Stochastic Spectral Methods for Uncertainty Quantification

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O. Le Maître & O. Knio Stochastic Spectral Methods



UQ in numerical simulations Proper Generalized Decompositions

Content :

UQ in numerical simulations

- Numerical Simulation
- Uncertainty propagation
- UQ methods



Polynomial Chaos expansions

- Stochastic discretization
- PC solution methods.
- Examples



Proper Generalized Decompositions

- Optimal Decompositions
- Algorithms
- An example

Numerical Simulation Uncertainty propagation UQ methods

The simulation of a physical system involves the basic steps :

Definition of a mathematical model : express basic physical principles (conservation laws, modeling of elementary processes, formulation, ...)

Prescription of the system investigated : definition of model inputs (geometry, forcing, ICs, BCs, model constants, ...)

Construction & resolution of the numerical model : discretization method, algorithms, approximate solvers, (parallel) implementation, ...

Analysis & post-treatment : recast model output in a format suitable to fair decision making.

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Prescription of the system investigated : definition of model inputs (geometry, forcing, ICs, BCs, model constants, ...) Usually cannot *exactly specified*, *e.g.* because of limited measurements / data, identification procedures, inherent variabilities,...

Construction & resolution of the numerical model : discretization method, algorithms, approximate solvers, (parallel) implementation, ...
 To obtain an *approximation* of the model solution within some prescribed accuracy.
 Verification & error analysis

Analysis & post-treatment : recast model output in a format suitable to fair decision making.
 One should quantify the impact of all sources of errors and uncertainty affecting the numerical predictions.
 Error & uncertainty quantification

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Reality : all these basic steps are mixed and strongly interrelated in engineering practice.

Numerical Simulation Uncertainty propagation UQ methods

Input-data uncertainty D

- Inherent variability (e.g. industrial processes, natural systems, variable environments,...)
- Epistemic uncertainty (e.g. incomplete identification/calibration, unobserved quantities, non-measurable model constants,...)

May not be reducible, even theoretically

• Probabilistic treatment of input uncertainty :

D defined on $(\Theta, \mathcal{A}, d\mu)$.

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Uncertainty propagation

Given the random input $D \in (\Theta, A, d\mu)$, and a model $\mathcal{M}(\cdot|D)$, the objective is to determine the model solution U:

U is random and defined on (Θ, A, dµ) :

 $U = U(\theta \in \Theta).$

• U and D are dependent random quantities, related by the model :

 $\mathcal{M}(U(\theta)|D(\theta)) = 0, \quad \forall \theta \in \Theta.$

Numerical Simulation Uncertainty propagation UQ methods

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Computational approaches (I) :

Deterministic Methods

- Local sensitivity analysis : adjoint, AD, ...
- Perturbation techniques : limited to low variance of the input.
- Neumann expansions : limited to low expansion order.
- Moments method : limited characterization of S, closure problem (non-Gaussian / non-linear problems).

Stochastic Methods

- Generate at random a sample set of inputs :
- Compute the corresponding sample set of model ouputs :

 $\mathcal{M}(U(\theta_i)|D(\theta_i))=0.$

 $S_D = \{ D(\theta_1), D(\theta_2), \ldots \}$ $S_U = \{ U(\theta_1), U(\theta_2), \ldots \}$

③ Use the sample set S_U to estimate moments, correlations, ...

$$\mathbb{E}\left\{S\right\} = \frac{1}{M}\sum_{i=1}^{M}U(\theta_i),\ldots$$

Robust and generic approach, no assumption regarding to U or D, reuse deterministic codes, but slow convergence of the random estimates with the sample set size (M).

Monte-Carlo

Numerical Simulation Uncertainty propagation UQ methods

Computational approaches (II) :

Solution spaces

We assume that $U(\theta) \in \mathbb{V}$, almost surely. The Hilbert space \mathbb{V} is equipped with the inner product and norm

$$(U, V)_{\mathbb{V}}, \quad \|U\| = (U, U)_{\mathbb{V}}^{1/2} \quad U, V \in \mathbb{V}.$$

Since U is random, ||U|| is a random variable :

We further assume that the solution norm is a second order random variable :

$$\mathbb{E}\left\{ \left\| oldsymbol{U}
ight\|_{\mathbb{V}}^2
ight\} = \int_{\Theta} \left\| oldsymbol{U}(heta)
ight\|_{\mathbb{V}}^2 oldsymbol{d} \mu(heta) < \infty.$$

We denote $L_2(\Theta, d\mu)$ the space of second order random variables defined on $(\Theta, A, d\mu)$, equipped with the inner product and norm

$$\langle u, v \rangle = \mathbb{E} \{ uv \} = \int_{\Theta} u(\theta) v(\theta) d\mu(\theta), \quad \|u\|_{L_2} = \langle u, u \rangle^{1/2} \quad u, v \in L_2(\Theta, d\mu).$$

Functional representation

The stochastic solution can be sought as an element of the tensored Hilbert space $X = L_2(\Theta, d\mu) \otimes \mathbb{V}$:

$$V \in X \Rightarrow V(\theta) = \sum_{\alpha} v_{\alpha}(\theta) V_{\alpha}, \quad v_{\alpha} \in L_{2}(\Theta, d\mu), \ V_{\alpha} \in \mathbb{V}.$$

- $v_{\alpha}(\theta)$ are random variables,
- V_{α} are the deterministic functions.

 $\|U\|_{\mathbb{V}}(\theta)$

Computational approaches (II) :

Functional representation

The stochastic solution can be sought as an element of the tensored Hilbert space $X = L_2(\Theta, d\mu) \otimes \mathbb{V}$:

$$V \in X \Rightarrow V(\theta) = \sum_{\alpha} f_{\alpha}(\theta) v_{\alpha}, \quad f_{\alpha} \in L_{2}(\Theta, d\mu), \ v_{\alpha} \in \mathbb{V}.$$

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For computational purposes, we need

- **1** to discretize the abstract probability space $(L_2(\Theta, d\mu))$,
- 2 to discretize the deterministic space V,
- Ito define the functional expansion,
- to introduce computational strategies for its determination.

The interest in the functional expansion comes from

- possibly high convergence with the number of modes : low storage, low computational cost, ...
- explicit mapping $D(\theta) \mapsto U(\theta)$:

detailed UQ, sensitivity analysis

• cheap (re)sampling of the stochastic solution :

surrogate model for subsequent use.

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2 Polynomial Chaos expansions

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UQ in numerical simulations Stochastic discretization Polynomial Chaos expansions PC solution methods Examples

Representation of Input Uncertainty

We assume the availability of a parametrization of the uncertain inputs in terms of a set of N independent real-valued second order random variables $\boldsymbol{\xi} = (\xi_1, \dots, \xi_N)$ defined on $(\Theta, \mathcal{A}, d\mu)$:

$$D(\theta) = D(\boldsymbol{\xi}(\theta)), \quad p_{\boldsymbol{\xi}}(\boldsymbol{y}) = \prod_{i=1}^{N} p_i(y_i),$$

where p_{ξ} is the joint density function of ξ , with support $\Xi \subseteq \mathbb{R}^{N}$.

- transformation of random variables,
- principal orthogonal decompositions,
- principal component analysis.

Example : Karhunen-Loeve decomposition of a Gaussian random field

$$\kappa(\boldsymbol{x},\theta) \approx \mathbb{E}\left\{\kappa\right\}(\boldsymbol{x}) + \sum_{i=1}^{N} \phi_i(\boldsymbol{x})\xi_i(\theta), \quad \xi_i \sim N(0,1), \quad \mathbb{E}\left\{\xi_i\xi_j\right\} = \delta_{ij}$$

Then, the solution $U(\theta)$ of $\mathcal{M}(U|D(\theta)) = 0$ can be identified with $\tilde{U}(\boldsymbol{\xi})$, the solution of

$$\mathcal{M}(\tilde{U}(\boldsymbol{\xi})|D(\boldsymbol{\xi}))=0.$$

In addition (dropping the tilde),

$$U(\boldsymbol{\xi}) = \sum_{\alpha} \Psi_{\alpha}(\boldsymbol{\xi}) u_{\alpha} \in L_{2}(\Xi, \boldsymbol{p}_{\boldsymbol{\xi}}) \otimes \mathbb{V},$$

where $\Psi_{\alpha}(\boldsymbol{\xi}) \in L_2(\Xi, \boldsymbol{p}_{\boldsymbol{\xi}})$ and $u_{\alpha} \in \mathbb{V}$.

Polynomial Chaos expansions (I) PC expansion corresponds to the case where, in

$$U(\boldsymbol{\xi}) = \sum_{lpha} \Psi_{lpha}(\boldsymbol{\xi}) u_{lpha},$$

the stochastic functions Ψ_{α} are orthogonal multivariate polynomials in $\boldsymbol{\xi}$. For i = 1, ..., N, consider the family of orthogonal polynomials $\{\psi_0^i, \psi_1^i, ...\}$ such that

$$\left\langle \psi_{\alpha}^{i},\psi_{\beta}^{i}\right\rangle _{i}=\int\psi_{\alpha}^{i}(\mathbf{y})\psi_{\beta}^{i}(\mathbf{y})\mathbf{p}_{i}(\mathbf{y})d\mathbf{y}=\left\langle \psi_{\alpha}^{i},\psi_{\alpha}^{i}\right\rangle \delta_{\alpha,\beta},\quad\psi_{\alpha}^{i}\in\mathsf{\Pi}_{\alpha}(\mathbb{R}).$$

Classical distributions [Xiu and Karniadakis, 2002]

p_i Gaussian : Hermite polynomials,

- p_i Uniform : Legendre polynomials,
- p_i Exponential : Laguerre polynomials.

Let $\boldsymbol{\alpha} = (\alpha_1 \dots \alpha_N) \in \mathbb{N}^N$ be a multi-index, and define

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{N} \psi^{i}_{\alpha_{i}}(\xi_{i}),$$

such that

$$\left\langle \Psi_{\boldsymbol{\alpha}}, \Psi_{\boldsymbol{\beta}} \right\rangle = \left\langle \Psi_{\boldsymbol{\alpha}}, \Psi_{\boldsymbol{\alpha}} \right\rangle \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \prod_{i=1}^{N} \left\langle \psi_{\alpha_{i}}^{i}, \psi_{\alpha_{i}}^{i} \right\rangle \delta_{\alpha_{i}\beta_{i}}.$$

Then,

$$L_2(\Xi, p_{\boldsymbol{\xi}}) = \operatorname{span}\{\Psi_{\boldsymbol{\alpha}}, \ \boldsymbol{\alpha} \in \mathbb{N}^N\} \quad \text{and} \quad U(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^N} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) U_{\boldsymbol{\alpha}}.$$

[Wiener,38], [Cameron and Martin,47]

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Polynomial Chaos expansions (II)

In practice, the PC expansion must be truncated

$$U(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^{\mathbb{N}}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) u_{\boldsymbol{\alpha}} \approx \sum_{\boldsymbol{\alpha} \in \mathcal{A}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) u_{\boldsymbol{\alpha}} = U^{|\mathcal{A}|}(\boldsymbol{\xi}) \in \mathbb{S}^{\mathcal{A}} \otimes \mathbb{V} \subset L_{2}(\Xi, p_{\boldsymbol{\xi}}) \otimes \mathbb{V}.$$

Classical choice for the finite multi-index set \mathcal{A} are

- partial degree truncation
- total degree truncation
- hyperbolic cross truncation

the objective being to control the increase of the basis dimension with both the expansion order ${\rm No}$ and ${\rm N}$:

$$|\mathcal{A}_{N_{O}}^{p}| = \left(N_{O}+1\right)^{N} \geq |\mathcal{A}_{N_{O}}^{p}| = \frac{(N_{O}+N)!}{N_{O}!N!} \geq |\mathcal{A}_{N_{O},q<1}^{h}|.$$

Having Defined the stochastic basis, it remains to determine the deterministic functions U_{α} , $\alpha \in A$. HINT :

- Minimize L_2 -distance $\mathbb{E}\left\{ \| U(\boldsymbol{\xi}) U^{|\mathcal{A}|}(\boldsymbol{\xi}) \|_{\mathbb{V}}^2 \right\}$ NISP, "Regression"
- Verify $||U(\boldsymbol{\xi}) U^{|\mathcal{A}|}(\boldsymbol{\xi})||_{\mathbb{V}} = 0$ over a set of selected points

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Collocation

• Reformulate model equations for the U_{α}

Stochastic Galerkin projection

 $\mathcal{A}_{N_{0}}^{p} = \{ \boldsymbol{\alpha} \in \mathbb{N}^{N}, \max_{i} \alpha_{i} \leq N_{0} \},\$ $\mathcal{A}_{N_{0}}^{t} = \{ \boldsymbol{\alpha} \in \mathbb{N}^{N}, |\boldsymbol{\alpha}| = \sum_{i} \alpha_{i} < N_{0} \},\$

 $\mathcal{A}^{h}_{\mathrm{No},q} = \{ \boldsymbol{\alpha} \in \mathbb{N}^{\mathrm{N}}, \sum_{i} \alpha^{q}_{i} \leq \mathrm{No}^{q} \},\$

Stochastic Spectral Methods

Stochastic discretization PC solution methods Examples

Non-intrusive methods

Use code as a black-box

- Compute/estimate spectral coefficients via a set of deterministic model solutions
- Requires a deterministic solver only

2 Let $s^{(i)}$ be the solution of the deterministic problem $\mathcal{M}\left(U^{(i)}|D(\xi^{(i)})\right) = 0$

3 $S_U \equiv \{U^{(1)}, \ldots, U^{(m)}\}$ sample set of model solutions

- Estimate expansion coefficients u_{α} from this sample set.
- Complex models, reuse of determinsitic codes, planification, ...
- Error control and computational complexity (curse of dimensionality), ...

Basics

Least square fit

"Regression" [Bervillier et al, 2006]

• Best approximation is defined by minimizing a (weighted) sum of squares of residuals :

$$R^{2}\left(\left\{U_{\boldsymbol{\alpha}},\boldsymbol{\alpha}\in\mathcal{A}\right\}\right)\equiv\sum_{i=1}^{m}w_{i}\left\|U^{(i)}-\sum_{\boldsymbol{\alpha}\in\mathcal{A}}u_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}\left(\boldsymbol{\xi}^{(i)}\right)\right\|_{\mathbb{V}}^{2}.$$

Advantages/issues

- Stability with ratio *m* to |A|
- Convergence with number of regression points m
- Selection of the regression points and "regressors" $\Psi_{oldsymbol{lpha}}$
- Error estimate, ...
- \Rightarrow current trend toward Bayesian identification of the U_{α} : regularized version of the least square problem [Rizzi et al, 2012]

Non intrusive spectral projection : Exploit the orthogonality of the spectral basis : NISP [OLM et al, 2001]

$$\mathbb{E}\left\{\Psi_{\boldsymbol{\alpha}}^{2}\right\}u_{\boldsymbol{\alpha}}=\langle U,\Psi_{\boldsymbol{\alpha}}\rangle=\int_{\Xi}U(\boldsymbol{\xi})\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\rho_{\boldsymbol{\xi}}(\boldsymbol{\xi})d\boldsymbol{\xi}.$$

Estimate integrals from a random sample sets (MC and variants) :

$$\langle U, \Psi_{\boldsymbol{\alpha}} \rangle \approx \frac{1}{m} \sum_{i=1}^{m} U(\boldsymbol{\xi}^{(i)}) \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(i)})$$



- Convergence rate
- Error estimate
- Optimal sampling strategy

Non intrusive projection

Approximate integrals by N-dimensional guadratures :

$$\langle U, \Psi_{\boldsymbol{\alpha}} \rangle \approx \sum_{i=1}^{N_{\boldsymbol{Q}}} w^{(i)} U^{(i)} \Psi_{\boldsymbol{\alpha}} \left(\boldsymbol{\xi}^{(i)} \right).$$

Owing to the product structure of \equiv the quadrature points $\boldsymbol{\xi}^{(i)}$ and weights $\boldsymbol{w}^{(i)}$ can be obtained by

full tensorization of n points 1-D quadrature (i.e. Gauss) :

ted 1-D quadrature formula (Féjer, Clenshaw-Curtis) using Smolyak formula : [Smolyak, 63]

The partial tensorization results in so-called Sparse-Grid cubature formula, that can be constructed adaptively to the integrants (anisotropic formulas) in order to account for variable behaviors along the stochastic directions Gerstner and Griebel, 2003]

Deterministic Quadratures

PC solution methods

$$N_Q = n^N$$

 $N_O << n^N$

Stochastic discretization PC solution methods Examples

Non intrusive projection





- Important development of sparse-grid methods
- Anisotropy and adaptivity
- Also (sparse grid) collocation methods (N-dimensional interpolation) Hussaini, 2003], [Nobile et al, 2008]

[Mathelin and

Galerkin projection

- Weak solution of the stochastic problem $\mathcal{M}(U(\xi); D(\xi)) = 0$
- Needs adaptation of deterministic codes
- Potentially more efficient than NI techniques.

Let $\mathbb{S}^{\mathbb{P}} \subset L^2(\Xi, p_{\xi})$ defined as

$$\mathbb{S}^P = \text{span}\{\Psi_0,\ldots,\Psi_P\},$$

where the { Ψ_k } are orthogonal functionals in $\boldsymbol{\xi}$, *e.g.* a PC basis truncated to an order No. We seek for the approximate stochastic model solution in $\mathbb{V} \otimes \mathbb{S}^P$.

$$U(\boldsymbol{\xi}) \approx U^{\mathrm{P}}(\boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\boldsymbol{\xi}).$$

Inserting $U^{\mathbb{P}}$ in the weak formulation yields the stochastic residual $\mathcal{R}(U^{\mathbb{P}}) = \mathcal{M}(U^{\mathbb{P}}(\boldsymbol{\xi})|D(\boldsymbol{\xi})) \in \mathbb{V}'$.

Galerkin projection

[Ghanem & Spanos, 1991]

In general, one cannot find $U^{\mathbb{P}} \in \mathbb{V} \otimes \mathbb{S}^{\mathbb{P}}$ such that

$$\mathcal{R}(U^{\mathbb{P}}) = 0$$

It is then required that $\mathcal{R}(\textit{U}^{P})$ is orthogonal to the stochastic approximation space :

$$\left\langle \left\langle \mathcal{M}(U^{\mathrm{P}}(\boldsymbol{\xi})|D(\boldsymbol{\xi})),v\right\rangle _{\mathbb{V}^{\prime}},eta(\boldsymbol{\xi})
ight
angle =0 \hspace{1em} oralleta\in\mathbb{S}^{\mathrm{P}} ext{ and }v\in\mathbb{V}.$$

- This weak formulation corresponds to the stochastic Galerkin formulation.
- $\bullet~$ The actual formulation is obtained in practice by projecting all model equations on $\mathbb{S}^{P}.$

The Galerkin projection results in a set of P + 1 coupled problems for the stochastic modes u_k of the solution.

Find $\{u_k, k = 0, \dots, P+1\} \in \mathbb{V}^{P+1}$ such that

$$\left\langle \left\langle \mathcal{M}\left(\sum_{k=0}^{P} u_{k} \Psi_{k}(\boldsymbol{\xi}) | D(\boldsymbol{\xi})\right), v \right\rangle_{\mathbb{V}'}, \Psi_{l}(\boldsymbol{\xi}) \right\rangle = 0, \quad \forall v \in \mathbb{V} \text{ and } l = 0, \dots, P.$$

- The size of the Galerkin problem increases with the stochastic basis dimension P + 1.
- Recall that $P + 1 = (N + N_0)!/N!N_0!$ for polynomial truncation at order No.
- This can be costly for complex problems requiring large parametrization and large expansion order.
- $P + 1 < N_Q$ so complexity potentially less than for NISP and other non-intrusive approaches.
- Galerkin solvers and algorithms targeting a complexity scaling with P + 1, whenever possible.
- Projections on the Ψ_l of the model equations can be problematic for **non-linear models**.

PC solution methods Examples

Case of linear modelsLinear problems are of practical importance in scientific computing, whether as stand-alone mathematical problems or as ingredients of numerical methods (*e.g.* iterative techniques for the resolution of non-linear problems).

We analyze the structure of the Galerkin problem arising from the projection of linear models, and examine implications regarding suitable solution strategies.

Consider a linear problem discretized at the deterministic level and recast in the matrix form

$$[A](\boldsymbol{\xi})\boldsymbol{U}(\boldsymbol{\xi})=\boldsymbol{B}(\boldsymbol{\xi}).$$

Seeking the solution $U(\boldsymbol{\xi})$ in $\mathbb{R}^m \otimes \mathbb{S}^P$, the Galerkin projection gives :

$$\sum_{i=0}^{\mathsf{P}} \langle \Psi_k, [A] \Psi_i \rangle \, \boldsymbol{u}_i = \langle \Psi_k, \boldsymbol{B} \rangle \,, \quad k \in \{0, \ldots, \mathsf{P}\}.$$

equivalent to the larger (block) system of linear equations

$$\begin{bmatrix} [A]_{00} & \dots & [A]_{0P} \\ \vdots & \ddots & \vdots \\ [A]_{P0} & \dots & [A]_{PP} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \vdots \\ \boldsymbol{u}_P \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_0 \\ \vdots \\ \boldsymbol{b}_P \end{pmatrix}$$

 $[A]_{ij}$ the $(m \times m)$ matrix given by $[A]_{ij} := \langle \Psi_i, [A] \Psi_j \rangle$, and $\boldsymbol{b}_i := \langle \Psi_i, \boldsymbol{B} \rangle$.

- The linear Galerkin problem couples all the stochastic modes *u_i* ∈ ℝ^{*m*} of the stochastic solution.
- It is not possible in general to compute independently the components **u**_i.
- The size of the spectral problem is large : $m \times \dim \mathbb{S}^{\mathbb{P}} = m \times (\mathbb{P} + 1)$.
- Resolution of the linear Galerkin system can be demanding.
- An understanding of the block structured system is instructive to design and apply well-suited numerical methods.

In general, the matrix [A] has a PC expansion

$$[\mathbf{A}](\boldsymbol{\xi}) = \sum_{i=0}^{P} [\mathbf{A}]_{i} \Psi_{i}(\boldsymbol{\xi}) \implies [\mathbf{A}]_{ij} = \left\langle \Psi_{i}, [\mathbf{A}] \Psi_{j} \right\rangle = \sum_{k=0}^{P} [\mathbf{A}]_{k} \left\langle \Psi_{i}, \Psi_{j} \Psi_{k} \right\rangle,$$

and the Galerkin system can be conveniently recast as

$$\begin{bmatrix} [\overline{A}]_{00} & \dots & [\overline{A}]_{0P} \\ \vdots & \ddots & \vdots \\ [\overline{A}]_{P0} & \dots & [\overline{A}]_{PP} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_{0} \\ \vdots \\ \boldsymbol{u}_{P} \end{pmatrix} = \begin{pmatrix} \overline{\boldsymbol{b}}_{0} \\ \vdots \\ \overline{\boldsymbol{b}}_{P} \end{pmatrix},$$

where $\overline{m{b}}_i:=\left< B, \Psi_i \right> / \left< \Psi_i^2 \right>$ and

$$[\overline{A}]_{ij} := \sum_{k=0}^{P} [A]_k C_{kji}, \quad C_{ijk} := \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k \Psi_k \right\rangle}.$$

The third-order tensor *C_{ijk}* plays a fundamental role in stochastic Galerkin methods, especially in non-linear problems.

- C_{ijk} is symmetric w.r.t. the two first indices, C_{ijk} = C_{jik}.
- It induces block-symmetry in the spectral problem, $[\overline{A}]_{ij} = [\overline{A}]_{ji}$
- Many of the $(P + 1)^3$ entries are zero with many simplifications.
- For instance the first block of the Galerkin system reduces to

$$[\overline{A}]_{00} = \sum_{k=0}^{P} [A]_k C_{k00} = [A]_0$$

and the sum for the upper-right block (and lower-left block) actually reduces to $[\overline{A}]_{0P} = [A]_{P} / \langle \Psi_{P}^{2} \rangle$.

Many other simplifications occur.

Stochastic discretization PC solution methods Examples

$$N = 4$$
-dim $S^{P} = 35$ - $S = 0.58$ $N = 6$ -dim $S^{P} = 84$ - $S = 0.41$





$$N = 8$$
-dim $S^P = 165$ - $S = 0.31$ $N = 10$ -dim $S^P = 286$ - $S = 0.23$



Illustration of the sparse structure of the matrices of the linear spectral problem for different dimensions, N, with No = 3. Matrix blocks $[\overline{A}]_{ij}$ that are generally non-zero appear as black squares.

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No = 2-dim
$$S^P$$
 = 21-S = 0.52 No = 3-dim S^P = 56-S = 0.49



No = 4-dim
$$S^P$$
 = 126-S = 0.54 No = 5-dim S^P = 252-S = 0.55



Illustration of the sparse structure of the matrices of the linear spectral problem for different expansion orders No, with N = 5. Matrix blocks $[\bar{A}]_{ij}$ that are generally non-zero appear as black squares.

- The main difficulty in solving discrete linear spectral problems is the size of the system.
- The structure and sparsity of the linear Galerkin problem suggests iterative solution strategies.
- Iterative solvers (e.g. conjugate gradient techniques for symmetric systems, and Krylov subspace methods) can be used.
- The efficiency of iterative solvers depends on the availability of appropriate preconditioners which need be adapted to the Galerkin problem.
- Construction of preconditioners to exploit the structure of the linear Galerkin problem.

Convection dispersion equation

Proposed by : J.-M. Martinez (CEA/DEN/DM2S/LGLS) and A. Cartalade (CEA/DEN/DM2S).

Stochastic discretization PC solution methods Examples

1-D Convection dispersion

Model equation

- Concentration C(x, t)
- IC and BC :
- Parameters: q > 0 the Darcy velocity (1m/day), φ the fluid fraction (given in]0, 1[), D₀ the molecular diffusivity (<< 1), and λ uncertain the hydrodynamic dispersion coefficient.

Uncertainty model

- λ follows an uncertain power-law :
- a and b independent random variables.
- log₁₀(a) ∼ U[-4, -2] and b ∼ U[-3.5, -1].

$$a(\xi_1) = \exp(\mu_1 + \sigma_1\xi_1), \quad b = \mu_2 + \sigma_2\xi_2, \quad \xi_1, \xi_2 \sim U[-1, 1].$$

 $\lambda(\xi_{1},\xi_{2}) = \exp(\mu_{1} + \sigma_{1}\xi_{1})\phi^{\mu_{2}+\sigma_{2}\xi_{2}} \approx \sum_{k} \lambda_{k}\Psi_{k}(\xi_{1},\xi_{2})$

[Debusschere et al, 2004]

A. Cartalade (CEA)

 $\phi \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left[qy - (\phi D_0 + \lambda |q|) \frac{\partial C}{\partial x} \right].$

C(x, t = 0) = 0, C(x = 0, t) = 1.

$$\lambda = \mathbf{a}\phi^{\mathbf{b}}$$

Stochastic discretization PC solution methods Examples

Convection dispersion equation

Solution method

- Wiener-Legendre expansion and Galerkin projection : $C(x, t, \xi_1, \xi_2) = \sum_{k=0}^{p} C_k(x, t) \Psi_k(\xi_1, \xi_2).$
- Finite volume deterministic discretization $\mathcal{O}(\Delta x^2)$.
- Implicit time scheme $\mathcal{O}(\Delta t^2)$ (block tri-diagonal system, mean operator preconditionner).
- upwind stabilization of convection term (velocity is certain).

Expectation & standard deviation at x = 0.5



Stochastic discretization PC solution methods Examples

Convection dispersion equation

Convergence of pdfs at x = 0.5



Stochastic discretization PC solution methods Examples

results

Convection dispersion equation



Stochastic discretization PC solution methods Examples

Stochactic spectral solvers for incompressible Navier-Stokes equations

Stochastic Navier-Stokes equations with uncertain viscosity and source term :

$$\frac{\partial \boldsymbol{U}}{\partial t} + \boldsymbol{U} \nabla \boldsymbol{U} = -\nabla \boldsymbol{P} + \boldsymbol{\nu} \nabla^2 \boldsymbol{U} + \boldsymbol{F}$$
$$\nabla \cdot \boldsymbol{U} = 0.$$

PC expansion of the solution :

$$(\boldsymbol{U},\boldsymbol{P})\approx(\boldsymbol{U}^{\mathrm{P}},\boldsymbol{P}^{\mathrm{P}})=\sum_{k=0}^{\mathrm{P}}(\boldsymbol{u}_{k},\boldsymbol{p}_{k})\Psi_{k}.$$

And the Galerkin projection on Ψ_{α} gives

$$\begin{aligned} \frac{\partial \boldsymbol{u}_{k}}{\partial t} + \sum_{i,j=0}^{P} \boldsymbol{C}_{kij} \boldsymbol{u}_{i} \boldsymbol{\nabla} \boldsymbol{u}_{j} &= -\boldsymbol{\nabla} \boldsymbol{p}_{k} + \sum_{i=0}^{P} \frac{\langle \boldsymbol{\nu} \boldsymbol{\Psi}_{i}, \boldsymbol{\Psi}_{k} \rangle}{\langle \boldsymbol{\Psi}_{k}, \boldsymbol{\Psi}_{k} \rangle} \nabla^{2} \boldsymbol{u}_{i} + \frac{\langle \boldsymbol{F}, \boldsymbol{\Psi}_{k} \rangle}{\langle \boldsymbol{\Psi}_{k}, \boldsymbol{\Psi}_{k} \rangle} \\ \boldsymbol{\nabla} \cdot \boldsymbol{u}_{k} &= 0. \end{aligned}$$

UQ in numerical simulations Stochastic discretization Polynomial Chaos expansions PC solution methods Examples

Galerkin projection of the Navier-Stokes Equation :

$$\frac{\partial \boldsymbol{u}_k}{\partial t} + \sum_{l,m} C_{klm} \boldsymbol{u}_l \nabla \boldsymbol{u}_m = -\nabla \boldsymbol{p}_k + \sum_{l,m} C_{klm} \boldsymbol{\nu}_l \nabla^2 \boldsymbol{u}_m + \boldsymbol{f}_k, \quad \nabla \cdot \boldsymbol{u}_k = 0$$

where $C_{klm} := \frac{\langle \Psi_l \Psi_m, \Psi_k \rangle}{\langle \Psi_k, \Psi_k \rangle}$ **Deterministic viscosity** and explicit treatment of the non-linearity Decoupling!

$$\frac{1}{\Delta t}\boldsymbol{u}_{k}^{n+1} - \nu \nabla^{2}\boldsymbol{u}_{k}^{n+1} + \boldsymbol{\nabla}\boldsymbol{p}_{k}^{n+1} = \frac{1}{\Delta t}\boldsymbol{u}_{k}^{n} - \sum_{i,j=0}^{P} C_{kjj}\boldsymbol{u}_{i}^{n}\boldsymbol{\nabla}\boldsymbol{u}_{j}^{n} + \frac{\langle \boldsymbol{F}, \boldsymbol{\Psi}_{k} \rangle}{\langle \boldsymbol{\Psi}_{k}, \boldsymbol{\Psi}_{k} \rangle} \\ \boldsymbol{\nabla} \cdot \boldsymbol{u}_{k}^{n+1} = 0.$$

Other treatments of the convective part :

- semi-implicit, $u_l^n \nabla u_m^{n+1}$, \longrightarrow set of linear non-symmetric coupled problems : stabilization,?
- alternative semi-implicit form :

$$\left(\sum_{l,m} C_{klm} \boldsymbol{u}_l \boldsymbol{\nabla} \boldsymbol{u}_m\right)^{n+1} \approx \boldsymbol{u}_0^n \boldsymbol{\nabla} \boldsymbol{u}_k^{n+1} + \sum_{l>0,m} C_{klm} \boldsymbol{u}_l^n \boldsymbol{\nabla} \boldsymbol{u}_m^n$$

 \rightarrow mean-flow based stabilization (*e.g. upwinding*).

Steady problem

Solve the nonlinear set of equations

$$\sum_{l,m} C_{klm} \left(\boldsymbol{u}_l \boldsymbol{\nabla} \boldsymbol{u}_m - \nu_l \boldsymbol{\nabla}^2 \boldsymbol{u}_m \right) + \boldsymbol{\nabla} \boldsymbol{p}_k = \boldsymbol{f}_k, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u}_k = 0.$$

- Large problem
- Iterative approach mandatory (Newton-like)
- Construction of approximate tangent operator (matrix-free)
- Derive appropriate preconditioners, *e.g.* based on time-stepper [olm, 2009]

Steady Flow around a circular cylinder - Vorticity formulation

Uncertain Reynolds : $\text{Re} = \text{Re}(\xi) \sim LN$ (Median above critical value) stochastic basis :

0.05

Numerical Method :

Wiener-Hermite

Newton Iterations (with Unstd. stoch. Stokes prec.) $\psi - \omega$ formulation + influence matrix for BCs

$$\boldsymbol{u}(\xi)\boldsymbol{\nabla}\omega(\xi)-rac{1}{\operatorname{Re}(\xi)}\nabla^{2}\omega(\xi)=0.$$

Centered Finite differences $O(\Delta x^2)$ Uniform mesh (512 × 360) and direct FFT-based solvers

Stochastic discretization PC solution methods Examples

Convergence of Newton iterates

 $\boldsymbol{u}(\xi)\boldsymbol{\nabla}\omega(\xi)-rac{1}{\operatorname{Re}(\xi)}\nabla^{2}\omega(\xi)=0.$



Convergence of the mean mode : (first 4 iterations)



Stochastic discretization PC solution methods Examples

First 4 stoch. modes :

$$\omega(\mathbf{x},\xi) = \sum_{k} \omega_k(\mathbf{x}) \Psi_k(\xi)$$



Near wake statistics :



Examples

Content :

UQ in numerical simulations

- Numerical Simulation
- Uncertainty propagation
- UQ methods



Polynomial Chaos expansions

- Stochastic discretization
- PC solution methods.
- Examples



Proper Generalized Decompositions

- Optimal Decompositions
- Algorithms
- An example

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Functional expansions

Recall that the stochastic solution is sought in $L_2(\Xi, p_{\xi}) \otimes \mathbb{V}$:

$$U(\boldsymbol{\xi}) = \sum_{\alpha} f_{\alpha}(\boldsymbol{\xi}) u_{\alpha}(\boldsymbol{\xi}), \quad f_{\alpha} \in L_{2}(\Xi, p_{\boldsymbol{\xi}}) \text{ and } u_{\alpha} \in \mathbb{V}.$$

The PC methods consist in :

① Discretization of $L_2(\Xi, p_{\xi})$ introducing a subspace $\mathbb{S}^{|\mathcal{A}|}$ spanned by a basis $\{\Psi_{\alpha}, \alpha \in \mathcal{A}\},\$

2 Determination of the "best" approximation $U^{|\mathcal{A}|}$ of $U(\xi)$ in the subspace $\mathbb{S}^{|\mathcal{A}|} \otimes \mathbb{V}$.

The *a priori* selection of the stochastic basis yields the question of the optimality of the PC approximation. Can we do better?

Instead, we could consider the stochastic subspace space $\mathbb{S}^{|\mathcal{A}|},$ and define the generic separated representation as

$$U^{|\mathcal{A}|}(\boldsymbol{\xi}) pprox U^{m}(\boldsymbol{\xi}) = \sum_{lpha=1}^{m} f_{lpha}(\boldsymbol{\xi}) u_{lpha}(\boldsymbol{\xi}), \quad f_{lpha} \in \mathbb{S}^{|\mathcal{A}|} \text{ and } u_{lpha} \in \mathbb{V},$$

where known of the U_{α} and λ_{α} are selected *a priori*, and we expect $m \ll |\mathcal{A}|$ if the approximation is reducible.

The reduced solution $U^m(\xi)$ is called the rank-*m* approximation, while $\{\lambda_1, \ldots, \lambda_m\}$ and $\{u_1, \ldots, u_m\}$ are the stochastic and deterministic reduced bases. The questions are then :

- how to define the (deterministic or stochastic) reduced basis?
- how to compute the reduced basis and the *m*-th order PGD of *U*?

Optimal *L*²-spectral decomposition :

If we define the rank-m approximation as the minimizer of

$$\mathcal{R}^2(\mathcal{U}^m(oldsymbol{\xi})) = \mathbb{E}\left\{ \left\| \mathcal{U}(oldsymbol{\xi}) - \sum_{lpha=1}^m \lambda_lpha(oldsymbol{\xi}) u_lpha
ight\|_{\mathbb{V}}^2
ight\},$$

POD, KL decomposition

it is well known that the optimum is the KL decomposition of U, that is the u_{α} are the *m* dominant eigenmodes of correlation operator of U, $C : \mathbb{V} \mapsto \mathbb{V}$ (symmetric positive operator) :

$$\forall \boldsymbol{v} \in \mathbb{V}, \quad (\boldsymbol{C}\boldsymbol{u}_{\alpha}, \boldsymbol{v})_{\mathbb{V}} = \gamma_{\alpha} \left(\boldsymbol{u}_{\alpha}, \boldsymbol{v}\right), \quad \lambda_{\alpha}(\boldsymbol{\xi}) \|\boldsymbol{u}_{\alpha}\|_{\mathbb{V}}^{2} = (\boldsymbol{U}, \boldsymbol{u}_{\alpha})_{\mathbb{V}}.$$

But the solution is needed to perform the decomposition !

- Solve the Galerkin problem in $\mathbb{V} \otimes \mathbb{S}^{|\mathcal{A}'|}$, with $|\mathcal{A}'| < |\mathcal{A}|$, to construct a deterministic basis $\{u_{\alpha}, \alpha = 1, \dots, m\}$; then solve the reduced problem for the $\{\lambda_{\alpha=1,\dots,m} \in \mathbb{S}^{|\mathcal{A}|}\}$.
- Solve the Galerkin problem in V^H ⊗ S^{|A|} to construct {λ_{α=1,...,m}}; then solve the reduced problem for the {u_{α=1,...,m} ∈ V^h} with dim V^H ≪ dim V^h.

See works by the groups of Ghanem and Matthies.

Observe : the above approaches mix L₂ and Galerkin optimality definitions !

An alternative definition of the optimality

Consider the family of variational problems : given $\xi \in \Xi$, find $u \in \mathbb{V}$ such that

$$a(u, v|\boldsymbol{\xi}) = b(v|\boldsymbol{\xi}) \quad \forall v \in \mathbb{V},$$

where the bilinear form $a(\cdot, \cdot | \boldsymbol{\xi})$ is a.s. symmetric and positive definite. Example : elliptic equation with random coefficient : $\mathbb{V} = H_0^1$

$$a(u, v | \boldsymbol{\xi}) = \int_{\Omega} k(\boldsymbol{\xi}) \nabla u \nabla v \, dx, \quad \epsilon < k(\xi) < \infty \ a.s. \text{ in } \Omega.$$

The Galerkin problem becomes : Find $U(\xi) \in L_2(\Xi, \rho_{\xi}) \otimes \mathbb{V}$ such that

$$A(U, V) = \mathbb{E} \{ a(U, V | \boldsymbol{\xi}) \} = B(V) = \mathbb{E} \{ b(V | \boldsymbol{\xi}) \} \quad \forall V \in L_2(\Xi, p_{\boldsymbol{\xi}}) \otimes \mathbb{V}.$$

Clearly, the bilinear form $A : (L_2(\Xi, \rho_{\xi}) \otimes \mathbb{V}) \times (L_2(\Xi, \rho_{\xi}) \otimes \mathbb{V}) \mapsto \mathbb{R}$ is symmetric positive definite, so the solution *U* is the minimizer of the energy functional

$$\mathcal{J}(V) \equiv \frac{1}{2}A(V, V) - B(V)$$

Introducing the reduced solution, U^m can be defined as

$$\mathcal{J}(\boldsymbol{U}^{m}) = \frac{1}{2}\boldsymbol{A}(\boldsymbol{U}^{m},\boldsymbol{U}^{m}) - \boldsymbol{B}(\boldsymbol{U}^{m}) = \min_{\left\{\boldsymbol{u}_{\alpha=1,\ldots,m}\right\}, \left\{\boldsymbol{\lambda}_{\alpha=1,\ldots,m}\right\}} \mathcal{J}\left(\sum_{\alpha=1}^{m} \boldsymbol{u}_{\alpha}\boldsymbol{\lambda}_{\alpha}\right).$$

(detailed analysis for elliptic problems in [Nouy and Falco, 2012])

The rank-m solution U^m is defined by

$$\mathcal{J}(U^m) = \frac{1}{2}A(U^m, U^m) - B(U^m) = \min_{\{u_{\alpha=1}, \dots, m\}, \{\lambda_{\alpha=1}, \dots, m\}} \mathcal{J}\left(\sum_{\alpha=1}^m u_{\alpha}\lambda_{\alpha}\right).$$

- The minimum is not unique (homogeneity)
- Minimizing ${\mathcal J}$ is equivalent to minimizing a Rayleigh quotient
- The reduced solution is optimal w.r.t the A-norm defined as

$$\|V\|_A^2 \equiv \mathbb{E}\left\{a(V, V)\right\} = A(V, V),$$

to be compared with the KL norm $\mathbb{E}\left\{ \|V\|_{\mathbb{V}}^{2}\right\} = \mathbb{E}\left\{ (V, V)_{\mathbb{V}} \right\}.$

Recursive construction :

For *i* = 1, 2, 3...

Sequential construction [Nouy, 2007]

 $u_i = \mathcal{D}(\lambda_i, U^{i-1})$

 $\lambda_i = \mathcal{S}(u_i, U^{i-1})$

$$\mathcal{J}(U^{i}) = \min_{\mathbf{v} \in \mathbb{V}, \beta \in \mathbb{S}^{P}} \mathcal{J}\left(\beta \mathbf{v} + \sum_{j=1}^{i-1} \lambda_{j} u_{j}\right) = \min_{\mathbf{v} \in \mathbb{V}, \beta \in \mathbb{S}^{P}} \mathcal{J}\left(\beta \mathbf{v} + U^{i-1}\right)$$

The optimal couple (λ_i, u_i) solves simultaneously

• a) deterministic problem

$$A(\lambda_i u_i, \lambda_i v) = B(\lambda_i v) - A(U^{i-1}, \lambda_i v), \quad \forall v \in \mathbb{V}$$

• b) stochastic problem

$$\boldsymbol{A}(\lambda_{i}\boldsymbol{u}_{i},\beta\boldsymbol{u}_{i})=\boldsymbol{B}(\beta\boldsymbol{u}_{i})-\boldsymbol{A}\left(\boldsymbol{U}^{i-1},\beta\boldsymbol{u}_{i}\right),\quad\forall\beta\in\mathbb{S}^{\mathrm{P}}$$

Example of stochastic elliptic problem :

• Deterministic problem : $u_i = \mathcal{D}(\lambda_i, U^{i-1})$

$$\int_{\Omega} \mathbb{E}\left\{\lambda_{i}^{2} k\right\} \nabla u_{i} \cdot \nabla v \mathrm{d} \boldsymbol{x} = \mathbb{E}\left\{-\int_{\Omega} \lambda_{i} k \nabla U^{i-1} \cdot \nabla v \mathrm{d} \boldsymbol{x} + \int_{\Omega} \lambda_{i} f v \mathrm{d} \boldsymbol{x}\right\}, \quad \forall v$$

• Stochastic problem :
$$\lambda_i = S(u_i, U^{i-1})$$

$$\mathbb{E}\left\{\lambda_{i}\beta\int_{\Omega}k\boldsymbol{\nabla}\boldsymbol{u}_{i}\cdot\boldsymbol{\nabla}\boldsymbol{u}_{i}\mathrm{d}\boldsymbol{x}\right\}=\mathbb{E}\left\{-\beta\int_{\Omega}k\boldsymbol{\nabla}\boldsymbol{U}^{i-1}\cdot\boldsymbol{\nabla}\boldsymbol{u}_{i}\mathrm{d}\boldsymbol{x}+\int_{\Omega}\boldsymbol{f}\boldsymbol{u}_{i}\mathrm{d}\boldsymbol{x}\right\},\quad\forall\beta.$$

Properties :

[Nouy, 2007, 2008]

• The couple (λ_i, u_i) is a fixed point of :

$$\lambda_i = S \circ \mathcal{D}(\lambda_i, \cdot), \quad u_i = \mathcal{D} \circ S(u_i, \cdot)$$

• Homogeneity property :

$$rac{\lambda_i}{c} = \mathcal{S}(cu_i, \cdot), \quad rac{u_i}{c} = \mathcal{D}(c\lambda_i, \cdot), \quad \forall c \in \mathbb{R} \setminus \{0\}.$$

 \Rightarrow arbitrary normalization of one of the two elements.

Algorithms inspired from dominant subspace methods Power-type, Krylov/Arnoldi, ... UQ in numerical simulations Polynomial Chaos expansions Proper Generalized Decompositions Algorithms An example

Power Iterations

Set / = 1

2 initialize λ (*e.g.* randomly)

- While not converged, repeat
 - a) Solve : $u = \mathcal{D}(\lambda, U^{l-1})$
 - b) Normalize u
 - c) Solve : $\lambda = S(u, U^{l-1})$

$$I e u_l = u, \lambda_l = \lambda$$

() *I* ← *I* + 1, if *I* < *m* repeat from step 2

Comments :

- Convergence criteria for the power iterations (subspace with dim > 1 or clustered eigenvalues)
 [Nouy, 2007, 2008]
- Usually few (4 to 5) inner iterations are sufficient

(power iterations)

Power Iterations with Update

[Nouy and olm, 2009]

(optional)

Same as Power Iterations, but after (u_l, λ_l) is obtained (step 4) update of the stochastic coefficients :

- Orthonormalyze $\{u_1, \ldots, u_l\}$
- Find $\{\lambda_1, \ldots, \lambda_l\}$ s.t.

$$A\left(\sum_{i=1}^{l} u_i \lambda_i, \sum_{i=1}^{l} u_i \beta_i\right) = B\left(\sum_{i=1}^{l} u_i \beta_i\right), \quad \forall \beta_{i=1,\ldots,l} \in \times \mathbb{S}^{\mathsf{P}}$$

Ontinue for next couple

Comments :

- Improves the convergence
- Low dimensional stochastic linear system $(I \times I)$
- Cost of update increases linearly with the order / of the reduced representation

UQ in numerical simulations Proper Generalized Decompositions

Algorithms

Arnoldi (Full Update version)

- Set / = 0
- **2** Initialize $\lambda \in \mathbb{S}^{P}$

3 For l' = 1, 2, ...

(Arnoldi iterations)

- Solve deterministic problem $u' = \mathcal{D}(\lambda, U')$
- Orthogonalize : $u_{l+l'} = u' \sum_{i=1}^{l+l'-1} (u', u_i)_{\Omega}$
- If $||u_{l+l'}||_{\mathbb{V}} \leq \epsilon$ or l+l' = m then break
- Normalize u_{l+l'}
- Solve $\lambda = \mathcal{S}(u_{l'}, U')$
- $\bigcirc I \leftarrow I + I'$

$$\textbf{9} \text{ Find } \{\lambda_1, \dots, \lambda_l\} \text{ s.t.}$$

$$A\left(\sum_{i=1}^l u_i \lambda_i, \sum_{i=1}^l u_i \beta_i\right) = B\left(\sum_{i=1}^l u_i \beta_i\right), \quad \forall \beta_{i=1,\dots,l} \in \mathbb{S}^P$$

(6) If l < m return to step 2.

[Tamellini et al. 2009]

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Summary

Resolution of a series of deterministic elliptic problems, with elliptic coefficients E {λ²k} and modified (deflated) rhs

dimension is dim \mathbb{V}^h

• Resolution of a series of linear stochastic equations

dimension is $\text{dim}\,\mathbb{S}^P$

- Update problems : system of linear equations for stochastic random variables dimension is m × dim S^P
- To be compared with the Galerkin problem dimension

 $\dim \mathbb{V}^h \times \dim \mathbb{S}^{\mathrm{P}}$

Weak modification of existing (FE/FV) codes (weakly intrusive)

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Example definition



- Rectangular domain 25,000×695 (m)
- 4 Geological layers with uncertain conductivities
- uncertainty on BCs
- 9 independent r.v. $\{\xi_1, ..., \xi_9\} \sim U[0, 1]^9$
- $\bullet~$ Stochastic space \mathbb{S}^{P} : Legendre polynomial up to order No
- dim $S^P = P + 1 = (9 + No)!/(9!No!)$

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Norm of residual and error as a function of m (No = 3)



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CPU times (No = 3)



Closing remarks

Polynomial Chaos expansions

- Fast convergence when the solution has smooth dependence with respect to ξ
- Adaptivity of the spectral basis to the solution
- Development of dedicated Galerkin solvers
- Treatment of non-linearities in Galerkin projection
- Preconditioning for non-intrusive methods
- Case of non-smooth solutions : multi-resolution.

Proper Generalized Decompositions

- Theoretically well grounded method for linear symmetric definite operators
- Yield close to optimal decomposition
- Connection with Greedy algorithms
- Non-intrusive versions possible
- Adaptation of algorithms and analysis to more general class of problems
- Application to non-linear problems [Nouy and Olm, 2010] *e.g.* Navier-Stokes [Tamellini Nouy and olm, 2013]

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Thanks for your attention

Spectral Methods for Uncertainty Quantification with applications in computational fluid dynamics

with Omar Knio Springer Series on Scientific Computation.



O. Le Maître & O. Knio Stochastic Spectral Methods