Méthodes Spectrales Non-Intrusives et de Galerkin pour la Quantification d'Incertitudes

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MOMAS-CALCUL - 05/05/10

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Outline

Simulation framework.

Basic ingredients

- Understanding of the physics involved (optional ?) :
  selection of the **mathematical model**.
- **Numerical method**(s) to solve the model.
- Specify a set of **data** :
  select a system among the class spanned by the model.

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Simulation errors

- **Model errors** : physical approximations and simplifications.
- **Numerical errors** : discretization, approximate solvers, finite arithmetics.
- **Data error** : boundary/initial conditions, model constants and parameters, external forcings, . . .

Sources of data uncertainty

- Inherent **variability** (*e.g.* industrial processes).
- **Epistemologic** uncertainty (*e.g.* model constants).
- **May not be fully reductible, even theoretically**.

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Probabilistic framework

- Define an abstract probability space $(\Omega, \mathcal{A}, d\mu)$.
- Consider **data** D as **random** quantity : $D(\omega), \ \omega \in \Omega$.
- **Simulation output** S is **random** and on $(\Omega, \mathcal{A}, d\mu)$.

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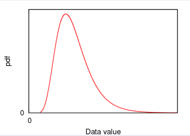
- **Simulation output** S is **random** and on $(\Omega, \mathcal{A}, d\mu)$.
- Data D and simulation output S are dependent random quantities (through the mathematical model $\mathcal{M}$) :

$$\mathcal{M}(S(\omega), D(\omega)) = 0, \quad \forall \omega \in \Omega.$$

Propagation and Quantification of data uncertainty

Data density



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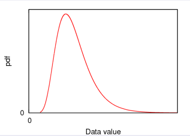

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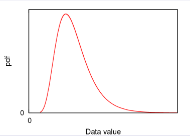

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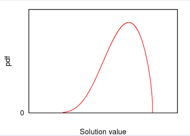

Propagation and Quantification of data uncertainty

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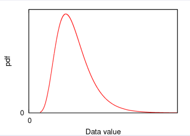

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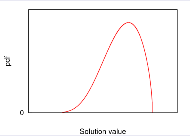

- **Variability** in model output : numerical error bars.
- Assessment of **predictability**.
- Support **decision making process**.
- What type of information (abstract quantities, confidence intervals, density estimations, structure of dependencies, ...) one needs ?

Deterministic methods

- Sensitivity analysis (adjoint based, AD, ...) : local.
- Perturbation techniques : limited to low order and simple data uncertainty.
- Neuman expansions : limited to low expansion order.
- Moments method : closure problem (non-Gaussian / non-linear problems).

Simulation techniques Monte-Carlo

Spectral Methods

Deterministic methods

Simulation techniques — Monte-Carlo

- Generate a sample set of data realizations and compute the corresponding sample set of model ouput.
- Use sample set based random estimates of abstract characterizations (moments, correlations, . . .).
- Plus : **Very robust** and re-use **deterministic codes** : (parallelization, complex data uncertainty).
- Minus : **slow convergence of the random estimates** with the sample set dimension.

Spectral Methods

Deterministic methods

Simulation techniques Monte-Carlo

Spectral Methods

- Parametrization of the data with random variables (RVs).
- $\perp$ projection of solution on the (L_2) space spanned by the RVs.
- Plus : **arbitrary level of uncertainty, deterministic approach, convergence rate, information contained**.
- Minus : **parametrizations** (limited # of RVs), **adaptation of simulation tools** (legacy codes), **robustness** (non-linear problems, non-smooth output, ...).
- **Not suited for model uncertainty**

Outline

1. **Introduction**
   - Simulation and errors
   - Data uncertainty
   - Alternative UQ methods
2. **Spectral UQ**
   - Generalized PC expansion
   - Application to spectral UQ
3. **Solution Methods**
   - Non-Intrusive Methods
   - Stochastic Galerkin Projection
4. **Conclusion**

Polynomial Chaos expansion **[Wiener-1938]**

Any well behaved RV $U(\omega)$ (*e.g.* 2nd-order one) defined on $(\Omega, \mathcal{A}, d\mu)$ has a **convergent expansion** of the form :

$$\begin{aligned} U(\omega) &= u_0\Gamma_0 + \sum_{i_1=1}^{\infty} u_{i_1}\Gamma_1(\xi_{i_1}(\omega)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} u_{i_1,i_2}\Gamma_2(\xi_{i_1}(\omega), \xi_{i_2}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} u_{i_1,i_2,i_3}\Gamma_3(\xi_{i_1}(\omega), \xi_{i_2}(\omega), \xi_{i_3}(\omega)) + \dots \end{aligned}$$

- $\{\xi_1, \xi_2, \dots\}$: **independent normalized Gaussian RVs**.
- Γ_p **polynomials with degree** p, orthogonal to $\Gamma_q, \forall q < p$.
- Convergence in the **mean square sense** (Cameron and Martin, 1947).

Polynomial Chaos expansion [Wiener-1938]

Truncated PC expansion at order No and N RVs :

$$U(\omega) \approx \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi(\omega)), \quad \xi = \{\xi_1, \dots, \xi_{\mathrm{N}}\}, \quad \mathrm{P} = \frac{(\mathrm{N}+\mathrm{No})!}{\mathrm{N}!\mathrm{No}!}.$$

- $\{u_k\}_{k=0,\dots,\mathrm{P}}$: **deterministic** expansion coefficients,
- $\{\Psi_k\}_{k=0,\dots,\mathrm{P}}$: $\perp$ **random polynomials** wrt the **inner product** involving the density of ξ :

$$\begin{aligned} E\left[\Psi_k \Psi_l\right] = \langle \Psi_k, \Psi_l \rangle &\equiv \int_\Omega \Psi_k(\xi(\omega))\Psi_l(\xi(\omega))d\mu(\omega) \\ &= \int \Psi_k(\xi)\Psi_l(\xi)p(\xi)d\xi = \delta_{kl}\left\langle \Psi_k^2 \right\rangle. \end{aligned}$$

Polynomial Chaos expansion [Wiener-1938]

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- $p(\boldsymbol{\xi}) = \prod_{i=1}^{n} \frac{\exp\left(-\xi_i^2/2\right)}{\sqrt{2\pi}} \Longrightarrow \Psi_k(\boldsymbol{\xi})$: **Hermite polynomials**
- $\{\Psi_0, \ldots, \Psi_{\mathrm{P}}\}$ is an orthogonal basis of $\mathcal{S}^{\mathrm{P}} \subset L_2(\Xi, p(\boldsymbol{\xi}))$.

Polynomial Chaos expansion [Wiener-1938]

Truncated PC expansion : $U(\omega) \approx \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi(\omega))$.

- Convention $\Psi_0 \equiv 1$: mean mode.
- **Expectation** of U :

$$E[U] \equiv \int_\Omega U(\omega) d\mu(\omega) \approx \sum_{k=0}^{\mathrm{P}} u_k \int_\Xi \Psi_k(\xi) p(\xi) d\xi = u_0.$$

- **Variance** of U :

$$V[U] = E[U^2] - E[U]^2 \approx \sum_{k=1}^{\mathrm{P}} u_k^2 \left\langle \Psi_k, \Psi_k \right\rangle .$$

- Extension to **random vectors & stochastic processes** :

$$\begin{pmatrix} U_1 \\ \vdots \\ U_m \end{pmatrix} (\omega, \boldsymbol{x}, t) \approx \sum_{k=0}^{\mathrm{P}} \begin{pmatrix} u_1 \\ \vdots \\ u_m \end{pmatrix}_k (\boldsymbol{x}, t)\, \Psi_k(\xi(\omega)).$$

Generalized PC expansion [Xiu and Karniadakis, 2002]

Askey scheme

Distribution of ξ_i	Polynomial familly
Gaussian	Hermite
Uniform	Legendre
Exponential	Laguerre
β-distribution	Jacobi

Also : discrete RVs (Poisson process).

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

where Ψ_k : classical (or mixture of) polynomials.

Data parametrization

Parametrization of D using $\mathrm{N} < \infty$ **independent** RVs with prescribed distribution $p(\xi)$:

$$D(\omega) \approx D(\boldsymbol{\xi}(\omega)), \quad \boldsymbol{\xi} = (\xi_1, \dots, \xi_{\mathrm{N}}) \in \Xi.$$

- Iso-probabilistic Transformation of random variables.
- Karhunen-Loève expansion : $D(\boldsymbol{x}, \omega)$ stochastic field/process.
- Independent components analysis.

Model

Solution expansion

Data parametrization

Model

We assume that for a.e. $\xi \in \Xi$, the problem $\mathcal{M}(S, D(\xi)) = 0$

1. is **well-posed**,
2. has a **unique solution**

and that

$\boxed{\text{the random solution } S(\xi) \in L_2(\Xi, p_\xi)}$:

$$E\left[S^2\right] = \int_\Omega S^2(\xi(\omega))d\mu(\omega) = \int_\Xi S^2(\xi)p(\xi)d\xi < +\infty.$$

Solution expansion

Data parametrization

Model

Solution expansion

Let $\{\Psi_0, \Psi_1, \ldots\}$ be a basis of $L_2(\Xi, p_\xi)$ then

$$S(\xi) = \sum_k s_k \Psi_k(\xi).$$

- Knowledge of the **spectral coefficients s_k** fully **determine the random solution**.
- Makes explicit the dependence between $D(\xi)$ and $S(\xi)$.

Data parametrization

Model

Solution expansion

Let $\{\Psi_0, \Psi_1, \ldots\}$ be a basis of $L_2(\Xi, p_\xi)$ then

$$S(\xi) = \sum_k s_k \Psi_k(\xi).$$

- Knowledge of the **spectral coefficients s_k** fully **determine the random solution**.
- Makes explicit the dependence between $D(\xi)$ and $S(\xi)$.
- **Need efficient procedure(s) to compute the s_k.**

Outline

Non-intrusive methods

Basics

Use code as a black-box

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

1. $\mathcal{S}_\Xi \equiv \{\xi^{(1)}, \ldots, \xi^{(m)}\}$ sample set of ξ
2. Let $s^{(i)}$ be the solution of the **deterministic** problem
$$\mathcal{M}\left(s^{(i)}, D(\xi^{(i)})\right) = 0$$
3. $\mathcal{S}_S \equiv \{s^{(1)}, \ldots, s^{(m)}\}$ sample set of model solutions
4. Estimate expansion coefficients s_k from this sample set.

- Complex models, reuse of determinsitic codes, planification, ...
- Error control and computational complexity (curse of dimensionality), ...

Least square fit "Regression"

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

$$R^2(s_0, \ldots, s_{\mathrm{P}}) \equiv \sum_{i=1}^{m} w_i \left(s^{(i)} - \sum_{k=0}^{\mathrm{P}} s_k \Psi_k \left(\xi^{(i)} \right) \right)^2 .$$

Advantages/issues

- Convergence with number of regression points m
- Selection of the regression points and "regressors" Ψ_k
- Error estimate

Non intrusive spectral projection : NISP

Exploit the orthogonality of the basis :

$$E\left[\Psi_k^2\right] s_k = \langle S, \Psi_k \rangle = \int_{\Xi} S(\xi)\Psi_k(\xi)p(\xi)d\xi.$$

Computation of $(\mathrm{P}+1)$ N-dimensional integrals

Non intrusive spectral projection : NISP

Exploit the orthogonality of the basis :

$$E\left[\Psi_k^2\right]s_k = \langle S, \Psi_k \rangle = \int_\Xi S(\xi)\Psi_k(\xi)p(\xi)d\xi.$$

Computation of $(\mathrm{P}+1)$ N-dimensional integrals

$$\langle S, \Psi_k \rangle \approx \sum_{i=1}^{N_Q} w^{(i)} S\left(\xi^{(i)}\right)\Psi_k\left(\xi^{(i)}\right).$$

Non intrusive projection

Random Quadratures

Approximate integrals from a (pseudo) random sample set $\mathcal{S}_S$:

$$\langle S, \Psi_k \rangle \approx \frac{1}{m} \sum_{i=1}^{m} w^{(i)} s^{(i)} \Psi_k \left(\xi^{(i)} \right).$$

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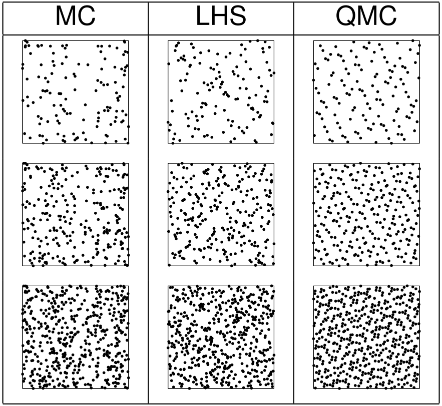


- Convergence rate
- Error estimate
- Optimal sampling strategy

Non intrusive projection — Deterministic Quadratures

Approximate integrals by N-dimensional quadratures :

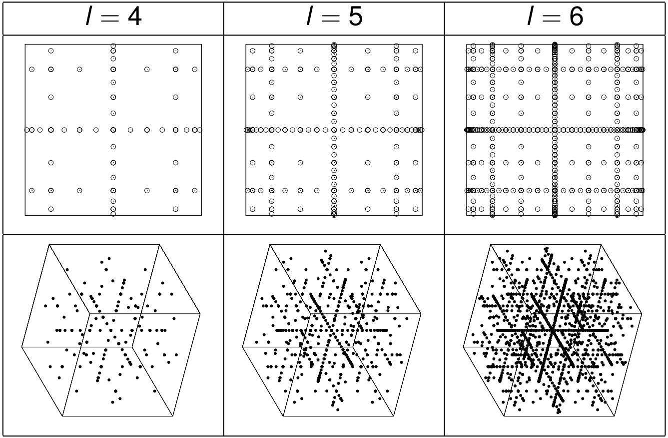
$$\langle S, \Psi_k \rangle \approx \sum_{i=1}^{N_Q} w^{(i)} s^{(i)} \Psi_k \left(\xi^{(i)} \right).$$

Quadrature points $\xi^{(i)}$ and weights $w^{(i)}$ obtained by

- **full tensorization** of n points 1-D quadrature (*i.e.* Gauss) :
  $$\boxed{N_Q = n^{\mathrm{N}}}$$
- **partial tensorization**
  of nested 1-D quadrature formula (Féjer, Clenshaw-Curtis) :
  $$\boxed{N_Q << n^{\mathrm{N}}}$$

Non intrusive projection

Deterministic Quadratures



- Important development of sparse-grid methods
- Anisotropic and adaptivity
- Extension to collocation approach ($\mathbb{N}$-dimensional interpolation)

Galerkin projection

- Weak solution of the stochastic problem $\mathcal{M}(S, D) = 0$.
- Needs adaptation of deterministic codes.
- Usually more efficient than NI techniques.
- Better suited to improvement (error estimate, optimal and basis reduction, ...), thanks to spectral theory and functional analysis.

Galerkin projection

Method of weighted residual

① Introduce truncated expansions in model equations

② Require residual to be $\perp$ to the stochastic subspace $\mathcal{S}^{\mathrm{P}}$

$$\left\langle \mathcal{M}\left(\sum_{k=0}^{\mathrm{P}} s_k \Psi_k(\xi), D(\xi)\right) \Psi_m(\xi) \right\rangle = 0 \quad \text{for } m = 0, \ldots, \mathrm{P}.$$

Set of $\mathrm{P}+1$ **coupled** problems.

Plus

- Implicitly account for modes' coupling.
- Often inherit properties of the deterministic model.

Minus

- Requires adaptation of deterministic solvers.
- Treatment of non-linearities.

Example of Galerkin projection

Convection dispersion equation — A. Cartalade (CEA)

- **1-D Convection dispersion :** concentration $C(x,t)$

$$\phi\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left[qC - (\phi d_m + \Lambda|q|)\frac{\partial C}{\partial x}\right].$$

- **IC and BC :** $C(x,t=0)=0$, $C(x=0,t)=1$ a.s.
- **Model coefficients :**

- $q>0$: Darcy velocity (1 m/day),
- ϕ : fluid fraction $0<\phi\leq 1$,
- d_m : molecular diffusivity ($<<1$),
- Λ : uncertain hydrodynamic dispersion coefficient.

Uncertainty model

Example of Galerkin projection

Model equation

Uncertainty model

- Λ follows an uncertain power-law : $\boxed{\Lambda = A\phi^B}$
- A and B independent random variables with p.d.f.
  $\log_{10} A \sim U[-4,-2]$ and $B \sim U[-3.5,-1]$
- Parametrization with two RV $\xi_1, \xi_2 \sim U[-1,1]$:

$$A(\xi_1) = \exp(\mu_1 + \sigma_1\xi_1) \qquad B = \mu_2 + \sigma_2\xi_2$$

- Expansion of Λ : (2-D Legendre basis)

$$\Lambda(\xi_1,\xi_2) \approx \sum_k \lambda_k \Psi_k(\xi_1,\xi_2)$$

Stochastic convection dispersion equation becomes :

$$\partial_t C + q\partial_x C - D(\xi)\partial_{xx} C = 0$$

Expansion of the solution : $C(\xi, t, x) \approx \sum_{k=0}^{\mathrm{P}} c_k(x,t)\Psi_k(\xi)$
Insert and project : for $m = 0, \dots, \mathrm{P}$

$$\sum_{k=0}^{\mathrm{P}} \partial_t c_k \langle \Psi_k, \Psi_m \rangle + q\partial_x c_k \langle \Psi_k, \Psi_m \rangle - \langle \Psi_k D(\xi), \Psi_m \rangle \partial_{xx} c_k = 0$$

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Insert and project : for $m = 0, \dots, \mathrm{P}$

$$\partial_t c_m + q\partial_x c_m - \sum_{k=0}^{\mathrm{P}} \frac{\langle \Psi_k D(\xi), \Psi_m \rangle}{\langle \Psi_m, \Psi_m \rangle} \partial_{xx} c_k = 0$$

Coupling of the stochastic modes $c_k(\boldsymbol{x}, t)$ through the stochastic dispersion operator.

Proceed with the deterministic discretization :

- Time derivative $\partial_t c_k = (c_k^{n+1} - c_k^n)/\Delta t + \mathcal{O}(\Delta t)$
- Implicit scheme with FV scheme with n_c spatial cells

$$\sum_{k=0}^{\mathrm{P}} \frac{\langle \Psi_k \mathbb{A}(\xi), \Psi_m \rangle}{\langle \Psi_m, \Psi_m \rangle} \boldsymbol{c}_k^{n+1} = \boldsymbol{b}(\boldsymbol{c}_m^n), \quad m = 0, \dots, \mathrm{P}$$

where $\boldsymbol{c}_k^n \in \mathbb{R}^{n_c}$ and $\mathbb{A}(\xi)$ is a random matrix in $\mathbb{R}^{n_c \times n_c}$

- Random matrix expansion $\mathbb{A}(\xi) = \sum_{k=0}^{\mathrm{P}} [A]_k \Psi_k(\xi)$

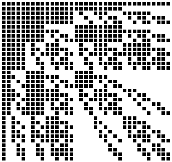
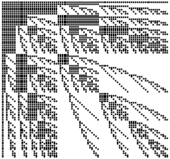
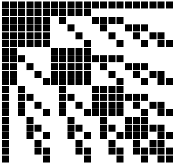
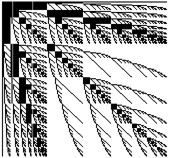
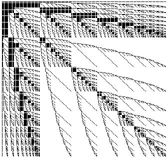
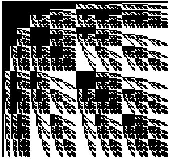
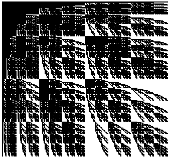
$$\sum_{k,l=0}^{\mathrm{P}} \mathcal{M}_{klm} [A]_k \boldsymbol{c}_l^{n+1} = \boldsymbol{b}(\boldsymbol{c}_m^n), \quad \mathcal{M}_{klm} := \frac{\langle \Psi_k \Psi_l, \Psi_m \rangle}{\langle \Psi_m, \Psi_m \rangle}$$

- **Linear system of $(\mathrm{P}+1) \times n_c$ equations.**

Structure of the Galerkin system :

- Usually the matrices $[A]_k$ inherit the structure of the determinstic problem
- The Galerkin product tensor $\mathcal{M}$ is sparse

(examples for $\mathrm{No} = 3$ -left- and $\mathrm{N} = 5$ -right-)

$\mathrm{N} = 4$-$\mathrm{P} = 35$	$\mathrm{N} = 6$-$\mathrm{P} = 84$	$\mathrm{No} = 2$-$\mathrm{P} = 20$	$\mathrm{No} = 3$-$\mathrm{P} = 55$
			
$\mathrm{N} = 8$-$\mathrm{P} = 164$	$\mathrm{N} = 10$-$\mathrm{P} = 285$	$\mathrm{No} = 4$-$\mathrm{P} = 126$	$\mathrm{No} = 5$-$\mathrm{P} = 251$
			

Resolution of the Galerkin system

$$\sum_{k=0}^{\mathrm{P}} \sum_{l=0}^{\mathrm{P}} \mathcal{M}_{klm} [A]_k \boldsymbol{c}_l^{n+1} = \boldsymbol{b}(\boldsymbol{c}_m^n), \quad \text{for } m = 0, \ldots, \mathrm{P}$$

Resolution of the Galerkin system

$$\sum_{l=0}^{\mathrm{P}} \mathcal{M}_{0lm}[A]_0 \boldsymbol{c}_l^{n+1} + \sum_{k=1}^{\mathrm{P}} \sum_{l=0}^{\mathrm{P}} \mathcal{M}_{klm}[A]_k \boldsymbol{c}_l^{n+1} = \boldsymbol{b}(\boldsymbol{c}_m^n), \quad \text{for } m = 0, \dots, \mathrm{P}$$

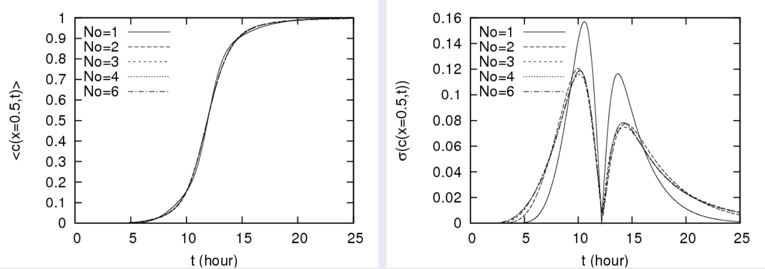
Resolution of the Galerkin system

$$[A]_0 \boldsymbol{c}_m^{n+1} = \boldsymbol{b}(\boldsymbol{c}_m^n) - \sum_{k=1}^{\mathrm{P}} \sum_{l=0}^{\mathrm{P}} \mathcal{M}_{klm} [A]_k \boldsymbol{c}_l^{n+1}, \quad \text{for } m = 0, \dots, \mathrm{P}$$

- Suggest Jacobi type iterations
- Factorization of $[A]_0 = E[\mathbb{A}]$ only
- Other iterative (Krylov-type) methods with preconditioner $\mathbb{P} = diag(E[\mathbb{A}])$
- Efficiency depends on the variability of $\mathbb{A}$.

Convection dispersion equation results

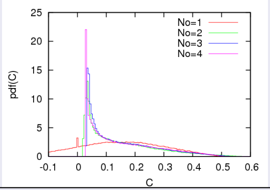
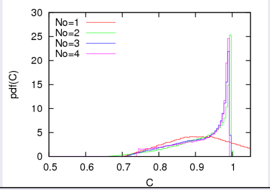
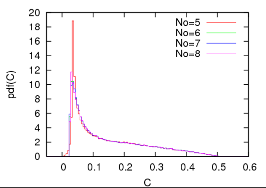
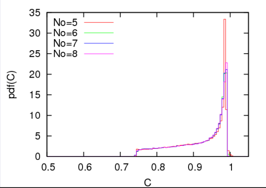
Expectation & standard deviation at $x = 0.5$



$\mathrm{No} = 1 \rightarrow P + 1 = 3$, $\mathrm{No} = 6 \rightarrow P + 1 = 145$.

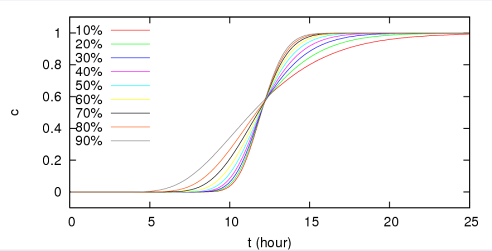
Convection dispersion equation results

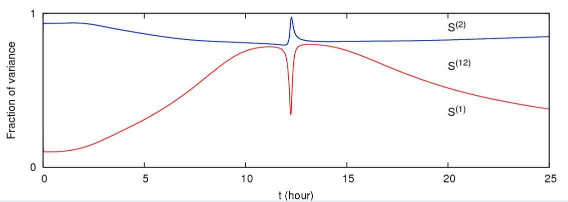
Convergence of pdfs at $x = 0.5$

$t = 10h.$	$t = 15h.$
	
	

Convection dispersion equation results

Further uncertainty analysis : quartiles & ANOVA (Sobol)





Conclusion

- Propagation des incertitudes = calculs intensifs
- HPC nécessaire (tant en intrusif que non intrusif)
- Non-intrusif : plateformes / lanceurs, planification, répartition de charge, . . .
- Galerkin : strategies de parallélisation appropriées (distribution de la résolution des modes / décomposition de domaine spatial), équilibrage et optimisation des volumes de communication entre processeurs
- Multi-résolution : procédures de type AMR au niveau stochastique, nombreux problèmes de Galerkin découplés, . . .
- Incertitudes de modélisation par MC

Fundings : GNR MoMaS and ANR

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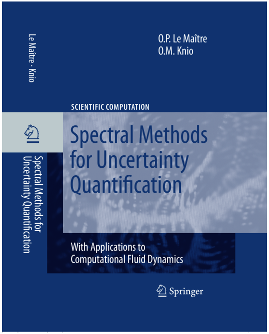

http://www.limsi.fr/Individu/olm