Generalized spectral decomposition and separated representations for the solution of uncertain advection-diffusion-reaction equations

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Outline

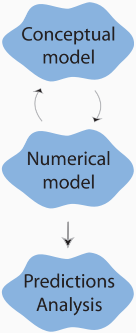
1. Uncertainty Quantification: spectral stochastic methods
2. Separated representations and Generalized Spectral Decomposition
3. Application to Couplex (Groundwater flow)
4. Application to a transient advection-diffusion-reaction

Uncertainty quantification

A critical issue in science and engineering

- More realistic predictions (improve predictibility)
- Analyze the impact of input uncertainty (hierarchization, confidence, ...)
- Comprehension and selection of models

Propagation of uncertainties: a probabilistic point of view



Probability space $(\Theta, \mathcal{B}, P)$

$$\mathcal{A}(u(\theta);\theta) = b(\theta), \quad \theta \in \Theta$$

Finite dimensional probability space $(\boldsymbol{\Xi}, \mathcal{B}_{\boldsymbol{\Xi}}, P_{\boldsymbol{\xi}})$

$$\mathcal{A}_N(u_N(\boldsymbol{\xi});\boldsymbol{\xi}) = b_N(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \in \boldsymbol{\Xi} \subset \mathbb{R}^s$$

Quantity of interest

$$Q(u_N(\boldsymbol{\xi}))$$

A functional approach to probability for uncertainty propagation

Functional representation of random variables $u : \boldsymbol{\Xi} \rightarrow \mathcal{V}$

$$u \in \mathcal{S}(\boldsymbol{\Xi}, dP_{\boldsymbol{\xi}}; \mathcal{V}) \qquad \boxed{u(\boldsymbol{\xi}) \approx \sum_\alpha u_\alpha \psi_\alpha(\boldsymbol{\xi})}$$

A tool for probabilistic and parametric analyses

- Information preserved
- A posteriori probabilistic analyses

  $\hookrightarrow$ *probability measure, sensitivity, reliability ...*
- Parametric analyses

  $\hookrightarrow$ *optimization, model validation, ...*

Construction of approximation spaces

$\mathcal{S}_P = span\{\psi_\alpha\}_{\alpha=1}^P \subset \mathcal{S}$

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

Computation of functional representations

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

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

$$u_\alpha = \sum_k \omega_k^\alpha u(\boldsymbol{\xi}_k) \quad \langle v, \mathcal{A}(u(\boldsymbol{\xi}_k))\rangle = \langle v, b(\boldsymbol{\xi}_k)\rangle \quad \forall v \in \mathcal{V}_N$$

Galerkin projection

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

Limitations

Dimensionality, Complexity, Solvers

Outline

Separated representations

Problem formulated on a tensor product space

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad \ll v, \mathcal{A}(u) \gg = \ll v, b \gg \quad \forall v \in \mathcal{V} \otimes \mathcal{S}$$

Separated representation of the solution

$$\boxed{u(\boldsymbol{\xi}) \approx u_m(\boldsymbol{\xi}) = \sum_{i=1}^{m} w_i \lambda_i(\boldsymbol{\xi}), \quad w_i \in \mathcal{V}, \quad \lambda_i \in \mathcal{S}}$$

Usually, accurate representation on low dimensional deterministic and stochastic approximation spaces

$$\mathcal{V}_m = span\{w_i\}_{i=1}^m \subset \mathcal{V} \quad \text{and} \quad \mathcal{S}_m = span\{\lambda_i\}_{i=1}^m \subset \mathcal{S}$$

Alternative solution techniques based on separated representations

Classical Spectral Decomposition (a posteriori construction)

$$\boxed{\|u - u_m\|^2 = \min_{w_i \in \mathcal{V}, \lambda_i \in \mathcal{S}} \|u - \textstyle\sum_{i=1}^m \lambda_i w_i\|^2} \quad \Rightarrow \quad \text{Eigenproblem on the correlation operator}$$

$$\|\cdot\|^2 = E(\|\cdot\|_{\mathcal{V}}^2)$$

Solution techniques based on classical spectral decomposition

- Approximation of the correlation operator by a first coarse resolution
  [Matthies 2005, Ghanem 2007]
- Classical spectral decomposition at each step of iterative solution techniques
  [Matthies & Zander 2009]

Generalized Spectral Decomposition (GSD) (a priori construction)

Separated representation without knowing u

- New definition of optimality
- Dedicated algorithms

Generalized Spectral Decomposition (GSD)

Progressive definition based on Galerkin orthogonality

Problem formulated on a tensor product Hilbert space

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad \ll v, \mathcal{A}(u) \gg = \ll v, b \gg \quad \forall v \in \mathcal{V} \otimes \mathcal{S}$$

Suppose that u_{m-1} is known. (w_m, λ_m) is defined as the optimal couple (w, λ) satisfying

$$\boxed{(w, \lambda) \in \mathcal{V} \times \mathcal{S}, \quad \ll v, \mathcal{A}(u_{m-1} + w\lambda) \gg = \ll v, b \gg \quad \forall v \in \{w\} \otimes \mathcal{S} + \mathcal{V} \otimes \{\lambda\}}$$

- $< w, \mathcal{A}(u_{m-1} + w\lambda) >_{\mathcal{V}} = < w, b >_{\mathcal{V}} \quad \Leftrightarrow \quad \boxed{\lambda = F_m^{\diamond}(w)}$
- $< \lambda, \mathcal{A}(u_{m-1} + w\lambda) >_{\mathcal{S}} = < \lambda, b >_{\mathcal{S}} \quad \Leftrightarrow \quad \boxed{w = F_m(\lambda)}$

Equivalent pseudo eigenproblems [N. 2008]

- w_m dominant eigenfunction of operator $\boxed{T_m(w) = F_m \circ F_m^{\diamond}(w)}$ and $\boxed{\lambda_m = F_m^{\diamond}(w_m)}$
- λ_m dominant eigenfunction of operator $T_m^{\diamond}(\lambda) = F_m^{\diamond} \circ F_m(\lambda)$ and $w_m = F_m(\lambda_m)$

Generalized Spectral Decomposition (GSD)

Progressive definition based on Galerkin orthogonality

Definition of the progressive generalized spectral decomposition $u_m = \sum_{i=1}^m w_i \lambda_i$

w_i is a dominant eigenfunction of $T_i(w) = F_i \circ F_i^{\diamond}(w)$ associated with eigenvalue $\sigma_i = \sigma_i(w_i) = \max_w \sigma_i(w)$, with $\sigma_i(w) = \ll wF_i^{\diamond}(w), \mathcal{A}(wF_i^{\diamond}(w)) \gg$, and $\lambda_i = F_i^{\diamond}(w_i)$

Theorem (Generalized spectral decomposition) (*elliptic symmetric case*)

If $\mathcal{A}$ is linear symmetric bounded elliptic operator on $\mathcal{V} \otimes \mathcal{S}$, it defines a norm $\|\cdot\|_{\mathcal{A}}$ and

$$(w_i, \lambda_i) \in \arg \min_{w \in \mathcal{V}, \lambda \in \mathcal{S}} \|u - u_{i-1} - w\lambda\|^2_{\mathcal{A}}, \qquad \sigma_i = \max_{w \in \mathcal{V}} \sigma_i(w)$$

$$\|u - u_m\|^2_{\mathcal{A}} = \|u\|^2_{\mathcal{A}} - \sum_{i=1}^{m} \sigma_i \xrightarrow[m \to \infty]{} 0$$

Proof: use the fact that the set of rank one separated functions $\mathcal{D} = \{w\lambda; w \in \mathcal{V}, \lambda \in \mathcal{S}\}$ *is weakly closed in* $\mathcal{V} \otimes \mathcal{S}$ *for the topology induced by* $\|\cdot\|_{\mathcal{A}}$

Generalized Spectral Decomposition (GSD)

Progressive definition based on Galerkin orthogonality

Definition of the progressive generalized spectral decomposition $u_m = \sum_{i=1}^{m} w_i \lambda_i$

w_i is a dominant eigenfunction of $T_i(w) = F_i \circ F_i^{\diamond}(w)$ associated with eigenvalue $\sigma_i = \sigma_i(w_i) = \max_w \sigma_i(w)$, with $\sigma_i(w) = \ll wF_i^{\diamond}(w), \mathcal{A}(wF_i^{\diamond}(w)) \gg$, and $\lambda_i = F_i^{\diamond}(w_i)$

A dedicated algorithm: Power iterations [N. 2007]

To compute the dominant eigenfunction w_i of T_i, construct the sequence

$$w^{k+1} = T_i(w^k) = F_i \circ F_i^{\diamond}(w^k)$$

Separation of difficulties (partly non-intrusive):

- Stochastic algebraic equations ($\lambda^k = F_i^{\diamond}(w^k)$)
- Deterministic problems ($w^{k+1} = F_i(\lambda^k)$)

Generalized Spectral Decomposition (GSD)

Alternative definitions and algorithms

- Different definitions of decompositions

	Simultaneous	Progressive
	Find $u_m = \sum_{i=1}^{m} w_i \lambda_i$ such that $\forall v_m \in \mathcal{V}_m \otimes \mathcal{S} + \mathcal{V} \otimes \mathcal{S}_m$,	Find (w, λ) such that $\forall v \in \{w\} \otimes \mathcal{S} + \mathcal{V} \otimes \{\lambda\}$,
Galerkin	$\ll v, \mathcal{A}(u_m) - b \gg = 0$	$\ll v, \mathcal{A}(u_m + \lambda w) - b \gg = 0$
Minimal residual	$\ll \mathcal{A}(v), \mathcal{A}(u_m) - b \gg = 0$	$\ll \mathcal{A}(v), \mathcal{A}(u_m + \lambda w) - b \gg = 0$

$\hookrightarrow$ Interpretation as pseudo eigenproblems

- Associated algorithms, inspired from solution techniques for classical eigenproblems
  - Progressive definition $\rightarrow$ Power iteration algorithm [N. 2007]
  - Simultaneous definition (optimal) $\rightarrow$ Subspace iterations [N. 2008]
  - Approximation of the optimal $\rightarrow$ Arnoldi algorithm [N. 2008]

Outline

Application to Couplex-1 (Groundwater flow)

Groundwater flow equation (hydraulic head u)

$$-\nabla(\kappa(x,\xi)\nabla u) = 0 \quad on \quad \Omega$$

$+$ boundary conditions

Geological layers with uncertain properties

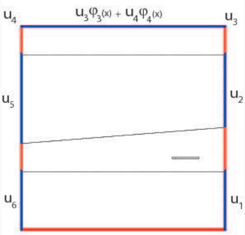
κ's probability laws

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

10 basic uniform random variables ξ,

$\Xi = (-1,1)^{10}$, uniform probability P_ξ

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	$U(285, 287)$

Weak formulation

$$\boxed{u = u_0 + \mathcal{V} \otimes \mathcal{S}} \quad \mathcal{V} = H_0^1(\Omega)\ \mathcal{S} = L^2(\boldsymbol{\Xi}, dP_{\boldsymbol{\xi}})$$

$$\boxed{\tilde{u} \in \mathcal{V} \otimes \mathcal{S}, \quad A(\tilde{u}, v) = -A(u_0, v) \quad \forall v \in \mathcal{V} \otimes \mathcal{S}}$$

$$A(u, v) := \ll v, \mathcal{A}(u) \gg = \int_{\boldsymbol{\Xi}} \int_{\Omega} \kappa(x, \mathbf{y}) \nabla v \cdot \nabla u \, dx \, dP_{\boldsymbol{\xi}}(\mathbf{y})$$

Discretization

Spatial approximation

P_1 finite elements (≈ 15000)

$$\boxed{\mathcal{V}_N \subset \mathcal{V}} \quad N \approx 7265$$

Stochastic approximation

Complete polynomial space on $\boldsymbol{\Xi} = (-1, 1)^{10}$, with degree $p = 3$

$$\boxed{\mathcal{S}_P = \mathbb{P}_3(\boldsymbol{\Xi}) \subset \mathcal{S}} \quad P = 285$$

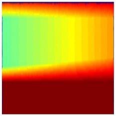
$$\boxed{dim(\mathcal{V}_N \otimes \mathcal{S}_P) = N \times P \approx 2.10^6}$$

Progressive Galerkin GSD

Computing (w_1, λ_1) by power iterations on $T_1 = F_1 \circ F_1^\diamond$

Initialize λ^0 and for $k \geqslant 1$, $w^k = F_1(\lambda^{k-1})$ and $\lambda^k = F_1^\diamond(w^k)$

$w^1 = F_1(\lambda^0)$



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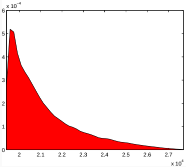
$\lambda^1 = F_1^\diamond(w^1)$



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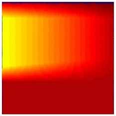
$w^2 = F_1(\lambda^1)$



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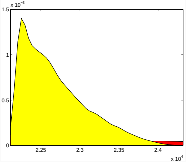
$\lambda^2 = F_1^\diamond(w^2)$



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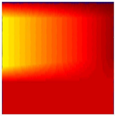
$w^3 = F_1(\lambda^2)$



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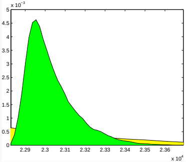
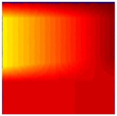
$\lambda^3 = F_1^\diamond(w^3)$



$\nearrow$

$w^4 = F_1(\lambda^3)$



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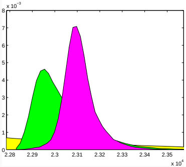
$\lambda^4 = F_1^\diamond(w^4)$

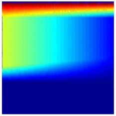


Progressive Galerkin GSD

Computing (w_2, λ_2) by power iterations on $T_2 = F_2 \circ F_2^\diamond$

Initialize λ^0 and for $k \geqslant 1$ $w^k = F_2(\lambda^{k-1})$ and $\lambda^k = F_2^\diamond(w^k)$

$w^1 = F_2(\lambda^0)$



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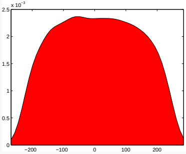
$\lambda^1 = F_2^\diamond(w^1)$



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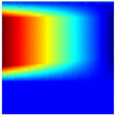
$w^2 = F_2(\lambda^1)$



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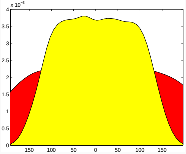
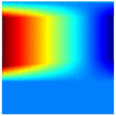
$\lambda^2 = F_2^\diamond(w^2)$



$\nearrow$

$w^3 = F_2(\lambda^2)$



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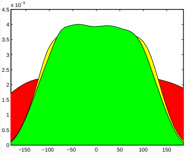
$\lambda^3 = F_2^\diamond(w^3)$



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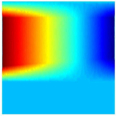
$w^4 = F_2(\lambda^3)$



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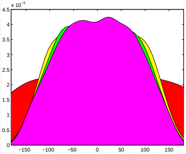
$\lambda^4 = F_2^\diamond(w^4)$

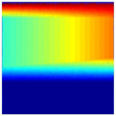


Progressive Galerkin GSD

Computing (w_3, λ_3) by power iterations on $T_3 = F_3 \circ F_3^{\diamond}$

Initialize λ^0 and for $k \geqslant 1$ $w^k = F_3(\lambda^{k-1})$ and $\lambda^k = F_3^{\diamond}(w^k)$

$w^1 = F_3(\lambda^0)$



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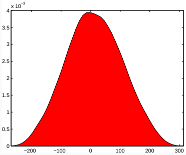
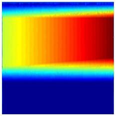
$\lambda^1 = F_3^{\diamond}(w^1)$



$\nearrow$

$w^2 = F_3(\lambda^1)$



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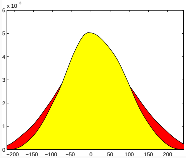
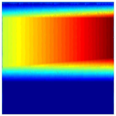
$\lambda^2 = F_3^{\diamond}(w^2)$



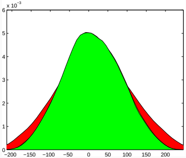
$\nearrow$

$w^3 = F_3(\lambda^2)$



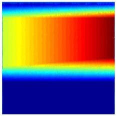
$\downarrow$

$\lambda^3 = F_3^{\diamond}(w^3)$



$\nearrow$

$w^4 = F_3(\lambda^3)$



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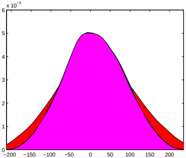
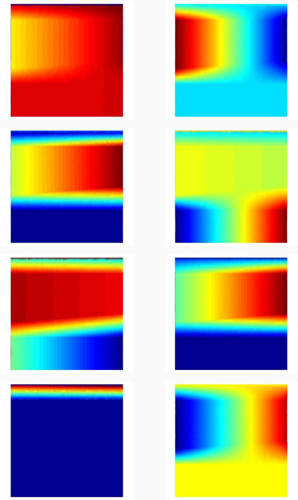
$\lambda^4 = F_3^{\diamond}(w^4)$



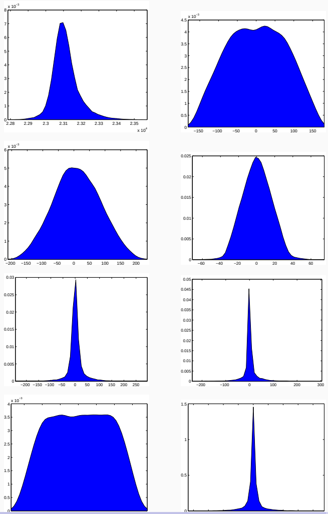
Progressive Galerkin GSD

First modes of the decomposition

Spatial modes $\{w_1, \ldots, w_8\}$



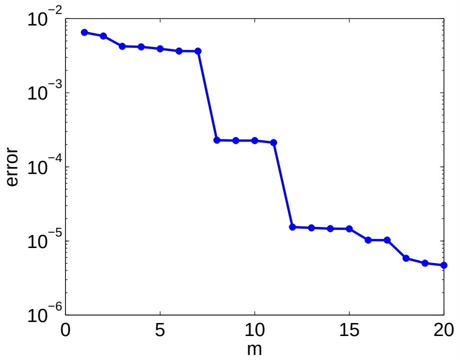
Stochastic modes $\{\lambda_1, \ldots, \lambda_8\}$



Progressive Galerkin GSD

Convergence of the decomposition (L^2-norm)

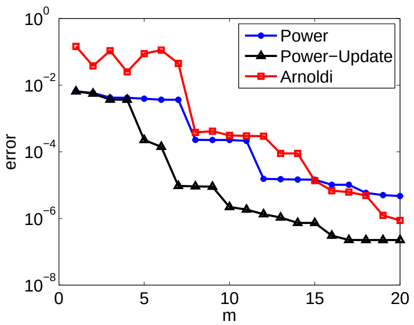
$\|u - u_m\|_{L^2}$



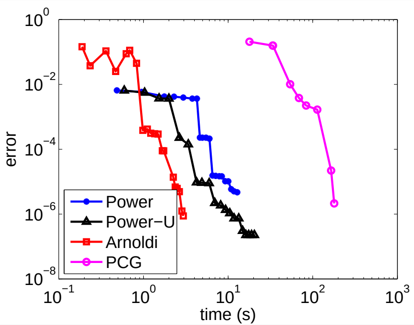
Different definitions of decomposition and associated algorithms
Convergence and computational efficiency

- ⋆ **Power iterations** (progressive definition)
- ▲ **Power iterations with update** of stochastic functions $\{\lambda_1, \ldots, \lambda_m\}$ (improves convergence of u_m)
- ■ **Arnoldi algorithm**: generate a "Krylov subspace" $\mathcal{V}_m = span\{w_1, \ldots, w_m\}$ of initial operator $T_1(w)$ and compute associated stochastic functions

Error vs m



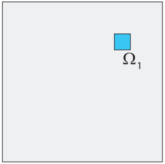
Error vs time



Outline

Application to an advection-diffusion-reaction equation

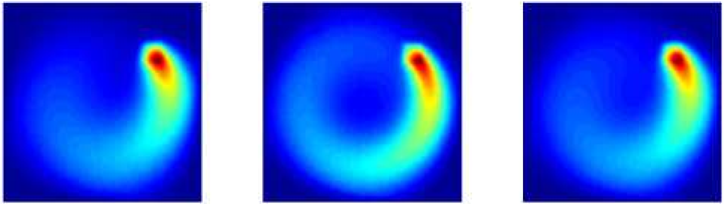
- $\partial_t u - a_1 \Delta u + a_2 c \cdot \nabla u + a_3 u = a_4 I_{\Omega_1}$ on $\Omega \times (0, T)$
- $u = 0$ on $\Omega \times \{0\}$
- $u = 0$ on $\partial\Omega \times (0, T)$



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

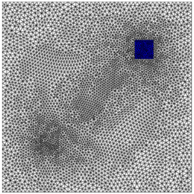
$$u(x,t,\boldsymbol{\xi}) \approx \sum_{i=1}^{m} w_i(x,t)\lambda_i(\boldsymbol{\xi})$$

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

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

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

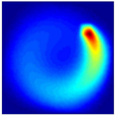


Computation of Generalized Spectral Decomposition

Arnoldi algorithm

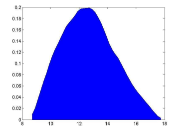
1. Initialize λ and for $k = 1 \dots m$, $w_k = \Pi_{k-1}^{\perp}(F_1(\lambda))$ and $\lambda = F_1^{\diamond}(w_k)$
2. Compute associated $\{\lambda_1, \dots, \lambda_m\}$

$w^1 = F_1(\lambda)$



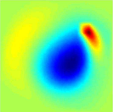
$\downarrow$

$\lambda = F_1^{\diamond}(w_1)$



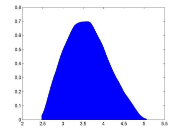
$\nearrow$

$w^2 = \Pi_1^{\perp}(F_1(\lambda))$



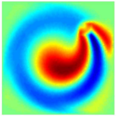
$\downarrow$

$\lambda = F_1^{\diamond}(w_2)$



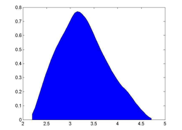
$\nearrow$

$w^3 = \Pi_2^{\perp}(F_1(\lambda))$



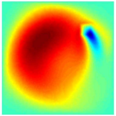
$\downarrow$

$\lambda = F_1^{\diamond}(w_3)$



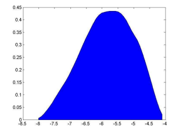
$\nearrow$

$w^4 = \Pi_3^{\perp}(F_1(\lambda))$



$\downarrow$

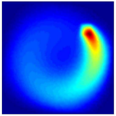
$\lambda = F_1^{\diamond}(w_4)$



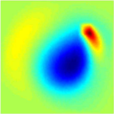
Arnoldi algorithm

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 $\{\lambda_1, \dots, \lambda_m\}$

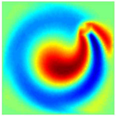
$w^1 = F_1(\lambda)$



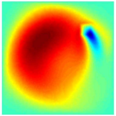
$w^2 = \Pi^{\perp}_1(F_1(\lambda))$



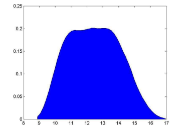
$w^3 = \Pi^{\perp}_2(F_1(\lambda))$



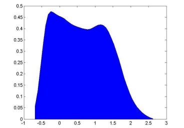
$w^4 = \Pi^{\perp}_3(F_1(\lambda))$



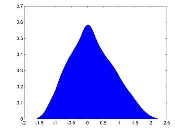
λ_1



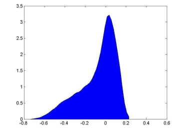
λ_2



λ_3

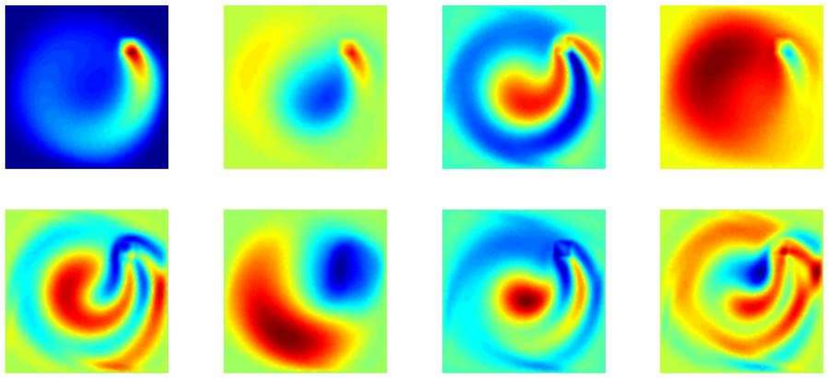


λ_4



Deterministic modes

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

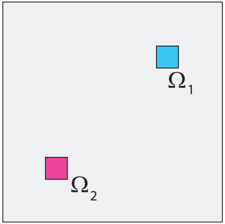


To compute these modes $\Rightarrow$ **only 8 deterministic problems**

Probability density function

Quantity of interest

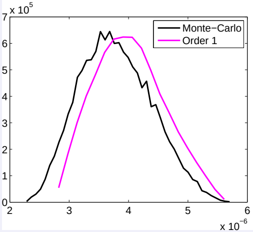
$$Q(\xi) = \int_0^T \int_{\Omega_2} u(x,t,\xi)\, dxdt$$



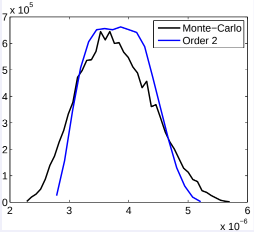
$$Q_m(\xi) = \int_0^T \int_{\Omega_2} u_m(x,t,\xi)\, dxdt$$

Probability density function of $Q_m(\xi)$

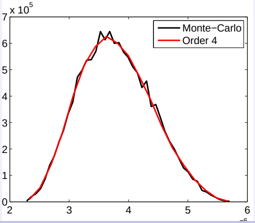
$m = 1$



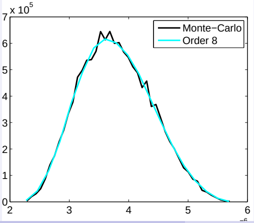
$m = 2$



$m = 4$



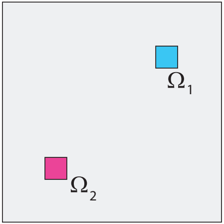
$m = 8$



Convergence properties of quantities of interest
Quantiles

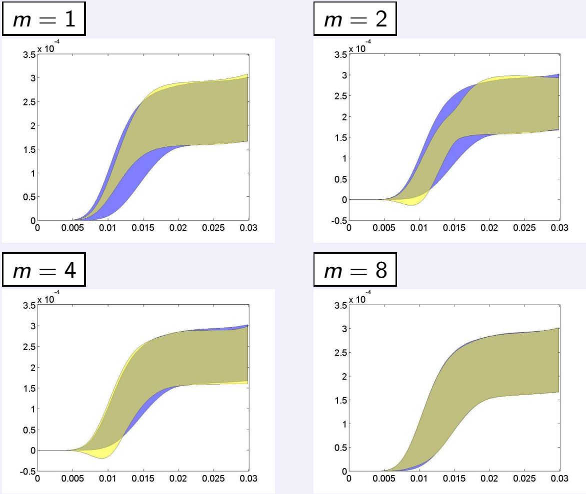
Quantity of interest

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



$$Q_m(t,\xi) = \int_{\Omega_2} u_m(x,t,\xi)\,dx$$

99% Quantiles of $Q_m(t,\xi)$



Conclusions

GSD method for stochastic problems ($\sim$ PGD method)

- Separation of difficulties: deterministic/stochastic separation

  partly non intrusive Galerkin stochastic method

- Reduced order model construction

  a priori construction of quasi-optimal reduced basis

- Separation in high-dimensional tensor product spaces :

  a way to circumvent the curse of dimensionality

$$u(\boldsymbol{\xi}) = \sum_{i=1}^{m} w_i \underbrace{\phi_i^1(\xi_1)\ldots\phi_i^s(\xi_s)}_{\Psi_i(\boldsymbol{\xi})} \in \mathcal{V} \otimes \underbrace{\mathcal{S}_1 \otimes \ldots \otimes \mathcal{S}_s}_{\mathcal{S}}$$

A priori construction of a hyperreduced approximation space

$$\boxed{\mathcal{S}_m = span\{\Psi_i\}_{i=1}^m \subset \mathcal{S}_P \subset \mathcal{S}}$$

$$\boxed{m \approx 10, 100 \quad \lll \quad P = 10^{10},\ 10^{100},\ \ldots}$$

[N., Archiv. Comp. 2009]

Open questions and perspectives

Open questions

- Mathematical framework for pseudo eigenproblems ?
- Optimality and convergence for non-symmetric problems ?
- Error control, Goal-oriented model reduction

Perspectives and application to Couplex (transport)

- Large scale application and long time simulation

  $\rightsquigarrow$ additional space/time separation $\boxed{u(x,t,\boldsymbol{\xi}) = \sum_{i=1}^{m} w_i(x)\beta_i(t)\lambda_i(\boldsymbol{\xi})}$
- Large number of random variables

  $\rightsquigarrow$ multidimensional separation
- Stabilization

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