_m \otimes \mathcal{S}$$
3. Compute
$$u_m \in \Pi_{U_m}(u) = \arg \min_{v \in \mathcal{V}_m \otimes \mathcal{S}} \|u - v\|_\star \quad (\text{i.e. } u_m = P_{\mathcal{V}_m} u)$$

Application to an advection-diffusion-reaction equation

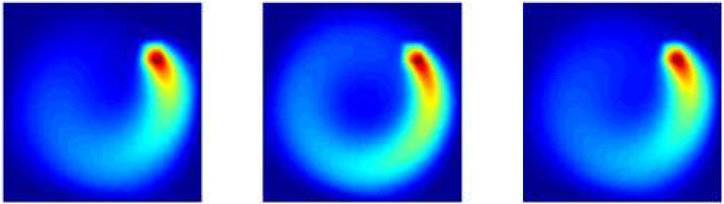
- $\partial_t u - a_1 \Delta u + a_2 c \cdot \nabla u + a_3 u = a_4 I_{\Omega_1}$ *on* $\Omega \times (0, T)$
- $u = 0$ *on* $\Omega \times \{0\}$
- $u = 0$ *on* $\partial\Omega \times (0, T)$



Uncertain parameters

$$a_i(\boldsymbol{\xi}) = \mu_{a_i}(1 + 0.2\xi_i), \quad \xi_i \in U(-1, 1), \quad \boxed{\boldsymbol{\Xi} = (-1, 1)^4}$$

Three samples of the solution $u(x, t, \boldsymbol{\xi})$



Application to an advection-diffusion-reaction equation

Separated representation of the solution

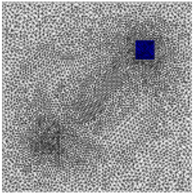
$$u(x,t,\boldsymbol{\xi}) \approx \sum_{i=1}^{M} w_i(x,t)\lambda_i(\boldsymbol{\xi})$$

$$w_i \in \mathcal{V} = L^2(0,T;H_0^1(\Omega)), \quad \lambda_i \in \mathcal{S} = L^2(\boldsymbol{\Xi}, dP_{\boldsymbol{\xi}})$$

Discretization

- Space : finite element (4640 nodes)
- Time : discontinuous Galerkin of degree 0 (80 time intervals)
- Stochastic : polynomial chaos of degree $p = 5$ in 4 dimension

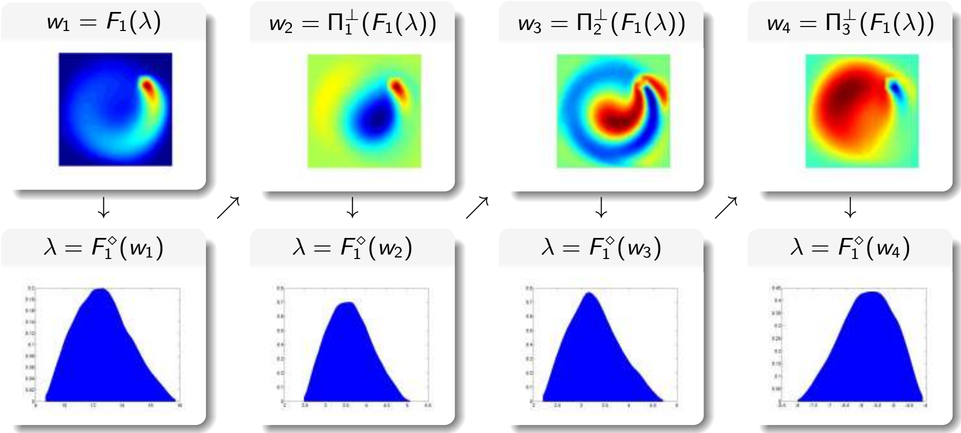
$$dim(\mathcal{V}_N) = 371200 \quad dim(\mathcal{S}_P) = 125$$



Computation of Generalized Spectral Decomposition

Arnoldi algorithm

1. Initialize λ and for $k = 1 \dots M$, $w_k = \Pi^{\perp}_{k-1}(F_1(\lambda))$ and $\lambda = F_1^{\diamond}(w_k)$
2. Compute associated $\{\lambda_1, \dots, \lambda_M\} = F^{\diamond}(\{w_1, \dots, w_M\})$

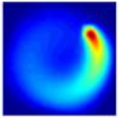


Computation of Generalized Spectral Decomposition

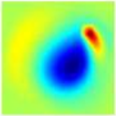
Arnoldi algorithm

1. Initialize λ and for $k = 1 \dots M$, $w_k = \Pi^{\perp}_{k-1}(F_1(\lambda))$ and $\lambda = F_1^{\diamond}(w_k)$
2. Compute associated $\{\lambda_1, \dots, \lambda_M\} = F^{\diamond}(\{w_1, \dots, w_M\})$

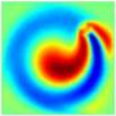
$w_1 = F_1(\lambda)$



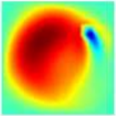
$w_2 = \Pi^{\perp}_1(F_1(\lambda))$



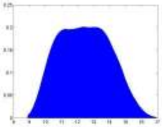
$w_3 = \Pi^{\perp}_2(F_1(\lambda))$



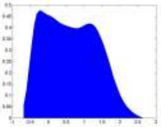
$w_4 = \Pi^{\perp}_3(F_1(\lambda))$



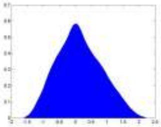
λ_1



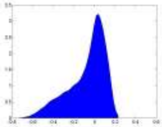
λ_2



λ_3

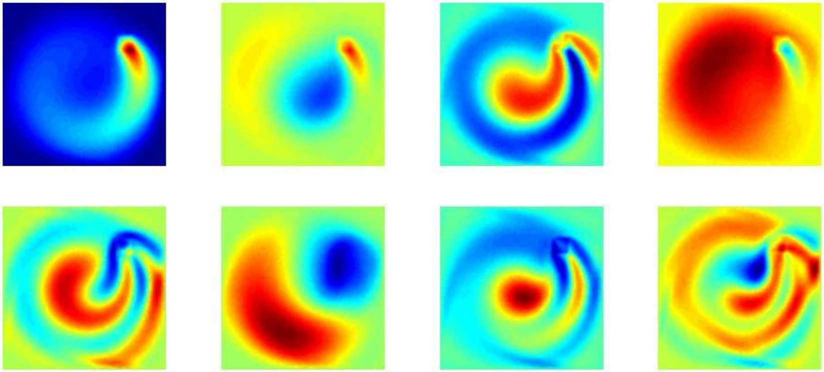


λ_4



Generalized Spectral Decomposition
Deterministic modes

8 first modes of the decomposition $\{w_1(x,t) ... w_8(x,t)\}$

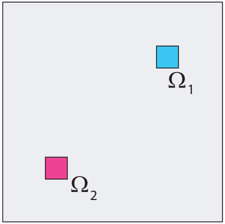


To compute these modes $\Rightarrow$ **only 8 deterministic problems**

Probability density function

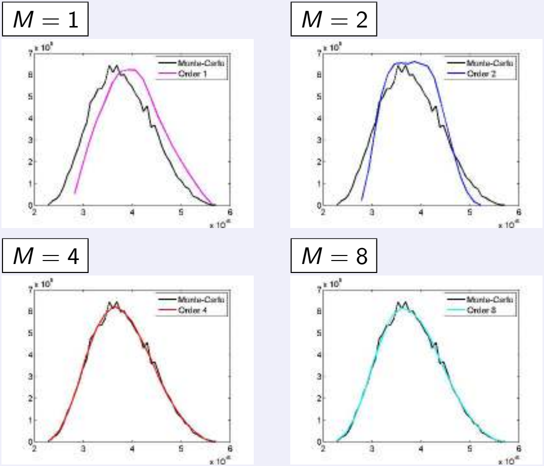
Quantity of interest

$$Q(\xi) = \int_0^T \int_{\Omega_2} u(x,t,\xi)\,dxdt$$



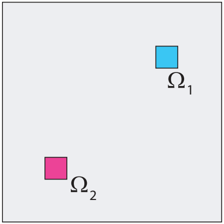
$$Q_M(\xi) = \int_0^T \int_{\Omega_2} u_M(x,t,\xi)\,dxdt$$

Probability density function of $Q_M(\xi)$



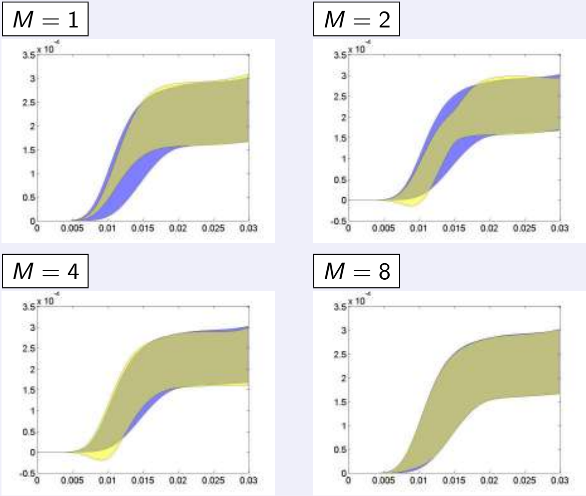
Quantity of interest

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



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

99% Quantiles of $Q_M(t, \boldsymbol{\xi})$



Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Tensor formats for stochastic parametric problems
with M. Chevreuil, L. Giraldi, O. Zahm

Hierarchical structure

$$\frac{\partial u}{\partial t} - \nabla \cdot (\kappa(\xi)\nabla u) + \gamma(\xi')u = f$$

$$u \in \underbrace{\underbrace{\mathcal{V}_x \otimes \mathcal{V}_y}_{\mathcal{V}_{x,y}} \otimes \mathcal{V}_t}_{\mathcal{V}} \otimes \underbrace{\underbrace{\mathcal{S}_{\xi_1} \otimes \ldots \otimes \mathcal{S}_{\xi_r}}_{\mathcal{S}_{\xi}} \otimes \underbrace{\mathcal{S}_{\xi'_1} \otimes \ldots \otimes \mathcal{S}_{\xi'_s}}_{\mathcal{S}_{\xi'}}}_{\mathcal{S}}$$

Idea

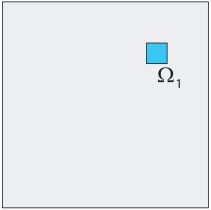
Exploit the specific tensor product structure of SPDEs in order to

- avoid the deterioration of convergence when dimension increases
- recover optimal model reduction obtained by Karhunen-Loeve type decomposition

$$u(x, y, t, \xi, \xi') = \sum_{i=1}^{m} v_i(x, y, t)\phi_i(\xi, \xi')$$

Illustration : stationary advection-diffusion-reaction equation

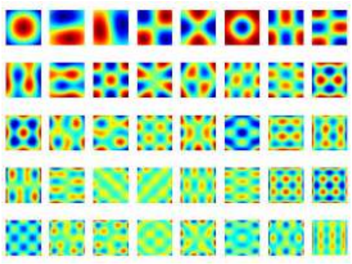
$$-\nabla \cdot (\kappa \nabla u) + c \cdot \nabla u + \gamma u = \delta I_{\Omega_1}(x) \quad on \quad \Omega$$



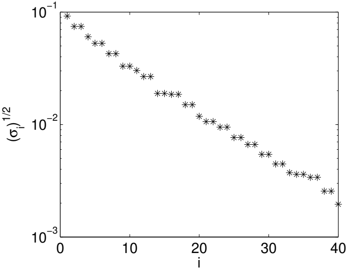
Random field

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

Spatial modes $\kappa_i(x)$



Amplitudes σ_i



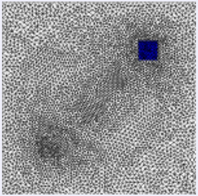
Stochastic approximation

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

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

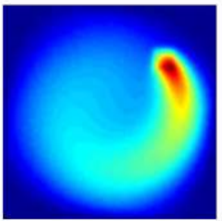
$$dim(\mathcal{S}_P) = 5^{40} \approx 10^{28}$$

Finite element mesh



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

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



A basic hierarchical format

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

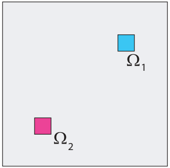
▸ Results

Convergence properties of quantities of interest

Probability of events

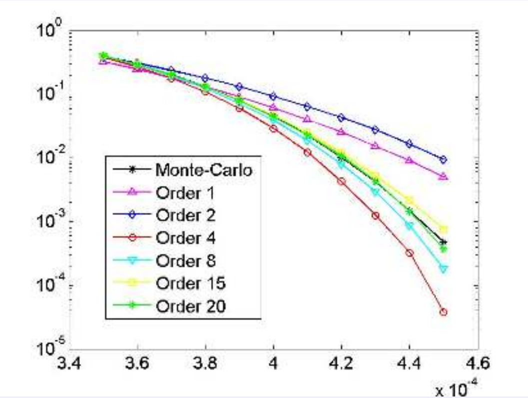
Quantity of interest

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



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

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



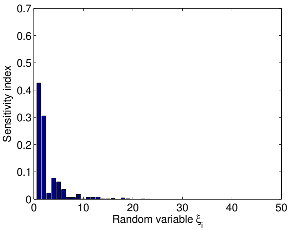
$$Q(\boldsymbol{\xi}) \approx Q_M(\boldsymbol{\xi}) \approx Q_{M,Z}(\boldsymbol{\xi}) = \sum_{k=1}^{Z} q_k \Psi_k(\boldsymbol{\xi}), \quad \Psi_k(\boldsymbol{\xi}) = \prod_{i=1}^{40} \phi_k^i(\xi_i)$$

First order Sobol sensitivity index with respect to parameter ξ_i

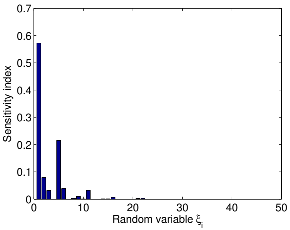
$$\boxed{S_i = \frac{Var(E(Q|\xi_i))}{Var(Q)}} \quad E(Q|\xi_i) = \sum_{k=1}^{Z} \alpha_k^i \phi_k^i(\xi_i), \quad \alpha_k^i = q_k \prod_{\substack{j=1 \\ j\neq i}}^{40} E(\phi_k^j(\xi_j))$$

First order Sobol sensivity indices S_i

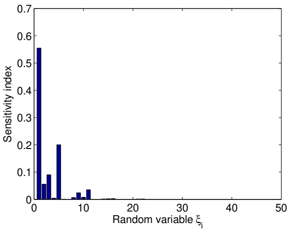
M=1



M=5



M=15

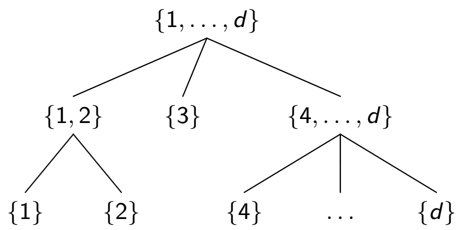


More hierarchical formats

Hierarchical canonical representation

With $V = V_1 \otimes \ldots \otimes V_d$, define a hierarchical tree T on $\{1, \ldots, d\}$. For $t \in T$, denote by $S(t)$ the set of successors of t.

$$
\begin{aligned}
V &= V_{t_0} \quad \text{(Level 0)} \\
&= \bigotimes_{t_1 \in S(t_0)} V_{t_1} \quad \text{(Level 1)} \\
&= \bigotimes_{t_1 \in S(t_0)} \Big(\bigotimes_{t_2 \in S(t_1)} V_{t_2} \Big) \quad \text{(Level 2)} \\
&= \ldots
\end{aligned}
$$



Let $\{m_t\}_{t \in T}$ be a set of decomposition ranks.

$$
\begin{aligned}
\mathcal{H}^T(V) &= \Big\{ v = \sum_{i_1=1}^{m_{t_0}} \bigotimes_{t_1 \in S(t_0)} \phi^{t_1}_{i_1} \; ; \; \phi^{t_1}_{i_1} \in \mathcal{H}^{T(t_1)}(V_{t_1}) \Big\} \\
&= \Big\{ v = \sum_{i_1=1}^{m_{t_0}} \bigotimes_{t_1 \in S(t_0)} \Big(\sum_{i_2=1}^{m_{t_1}} \bigotimes_{t_2 \in S(t_1)} \phi^{t_2}_{i_1, i_2} \Big) \; ; \; \phi^{t_2}_{i_1, i_2} \in \mathcal{H}^{T(t_2)}(V_{t_2}) \Big\} = \ldots
\end{aligned}
$$

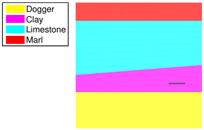
Example: stochastic groundwater flow equation (Couplex)

Groundwater flow equation (hydraulic head u)

$$\boxed{-\nabla \cdot (\kappa(x,\xi)\nabla u) = 0 \quad x \in \Omega,\ \xi \in \Xi}$$

$+$ boundary conditions

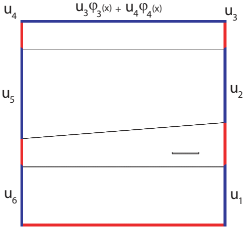
Geological layers with uncertain properties



κ's probability laws

Layer	Law
Dogger	$LU(5, 125)$
Clay	$LU(3.10^{-7}, 3.10^{-5})$
Limestone	$LU(1.2, 30)$
Marl	$LU(10^{-5}, 10^{-4})$

Uncertain BCs



Neumann homogeneous

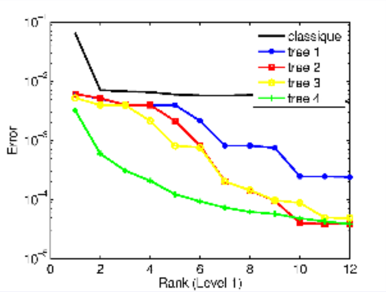
Dirichlet

	Law
u_1	$U(288, 290)$
u_2	$U(305, 315)$
u_3	$U(330, 350)$
u_4	$U(170, 190)$
u_5	$U(195, 205)$
u_6	$U(285, 287)$

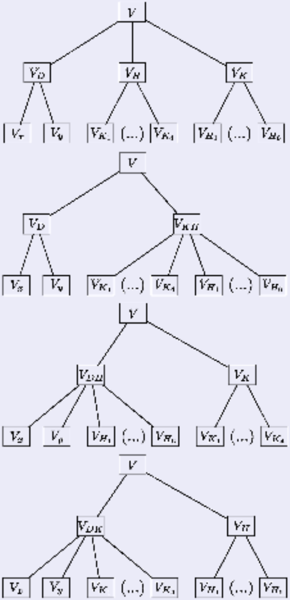
10 basic uniform random variables ξ,
$\Xi = (-1,1)^{10}$, uniform probability measure μ

$$V = \underbrace{V_x \otimes V_y}_{V_D \text{ (Space)}} \otimes \underbrace{S_{\xi_1} \otimes \ldots \otimes S_{\xi_4}}_{V_K \text{ (Diffusion)}} \otimes \underbrace{S_{\xi'_1} \otimes \ldots \otimes S_{\xi'_6}}_{V_H \text{ (BCs)}}$$

Progressive construction of level 1 decomposition: error versus rank at level 1



Trees 1 to 4



Outline

1. Uncertainty quantification with functional approaches
2. Strategies for complexity reduction
3. Tensor-based methods
4. Optimal model order reduction
5. Tensor formats for stochastic problems
6. Non intrusive tensor methods
7. References

Non intrusive sparse approximations

Aim

Compute an approximation of $u \in \mathcal{S}_P$ using a few samples $\{u(y^k)\}_{k=1}^{Q}$.

Regression in $\mathcal{S}_P = span\{\psi_i\}_{i=1}^P$

Approximation $v(\xi) = \sum_{i=1}^P v_i \psi_i(\xi)$ defined by

$$\boxed{\min_{v \in \mathcal{S}_P} \|u - v\|_Q^2} \quad \text{with} \quad \|u - v\|_Q^2 = \sum_{k=1}^{Q} |u(\xi^k) - v(\xi^k)|^2$$

or equivalently by

$$\boxed{\min_{\mathbf{v} \in \mathbb{R}^P} \|\mathbf{u} - \mathbf{\Phi}\mathbf{v}\|_2^2} \quad \text{with } \mathbf{v} = (v_i)_i, \ \mathbf{\Phi} = (\psi_i(\xi^k))_{k,i}$$

Regularized regression

$$\boxed{\min_{v \in \mathcal{S}_P} \|u - v\|_Q^2 + \lambda \mathcal{R}(v)} \quad \text{Choice of } \mathcal{R} \text{ ?}$$

Non intrusive sparse approximations

Ideal sparse regression

For a given precision ϵ, ideal sparse regression problem:

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{v}\|_0 \quad \text{subject to} \quad \|\mathbf{u}-\mathbf{\Phi v}\|_2^2 \leq \epsilon} \quad \text{with } \|\mathbf{v}\|_0 = \#\{i; v_i \neq 0\}$$

Approximate sparse regression (Basis Pursuit Denoising)

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{v}\|_1 \quad \text{subject to} \quad \|\mathbf{u}-\mathbf{\Phi v}\|_2^2 \leq \epsilon}$$

which for some $\lambda(\epsilon)$ is equivalent to

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{u}-\mathbf{\Phi v}\|_2^2 + \lambda\|\mathbf{v}\|_1}$$

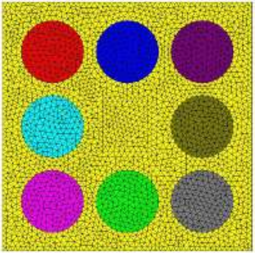
Illustration: diffusion problem with multiple inclusions

$$\begin{cases} -\nabla \cdot (\kappa \nabla u) = I_D(x) \quad on \quad \Omega = (0,1)\times(0,1) \\ u = 0 \quad on \quad \partial\Omega \end{cases}$$

with

$$\kappa(x,\xi) = \begin{cases} 1 & if \ x \in \Omega_0 \\ 1 + 0.1\xi_i & if \ x \in \Omega_i, \ i = 1...8 \end{cases}$$

with $\xi_i \in U(-1,1)$. $\Xi = (-1,1)^8$.



Approximation of a Quantity of Interest $I(u)$ in $\mathcal{S}_P \subset L^2_\mu(\Xi)$

$$I(u)(\xi) = \int_D u(x,\xi)dx, \quad D = (0.4,0.6)\times(0.4,0.6)$$

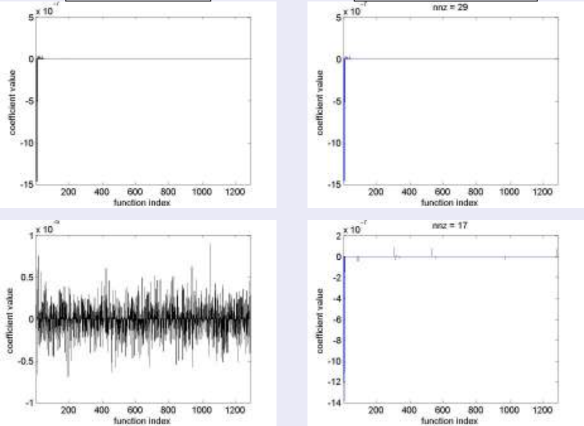
$$\boxed{\mathcal{S}_P = \mathbb{P}_4(\Xi), \quad dim(\mathcal{S}_P) = 1286}$$

$I(\xi) \approx \sum_\alpha I_\alpha \psi_\alpha(\xi)$: coefficients $\{I_\alpha\}$ obtained by regression

Least-square | ℓ_1-regularization

$Q = 2000$

$Q = 50$



Non intrusive sparse approximations

Issues

- Algorithms limited to approximation spaces with low dimension P
- Selection of good bases ?

Non intrusive sparse tensor approximations
with P. Rai, M. Chevreuil, J. Sen Gupta

Adaptive sparse tensor approximation

- Greedy construction of a basis $\{w_i\}_{i=1}^m$ selected in a tensor subset $\mathcal{M}$
- Compute $u_m = \sum_{i=1}^m \alpha_i w_i$ using regularized regression

Algorithm

Let $u_0 = 0$. For $m \geq 1$,

- Compute a correction $w_m \in \mathcal{M}$ defined by

$$w_m \in \arg\min_{w \in \mathcal{M}} \|u - u_{m-1} - w\|_Q^2$$

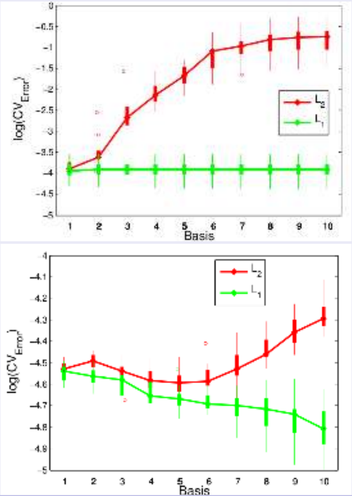
  Computed using alternating minimization on the parameters of $\mathcal{M}$.

- Set $U_m = span\{w_i\}_{i=1}^m$ (reduced approximation space)
- Compute $u_m = \sum_{i=1}^m c_i w_i \in U_m$ using sparse regularization

$$\min_{\mathbf{c} \in \mathbb{R}^m} \|u - \sum_{i=1}^m c_i w_i\|_Q^2 + \lambda \|\mathbf{c}\|_s$$

Illustration: diffusion problem with multiple inclusions

Error with ℓ_1 and ℓ_2 regularized update for $Q = 56$ (top) and $Q = 1000$ (bottom)



Error estimated using cross validation

Error with ℓ_1-regularized update for different sample sizes.

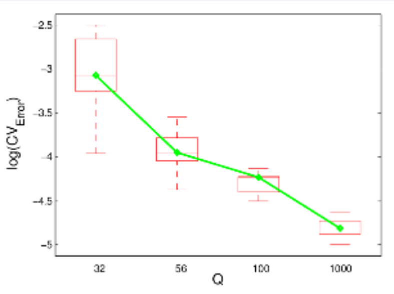


Illustration: advection-diffusion equation with random field

Stationary advection diffusion reaction stochastic equation

$$-\nabla \cdot (\mu(x,\xi)\nabla u) + c \cdot \nabla u + \kappa u = I_{\Omega_1}$$
$$+ \text{ homogeneous BCs}$$

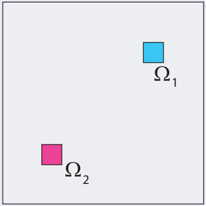
- random diffusion field

$$\mu(x,\xi) = \mu_0 + \sum_{i=1}^{100} \sqrt{\sigma_i}\mu_i(x)\xi_i$$

- approximation space

$$\mathcal{V}_N \otimes \underbrace{\mathbb{P}_p(\Xi_1) \otimes \ldots \otimes \mathbb{P}_p(\Xi_{100})}_{\mathcal{S}_P}$$

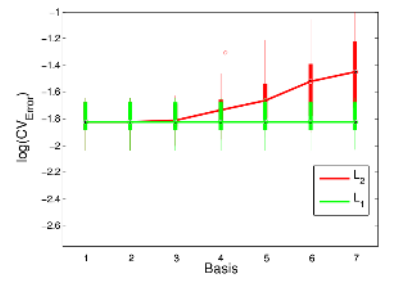
Problem and QoI



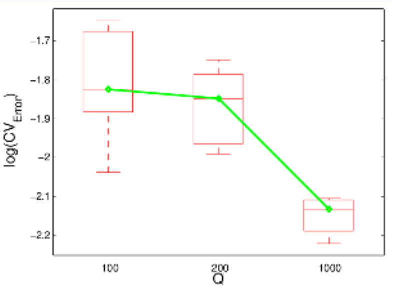
$$I(\xi) = \int_{\Omega_2} u(x,\xi)dx$$

Error computed by cross-validation

Error of ℓ_1 and ℓ_2-regularized updates for sample size $Q = 100$



Error with ℓ_1-regularized update for different sample sizes



Some conclusions and challenges

Tensor based and sparse approximation methods

- A route to circumvent the curse of dimensionality
- A non linear approximation world !

Some challenges

- Efficient algorithms for the construction of optimal approximations
- Robust non intrusive constructions of tensor approximations
- Adaptive search of optimal tensor formats
- Suitable change of variables for obtaining low rank decompositions
- Goal-oriented decompositions : take into account probabilistic quantities of interest (probability of events, moments, ...)
- Multiscale decompositions: one-scale decomposition has too much information to capture

Thank you for your attention

A. Nouy.

A generalized spectral decomposition technique to solve a class of linear stochastic partial differential equations.

Computer Methods in Applied Mechanics and Engineering, 196(45-48):4521–4537, 2007.

A. Nouy.

Generalized spectral decomposition method for solving stochastic finite element equations: invariant subspace problem and dedicated algorithms.

Computer Methods in Applied Mechanics and Engineering, 197:4718–4736, 2008.

A. Nouy and O.P. Le Maître.

Generalized spectral decomposition method for stochastic non linear problems.

Journal of Computational Physics, 228(1):202–235, 2009.

A. Nouy.

Recent developments in spectral stochastic methods for the numerical solution of stochastic partial differential equations.

Archives of Computational Methods in Engineering, 16(3):251–285, 2009.

A. Nouy.

Proper Generalized Decompositions and separated representations for the numerical solution of high dimensional stochastic problems.

Archives of Computational Methods in Engineering, 17(4):403–434, 2010.

A. Nouy.

A priori model reduction through proper generalized decomposition for solving time-dependent partial differential equations.

Computer Methods in Applied Mechanics and Engineering, 199(23-24):1603–1626, 2010.

A. Falco and A. Nouy.

A Proper Generalized Decomposition for the solution of elliptic problems in abstract form by using a functional Eckart-Young approach.

Journal of Mathematical Analysis and Applications, 376(2):469–480, 2011.

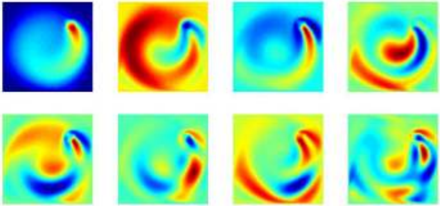
A. Falco and A. Nouy.

Proper Generalized Decomposition for nonlinear convex problems in tensor Banach spaces.

Numerische Mathematik, (2012).

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

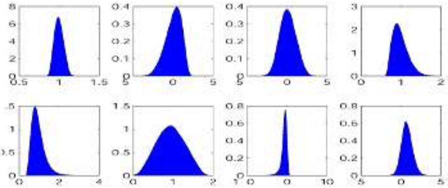
Spatial modes $W = \{w_1(x)...w_8(x)\}$



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

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

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



Separated representation of random variables

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

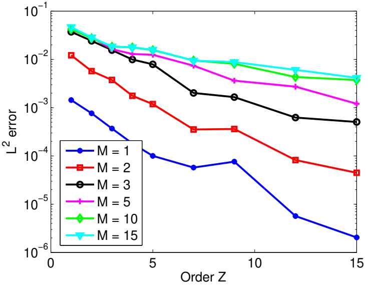
Convergence of multidimensional separated representations

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

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

$$\Lambda(\boldsymbol{\xi}) \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \Psi_k(\boldsymbol{\xi}), \quad \phi_k^0 \in \mathbb{R}^M, \quad \Psi_k(\boldsymbol{\xi}) = \phi_k^1(\xi_1)...\phi_k^{40}(\xi_{40}) \in \mathcal{S}_P$$

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



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

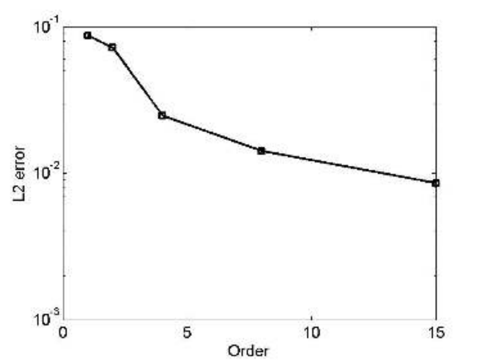
For a precision of 10^{-2}: $\boxed{Z \approx 10}$
to be compared with $\boxed{P = 10^{28}}$

Convergence of generalized spectral decomposition

Mean square convergence

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

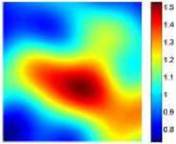
$\|u_M - u\|^2_{L^2}$ $(N_s = 500)$



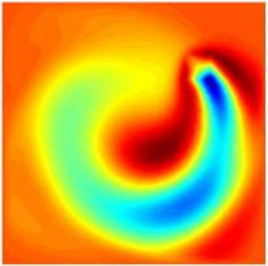
Convergence properties of generalized spectral decomposition

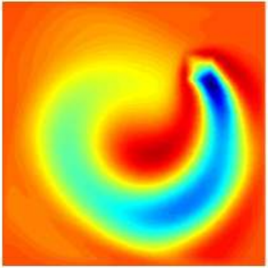
Samples

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

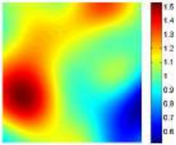


$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$ $u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$

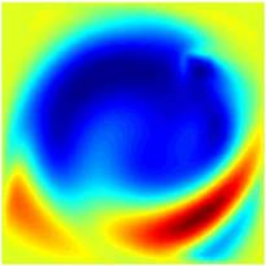




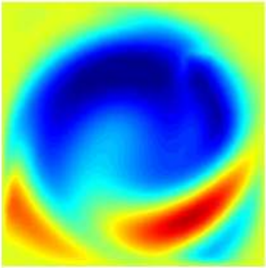
Sample of $\kappa(x, \boldsymbol{\xi})$



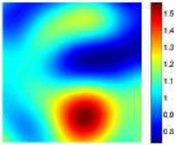
$u_{ref}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$



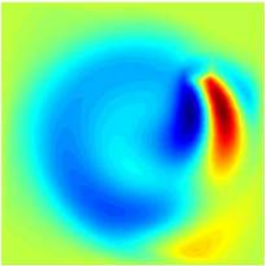
$u_{15}(x, \boldsymbol{\xi}) - u(x, \boldsymbol{\mu}_{\boldsymbol{\xi}})$

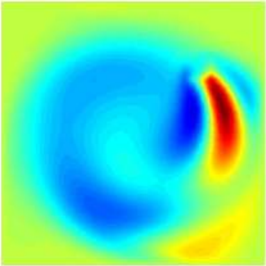


Sample of $\kappa(x, \boldsymbol{\xi})$



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

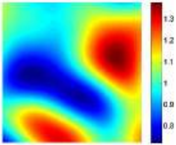




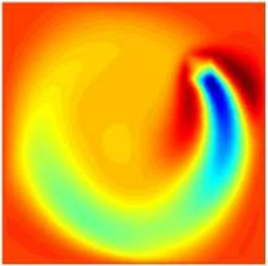
Convergence properties of generalized spectral decomposition

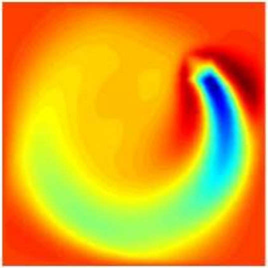
Samples

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



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



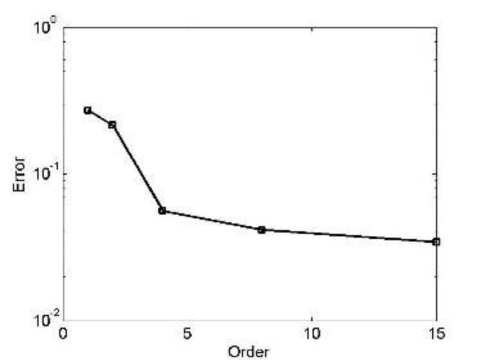


Convergence properties of generalized spectral decomposition

Uniform convergence

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

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

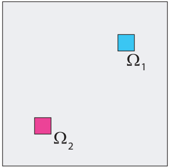


Convergence properties of quantities of interest

Probability density function

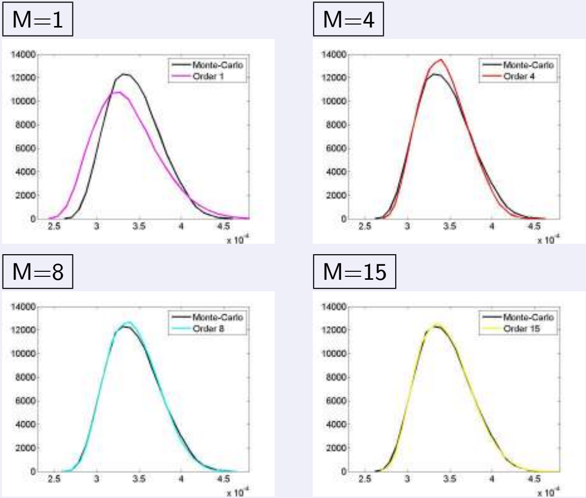
Quantity of interest

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



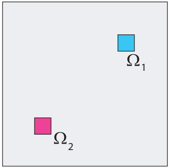
$$Q_M(\boldsymbol{\xi}) = \int_{\Omega_2} u_M(x, \boldsymbol{\xi})\, dx$$

Probability density function of $Q(\boldsymbol{\xi})$



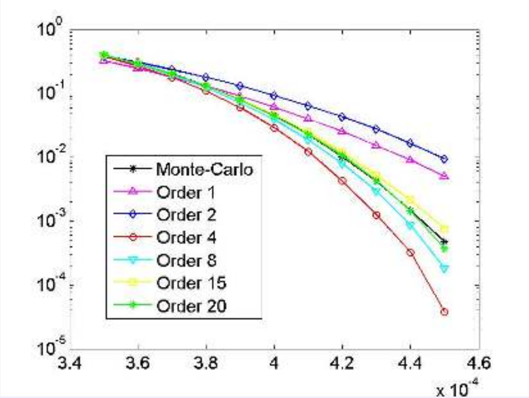
Quantity of interest

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



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

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



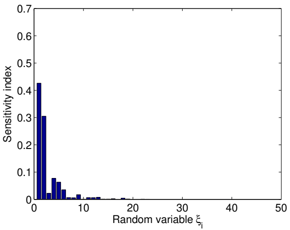
$$Q(\boldsymbol{\xi}) \approx Q_M(\boldsymbol{\xi}) \approx Q_{M,Z}(\boldsymbol{\xi}) = \sum_{k=1}^{Z} q_k \Psi_k(\boldsymbol{\xi}), \quad \Psi_k(\boldsymbol{\xi}) = \prod_{i=1}^{40} \phi_k^i(\xi_i)$$

First order Sobol sensitivity index with respect to parameter ξ_i

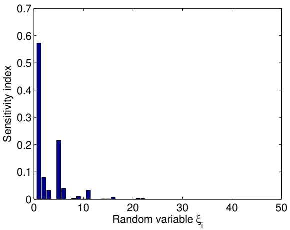
$$\boxed{S_i = \frac{Var(E(Q|\xi_i))}{Var(Q)}} \quad E(Q|\xi_i) = \sum_{k=1}^{Z} \alpha_k^i \phi_k^i(\xi_i), \quad \alpha_k^i = q_k \prod_{\substack{j=1 \\ j \neq i}}^{40} E(\phi_k^j(\xi_j))$$

First order Sobol sensivity indices S_i

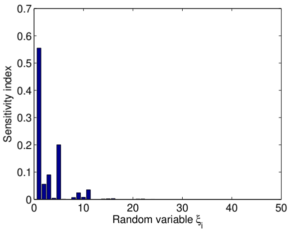
M=1



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

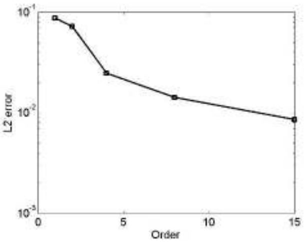
$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^{M} \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

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

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

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

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



Return

Results... in brief

Deterministic/stochastic separation

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

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

Random variables separation

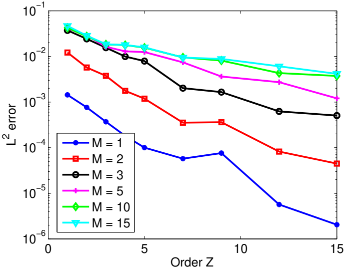
$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^{M} \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

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

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

- $dim(\mathcal{V}_M) \approx 15$ $\ll 4435 = dim(\mathcal{V}_N)$
- $dim(\mathcal{S}_Z) \approx 10$ $\ll 10^{28} = dim(\mathcal{S}_P)$

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



Results... in brief

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

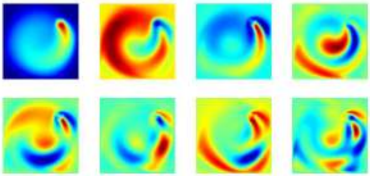
$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^{M} \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

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

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

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

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



Return

Results... in brief

Deterministic/stochastic separation

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

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

Random variables separation

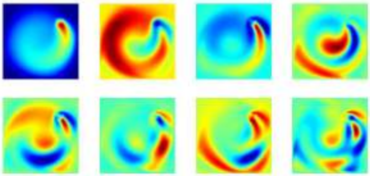
$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^{M} \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

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

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

- $dim(\mathcal{V}_M) \approx 15$ $\ll 4435 = dim(\mathcal{V}_N)$
- $dim(\mathcal{S}_Z) \approx 10$ $\ll 10^{28} = dim(\mathcal{S}_P)$
- 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 $\{w_1(x)...w_8(x)\}$



Return