Uncertainty Quantification in Thermofluid Systems

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A short course.

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Plan

- Lecture 1
  - Fundamentals, UQ, spectral stochastic expansions
- Lecture 2
  - Uncertainty propagation, intrusive/non-intrusive
- Lecture 3
  - Challenges with non-linearity, Multiwavelet expansions
- Lecture 4
  - Bayesian inference and model construction

Lecture 1

- Fundamental context, uncertain parameters, validation
- Review Uncertainty Quantification (UQ) methods :
  - sensitivity analysis/error propagation, evidence theory, stochastic framework
- Stochastic UQ
  - Sampling parametric pdfs, sampling challenge
  - Polynomial Chaos (PC) theory for representation of Random Variables (RVs) and Random Fields (RFs)
    - PC basics
    - Multidimensional PC
    - PC Expansion (PCE) construction for an RV
    - PCE construction for a RF

The Validation Challenge

- Validation of a computational model :
  - Establish "agreement" between predictions and empirical observations
- Establishing model validity requires "error bars" on computational predictions
  - Disagreement without error bars cannot be used to conclude that a particular model is not valid
  - Disagreement within the range of uncertainty of the results can be due to parametric uncertainty

The Case for Uncertainty Quantification

- UQ is needed for :
  - validation of scientific models
  - validation of predictive codes
  - engineering design optimization
  - assessment of confidence in computational predictions
  - enabling decision-making strategies based on predictive models
  - assimilation of observational data and model construction in noisy environments
  - multiscale/multiphysics modeling

Sources of Uncertainty

- model structure
  - participating physical processes
  - governing equations
  - constitutive relations
- model parameters
  - transport properties
  - thermodynamic properties
  - constitutive relations
  - rate coefficients
- initial and boundary conditions
- geometry

Focus on parametric UQ

Elements of a UQ strategy

- Estimation of model/parametric uncertainties based on data
  - Deterministic framework
    - Regresssion analysis, fitting, parameter estimation
  - Probabilistic framework
    - Bayesian inference of uncertain models/parameters
- Forward propagation of uncertainty in computational models
  - Local sensitivity analysis (SA) and error propagation
  - Fuzzy logic
  - Evidence theory — interval math
  - Probabilistic framework — Global SA / stochastic UQ
    - Sampling based — non-intrsive
    - Direct — intrusive

Local Sensitivity Analysis & Error Propagation

- Forward methods
  - Advantageous when dealing with a small number of parameters and many output observables
  - Extrapolation based on Taylor series used to evaluate variance in observables given that of parameters
    - Challenges with models with

      significant non-linearity

      large uncertainty

      parametric uncertainties of different order
    - No information on shapes/tails of PDFs of output observables
- Adjoint methods
  - Advantageous when dealing with a small number of observables and many input parameters

Global Sensitivity Analysis

- Random sampling-based
  - Define parametric PDFs
  - Sample them (MC, LHS, Quasi-Random, ...)
  - Run forward model for each sample
  - Evaluate statistics/PDFs of output observables
  - Sensitivity information
    - Scatter plots; Correlation measures; Regression
    - Measures of Importance; Sobol' sensitivity indices, ...
- Response surface construction through factorial designs
  - followed by sensitivity/UQ
- Anal. of Variance (ANOVA) – High Dim. Model Rep. (HDMR)

UQ based on Probability Theory

- Conception of probability as a degree of belief or certainty
  - Uncertain quantity $\equiv$ Random Variable/Process
  - This is the *Bayesian* understanding of probability by Bayes (1702-1761) and Laplace (1749-1827)

    "A Philosophical Essay on Probabilities", Pierre Simon - Marquis de Laplace, Dover Pub.
  - Encompasses both Aleatoric and Epistemic uncertainty
    - Aleatoric uncertainty: due to variability
    - Epistemic uncertainty: due to lack of knowledge
  - Distinct from the *frequentist* viewpoint

Basic Sampling Methods for Stochastic UQ

- Decide, e.g. based on sensitivity analysis, on the smallest relevant set of "important" parameters that are uncertain
- Evaluate/define the probability density functions (PDFs) that best describe the uncertainty in these model parameters
- Generate samples from these PDFs, e.g.
  - Monte Carlo (MC) sampling
  - Latin Hypercube Sampling (LHS)
- For each parameter sample, run the forward model and generate a sample of the model outputs
- Collect statistics of interest on realizations of model outputs
  - Means, variances, other moments, PDFs
- Sandia's DAKOTA toolkit useful for such sampling studies

  — www.cs.sandia.gov/DAKOTA/software.html

Challenges with Random Sampling-based UQ

- Random sampling (MC,LHS) typically requires many thousands of samples for reliable statistics
  - This is feasible for simple forward models
  - It is not feasible for complex computational problems

Spectral Methods for Forward Stochastic UQ

- Goal:
  - Represent model parameters as random variables/processes
  - Evaluate corresponding stochastic model outputs
- Representation of random quantities using spectral expansions provides means for:
  - reformulation of the governing equations and direct evaluation of the uncertain model outputs
  - extracting sensitivity information from sampled realizations of uncertain quantities
- Requirement: random variables in L_2, i.e. with finite variance

Background: One-Dimensional Hermite Polynomials

$$\psi_0(x) = 1$$

$$\psi_k(x) = (-1)^k e^{x^2/2} \frac{\mathrm{d}^k}{\mathrm{d}x^k} e^{-x^2/2}, \qquad k = 1, 2, \ldots$$

$$\psi_1(x) = x, \quad \psi_2(x) = x^2 - 1, \quad \psi_3(x) = x^3 - 3x, \ \ldots$$

The Hermite polynomials form an orthogonal basis over $[-\infty, \infty]$ with respect to the inner product

$$\langle \psi_i \psi_j \rangle \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_i(x) \psi_j(x) w(x) dx = \delta_{ij} \left\langle \psi_i^2 \right\rangle$$

where $w(x)$ is the weight function

$$w(x) = e^{-x^2/2}$$

Note that $\frac{e^{-x^2/2}}{\sqrt{2\pi}}$ is the density of a standard normal random variable

1D Hermite Polynomials and Gaussian Random Variables

Thus, given a probability space (Θ, σ, P):

if $\xi(\theta) : \Theta \longrightarrow \mathbb{R}$ is a standard normal RV, $\xi \sim \mathcal{N}(0,1)$, we have

$$p(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2}$$

and the following inner product over the event space Θ is given by:

$$\begin{aligned}\left\langle \psi_i(\xi(\theta))\psi_j(\xi(\theta))\right\rangle &\equiv \int_\Theta \psi_i \psi_j dP \\ &= \int_{-\infty}^{\infty} \psi_i(\xi)\psi_j(\xi)p(\xi)\mathrm{d}\xi = \delta_{ij}\left\langle \psi_i^2 \right\rangle\end{aligned}$$

Hence the association bet. Hermite polynomials and Gaussian RVs

Polynomial Chaos Expansion

An L_2 random variable $u(\theta)$ can be described by a Polynomial Chaos (PC) expansion in terms of: the infinite-dimensional i.i.d. Gaussian basis $\boldsymbol{\xi} = \{\xi_i(\theta)\}_{i=1}^{\infty}$;

$$\begin{aligned} u(\theta) \;=\; & a_0\Gamma_0 + \sum_{i_1=1}^{\infty} a_{i_1}\Gamma_1(\xi_{i_1}(\theta)) \\ & + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{\infty} a_{i_1 i_2}\Gamma_2(\xi_{i_1}(\theta),\xi_{i_2}(\theta)) \\ & + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{\infty}\sum_{i_3=1}^{\infty} a_{i_1 i_2 i_3}\Gamma_3(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta)) + \ldots \end{aligned}$$

where Γ_p is the Polynomial Chaos of order p, $\Gamma_0 = 1$, and

$$\Gamma_p(\xi_{i_1},\ldots,\xi_{i_p}) = (-1)^p e^{\frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{\xi}} \frac{\partial^p}{\partial\xi_{i_1}\ldots\partial\xi_{i_p}} e^{-\frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{\xi}}$$

Notes on the PC construction

- The Polynomial Chaoses are by construction orthogonal with respect to the Gaussian probability measure
- They are thus identical with the corresponding multidimensional Hermite Polynomials
- The first four PCs are given by

$$
\begin{aligned}
\Gamma_0 &= 1 \\
\Gamma_1(\xi_i) &= \xi_i \\
\Gamma_2(\xi_{i_1}, \xi_{i_2}) &= \xi_{i_1}\xi_{i_2} - \delta_{i_1 i_2} \\
\Gamma_3(\xi_{i_1}, \xi_{i_2}, \xi_{i_3}) &= \xi_{i_1}\xi_{i_2}\xi_{i_3} - \xi_{i_1}\delta_{i_2 i_3} - \xi_{i_2}\delta_{i_1 i_3} - \xi_{i_3}\delta_{i_1 i_2} \\
&\dots
\end{aligned}
$$

R.G. Ghanem and P.D. Spanos, "Stochastic Finite Elements, A Spectral Approach", Dover Pub., 2003.

A more compact notation ... and finite dimensionality and order

- An L_2 random variable $u(\boldsymbol{x}, t, \theta)$ can be described by a PC expansion in terms of:
  - Hermite polynomials Ψ_k, $k = 1, \ldots, \infty$;
  - the associated infinite-dimensional Gaussian basis $\{\xi_i(\theta)\}_{i=1}^{\infty}$;
  - spectral mode strengths $u_k(\boldsymbol{x}, t)$, $k = 1, \ldots, \infty$.

- Truncated to finite dimension n and order p, the PC expansion for u is written as

$$u(\boldsymbol{x}, t, \theta) \simeq \sum_{k=0}^{P} u_k(\boldsymbol{x}, t) \Psi_k(\boldsymbol{\xi}(\theta))$$

where $\boldsymbol{\xi}(\theta) = \{\xi_1(\theta), \cdots, \xi_n(\theta)\}$, and $P + 1 = \frac{(n+p)!}{n!p!}$

A Sequence of 2D Hermite Polynomials

i	p	Ψ_i
0	0	1
1	1	ξ_1
2	1	ξ_2
3	2	$\xi_1^2 - 1$
4	2	$\xi_1 \xi_2$
5	2	$\xi_2^2 - 1$
...	...	...

The multidimensional Hermite polynomial $\Psi_i(\xi_1, \ldots, \xi_n)$ is a tensor product of the 1D Hermite polynomials, with a suitable multi-index $\boldsymbol{\alpha^i} = (\alpha_1^i, \alpha_2^i, \ldots, \alpha_n^i)$,

$$\Psi_i(\xi_1, \ldots, \xi_n) = \prod_{k=1}^{n} \psi_{\alpha_k^i}(\xi_k)$$

Multidimensional Inner Products — Orthogonality

$$\left\langle \Psi_i \Psi_j \right\rangle \equiv \int \ldots \int \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) g(\xi_1) g(\xi_2) \cdots g(\xi_n) \mathrm{d}\xi_1 \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_n$$

$$= \prod_{k=1}^{n} \left\langle \psi_{\alpha_k^i}(\xi_k) \psi_{\alpha_k^j}(\xi_k) \right\rangle = \delta_{ij} \left\langle \Psi_i^2 \right\rangle$$

where,

$$g(\xi) = \frac{e^{-\xi^2/2}}{\sqrt{2\pi}}$$

such that,

$$u = \sum_{k=0}^{P} u_k \Psi_k \qquad \Rightarrow \qquad \langle \Psi_i u \rangle = \sum_{k=0}^{P} u_k \langle \Psi_i \Psi_k \rangle = u_i \left\langle \Psi_i^2 \right\rangle$$

$$\Rightarrow \qquad u_i = \frac{\langle u \Psi_i \rangle}{\left\langle \Psi_i^2 \right\rangle}$$

Constructing a 1D PCE for a RV with a given PDF

Given RV $z \in \mathbb{R}$ with PDF: $g(z)$, CDF: $G(z)$

Define a 1D PCE :

$$z = \sum_{i=0}^{\infty} z_i \psi_i(\xi)$$

where ξ has PDF: $f(\xi)$, CDF: $F(\xi)$

Define a uniformly distributed RV $u \sim U(0,1)$, s.t.

$$z = G^{-1}(u), \qquad \xi = F^{-1}(u)$$

and evaluate the z_i via integrals over u :

$$z_i = \frac{\langle z\psi_i \rangle}{\langle \psi_i^2 \rangle} = \frac{1}{\langle \psi_i^2 \rangle} \int_0^1 \underbrace{G^{-1}(u)}_{z(\theta)} \, \psi_i(\underbrace{F^{-1}(u)}_{\xi(\theta)}) \underbrace{du}_{dP}$$

Constructing an nD PCE for a RV with a given PDF

- No general procedure.
- Given RV $z \in \mathbb{R}$ with PDF: $g(z)$, define:

$$z = \sum_{i=0}^{P} z_i \Psi_i(\xi_1, \xi_2, \ldots, \xi_n), \qquad P + 1 = \frac{(n+p)!}{n!p!}$$

- Can choose $\{n, p\}$ and the mode strengths by ensuring accurate capture of
  - the PDF $g(z)$
  - select moments of z
  - some observable of interest $\phi(z)$

Constructing an nD PCE for a stochastic process/random field

Let $M(\boldsymbol{x}, \theta) : D \times \Theta \to \mathbb{R}$ be an L^2 random field on D with mean $\mu(\boldsymbol{x})$, and a continuous covariance function, then M admits the following representation, the Karhunen-Loève (KL) expansion:

$$M(\boldsymbol{x}, \theta) = \mu(\boldsymbol{x}) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \xi_i(\theta) \phi_i(\boldsymbol{x})$$

where λ_i and $\phi_i(\boldsymbol{x})$ are eigenvalues and eigenfunctions of the covariance kernel C,

$$\begin{aligned} C(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \mathbb{E}[(M(\boldsymbol{x}_1, \theta) - \mu(\boldsymbol{x}_1))(M(\boldsymbol{x}_2, \theta) - \mu(\boldsymbol{x}_2)] \\ &= \sum_{i=1}^{\infty} \lambda_i \phi_i(\boldsymbol{x}_1) \phi_i(\boldsymbol{x}_2). \end{aligned}$$

The λ_i and $\phi_i(\boldsymbol{x})$ are the solution of the integral equation:

$$\int_D C(\boldsymbol{x}_1, \boldsymbol{x}_2) \phi_i(\boldsymbol{x}_1) \mathrm{d}\boldsymbol{x}_1 = \lambda_i \phi_i(\boldsymbol{x}_2)$$

More about KLE

The random variables $\{\xi_i(\theta)\}_{i=1}^{\infty}$ are uncorrelated with zero mean and unit variance

$$\langle \xi_i \rangle = 0, \quad \left\langle \xi_i \xi_j \right\rangle = \delta_{ij}, \qquad \forall i, j$$

and are in general non-Gaussian

$$\xi_i(\theta) = \frac{1}{\sqrt{\lambda_i}} \int_D (M(\boldsymbol{x}, \theta) - \mu(\boldsymbol{x}))\phi_i(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

If M is also a Gaussian process, then the ξ_i are i.i.d. Gaussians, $\xi_i \sim \mathcal{N}(0,1)\ \forall i$.

The KLE is *optimal*: of all possible orthonormal bases for $L^2(\Theta \times D)$ the above $\{\phi(\boldsymbol{x})\}$ minimize the mean-square error in a finite linear representation of $M(\cdot)$.

KLE to PCE

If M is a Gaussian process, then the KLE is the 1st-order nD PCE for M in terms of the ξ_i.

Otherwise, the Rosenblatt transform can be used to transform the uncorrelated non-Gaussian $\boldsymbol{\xi}$ into a set of i.i.d. uniform RVs, which can be further projected onto a PCE in terms of i.i.d. Gaussians.

Thus the KLE of any L^2 random-field/stochastic-process can be transformed into a corresponding Wiener-Hermite PCE

Closure — Lecture 1

- Covered
  - Motivation and background for stochastic UQ
  - Spectral representation of random variables and processes
  - Construction of PC and KL expansions
- Next
  - Use of PCEs for propagating uncertainty through computational models
  - Intrusive (direct) and non-intrusive (sampling-based) approaches
  - Applications to Navier-Stokes equations, and chemically reacting flow