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Uncertainty Quantification in Computational Models

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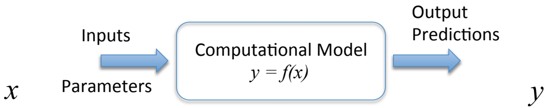
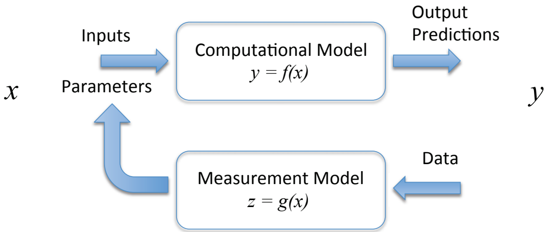
Uncertainty Quantification and Computational Science



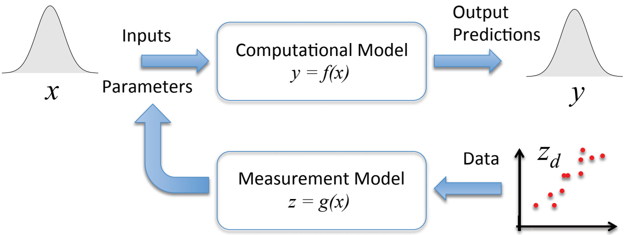
Forward problem

Uncertainty Quantification and Computational Science



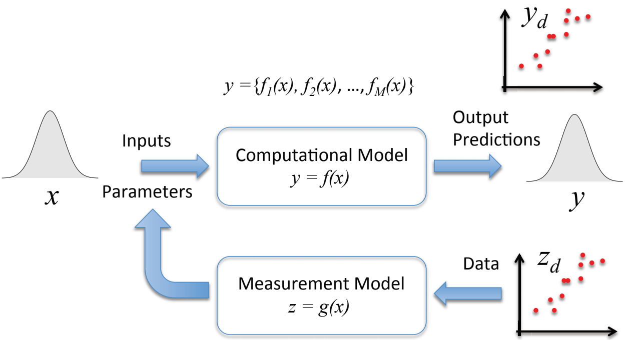
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

Outline

Forward propagation of parametric uncertainty

Forward model: $y = f(x)$

- Local sensitivity analysis (SA) and error propagation

$$\Delta y = \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} \Delta x$$

  This is ok for:

  - small uncertainty
  - low degree of non-linearity in $f(x)$

- Non-probabilistic methods
  - Fuzzy logic
  - Evidence theory – Dempster-Shafer theory
  - Interval math

- Probabilistic methods – this is our focus

Probabilistic Forward UQ – $y = f(x)$

Represent uncertain quantities using probability theory

- Random sampling, MC, QMC
  - Generate random samples $\{x^i\}_{i=1}^N$ from the PDF of x, $p(x)$
  - Bin the corresponding $\{y^i\}$ to construct $p(y)$
  - Not feasible for computationally expensive $f(x)$
    - slow convergence of MC/QMC methods
      $\Rightarrow$ very large N required for reliable estimates
- Build a cheap surrogate for $f(x)$, then use MC
  - Collocation – interpolants
  - Regression – fitting
- Galerkin methods
  - Polynomial Chaos (PC)
  - Intrusive and non-intrusive PC methods

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
  - as a function on a probability space

- Constraining the analysis to RVs with finite variance
  - $\Rightarrow$ Represent RV as a spectral expansion in terms of orthogonal functions of standard RVs
    - Polynomial Chaos Expansion

- Enables the use of available functional analysis methods for forward UQ

Polynomial Chaos Expansion (PCE)

- Model uncertain quantities as random variables (RVs)
- Given a *germ* $\boldsymbol{\xi}(\omega) = \{\xi_1, \cdots, \xi_n\}$ – a set of *i.i.d.* RVs
  - where $p(\boldsymbol{\xi})$ is uniquely determined by its moments

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

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

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

With dimension n and total order p: $$P + 1 = \frac{(n+p)!}{n!p!}$$

Orthogonality and Projection

By construction, the $\Psi_k()$ are orthogonal w.r.t. the density of ξ

$$\langle f(\boldsymbol{\xi})\rangle \equiv \int_{\Xi} f(\boldsymbol{\xi}) p(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \qquad \langle \Psi_i \Psi_j \rangle = \delta_{ij} \langle \Psi_i^2 \rangle$$

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

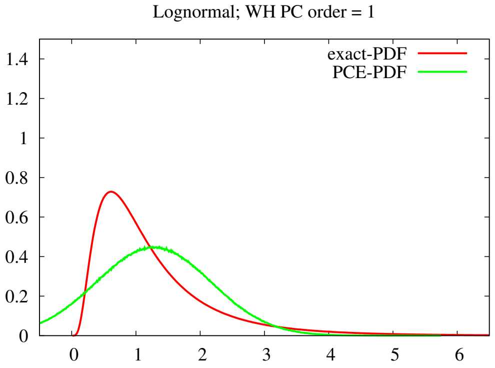
Examples:

- Hermite polynomials with Gaussian basis
- Legendre polynomials with Uniform basis, ...
- Global versus Local PC methods
    - Adaptive domain decomposition of the support of ξ

PC Illustration: WH PCE for a Lognormal RV

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

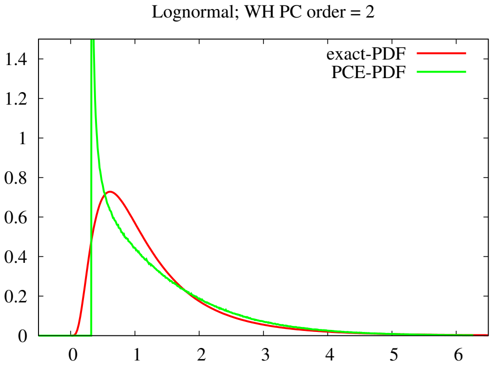
$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi) = u_0 + u_1 \xi$$



PC Illustration: WH PCE for a Lognormal RV

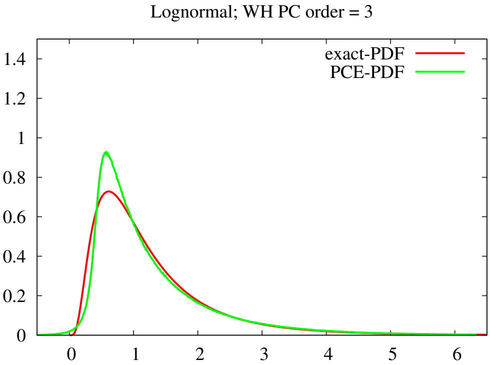
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 2

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



PC Illustration: WH PCE for a Lognormal RV

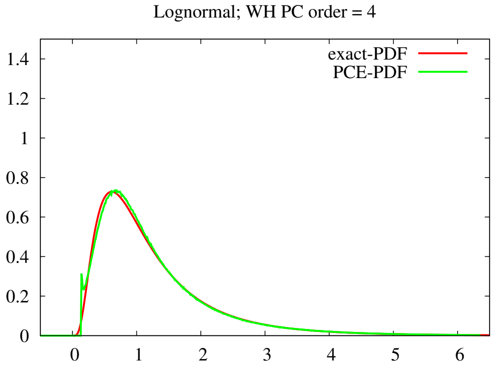
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 3



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV

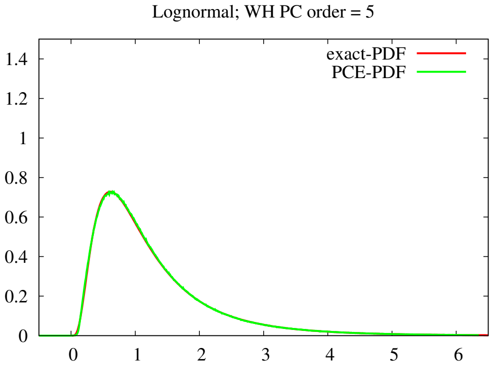
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4



$$\begin{aligned} u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\ &= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3) \end{aligned}$$

PC Illustration: WH PCE for a Lognormal RV

- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 5



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3) \\
&\quad + u_5(\xi^5 - 10\xi^3 + 15\xi)
\end{aligned}
$$

Random Fields (RFs)

- A random field $Z(x,\omega)$ is a function on a product space $D \times \Omega$
  - a RV at any $x \in D$
  - an infinite dimensional object
- In many physical systems, uncertain field quantities, described by RFs, have an underlying *smoothness* due to correlations
  - Can be represented with a small no. of stochastic degrees of freedom
- ℓ_2-Optimal representation – second-order statistics
  - Karhunen-Loève expansion (KLE)

Random Fields Representation – KLE

- KLE for a RF with a continuous covariance function

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

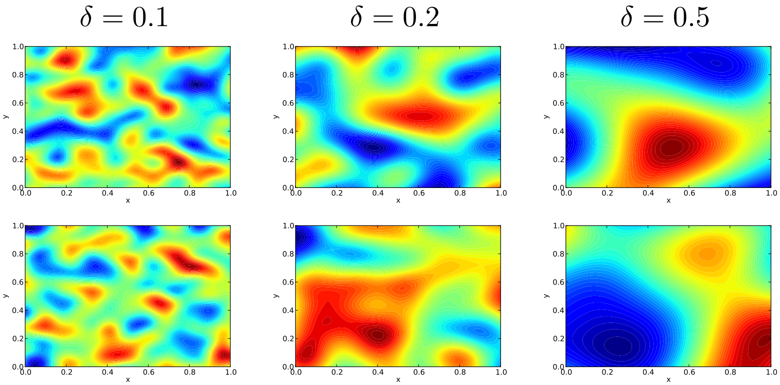
- $\mu(x)$ is the mean of $Z(x,\omega)$ at x
- λ_i and $\phi_i(x)$ are the eigenvalues and eigenfunctions of the covariance

$$C(x_1,x_2) = \langle [Z(x_1,\omega) - \mu(x_1)][Z(x_2,\omega) - \mu(x_2)] \rangle$$

- The ζ_i are uncorrelated zero-mean unit-variance RVs

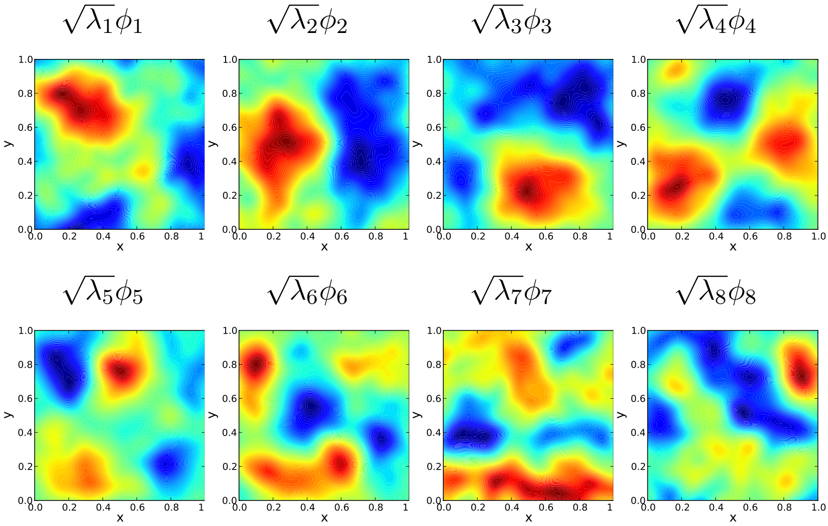
$$\zeta_i(\omega) = \frac{1}{\sqrt{\lambda_i}} \int_D Z(x,\omega)\phi_i(x)\mathrm{d}x$$

RF – 2D Gaussian Process

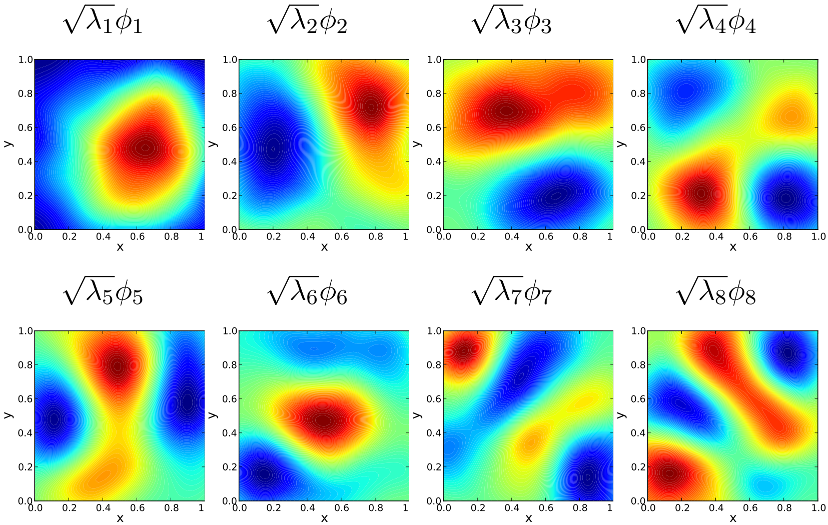


- 2D Gaussian Process with covariance:
  $Cov(x_1, x_2) = exp(-||x_1 - x_2||^2/\delta^2)$
- Realizations smoother as covariance length δ increases

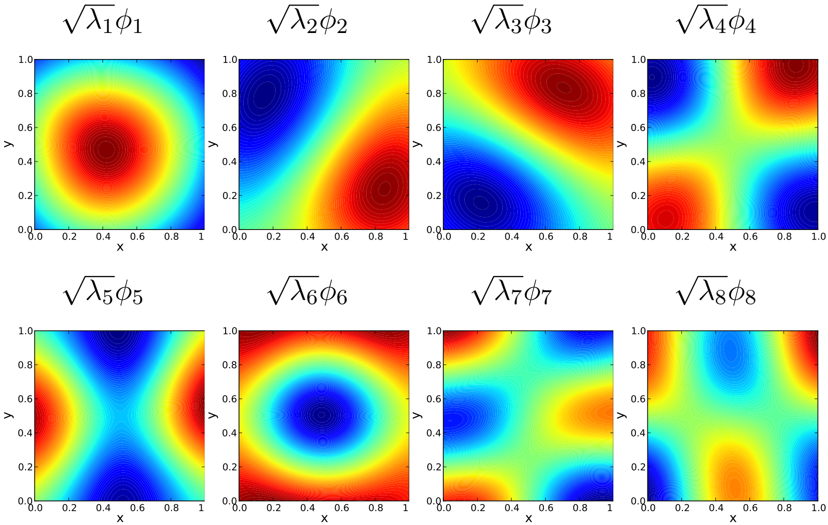
RF Illustration: 2D KL - Modes for $\delta = 0.1$



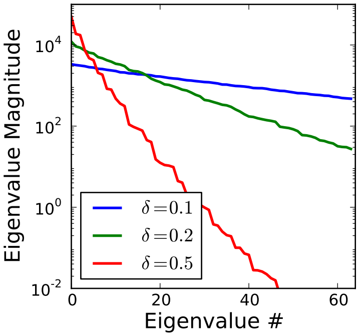
RF Illustration: 2D KL - Modes for $\delta = 0.2$



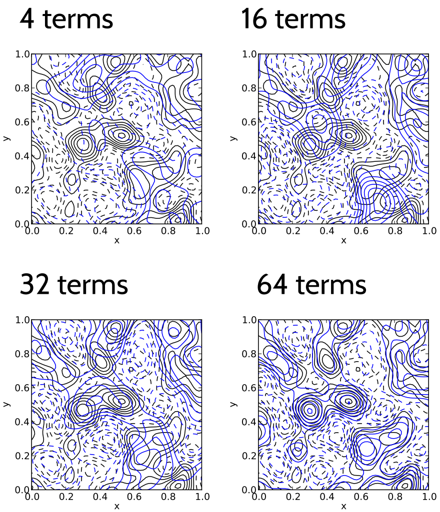
RF Illustration: 2D KL - Modes for $\delta = 0.5$



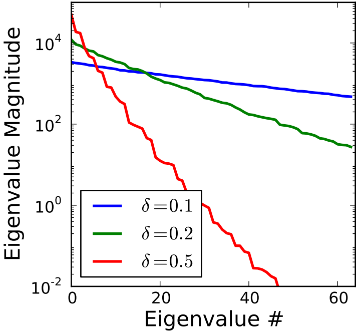
RF Illustration: 2D KL - eigenvalue spectrum

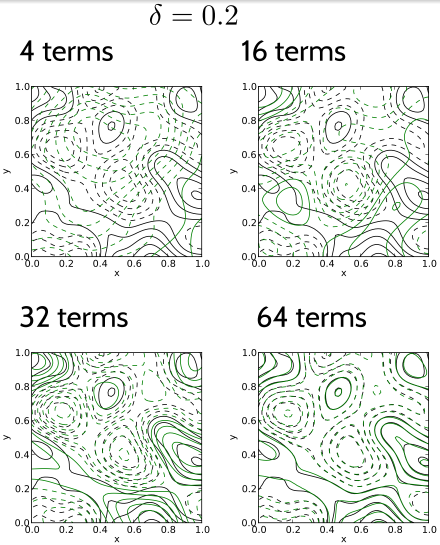


$\delta = 0.1$

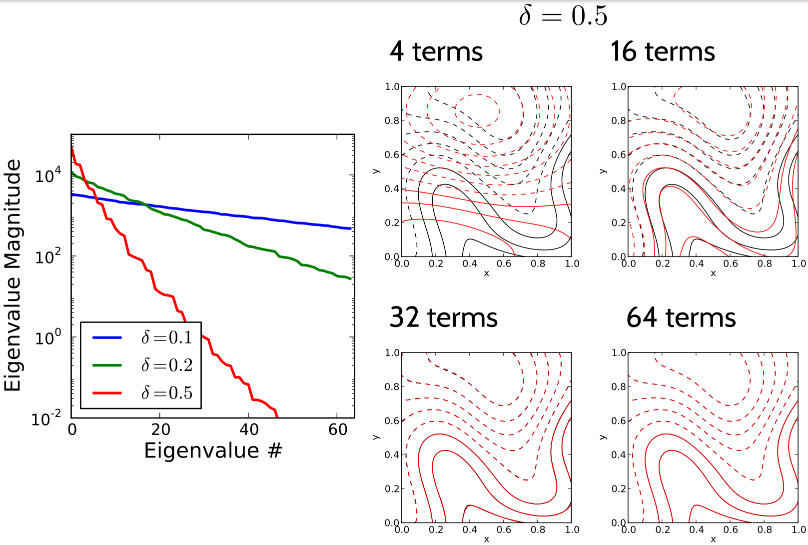


RF Illustration: 2D KL - eigenvalue spectrum

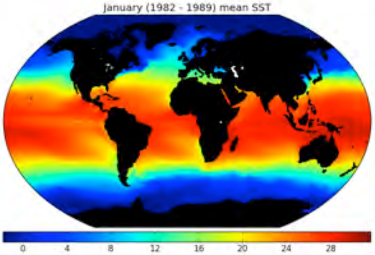




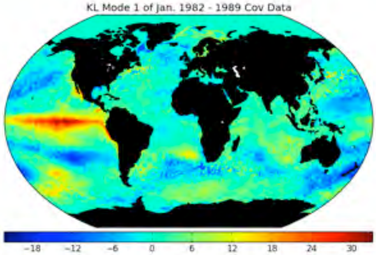
RF Illustration: 2D KL - eigenvalue spectrum



Random Field – SST Variability – work with NOAA



Mean SST



1^{st} KL mode

- Sea Surface Temperature (SST) variability – satellite data
- Large-scale RF KLE for global SST variability
  - 1/4-degree spatial resolution
  - Trilinos / parallelized block Krylov Schur solver – NERSC
  - 25 modes sufficient to capture most of the energy in the signal

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
- Utility
    - Moments: $\mathsf{E}(u) = u_0$, $\mathsf{var}(u) = \sum_{k=1}^{P} u_k^2 \langle \Psi_k^2 \rangle$, ...
    - Global Sensitivities – fractional variances, Sobol' indices
    - Surrogate for forward model

Requirement:

- RVs in L^2, *i.e.* with finite variance, on $(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$

Intrusive PC UQ – Stochastic Galerkin – *no sampling*

- Given model equations: $\mathcal{M}(u(\boldsymbol{x},t);\lambda) = 0$
- 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
- New set of equations: $\mathcal{G}(U(\boldsymbol{x},t),\Lambda) = 0$
  - with $U = [u_0, \ldots, u_P]^T$, $\Lambda = [\lambda_0, \ldots, \lambda_P]^T$
- Solving this deterministic system once provides the full specification of uncertain model ouputs

Example – *Intrusive* Galerkin PC ODE System

$$\frac{du}{dt} = f(u;\lambda)$$

$$\lambda = \sum_{i=0}^{P} \lambda_i \Psi_i \qquad u(t) = \sum_{i=0}^{P} u_i(t)\Psi_i$$

$$\frac{du_i}{dt} = \frac{\langle f(u;\lambda)\Psi_i\rangle}{\langle \Psi_i^2\rangle} \qquad i = 0,\ldots,P$$

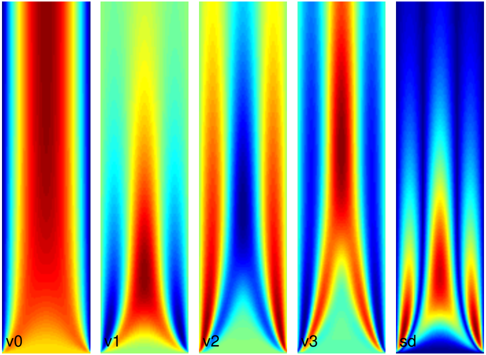
Say $f(u;\lambda) = \lambda u$, then

$$\frac{du_i}{dt} = \sum_{p=0}^{P}\sum_{q=0}^{P} \lambda_p u_q C_{pqi}, \quad i = 0,\cdots,P$$

where the tensor $C_{pqi} = \langle \Psi_p \Psi_q \Psi_i\rangle / \langle \Psi_i^2 \rangle$ is readily evaluated

Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Viscosity PCE
  - $\nu = \nu_0 + \nu_1 \xi$
- Streamwise velocity
  - $\mathrm{v} = \sum_{i=0}^{P} \mathrm{v}_i \Psi_i$
  - v_0: mean
  - v_i: i-th order mode
  - $\sigma^2 = \sum_{i=1}^{P} \mathrm{v}_i^2 \langle \Psi_i^2 \rangle$



v_0 v_1 v_2 v_3 σ

(Le Maître *et al.*, J. Comput. Phys., 2001)

Intrusive PC – UQ Pros/Cons

Pros:

- Tailored solvers can deliver superior performance

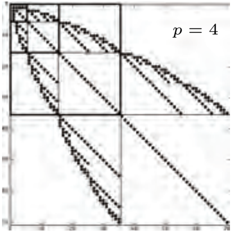
Cons:

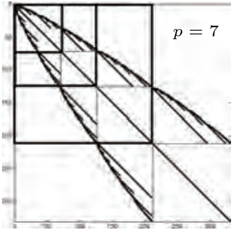
- Reformulation of governing equations
- New discretizations
- New numerical solution method
  - Consistency, Convergence, Stability
  - Global vs. multi-element local PC constructions
- New solvers and model codes
  - Opportunities for automated code transformation
  - New preconditioners

Intrusive PC UQ – Boundary Value Problem

B. Sousedík, R. Ghanem, USC; E. Phipps, SNL

- 2D linear elliptic BVP, N d.o.f.
- Uncertain diffusivity – random field
- FEM spatial discretization
- PCE stochastic representation
  - dim: $n = 4$, ord: $p = 4, 7$
    $Q = (n + p)!/n!p! = 70, 330$
- Stochastic Galerkin Matrix $QN \times QN$
  - $Q \times Q$ blocks, each of size $N \times N$
  - Each block has the sparsity structure of the deterministic FEM problem matrix
- With smart preconditioners ++ :
  - UQ prob. Cost $\sim \mathcal{O}(\text{det. prob.})$





(Sousedík, Ghanem, and Phipps, *Numer. Linear Algebra Appl.* 2010; *IJUQ*)

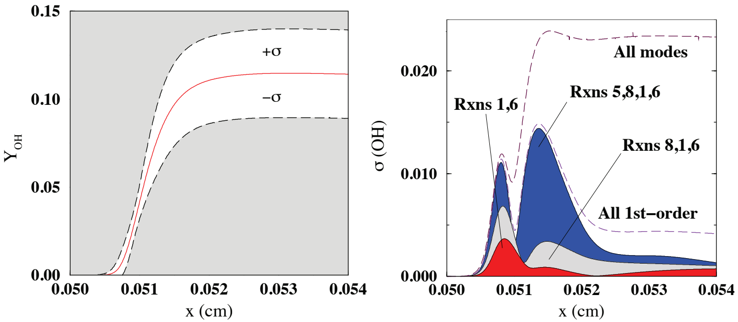
Non-intrusive PC UQ

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

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

- 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

Non-intrusive PC UQ – 1D H_2-O_2 SCWO Flame



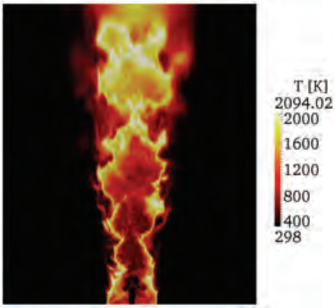
- Fast growth in OH uncertainty in the primary reaction zone
- Constant uncertainty and mean of OH in post-flame region
- Uncertainty in pre-exponential of Rxn.5 (H_2O_2+OH=H_2O+HO_2) has largest contribution to uncertainty in predicted OH

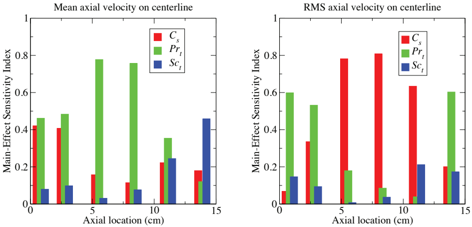
(Reagan *et al.* Comb. Flame, 2003)

UQ in LES computations: turbulent bluff-body flame

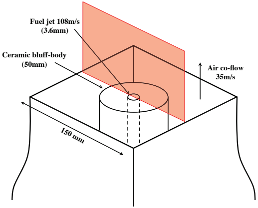
with M. Khalil, G. Lacaze, & J. Oefelein, Sandia Nat. Labs

- CH_4-H_2 jet, air coflow, 3D flow
- Re=9500, LES subgrid modeling
- 12×10^6 mesh cells, 1024 cores
- 3 days run time, 2×10^5 time steps
- 3 uncertain parameters (C_s, Pr_t, Sc_t)
- 2^{nd}-order PC, 25 sparse-quad. pts





Main-Effect Sensitivity Indices



J. Oefelein & G. Lacaze, SNL

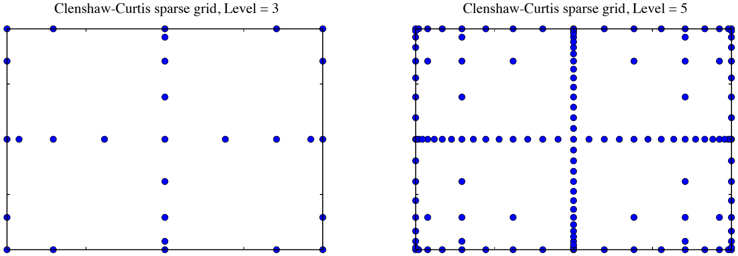
PC and High-Dimensionality

Dimensionality n of the PC basis: $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_n\}$

- $n \approx$ number of uncertain parameters
- $P + 1 = (n+p)!/n!p!$ grows fast with n

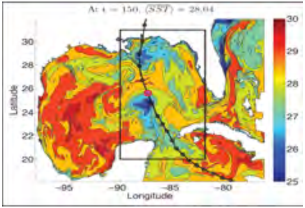
Impacts:

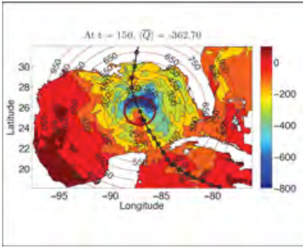
- Size of intrusive PC system
- Hi-D projection integrals $\Rightarrow$ large # non-intrusive samples
  - Sparse quadrature methods



UQ in Ocean Modeling – Gulf of Mexico

A. Alexanderian, J. Winokur, I. Sraj, O.M. Knio, Duke Univ.; A. Srinivasan, M. Iskandarani, Univ. Miami; W.C. Thacker, NOAA





- Hurricane Ivan, Sep. 2004
- HYCOM ocean model (hycom.org)
- 4 uncertain parameters, *i.i.d.* U
  - subgrid mixing & wind drag params
- 385 sparse quadrature samples

(Alexanderian *et al.*, Winokur *et. al.*, *Comput. Geosci.*, 2012, 2013)

PC Sparse Quadrature in hiD – Climate land model

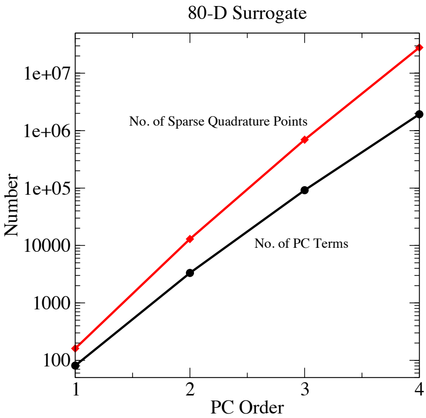
Full quadrature: $N = (N_{\text{1D}})^n$

Sparse Quadrature

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

Number of points can still be excessive in hi-D

- Large no. of terms
- Reduction/sparsity



Other non-intrusive methods

- Response surface employing PC or other functional basis
- Collocation: Fit interpolant to samples
  - Oscillation concern in multi-D
- Regression: Estimate best-fit response surface
  - Least-squares
    - Sparsity via ℓ_1 constraints; compressive sensing
  - Bayesian inference
    - Sparsity via Laplace priors; Bayesian compressive sensing
  - Useful when quadrature methods are infeasible, e.g.:
    - Samples given *a priori*
    - Can't choose sample locations
    - Can't take enough samples
    - Forward model is noisy

Inverse UQ – Estimation of Uncertain Parameters

Forward UQ requires specification of uncertain inputs

Probabilistic setting

- Require joint PDF on input space
- Statistical inference – an inverse problem

Bayesian setting

- Given Data: PDF on uncertain inputs can be estimated using Bayes formula
  - Bayesian Inference
- Given Constraints: PDF on uncertain inputs can be estimated using the Maximum Entropy principle
  - MaxEnt Methods

Bayes formula for Parameter Inference

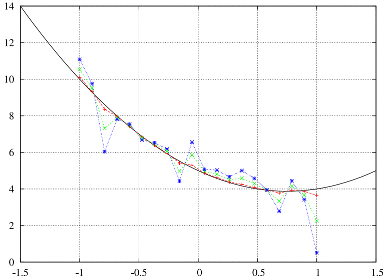
- Data Model (fit model + noise model): $y = f(\lambda) * g(\epsilon)$
- Bayes Formula:

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

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}}\;\overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

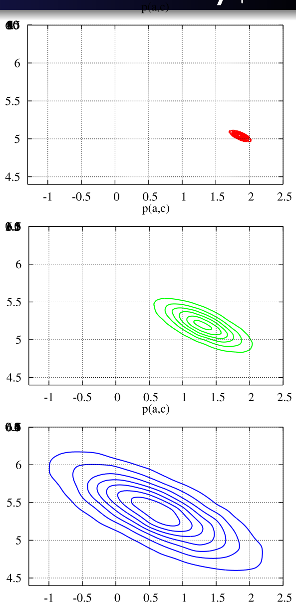
- Prior: knowledge of λ prior to data
- Likelihood: forward model and measurement noise
- Posterior: combines information from prior and data
- Evidence: normalizing constant for present context

Bayesian inference illustration: noise↑ ⇒ uncertainty↑



- data: $y = 2x^2 - 3x + 5 + \epsilon$
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$, $\sigma = \{0.1, 0.5, 1.0\}$
- Fit model $y = ax^2 + bx + c$

Marginal posterior density $p(a, c)$:



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

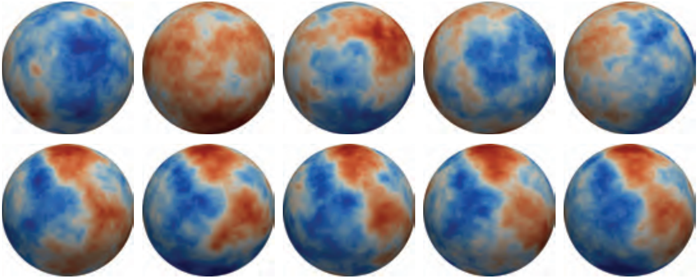
Surrogate Models for Bayesian Inference

- Need an inexpensive response surface for
  - Observables of interest y
  - as functions of parameters of interest x
- Gaussian Process (GP) surrogate
  - GP goes through all data points with probability 1.0
  - Uncertainty between the points
- Fit a convenient polynomial to $y = f(x)$
  - over the range of uncertainty in x
  - Employ a number of samples (x_i, y_i)
  - Fit with interpolants, regression, ... global/local
  - With uncertain x :
    - Construct Polynomial Chaos response surface

(Marzouk *et al.* JCP 2007; Marzouk & Najm JCP 2009)

Extreme-scale Seismic Inversion

T. Bui-Thanh, O. Ghattas, J. Martin, & G. Stadler, UT Austin



- linearized 3D global seismic inversion
- 1.07M earth model parameters
- 630M wave propagation unknowns
- 100K cores on Jaguar (ORNL)
- 2000× reduction in effective problem dimension due to low rank approx

- *Top row:* Prior samples
- *Bottom row:* Posterior samples
- Difference between rows indicates information gained from (and uncertainty reduced due to) data
- Gordon Bell Prize finalist, SC12

(Bui-Thanh *et al.* Proc. IEEE/ACM SC12; SISC 2013)

UQ from a Computational Perspective

- UQ involves significant computational cost
  - Generally (many times)$\times$ the deterministic code
  - Run case cannot be the single largest capability problem
- UQ enables extraction of additional information on the physical system at hand
  - Effectively a parametric study over uncertain model inputs
  - Enhances scientific discovery from computations
- Computational elements of interest
  - Scalability and Performance
  - Fault tolerance
  - Code failures

Computational Character of UQ Codes

- Bayesian inference
  - MCMC algorithms, serial, parallelism
  - many model samples
  - high dimensional parameter space
- Intrusive UQ methods
  - new math, algorithms, solvers, code
  - compiler relevance: automatic source code transformation
- non-intrusive UQ methods
  - deterministic sampling
  - high-dimensional integrals
  - embarrassingly parallel

High dimensionality challenge – Forward UQ

Consider a forward model

$$y = f(x)$$

Let $x \in \mathbb{R}^n$ be uncertain, represented as a random vector,

$$x \sim p(x)$$

Estimate moments of y

$$\mathcal{M}^q = \int [f(x)]^q p(x) \mathrm{d}x$$

Forward UQ is an integration problem.

Integration in High Dimensions

- Monte Carlo (MC) methods
  - well suited for high-D integrals – convergence rate independent of dimensionality
  - nonetheless they require large numbers of samples for good accuracy
- Quadrature
  - Tensor product quadrature is useless in hi-D
    - Say m points in each of n dimensions: m^n points
  - Adaptive sparse quadrature
    - Much more feasible
    - Can beat MC – dep. on smoothness of integrand
  - Greedy algorithms
- Dimensionality reduction
  - Low rank and sparse representations
  - Global sensitivity analysis

Model Complexity challenge

- If a single model run is a challenge then UQ is infeasible
- Most physical model output quantities of interest depend on only a "small" number of parameters, however:
  - Global sensitivity analysis itself requires many samples
  - Even after reduction of dimensionality to, say, 5 parameters, O(100) samples may be necessary
- Large number of independent samples
  - ideally suited for HPC
- Multifidelity UQ methods are useful – forward UQ
  - Use combinations of many low-resolution/low-fidelity runs with a few high-resolution/high-fidelity runs
- Parallel MCMC methods – inverse UQ

Data Scarcity Challenge

- Even in a “big-Data” context, it’s common to find no information in the data on many *big-model* parameters
  - Situation is typical in statistical inversion for field quantities
  - Bayesian inference of optimal random field constructions
  - Use adaptive MCMC methods that focus on data-informed parameters
- Usually, raw data is not published
  - Published “data” is essentially processed data products, being statistics on
    - the data, or functions of fitted model parameters
  - Use Maximum-Entropy and Approximate Bayesian Computation (ABC) methods – DFI
    - Discover posterior density on model parameters consistent with published statistics

Bayesian inference – High Dimensionality Challenge

- Judgement on local/global posterior peaks is difficult
    - Multiple chains
    - Tempering
- Choosing a good starting point is very important
    - An initial optimization strategy is useful, albeit not trivial
- Choosing good MCMC proposals, and attaining good mixing, is a signficant challenge
    - Likelihood-informed proposals
    - Dimention adaptive
    - Adaptive proposal learning from MCMC samples
    - Hessian informs best local multivariate normal approximation of posterior
    - Adaptive, Geometric, Langevin MCMC . . .

Bayesian inference – Model Error Challenge

- Quantifying model error, as distinct from data noise, is important for assessing confidence in model validity
- Available statistical methods for accounting for model error have shortcomings when applied to physical models
- New methods are needed/under-development for assessing how best to model model error such that
  - physical constraints are satisfied
  - feasible disambiguation of model-error/data-noise
  - calibrated model error terms adequately impact all model outputs of interest
  - uncertainties in predictions from calibrated model reflect the range of discrepancy from the truth

Model Evidence and Complexity

Let $\mathcal{M} = \{M_1, M_2, \ldots\}$ be a set of models of interest

- Parameter estimation from data is conditioned on the model

$$p(\theta|D, M_k) = \frac{p(D|\theta, M_k)\pi(\theta|M_k)}{p(D|M_k)}$$

Evidence (marginal likelihood) for M_k:

$$p(D|M_k) = \int p(D|\theta, M_k)\pi(\theta|M_k)\mathrm{d}\theta$$

Model evidence is useful for model selection

- Optimal complexity – Occam's razor principle
- Compromise between fitting data and model complexity
- Avoid overfitting

Closure

- Probabilistic UQ framework – PC & KLE
- Forward UQ
  - Polynomial Chaos representation of random variables
  - Intrusive and non-intrusive forward PC UQ methods
- Inverse UQ
  - Parameter estimation via Bayesian inference
- UQ and HPC
  - Scalability, Performance, Fault tolerance, Code failures
- UQ Challenges
  - High dimensionality
  - Model complexity
  - Data scarcity
  - Model error