# Challenges in Uncertainty Quantification in Computational Models

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#### Outline



## Introduction



#### Uncertainty Quantification Basics

- Forward Uncertainty Propagation
- Statistical Inverse Problems

#### Uncertainty Quantification Challenges – a Selection

- Characterization of Uncertain Inputs
- High-dimensionality
- Discontinuities
- Oscillatory Dynamics



### The Case for Uncertainty Quantification (UQ)

UQ is needed in:

- Assessment of confidence in computational predictions
- Validation and comparison of scientific/engineering models
- Design optimization
- Use of computational predictions for decision-support
- Assimilation of observational data and model construction
- Multiscale and multiphysics model coupling

#### **Overview of UQ Methods**

Estimation of model/parametric uncertainty

- Expert opinion, data collection
- Regression analysis, fitting, parameter estimation
- Bayesian inference of uncertain models/parameters

Forward propagation of uncertainty in models

- Local sensitivity analysis (SA) and error propagation
- Fuzzy logic; Evidence theory interval math
- Probabilistic framework Global SA / stochastic UQ
  - Random sampling, statistical methods
  - Galerkin methods
    - Polynomial Chaos (PC) intrusive/non-intrusive
  - Collocation, interpolants, regression, fitting ... PC/other

# Probabilistic Forward UQ & Polynomial Chaos Representation of Random Variables

- With y = f(x), x a random variable, estimate the RV y
- Can describe a RV in terms of its density, moments, characteristic function, or most fundamentally as a function on a probability space
- Constraining the analysis to RVs with finite variance, enables the representation of a RV as a spectral expansion in terms of orthogonal functions of standard RVs.
  - Polynomial Chaos
- Enables the use of available functional analysis methods for forward UQ

Forward Invers

#### Polynomial Chaos Expansion (PCE)

- Model uncertain quantities as random variables (RVs)
- Given a germ ξ(ω) = {ξ<sub>1</sub>, · · · , ξ<sub>n</sub>} a set of *i.i.d.* RVs
   where p(ξ) is uniquely determined by its moments

#### Any RV in $L^2(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$ can be written as a PCE:

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

-  $u_k(\mathbf{x}, t)$  are mode strengths -  $\Psi_k()$  are functions orthogonal w.r.t.  $p(\boldsymbol{\xi})$ 

With dimension n and order p:

$$P+1 = \frac{(n+p)!}{n!p!}$$

# Orthogonality

By construction, the functions  $\Psi_k()$  are orthogonal with respect to the density of  $\boldsymbol{\xi}$ 

$$u_k(\boldsymbol{x},t) = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \int u(\boldsymbol{x},t;\lambda(\boldsymbol{\xi})) \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

Examples:

- Hermite polynomials with Gaussian basis
- Legendre polynomials with Uniform basis, ...
- Global versus Local PC methods
  - Adaptive domain decomposition of the support of  $\boldsymbol{\xi}$

Forward Inverse



- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 1

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$$
$$= u_0 + u_1 \xi$$



Forward Inverse



- Wiener-Hermite
   PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 2

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$$
  
=  $u_0 + u_1 \xi + u_2(\xi^2 - 1)$ 



Forward Inverse

#### PC Illustration: WH PCE for a Lognormal RV



1.4 Wiener-Hermite 1.2 PCE constructed for a Lognormal RV 0.8 PCE-sampled PDF superposed on true 0.6 PDF 0.4 Order = 3 0.2 0 2 3 0 4 5 6  $u = \sum u_k \Psi_k(\xi)$ k=0 $= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi)$ 

Forward Inverse





Forward Inverse





Forward Inverse



- Fifth-order Wiener-Hermite PCE represents the given Lognormal well
- Higher order terms are negligible

### Random Fields – KLE

- Smooth random fields can be repesented with a small no. of stochastic degrees of freedom
- Karhunen-Loeve Expansion (KLE) for a RF with a continuous covariance function

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

- $\mu(x)$  is the mean of  $M(x, \omega)$  at x
- $\lambda_i$  and  $\phi_i(x)$  are the eigenvalues and eigenfunctions of the covariance  $C(x_1, x_2) = \langle [M(x_1, \omega) \mu(x_1)][M(x_2, \omega) \mu(x_2)] \rangle$
- The  $\eta_i$  are uncorrelated zero-mean unit-variance RVs
- KLE  $\Rightarrow$  representation of random fields using PC

Forward Inverse

#### **RF Illustration: KL of 2D Gaussian Process**

 $\delta = 0.1$ 



 $\delta = 0.5$ 



- 2D Gaussian Process with covariance:  $Cov(x_1, x_2) = exp(-||x_1 - x_2||^2/\delta^2)$
- Realizations smoother as covariance length  $\delta$  increases

#### RF Illustration: 2D KL - Modes for $\delta = 0.1$



#### RF Illustration: 2D KL - Modes for $\delta = 0.2$



#### RF Illustration: 2D KL - Modes for $\delta = 0.5$



Forward Inverse

### RF Illustration: 2D KL - eigenvalue spectrum



Forward Inverse

### RF Illustration: 2D KL - eigenvalue spectrum



Forward Inverse

### RF Illustration: 2D KL - eigenvalue spectrum



#### Essential Use of PC in UQ

Strategy:

- Represent model parameters/solution as random variables
- Construct PCEs for uncertain parameters
- Evaluate PCEs for model outputs

Advantages:

- Computational efficiency
- Sensitivity information

Requirement:

• Random variables in  $L^2$ , i.e. with finite variance

Forward Inverse

 $\mathcal{M}(u(\boldsymbol{x},t);\lambda) = 0$ 

#### Intrusive PC UQ: A direct non-sampling method

- Given model equations:
- Express uncertain parameters/variables using PCEs

$$u = \sum_{k=0}^{P} u_k \Psi_k; \quad \lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$$

Substitute in model equations; apply Galerkin projection

$$\mathcal{G}(U(\boldsymbol{x},t),\Lambda)=0$$

New set of equations: - with  $U = [u_0, \ldots, u_P]^T$ ,  $\Lambda = [\lambda_0, \ldots, \lambda_P]^T$ 

 Solving this system once provides the full specification of uncertain model ouputs

Forward Inverse

### Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Viscosity PCE

 $-\nu = \nu_0 + \nu_1 \xi$ 

Streamwise velocity

$$\begin{array}{l} - \ \mathbf{v} = \sum_{i=0}^{P} \mathbf{v}_{i} \Psi_{i} \\ - \ \mathbf{v}_{0} \text{: mean} \\ - \ \mathbf{v}_{i} \text{: } i\text{-th order mode} \\ - \ \sigma^{2} = \sum_{i=1}^{P} \mathbf{v}_{i}^{2} \left\langle \Psi_{i}^{2} \right\rangle \end{array}$$



#### Non-intrusive Spectral Projection (NISP) PC UQ

- Sampling-based
- Relies on black-box utilization of the computational model
- Evaluate projection integrals numerically
- For any quantity of interest  $\phi(\mathbf{x}, t; \lambda) = \sum_{k=0}^{P} \phi_k(\mathbf{x}, t) \Psi_k(\boldsymbol{\xi})$

$$\phi_k(\boldsymbol{x},t) = \frac{1}{\langle \Psi_k^2 \rangle} \int \phi(\boldsymbol{x},t;\lambda(\boldsymbol{\xi})) \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad k = 0,\ldots, P$$

Integrals can be evaluated using

- A variety of (Quasi) Monte Carlo methods
  - Slow convergence;  $\sim$  indep. of dimensionality
- Quadrature/Sparse-Quadrature methods
  - Fast convergence; depends on dimensionality

#### 1D H<sub>2</sub>-O<sub>2</sub> SCWO Flame NISP UQ/Chemkin-Premix



- Fast growth in OH uncertainty in the primary reaction zone
- Constant uncertainty and mean of OH in post-flame region
- Uncertainty in pre-exponential of Rxn.5 (H<sub>2</sub>O<sub>2</sub>+OH=H<sub>2</sub>O+HO<sub>2</sub>) has largest contribution to uncertainty in predicted OH

#### Other non-intrusive methods

- Response surface employing PC or other functional basis
- Collocation: Fit interpolant to samples
  - Oscillation concern
- Regression: Estimate best-fit response surface
  - Least-squares
  - Bayesian inference

• Useful when quadrature methods are infeasible, e.g. when

- Can't choose sample locations; samples given a priori
- Can't take enough samples
- Forward model is noisy

#### Inverse UQ – Estimation of Uncertain Inputs

- Forward UQ requires specification of uncertain inputs
- Probabilistic setting
  - Require joint PDF on input space
- Bayesian setting
  - PDF on uncertain inputs can be found given data
  - Probabilistic inference an inverse problem
- Uncertainty in computational predictions can depend strongly on detailed structure of the parametric PDF

#### The strong role of detailed input PDF structure



- Simple nonlinear algebraic model  $(u, v) = (x^2 y^2, 2xy)$
- Two input PDFs, p(x, y)
  - same nominals/bounds
  - different correlation structure
- Drastically different output PDFs
  - different nominals and bounds

Forward Inverse

#### Bayes formula for Parameter Inference

- Data Model (fit model + noise model):  $y = f(\lambda) * g(\epsilon)$
- Bayes Formula:

$$p(\lambda, y) = p(\lambda|y)p(y) = p(y|\lambda)p(\lambda)$$



- Prior: knowledge of  $\lambda$  prior to data
- Likelihood: forward model and measurement noise
- Posterior: combines information from prior and data
- Evidence: normalizing constant for present context

Forward Inverse

# Exploring the Posterior

 Given any sample λ, the un-normalized posterior probability can be easily computed

 $p(\lambda|y) \propto p(y|\lambda)p(\lambda)$ 

- Explore posterior w/ Markov Chain Monte Carlo (MCMC)
  - Metropolis-Hastings algorithm:
    - Random walk with proposal PDF & rejection rules
  - Computationally intensive,  $\mathcal{O}(10^5)$  samples
  - Each sample: evaluation of the forward model
    - Surrogate models
- Evaluate moments/marginals from the MCMC statistics

### UQ Challenges - Characterization of Uncertain Inputs

- Computational Model  $\mathcal{M}(u, \lambda) = 0$ 
  - Uncertain input parameter  $\lambda$
  - Experimental Measurement  $F(y, \lambda) = 0$
- Uncertain model inputs can be estimated from data on y
  - Regression
  - Bayesian inference
- Quite frequently, we have partial data/information
  - Partial missing data, e.g. failed measurements
  - Full data loss No data, but have summary information, e.g. moments and/or quantiles on
    - data processed data products
    - fitted parameters

#### **Dealing with Partial Data – Imputation**

Bayesian Multiple Imputation (Rubin, 1987)

- Use the posterior predictive conditioned on observed data to generate replicates of the missing data z<sup>t</sup><sub>mis</sub>, t = 1,...,m
- For each full data set, (*z*<sub>obs</sub>, *z*<sup>*t*</sup><sub>mis</sub>) apply Bayesian inference to get a posterior density on the model parameters
- Marginalize over the missing data to get the observed data posterior  $p(\beta|z_{\rm obs})$

$$p(eta|z_{
m obs}) = \int q(eta|z_{
m mis}, z_{
m obs}) f(z_{
m mis}|z_{
m obs}) dz_{
m mis}$$

#### Parameter Estimation in the Absence of Data

- Frequently:
  - we know summary statistics about data or parameters from previous work
  - the raw data used to arrive at these statistics is not available
- How can we construct a joint PDF on the parameters?
- In the absence of data, the structure of the fit model, combined with the summary statistics, implicitly inform the joint PDF on the parameters
- Goal: Make available information explicit in the joint PDF

#### Data Free Inference (DFI)

 Discover a consensus joint PDF on the parameters consistent with given information in the absence of data

Characterization hi-D Discont Osc

#### Generate ignition "data" using a detailed model+noise

- Ignition using a detailed chemical model for methane-air chemistry
- Ignition time versus Initial Temperature
- Multiplicative noise error model
- 11 data points:

$$\begin{array}{rcl} d_i & = & t_{\mathrm{ig},i}^{\mathsf{GRI}}(1+\sigma\epsilon_i) \\ \epsilon & \sim & N(0,1) \end{array}$$



#### Fitting with a simple chemical model

• Fit a global single-step irreversible chemical model

 $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ 

$$\mathfrak{R} = [CH_4][O_2]k_f$$
  
$$k_f = A \exp(-E/R^o T)$$

- Infer 3-D parameter vector  $(\ln A, \ln E, \ln \sigma)$
- Use an adaptive MCMC procedure
- Start at the maximum likelihood estimate

### **Bayesian Inference Posterior and Nominal Prediction**



#### DFI Challenge — Chemical Model Problem

Discarding initial data, reconstruct marginal  $(\ln A, \ln E)$  posterior using the following information

- Form of fit model
- Range of initial temperature
- Nominal fit parameter values of  $\ln A$  and  $\ln E$
- Marginal 5% and 95% quantiles on  $\ln A$  and  $\ln E$

Further, for now, presume

- Multiplicative Gaussian errors
- N = 8 data points

### **DFI** Algorithm Structure

Basic idea:

- Explore the space of hypothetical data sets
  - MCMC chain on the data
  - Each state defines a data set
- For each data set:
  - MCMC chain on the parameters
  - Evaluate statistics on resulting posterior
  - Accept data set if posterior is consistent with given information
- Evaluate pooled posterior from all acceptable posteriors Logarithmic pooling:

$$p(\lambda|y) = \left[\prod_{i=1}^{K} p(\lambda|y_i)\right]^{1/K}$$

#### 2D Marginal Pooled Posteriors vs. Reference Posterior



#### Empirical Convergence of 3D Pooled Posteriors

- Kullback-Leibler divergence between posteriors of successively increased data volumes
- Combinatorial choices of chains pooled at each stage
  - statistical scatter of KLdiv
- Overall convergence evident  $\propto 1/N$



### Challenges in PC UQ – High-Dimensionality

- Dimensionality *n* of the PC basis:  $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}$ 
  - number of degrees of freedom
  - P + 1 = (n + p)!/n!p! grows fast with n
- Impacts:
  - Size of intrusive system
  - # non-intrusive (sparse) quadrature samples
- Generally  $n \approx$  number of uncertain parameters
- Reduction of n:
  - Sensitivity analysis
  - Dependencies/correlations among parameters
  - Dominant eigenmodes of random fields
  - Manifold learning: Isomap, Diffusion maps
  - Sparsification: Compressed Sensing, LASSO

# PC Quadrature in hiD

Full quadrature:  $N = (N_{1D})^n$ 

#### Sparse Quadrature

- Wide range of methods
- Nested & hierarchical
- Clenshaw-Curtis:  $N = O(n^p)$
- Adaptive greedy algorithms

Number of points can still be excessive in hi-D

- Large no. of terms
- Reduction/sparsity



#### PC coefficients via sparse regression

PCE:

$$y = f(x) \simeq \sum_{k=0}^{K-1} c_k \Psi_k(x)$$

with  $x \in \mathbb{R}^n$ ,  $\Psi_k$  max order p, and K = (p + n)!/p!/n!

- *N* samples  $(x_1, y_1), ..., (x_N, y_N)$
- Estimate *K* terms  $c_0, \ldots, c_{K-1}$ , s.t.

$$\min ||\mathbf{y} - \mathbf{A}\mathbf{c}||_2^2$$

where  $y \in \mathbb{R}^N$ ,  $\boldsymbol{c} \in \mathbb{R}^K$ ,  $\boldsymbol{A}_{ik} = \Psi_k(x_i)$ ,  $\boldsymbol{A} \in \mathbb{R}^{N imes K}$ 

With  $N \ll K \Rightarrow$  under-determined

Need some form of regularization

## Regularization – Compressive Sensing (CS)

•  $\ell_2$ -norm — Tikhonov regularization; Ridge regression:

$$\min \{ \| \mathbf{y} - \mathbf{A}\mathbf{c} \|_2^2 + \| \mathbf{c} \|_2^2 \}$$

•  $\ell_1$ -norm — Compressive Sensing; LASSO; basis pursuit

$$\min \{ \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{c} \|_{2}^{2} + \| \boldsymbol{c} \|_{1} \}$$

$$\min \{ \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{c} \|_{2}^{2} \} \quad \text{subject to } \| \boldsymbol{c} \|_{1} \le \epsilon$$

$$\min \{ \| \boldsymbol{c} \|_{1} \} \quad \text{subject to } \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{c} \|_{2}^{2} \le \epsilon$$

 $\Rightarrow$  discovery of sparse signals



### **Bayesian Regression**

Bayes formula

$$p(\boldsymbol{c}|\boldsymbol{D}) \propto p(\boldsymbol{D}|\boldsymbol{c})\pi(\boldsymbol{c})$$

- Bayesian regression: prior as a regularizer, e.g.
  - Log Likelihood  $\Leftrightarrow \|y Ac\|_2^2$
  - Log Prior  $\Leftrightarrow \|\boldsymbol{c}\|_p^p$
- Laplace sparsity priors  $\pi(c_k|\alpha) = \frac{1}{2\alpha}e^{-|c_k|/\alpha}$
- LASSO (Tibshirani 1996) ... formally:

$$\min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_1 \right\}$$

Solution  $\sim$  the posterior mode of c in the Bayesian model

$$y \sim \mathcal{N}(oldsymbol{Ac}, I_N), \qquad c_k \sim rac{1}{2lpha} e^{-|c_k|/lpha}$$

Bayesian LASSO (Park & Casella 2008)

#### Bayesian Compressive Sensing (BCS)

- BCS (Ji 2008; Babacan 2010)— hierarchical priors:
  - Gaussian priors  $\mathcal{N}(0, \sigma_k^2)$  on the  $c_k$
  - Gamma priors on the  $\sigma_k^2$
  - $\Rightarrow$  Laplace sparsity priors on the  $c_k$
- Evidence maximization establishes ML estimates of the  $\sigma_k$ 
  - many of which are found  $\approx 0 \Rightarrow c_k \approx 0$
  - iteratively include terms that lead to the largest increase in the evidence
- iterative BCS (iBCS) (Sargsyan 2012):
  - adaptive iterative order growth
  - BCS on order-p Legendre-Uniform PC
  - repeat with order-*p* + 1 terms added to surviving *p*-th order terms

### CS and BCS

#### Oscillatory Genz function

• 
$$f(x) = \cos(2\pi r + \sum_{i=1}^{n} a_i x_i); \quad a_i \propto 1/i^2; \quad r = 0$$

• Legendre-Uniform PC, 10<sup>th</sup>-order in 5d; (5,6)<sup>th</sup>-order in 10d



#### Oscillatory function – BCS number of terms



#### Challenges in PC UQ – Non-Linearity

- Bifurcative response at critical parameter values
  - Rayleigh-Bénard convection
  - Transition to turbulence
  - Chemical ignition
- Discontinuous  $u(\lambda(\boldsymbol{\xi}))$ 
  - Failure of global PCEs in terms of smooth  $\Psi_k()$
  - ⇔ failure of Fourier series in representing a step function
- Local PC methods
  - Subdivide support of  $\lambda(\boldsymbol{\xi})$  into regions of smooth  $u \circ \lambda(\boldsymbol{\xi})$
  - Employ PC with compact support basis on each region
  - A spectral-element vs. spectral construction
  - Domain mapping

#### Multi-Block Multiwavelet PC UQ in Ignition



- H<sub>2</sub>-O<sub>2</sub> supercritical water oxidation model
- Empirically-based uncertainty in all 7 reactions
- Adaptive refinement of MW block decomposition

(Le Maître, 2004, 2007)

Challenges in hi-dimensional contexts

#### Uncertainty in Discontinuous Climate Response



- Atlantic meridional ocean circulation (AMOC)
- Predicted response to increasing CO<sub>2</sub> (Webster, 2007)
- Circulation ON/OFF response over parameter space
  - Rate of CO<sub>2</sub> increase
  - Climate sensitivity

#### Domain Mapping for Discontinuous Response



- Initial set of computational samples
- Discover uncertain discontinuity with Bayesian inference
- Map sub-domains to unit hypercubes; Rosenblatt transform
- PC quadrature in mapped domains; map back
- Marginalize over uncertain curve (Sargsyan, 2012)

#### Challenges in PC UQ – Time Dynamics

- Systems with limit-cycle or chaotic dynamics
- Large amplification of phase errors over long time horizon
- PC order needs to be increased in time to retain accuracy
- Time shifting/scaling remedies
- Futile to attempt representation of detailed turbulent velocity field ν(x, t; λ(ξ)) as a PCE
  - Fast loss of correlation due to energy cascade
  - Problem studied in 60's and 70's
- Focus on flow statistics, e.g. Mean/RMS quantities
  - Well behaved
  - Argues for non-intrusive methods with DNS/LES of turbulent flow

#### Closure

- Probabilistic UQ framework
- Forward UQ
  - Polynomial Chaos representation of random variables
  - Intrusive and non-intrusive forward PC UQ methods
- Inverse UQ
  - Bayesian methods
- Highlighted UQ Challenges
  - Missing data Imputation / DFI
  - High dimensionality
  - Non-linearity
  - Long term oscillatory dynamics