Methods for Uncertainty Propagation and Quantification in Numerical Models

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Materials of this lecture are taken from the book :
Spectral Methods for Uncertainty Quantification with applications in computational fluid dynamics with Omar Knio, Springer (2010).

6 Conclusion

- Selection of a **mathematical model** :
retain essential physical processes.
- Selection of a **numerical method** :
to solve the model equations.
- Define all **input-data** needed :
select a specific system in the class spanned by the model.

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

100

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- **Epistemic** uncertainty (e.g. model constants).
- May not be fully reducible, even theoretically.

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- Consider **input-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 of data uncertainty

Data density

$$\mathcal{M}(S, D) = 0$$

Solution density

$$\mathcal{M}(S, D) = 0$$

- **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.
- **Neumann 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 output**.
- 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

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Page 10 of 10

Discussion

- Parameterization 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 : parameterizations (limited # of RVs), adaptation of simulation tools (legacy codes), robustness (non-linear problems, non-smooth output, ...).
- Not suited for model uncertainty

Q: What is the difference between a "strong" and a "weak" form of a vowel?

Polymers

Method

- Stochastic conduction process

Discussion

Polynomial Chaos expansions

Polynomial Chaos expansions

[Wiener, 1938]

Truncated PC expansion at order N_0 and using N RVs :

$$U(\omega) \approx \sum_{k=0}^P u_k \Psi_k(\xi(\omega)), \quad \xi = \{\xi_1, \dots, \xi_N\}, \quad P = \frac{(N + N_0)!}{N!N_0!}.$$

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

$$\begin{aligned}\mathbb{E}\{\Psi_k\Psi_l\} &= \langle\Psi_k,\Psi_l\rangle \quad \equiv \quad \int_{\Omega}\Psi_k(\xi(\omega))\Psi_l(\xi(\omega))d\mu(\omega) \\ &= \int\Psi_k(\xi)\Psi_l(\xi)p(\xi)d\xi = \delta_{kl}\langle\Psi_k,\Psi_k\rangle.\end{aligned}$$

Polynomial Chaos expansions

[Wiener, 1938]

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- Gaussian RVs : $p(\xi) = \prod_{i=1}^N \frac{\exp(-\xi_i^2/2)}{\sqrt{2\pi}} \implies$ Hermite polynomials
(Wiener-Hermite expansions)
- $\{\Psi_0, \dots, \Psi_P\}$ is an orthogonal basis of $\mathcal{S}^P \subset L^2(\mathbb{R}^N, p(\xi))$.

Polynomial Chaos expansions

[Wiener, 1938]

Truncated PC expansion :

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

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

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

- **Variance** of U :

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

- Extension to random vectors & stochastic processes :

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

Generalized PC expansion

[Xiu & Karniadakis, 2002]

Askey scheme

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

Also : discrete RVs (Poisson process).

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

where Ψ_k : classical (or product of) polynomials :
spectral expansions

Instead of a spectral expansion over Ξ one can use **Piecewise polynomial expansion** on a mesh Σ of Ξ

- $\Xi = \bigcup_{SE \in \Sigma} \Xi_{SE}, \Xi_{SE} \cap \Xi_{SE'} = \emptyset$ for $SE \neq SE'$
- $\mathcal{S} = \left\{ U \in L^2(\Xi, p_\xi), U(\xi \in \Xi_{SE}) \in \mathbb{P}_{N_0}^N(\Xi_{SE}) \right\}$

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

- ψ_k are orthogonal with :

- 1 Support of Ψ_k limited to an element : **Stochastic multi-element method** [Deb et al., 2001], [Wang and Karniadakis, 2005]
Fully decouple the approximation problem for $\neq$ elements
- 2 Hierarchical orthogonal Ψ_k : **Stochastic Multiwavelet method** [Olm et al., 2004, 2006, 2009]
Couple the approximation problem, well suited for adaptive strategy (MRA)

[Ghanem & Spanos, 1991]

Input-data parametrization

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

$$D(\omega) \approx D(\xi(\omega)), \quad \xi = (\xi_1, \dots, \xi_N) \in \Xi.$$

- Iso-probabilistic transformations of RVs,
- Karhunen-Loève expansion : $D(\mathbf{x}, \omega)$ stochastic field/process,
- Identification (e.g. Bayesian).

Model

Solution expansion

[Ghanem & Spanos, 1991]

Input-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

the random solution $S(\xi) \in L^2(\Xi, p_\xi)$:

$$\mathbb{E} \{ S^2 \} = \int_{\Omega} S^2(\xi(\omega)) d\mu(\omega) = \int_{\Xi} S^2(\xi) p(\xi) d\xi < +\infty.$$

Solution expansion

[Ghanem & Spanos, 1991]

Input-data parametrization

Model

Solution expansion

Let $\{\psi_0, \psi_1, \dots\}$ 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 $S(\xi)$.

[Ghanem & Spanos, 1991]

Input-data parametrization

Model

Solution expansion

Let $\{\psi_0, \psi_1, \dots\}$ 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 .

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 $\mathcal{S}_{\Xi} \equiv \{\xi^{(1)}, \dots, \xi^{(m)}\}$ 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 $\mathcal{S}_{\mathcal{S}} \equiv \{s^{(1)}, \dots, s^{(m)}\}$ sample set of model solutions
 - 4 Estimate expansion coefficients s_k from this sample set.
- Complex models, reuse of deterministic codes, planification, ...
 - Error control and computational complexity (curse of dimensionality), ...

Non-Intrusive methods

Non intrusive projection

Random Quadratures

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

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

MC	LHS	QMC

- Convergence rate
- Error estimate
- Optimal sampling strategy

Non-Intrusive methods

Non intrusive projection

Deterministic Quadratures

See other lecture(s)

- Important development of sparse-grid methods
- Anisotropic and adaptivity
- Extension to collocation approach (N-dimensional interpolation)

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

$$\left\langle \mathcal{M} \left(\sum_{k=0}^P s_k \psi_k(\xi), D(\xi) \right), \psi_m(\xi) \right\rangle = 0 \quad \text{for } m = 0, \dots, P.$$

Set of $P + 1$ 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.

1 Introduction

- Simulation and errors
- Input-data uncertainty
- Alternative UQ methods

2 Spectral UQ

- Polynomial Chaos expansions
- Application to spectral UQ

3 Solution methods

- Non-Intrusive methods
- Galerkin projection

4 Application to conduction

- Stochastic conduction problem
- Heat exchanger

5 Application to natural convection

- Boussinesq equations
- Results

6 Conclusion

Consider the linear steady heat equation in an isotropic two-dimensional domain Ω , with boundary $\partial\Omega$.

$\mathbf{x} \in \Omega \mapsto u(\mathbf{x}) \in \mathbb{R}$ is the temperature field satisfying :

$$\nabla \cdot (\nu(\mathbf{x}) \nabla u(\mathbf{x})) = -f(\mathbf{x}) \quad + BC$$

where $\nu > 0$ is the thermal conductivity and $f \in L_2(\Omega)$ is a source term.

We consider **homogeneous Dirichlet and Neumann conditions** over the respective portions Γ_d and Γ_n of the domain boundary $\partial\Omega = \Gamma_d \cup \Gamma_n$, i.e.

$$u(\mathbf{x}) = 0, \quad \mathbf{x} \in \Gamma_d \quad \frac{\partial u}{\partial \eta} = 0, \quad \mathbf{x} \in \Gamma_n.$$

Stochastic conduction problem

$P - 1$ Finite Element discretization Let $\mathcal{T} = \{\Sigma_1, \dots, \Sigma_{ne}\}$ be a triangulation of Ω with ne non-overlapping triangular elements Σ_i . The $P - 1$ finite element space $\mathcal{V}^h$ consists in linear functions in each Σ_i , that are continuous across inter-element boundaries. A function $v \in \mathcal{V}^h$ is completely defined by its values at the mesh nodes, and v can be expressed as

$$v^h(\mathbf{x}) = \sum_{i \in \mathcal{N}} v_i^h \Phi_i(\mathbf{x}),$$

where $\mathcal{N}$ is the set of nodes which are not lying on Γ_d and $\Phi_i(\mathbf{x})$ are the shape functions associated to these nodes.

$$\mathcal{V}^h = \text{span} \{ \Phi_i \}_{i \in \mathcal{N}}.$$

Left : sketch of the domain Ω and decomposition of the boundary $\partial\Omega$ into Dirichlet Γ_d and Neumann Γ_n regions. Right : example of a finite-element mesh with 508 elements and 284 nodes.

Consider the case of **random conductivity and source term**, defined on an abstract probability space (Θ, Σ, P) :

$$\nu \rightarrow \nu(\mathbf{x}, \theta), \quad f \rightarrow F(\mathbf{x}, \theta).$$

Then, $u \rightarrow U(\mathbf{x}, \theta)$ satisfies almost surely the stochastic problem

$$\left\{ \begin{array}{ll} \nabla \cdot (\nu(\mathbf{x}, \theta) \nabla U(\mathbf{x}, \theta)) = -F(\mathbf{x}, \theta) & \mathbf{x} \in \Omega \\ U(\mathbf{x}, \theta) = 0 & \mathbf{x} \in \Gamma_d, \\ \frac{\partial U(\mathbf{x}, \theta)}{\partial n} = 0 & \mathbf{x} \in \Gamma_n. \end{array} \right.$$

The functional space for $U(\mathbf{x}, \theta)$ will be $\mathcal{V} \otimes L_2(\Theta, P)$. In other words,

$$U(\cdot, \theta) \in \mathcal{V}, \quad U(\mathbf{x}, \cdot) \in L_2(\Theta, P),$$

The variational form of the stochastic problem is :

Find $U \in \mathcal{V} \otimes L_2(\Theta, P)$ such that

$$A(U, V) = B(V) \quad \forall V \in \mathcal{V} \otimes L_2(\Theta, P),$$

where

$$A(U, V) \equiv \mathbb{E} \{a(U, V)\} = \int_{\Theta} \left[\int_{\Omega} \nu(\mathbf{x}, \theta) \nabla U(\mathbf{x}, \theta) \cdot \nabla V(\mathbf{x}, \theta) d\mathbf{x} \right] dP(\theta),$$

and

$$B(V) \equiv \mathbb{E} \{b(V)\} = \int_{\Theta} \left[\int_{\Omega} F(\mathbf{x}, \theta) V(\mathbf{x}, \theta) d\mathbf{x} \right] dP(\theta).$$

introducing the deterministic discretization in $\mathcal{V}^h$ it comes

$$U^h(\mathbf{x}, \theta) = \sum_{i \in \mathcal{N}} U_i(\theta) \Phi_i(\mathbf{x}) \in (\mathcal{V}^h \otimes L_2(\Theta, P)) .$$

It shows that the semi-discrete solution consists in $n = \text{Card}(\mathcal{N})$ random variables $U_i(\theta)$. They satisfy

$$\sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} \mathbb{E} \{ A_{i,j}(\theta) U_i(\theta) V_j(\theta) \} = \sum_{i \in \mathcal{N}} \mathbb{E} \{ B_i(\theta) V_i(\theta) \}, \quad \forall V_i(\theta) \in L_2(\Theta, P), \quad i \in \mathcal{N},$$

where

$$A_{i,j}(\theta) = \int_{\Omega} \nu(\mathbf{x}, \theta) \nabla \Phi_i(\mathbf{x}) \cdot \nabla \Phi_j(\mathbf{x}) d\mathbf{x},$$

and

$$B_i(\theta) = \int_{\Omega} f(\mathbf{x}, \theta) \Phi_i(\mathbf{x}) d\mathbf{x}.$$

Stochastic conduction problem

We assume ν and F parameterized with N independent r.v.
 $\xi = \{\xi_1 \cdots \xi_N\}$ defined on (Θ, Σ, P) :

$$\nu(\mathbf{x}, \theta) = \nu(\mathbf{x}, \xi(\theta)), \quad F(\mathbf{x}, \theta) = F(\mathbf{x}, \xi(\theta)).$$

Examples of parameterization will be shown later. The **space of second-order random functionals** in ξ is spanned by the Polynomial Chaos basis :

$$\mathcal{S} = \text{span}\{\psi_k(\xi)\}_{k=0}^{k=\infty} = L_2(\mathbb{R}^2, p_\xi),$$

where the ψ_i 's form a set of orthogonal multidimensional polynomials in ξ :

$$\langle \psi_i, \psi_j \rangle = \int_{\Xi} \psi_i(\eta) \psi_j(\eta) p_\xi(\eta) d\eta = \delta_{ij} \langle \psi_i^2 \rangle.$$

Provided that ν and F are second-order quantities, they have orthogonal representations :

$$\nu(\mathbf{x}, \xi) = \sum_{k=0}^{\infty} \nu_k(\mathbf{x}) \psi_k(\xi), \quad F(\mathbf{x}, \xi) = \sum_{k=0}^{\infty} f_k(\mathbf{x}) \psi_k(\xi).$$

Similarly, the expansion of the discrete solution U^h is

$$U^h(\mathbf{x}, \xi) = \sum_{i \in \mathcal{N}} \left(\sum_{k=0}^{\infty} u_{i,k} \psi_k(\xi) \right) \Phi_i(\mathbf{x}).$$

The stochastic expansions are truncated to a finite polynomial order N_0 .

Different orders of truncation may be considered for the conductivity, source and solution.

For simplicity, we use the same truncation order N_0 . It corresponds to a stochastic approximation space

$$\mathcal{S}^P \equiv \text{span}\{\psi_0, \dots, \psi_P\} \subset \mathcal{S}, \quad P + 1 = \frac{(N_0 + N)!}{N_0!N!}.$$

The Galerkin problem is obtained by inserting the expansions of ν , F , U^h and test functions $V \in \mathcal{V}^h \otimes \mathcal{S}^P$ into the variational form of the semi discrete stochastic problem. This results in :

Find $u_{i,k}$, $i \in \mathcal{N}$ and $k = 0, \dots, P$, such that

$$\sum_{i,j \in \mathcal{N}} \sum_{k,l,m=0}^P \langle \Psi_k \Psi_l \Psi_m \rangle A_{i,j}^k u_{i,l} v_{j,m} = \sum_{i \in \mathcal{N}} \sum_{k=0}^P b_i^k v_{i,k},$$

$$\forall v_{i,k}, \quad i \in \mathcal{N}, \quad k = 0, \dots, P$$

where

$$A_{i,j}^k \equiv \int_{\Omega} \nu_k(\mathbf{x}) \nabla \Phi_i(\mathbf{x}) \cdot \nabla \Phi_j(\mathbf{x}) d\mathbf{x}, \quad b_i^k \equiv \langle \Psi_k^2 \rangle \int_{\Omega} f_k(\mathbf{x}) \Phi_i(\mathbf{x}) d\mathbf{x}.$$

It involves $n \times (P + 1)$ deterministic quantities

Denote $\mathbf{u}_k := (u_{1,k} \dots u_{n,k})^t \in \mathbb{R}^n$ the vector of nodal values of the k -th stochastic mode of the solution.

With this notation, the Galerkin problem becomes :

Find $\mathbf{u}_0, \dots, \mathbf{u}_P$ such that for all $k = 0, \dots, P$

$$\sum_{l=0}^P \sum_{m=0}^P \langle \psi_k \psi_l \psi_m \rangle [A^l] \mathbf{u}_m = \mathbf{b}_k,$$

where the matrix $[A^l]$ has for coefficients $A_{i,j}^l$ and the vector

$$\mathbf{b}_k = (b_1^k \dots b_n^k)^t.$$

Stochastic conduction problem

Denote $\mathbf{u}_k := (u_{1,k} \dots u_{n,k})^t \in \mathbb{R}^n$ the vector of nodal values of the k -th stochastic mode of the solution.

This set of systems can be formally expressed as a single system $[\mathcal{A}]\mathbf{u} = \mathbf{B}$ where the global system matrix $[\mathcal{A}]$ has the block structure, corresponding to :

$$\begin{pmatrix} \mathcal{A}_{0,0} & \dots & \mathcal{A}_{0,P} \\ \vdots & \ddots & \vdots \\ \mathcal{A}_{P,0} & \dots & \mathcal{A}_{P,P} \end{pmatrix} \begin{pmatrix} \mathbf{u}_0 \\ \vdots \\ \mathbf{u}_P \end{pmatrix} = \begin{pmatrix} \mathbf{b}_0 \\ \vdots \\ \mathbf{b}_P \end{pmatrix}.$$

The matrix blocks are given by :

$$\mathcal{A}_{i,j} = \sum_{m=0}^P [\mathbf{A}^m] \langle \Psi_i \Psi_j \Psi_m \rangle \quad 0 \leq i, j \leq P.$$

The system $[\mathcal{A}]\mathbf{u} = \mathbf{B}$ is called the spectral or Galerkin problem.

Solution method :

- The matrix $[\mathcal{A}]$ of the Galerkin problem has a block symmetric structure, $\mathcal{A}_{i,j} = \mathcal{A}_{j,i}$, since $\langle \Psi_i \Psi_j \Psi_m \rangle = \langle \Psi_j \Psi_i \Psi_m \rangle$.
- The blocks are in fact symmetric because $A_{i,j}^k = A_{j,i}^k$, so **the matrix $[\mathcal{A}]$ is symmetric.**
- Standard solution techniques for (large) symmetric linear systems can be reused.
- Due to the size of the system, sparse storage is mandatory, even-though many blocks are zero.

Existence and uniqueness of the solution :

Properties of the Galerkin system have been the focus of many

works. *e.g.* [Babuska, 2002], [Babuska, 2005], [Frauenfelder, 2005], [Matthies, 2005]

- For Dirichlet boundary conditions, the Galerkin system for stochastic elliptic problems has a **unique solution** provided that the **random conductivity field satisfies some probabilistic (sufficient) conditions**.
- For the deterministic discretization with $P - 1$ finite-elements, these probabilistic conditions reduce to

$$\frac{1}{\nu(\mathbf{x}, \xi)} \in L_2(\Xi, P_\Xi), \forall \mathbf{x} \in \Omega$$

- For Neumann boundary conditions only, $U(\mathbf{x}, \xi)$ is defined up to an arbitrary random variable and **an integral constraint on the source term** is necessary for homogeneous conditions,

$$\int_{\Omega} F(\mathbf{x}, \xi) d\mathbf{x} = 0 \quad a.s.$$

Stochastic conduction problem

We consider $\Omega = [0, 1]^2$, with Dirichlet boundary conditions over 3 edges and a Neumann condition over the left edge $x = 1$.

Left : computational domain Ω and decomposition of the boundary $\partial\Omega$ into Dirichlet Γ_d and Neumann Γ_n parts.

Right : typical finite-element triangulation of Ω using 512 elements and 289 nodes.

Stochastic conduction problem

Consider first the case of a uniform deterministic source term and constant random conductivity

$$F(\mathbf{x}, \theta) = f(\mathbf{x}) = 1, \quad \nu(\mathbf{x}, \theta) = \beta(\theta).$$

- The random conductivity β is assumed to be log-normal, with unit median value $\bar{\beta} = 1$ and coefficient of variation $C \geq 1$.
- β is parametrized with a unique normalized Gaussian variable $\xi_1(\theta)$ so $N = 1$, and the PC basis is made of the one-dimensional Hermite polynomials.

$$\beta(\xi_1) = \exp(\mu_\beta + \sigma_\beta \xi_1), \quad \mu_\beta = \log(\bar{\beta}) \text{ and } \sigma_\beta = \frac{\log C}{2.85}.$$

- The PC coefficients β_k have closed form expressions [Ghanem, 1999] :

$$\beta(\xi_1) = \sum_{k=0}^{\infty} \beta_k \Psi_k(\xi_1), \quad \beta_k = \exp(\mu_\beta + \sigma_\beta^2/2) \frac{\sigma_\beta^k}{\langle \Psi_k^2 \rangle}.$$

Stochastic modes of the solution for $No = 4$

U_0^h

U_1^h

U_2^h

U_3^h

U_4^h

Standard deviation

Convergence with the expansion order

β being log-normal, so is its inverse, and the expansion of $1/\beta$ is consequently given by :

$$\left(\frac{1}{\beta}\right)_k = \exp(-\mu_\beta + \sigma_\beta^2/2) \frac{(-\sigma_\beta)^k}{\langle \psi_k^2 \rangle}.$$

The spectrum of the numerical solution should decay as $|\sigma_\beta|^k/k!$.

Normalized spectra of the random solution u_k^h at node $\mathbf{x} = (1, 0.5)$ as computed using different expansion orders.

Convergence of pdf

Computed probability density functions of U^h at $\mathbf{x} = (1, 0.5)$ for different expansion orders N_o as indicated. Top plot : $N_o = 1, \dots, 6$. Bottom plot : same pdfs in log scale for $N_o = 2, \dots, 6$ together with the theoretical pdf.

- ν^1 and ν^2 are two independent log-normal random variables with respective medians $\bar{\nu}^1$ and $\bar{\nu}^2$, and coefficients of variation C^1 and C^2 .
- Two normalized Gaussian variables ξ_1 and ξ_2 are used to parametrize the conductivity field.
- The stochastic dimension is $N = 2$, and the stochastic basis consists of two-dimensional Hermite polynomials.

The expansion on $\mathcal{S}^{\mathbf{p}}$ of the random conductivity field,

$$\nu(\mathbf{x}, \boldsymbol{\xi}) = \sum_{k=0}^P \nu_k(\mathbf{x}) \Psi_k(\boldsymbol{\xi}), \quad (1)$$

has many zero modes $\nu_k(\mathbf{x})$ (due to the independence over distinct sub-domain). Consequently, some elementary matrices $[A']$ are zero, resulting in a sparse block structure for the Galerkin system.

The sparsity of the full Galerkin matrix system $[A]$ for $N_0 = 4, \dots, 6$ ($\dim \mathcal{S} = P + 1 = 15, 21$ and 28).

Uncertainty in U^h along the line $y = 0.5$. Left : two random conductivities ($N = 2, P = 20$). Right : single random conductivity ($N = 1, P = 5$).

Stochastic modes

$$\Psi_0 = \psi_0(\xi_1)\psi_0(\xi_2)$$

$$\Psi_1 = \psi_1(\xi_1)\psi_0(\xi_2) \quad \Psi_2 = \psi_0(\xi_1)\psi_1(\xi_2)$$

Stochastic conduction problem

$$\Psi_3 = \psi_2(\xi_1)\psi_0(\xi_2) \quad \Psi_4 = \psi_1(\xi_1)\psi_1(\xi_2) \quad \Psi_5 = \psi_0(\xi_1)\psi_2(\xi_2)$$

$$\Psi_6 = \psi_3(\xi_1)\psi_0(\xi_2) \quad \Psi_7 = \psi_2(\xi_1)\psi_1(\xi_2) \quad \Psi_8 = \psi_1(\xi_1)\psi_2(\xi_2) \quad \Psi_9 = \psi_0(\xi_1)\psi_3(\xi_2)$$

Modes $u_k(\mathbf{x})$ of the stochastic solution for the nonuniform conductivity problem.

Heat exchanger

Table 5.1 Distributions of the random quantities for the problem of Sect. 5.1.5, and associated random variables

Log normal	Median value	COV	Gaussian variable
ν^1	1	$\sqrt{5}$	ξ_1
ν^2	10^{-2}	$\sqrt{5}$	ξ_2
W_n	125	$\sqrt{2}$	ξ_3
Uniform	Lower bound	Upper bound	Uniform variable
T_c	5	10	ξ_4
T_e	10	30	ξ_5

Heat exchanger : FE meshes and solution

Fig. 5.16 Probability density function of temperature at x_{max} ; *left*: linear scale; *right*: logarithmic scale. Results are shown for the coarse and fine finite-element meshes. In both cases, an expansion with $No = 4$ expansion (126 spectral modes) is used

Fig. 5.17 Probability density functions of W_e^h across the external boundary, Γ_e , of the casing for the problem of Sect. 5.1.5; *left*: linear scale; *right*: logarithmic scale. Results are shown for the coarse and fine finite-element meshes. In both cases, an expansion with $No = 4$ expansion (126 spectral modes) is used

Fig. 5.20 Probability density functions of η_c^h and η_e^h of problem in Sect. 5.1.5 for the coarse (*left*) and fine (*right*) finite-element meshes. Solutions with $No = 4$ (126 spectral modes) are used

Pdfs of T_{max} , flux at "cold" boundary and of efficiencies.

Heat exchanger

Heat exchanger

Heat exchanger

Table 5.2 Total sensitivity indices of the random fluxes and efficiencies

Quantity	$\mathcal{T}_{v^1}$	$\mathcal{T}_{v^2}$	$\mathcal{T}_{W_n}$	$\mathcal{T}_{T_c}$	$\mathcal{T}_{T_e}$	Total
W_n	0.0000	0.0000	1.0000	0.0000	0.0000	1.0000
W_c	0.0254	0.0481	0.9185	0.0006	0.0114	1.0041
W_e	0.2729	0.5116	0.1298	0.0076	0.1216	1.0435
T_{max}	0.0132	0.8082	0.1910	0.0016	0.0008	1.0147
η_1	0.2980	0.5747	0.0121	0.0080	0.1437	1.0364
η_2	0.3137	0.6000	0.0128	0.0095	0.1510	1.0869

1 Introduction

- Simulation and errors
- Input-data uncertainty
- Alternative UQ methods

2 Spectral UQ

- Polynomial Chaos expansions
- Application to spectral UQ

3 Solution methods

- Non-Intrusive methods
- Galerkin projection

4 Application to conduction

- Stochastic conduction problem
- Heat exchanger

5 Application to natural convection

- Boussinesq equations
- Results

6 Conclusion

Natural convection

Boussinesq approximation

Governing equations

- Momentum :

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{\text{Pr}}{\sqrt{\text{Ra}}} \nabla^2 \mathbf{u} + \text{Pr} \theta \mathbf{y}$$

- Mass :

$$\nabla \cdot \mathbf{u} = 0$$

- Energy :

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{\sqrt{\text{Ra}}} \nabla^2 \theta$$

Uncertain boundary conditions

Natural convection

Boussinesq approximation

Governing equations

Uncertain boundary conditions

Natural convection

Boussinesq approximation

Governing equations

Uncertain boundary conditions

- $\mathbf{u} = 0$ on Γ .
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.

Natural convection

Boussinesq approximation

Governing equations

Uncertain boundary conditions

- $\mathbf{u} = 0$ on Γ .
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.
- $\theta(x = 1, y, \omega) = -1/2 + \theta'(y, \omega)$.

Natural convection

Boussinesq approximation

Governing equations

Uncertain boundary conditions

- $\mathbf{u} = 0$ on Γ .
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.
- $\theta(x = 1, y, \omega) = -1/2 + \theta'(y, \omega)$.

$$\mathbb{E} \{ \theta'(y) \theta'(y') \} = \sigma_\theta^2 \exp[-|y - y'|/L], \quad \theta' \sim N(0, \sigma_\theta^2).$$

BC and solution representations

Galerkin projection

Implementation and solver

Discretization

- Uniform grid, staggered arrangement and 2nd order F-Diff.
- Semi-**explicit** second order Adams-Bashford time-scheme

Incompressibility Treatment

- Prediction / Projection method [Chorin, 1971]
- FFT based solver for the elliptic pressure equations

CPU : essentially projection of **uncoupled** modes :

Stochastic CPU $\simeq (P + 1) \times$ deterministic CPU.

Convergence and performance

(unsteady solver)

- $N = 4 \sim 6$ is enough for $L \geq 1/3$
- $N_0 = 3 \rightarrow$ relative error on variance $< 10^{-4}$
- ~ 1000 times more efficient than MC (LHS)
- ~ 10 times more efficient than NISP + GH quadrature (sparse grid ?)
- Parallelization

[olm et al., 2001]

Parallelization

Structure of $\langle \Psi | \Psi_m, \Psi_k \rangle$

- Distribution of modes resolution
- **Not scalable** with increasing P
- assembly of rhs requires too many communications
- load balancing
- Domain decomposition ?

Velocity modes

$$\text{Ra} = 10^6, L = 1 \quad - \quad \sigma_\theta = 0.25.$$

Uncertainty bars

$$L = 1.$$

[olm et al., 2002]

Temperature modes

$$Ra = 10^6, L = 1 - \sigma_\theta = 0.25.$$

Heat-transfer density

[olm et al., 2002]

- Functional approximation provides rich information
- For complex & very high-dimensional problems Monte-Carlo and sampling approaches remain the only alternative
- Non smooth dependences require other type of bases : piecewise polynomial approximations & multiwavelets
- High-dimensional problems calls for adaptive methods
- Reduced basis approaches for complexity reduction : Greedy, PGD, ...
- Do not address model uncertainty

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