Polynomial Chaos Based Uncertainty Propagation

Lecture 2: Forward Propagation and Inverse Problems

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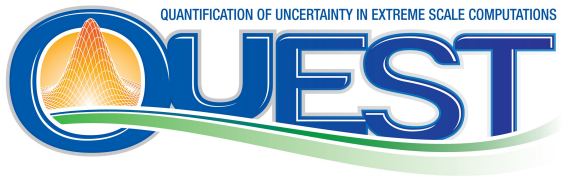

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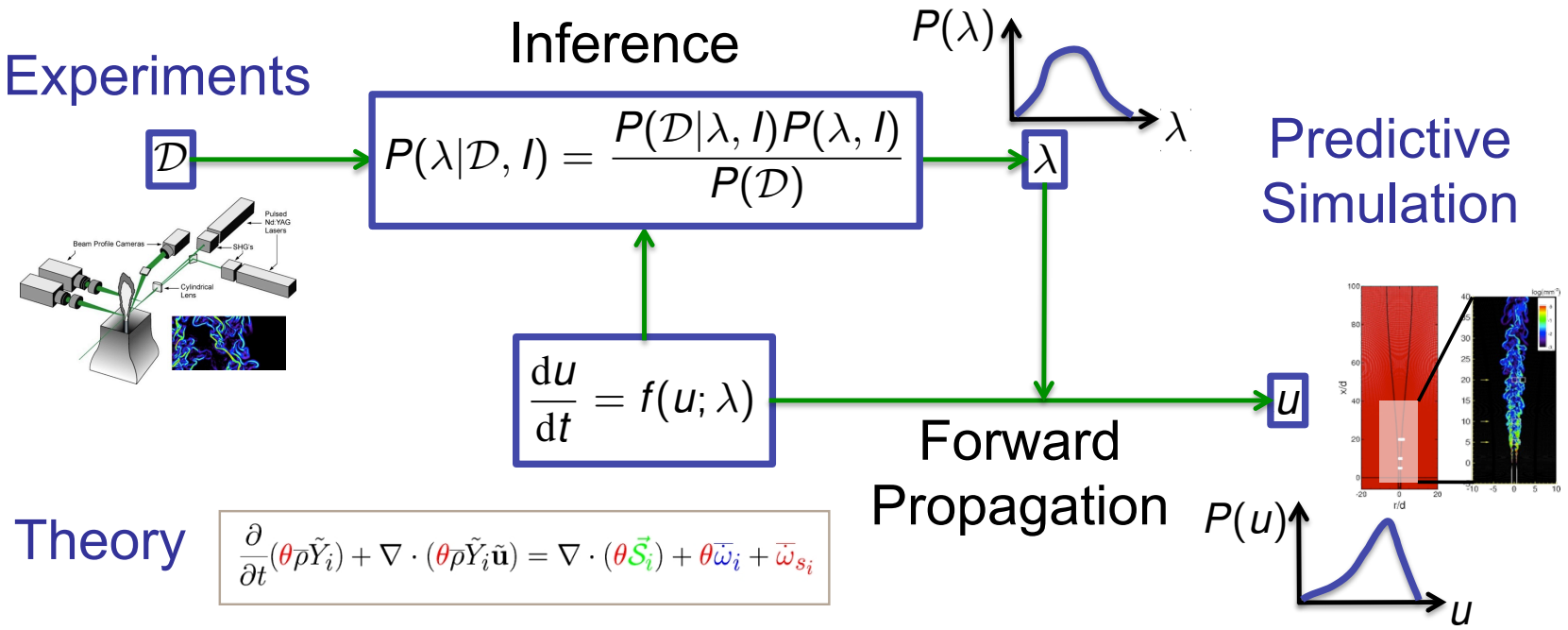
Goals of this tutorial

- 2 Lectures
  - Lecture 1: Context and Fundamentals
  - Lecture 2: Forward Propagation and Inverse Problems
    - Intrusive Approaches
    - Non-Intrusive Approaches
    - High-dimensional Systems
    - Sensitivity Analysis
    - Inverse Problems

Outline

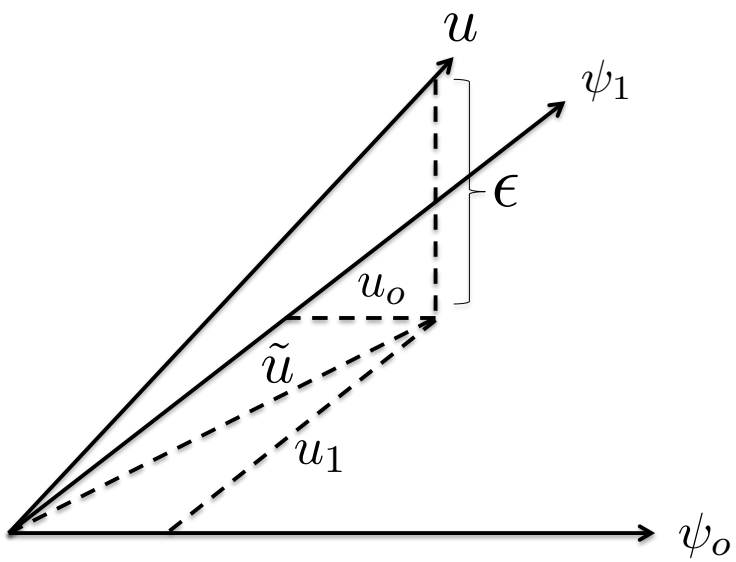
This section focuses on propagating uncertainty through computational models.



- Assume uncertain parameters λ have been characterized with PCEs
- The goal is to obtain PCEs for output quantities u

Propagation of Uncertain Inputs Represented with PCEs

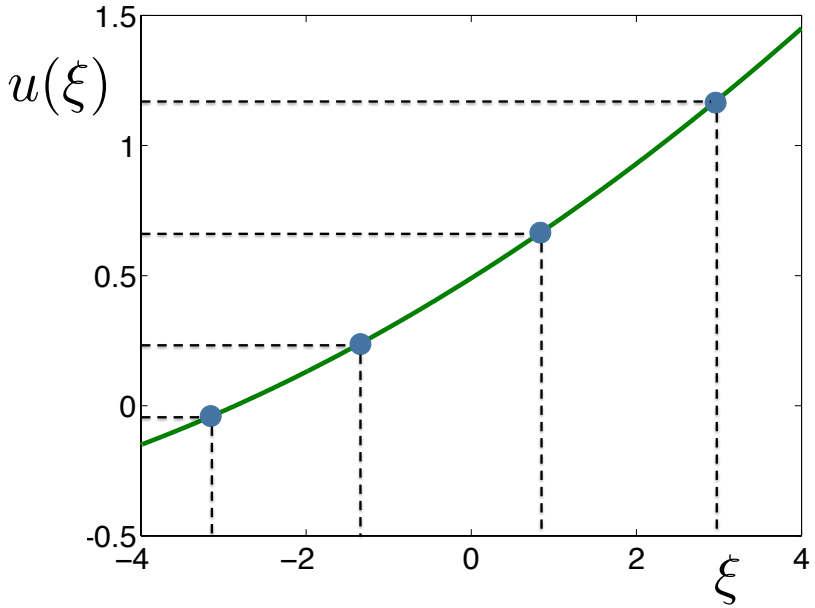
Galerkin Projection



$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

Residual orthogonal to space covered by basis functions

Collocation



Match PCE to random variable at chosen sample points: interpolation or regression

Galerkin projection methods are either intrusive or non-intrusive

- Use same projection but in different ways

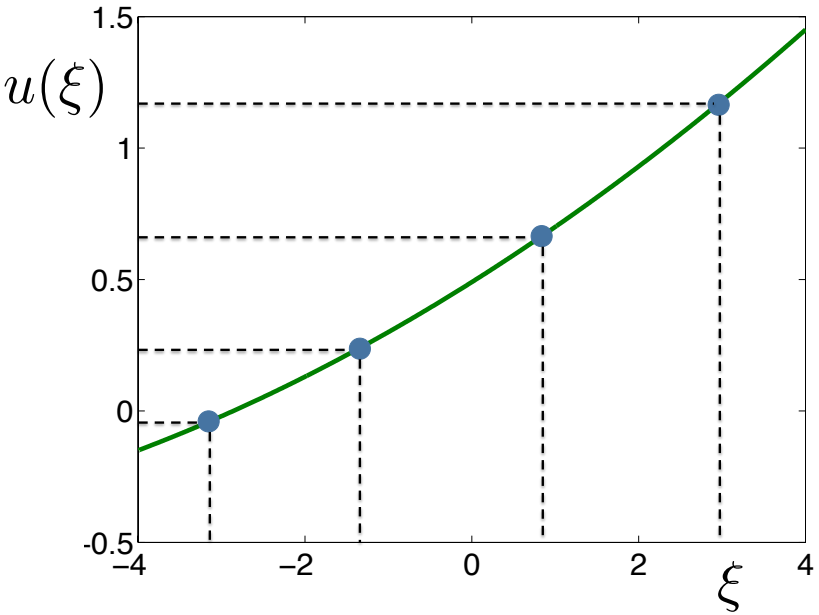
$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

- Intrusive methods apply Galerkin projection to governing equations
  - Results in set of equations for the PC coefficients
  - Requires redesign of computer code
  - PCEs for all uncertain variables in system
- Non-intrusive approaches apply Galerkin projection to outputs of interest
  - Sampling to evaluate projection operator
  - Can use existing code as black box
  - Only computes PCEs for quantities of interest

Collocation approaches are non-intrusive and minimize errors at sample points

$$\sum_{k=0}^{P} u_k \Psi_k(\xi_i) = u(\xi_i)$$

$$i = 1, \ldots, N_c$$



- Use functional representation point of view
- Can use interpolation, e.g. Lagrange interpolants
- Or use regression approaches: $P + 1$ degrees of freedom to fit N_c points
- Can position points where most accuracy desired

Remainder of this section focuses on Galerkin projection methods

- Intrusive Galerkin projection
- Non-intrusive Galerkin projection

Intrusive Galerkin projection reformulates original equations

- Assume $v = f(u; a, \lambda)$, with
  - a deterministic parameter(s)
  - λ uncertain parameter(s)
  - u, v variables of interest (deterministic or uncertain)
- Represent uncertain variables with PCEs

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \qquad v = \sum_{k=0}^{P} v_k \Psi_k(\xi)$$

- Apply Galerkin projection to get PC coefficients of v

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle f(u; a, \lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

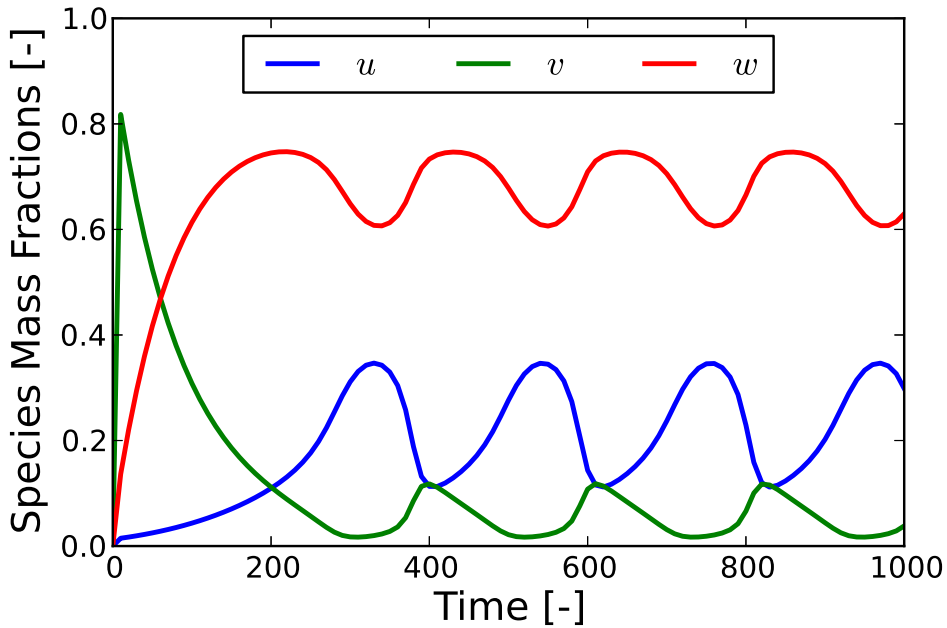
- Results in larger, but deterministic set of equations

Surface Reaction Model

3 ODEs for a monomer (u), dimer (v), and inert species (w) adsorbing onto a surface out of gas phase.

$$\begin{aligned}
\frac{\mathrm{d}u}{\mathrm{d}t} &= az - cu - 4duv \\
\frac{\mathrm{d}v}{\mathrm{d}t} &= 2bz^2 - 4duv \\
\frac{\mathrm{d}w}{\mathrm{d}t} &= ez - fw \\
z &= 1 - u - v - w
\end{aligned}$$

$$u(0) = v(0) = w(0) = 0.0$$

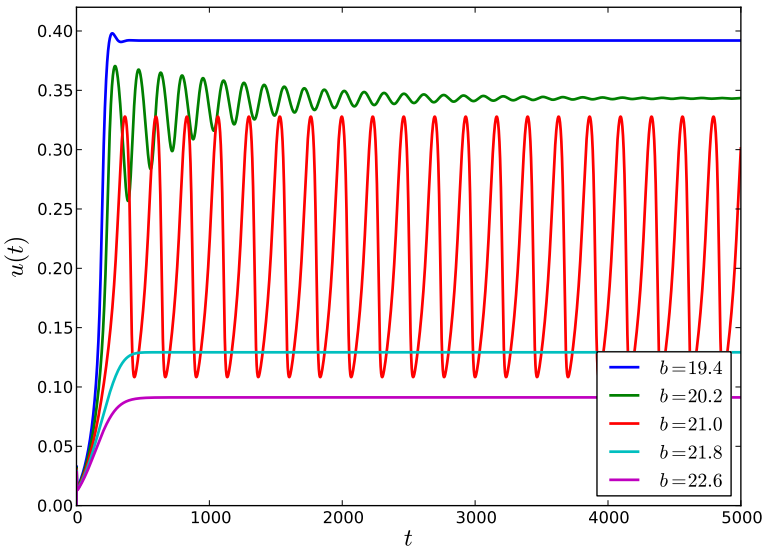


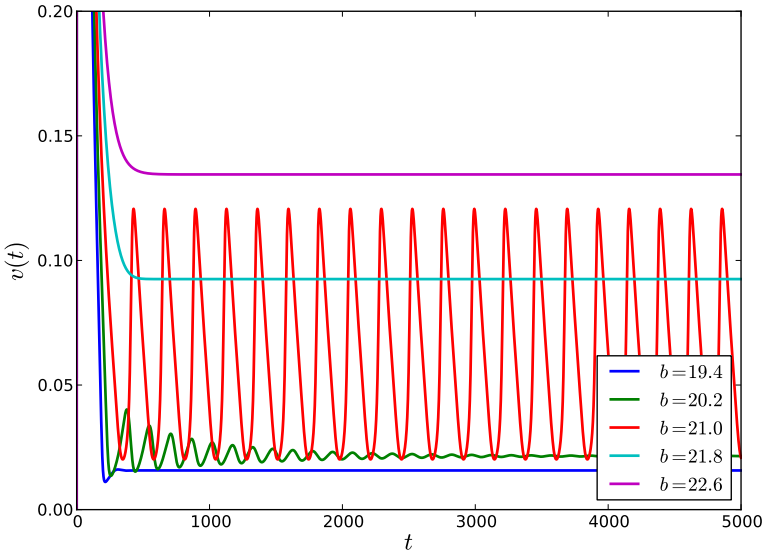
Oscillatory behavior for $b \in [20.2, 21.2]$

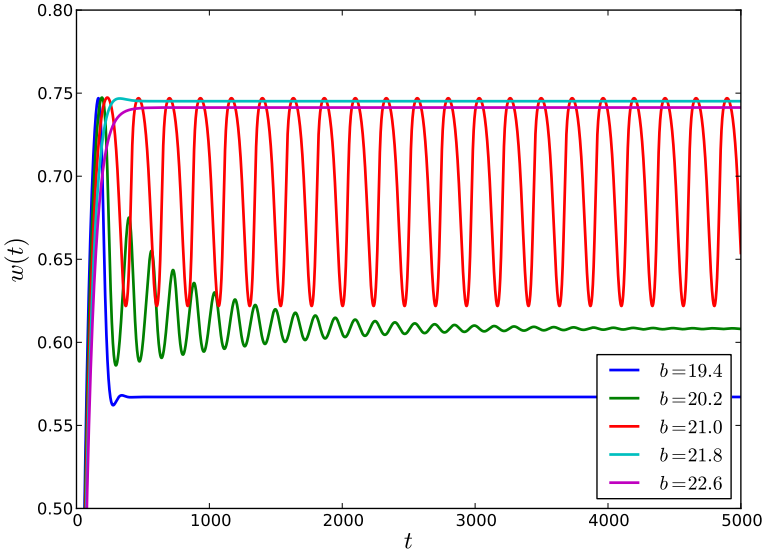
$$\begin{aligned}
a &= 1.6 \quad b = 20.75 \quad c = 0.04 \\
d &= 1.0 \quad e = 0.36 \quad f = 0.016
\end{aligned}$$

[Vigil *et al.*, Phys. Rev. E., 1996; Makeev *et al.*, J. Chem. Phys., 2002]

Surface reaction model shows wide range of dynamics







$$a = 1.6 \quad b = [19.4 \ldots 22.6]$$
$$c = 0.04 \quad d = 1.0$$
$$e = 0.36 \quad f = 0.016$$

Surface Reaction Model: Intrusive Spectral Propagation (ISP) of Uncertainty

- Assume PCE for uncertain parameter b and for the output variables, u, v, w
- Substitute PCEs into the governing equations
- Project the governing equations onto the PC basis functions
  - Multiply with Ψ_k and take the expectation
- Apply pseudo-spectral approximations where necessary

Surface Reaction Model: Specify PCEs for inputs and outputs

Represent uncertain inputs with PCEs with known coefficients:

$$b = \sum_{i=0}^{P} b_i \Psi_i(\xi)$$

Represent all uncertain variables with PCEs with unknown coefficients:

$$u(t) = \sum_{i=0}^{P} u_i(t)\Psi_i(\xi) \qquad v(t) = \sum_{i=0}^{P} v_i(t)\Psi_i(\xi)$$

$$w(t) = \sum_{i=0}^{P} w_i(t)\Psi_i(\xi) \qquad z(t) = \sum_{i=0}^{P} z_i(t)\Psi_i(\xi)$$

Surface Reaction Model: Substitute PCEs into governing equations and project onto basis functions

$$\frac{\mathrm{d}u}{\mathrm{d}t} = az - cu - 4duv$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} u_i\Psi_i = a\sum_{i=0}^{P} z_i\Psi_i - c\sum_{i=0}^{P} u_i\Psi_i - 4d\sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j$$

$$\left\langle \Psi_k \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} u_i\Psi_i \right\rangle = \left\langle a\Psi_k \sum_{i=0}^{P} z_i\Psi_i \right\rangle - \left\langle c\Psi_k \sum_{i=0}^{P} u_i\Psi_i \right\rangle$$

$$- \left\langle 4d\Psi_k \sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j \right\rangle$$

Surface Reaction Model: Reorganize terms

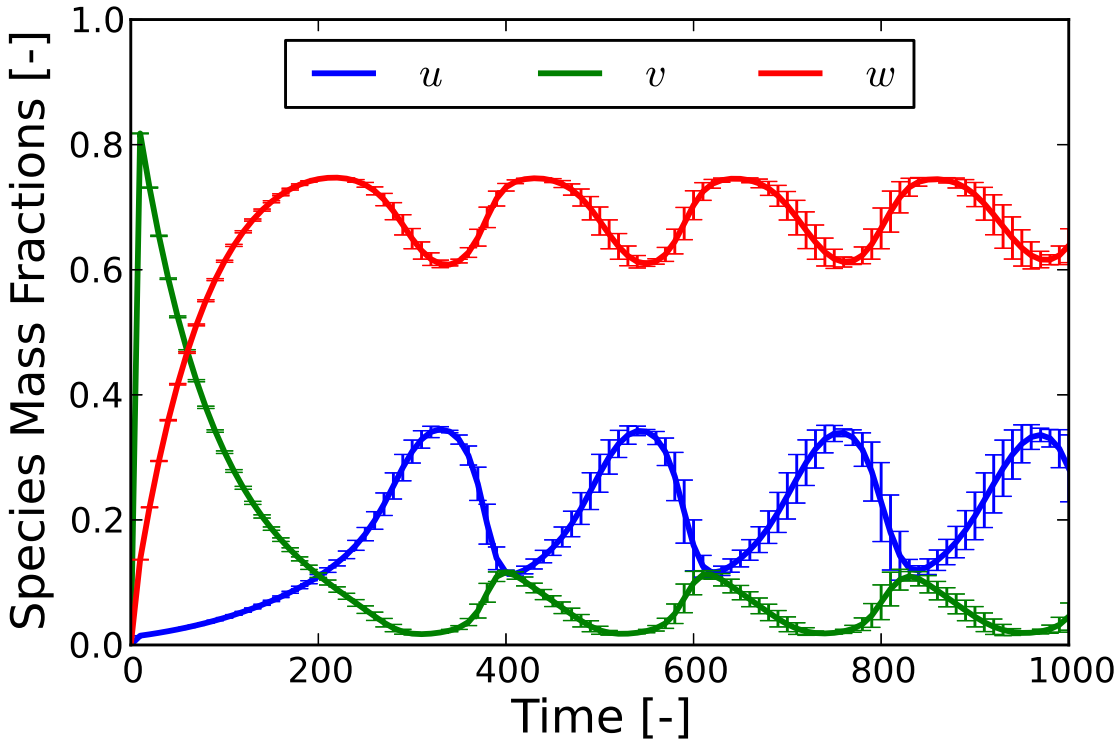
$$\frac{\mathrm{d}}{\mathrm{d}t} u_k \left\langle \Psi_k^2 \right\rangle = a z_k \left\langle \Psi_k^2 \right\rangle - c u_k \left\langle \Psi_k^2 \right\rangle - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \left\langle \Psi_i \Psi_j \Psi_k \right\rangle$$

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k = a z_k - c u_k - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k = a z_k - c u_k - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j C_{ijk}$$

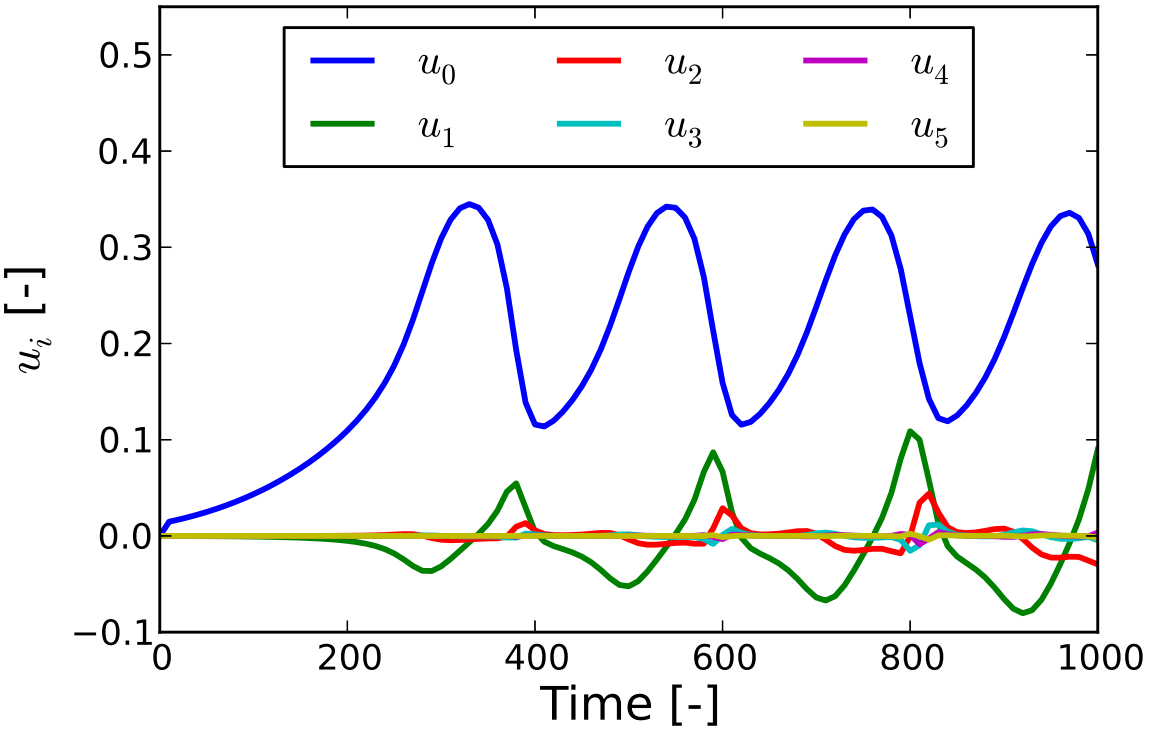
- Triple products $C_{ijk} = \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle}$ can be pre-computed and stored for repeated use

Surface Reaction Model: ISP results



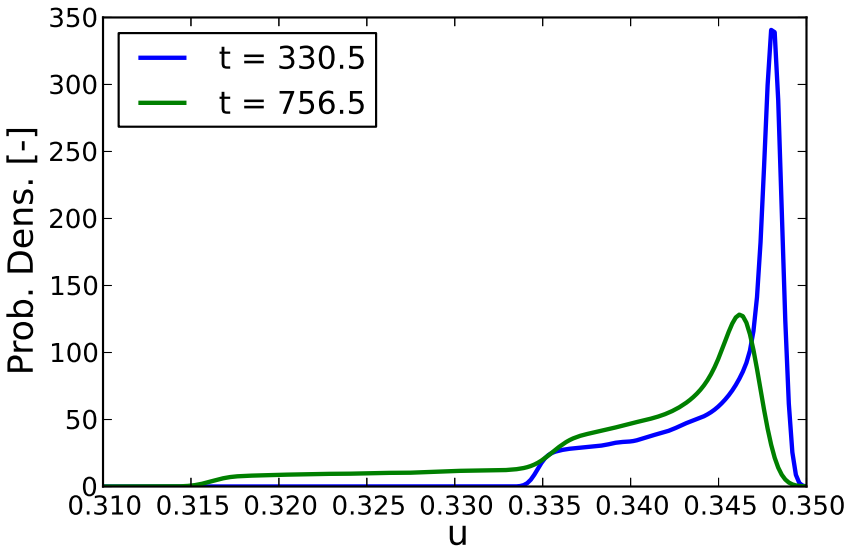
- Assume 0.5% uncertainty in *b* around nominal value
- Legendre-Uniform intrusive PC
- Mean and standard deviation for *u*, *v*, and *w*
- Uncertainty grows in time

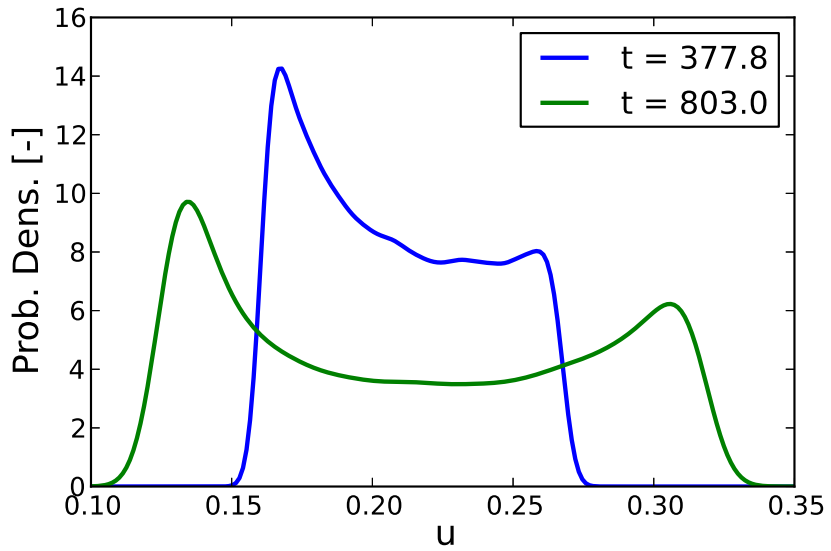
Surface Reaction Model: ISP results



- Modes of *u*
- Modes decay with higher order
- Amplitudes of oscillations of higher order modes grow in time

Surface Reaction Model: ISP results: PDFs





- Pdfs of u at maximum mean (left) and maximum standard deviation (right)
- Distributions get broader and multimodal as time increases
  - Effect of accumulating uncertainty in phase of oscillation

Remainder of this section focuses on Galerkin projection methods

- Intrusive Galerkin projection
- Non-intrusive Galerkin projection

Non-intrusive Galerkin projection

$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \int u\Psi_k(\xi) w(\xi) d\xi, \quad k = 0, \ldots, P$$

Evaluate projection integrals numerically

- Pick samples of uncertain parameters, e.g. $b(\xi) = \sum b_k \psi_k(\xi)$ by sampling ξ
- Run deterministic forward model for each of the sampled input parameter values $b^i = b(\xi^i)$
- Integration using random sampling or quadrature methods

Reconstruct uncertain model output

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

Random sampling approaches for Galerkin projection

- Evaluate integral through sampling

$$\int u\Psi_k(\xi)w(\xi)d\xi = \frac{1}{N_s}\sum_{i=1}^{N_s} u(\xi^i)\Psi_k(\xi^i)$$

- Samples are drawn according to the distribution of ξ
  - Monte-Carlo (MC)
  - Latin-Hypercube-Sampling (LHS)
- Pros:
  - Can be easily made fault tolerant
  - Sometimes random samples is all we have
- Cons: slow convergence, but less dependent on number of stochastic dimensions

Quadrature approaches for Galerkin projection

- Use numerical quadrature rules to evaluate integrals

$$\int u\Psi_k(\xi)w(\xi)d\xi = \sum_{i=1}^{N_q} q^i u(\xi^i)\Psi_k(\xi^i)$$

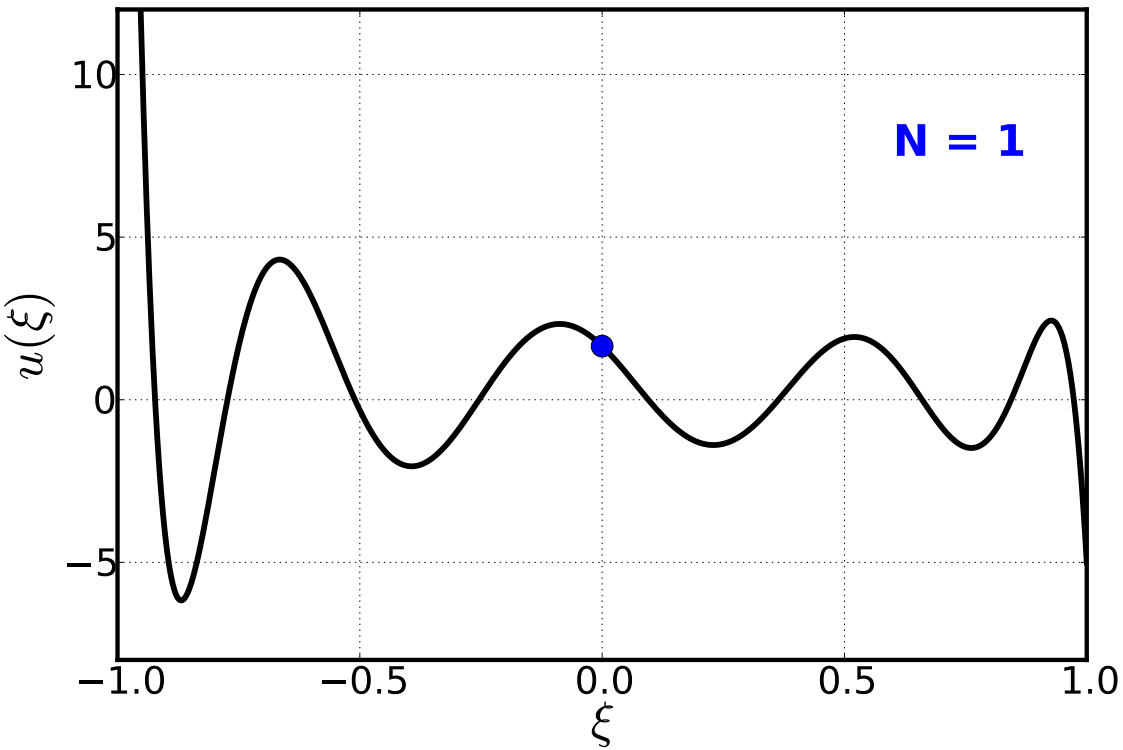
- The N_q ξ^i are quadrature points, with corresponding weights q^i
- Choice of quadrature points important for accuracy
  - Also referred to as *deterministic sampling* approach
- Pros:
  - Can use existing codes as black box to evaluate $u(\xi^i)$
  - Embarrassingly parallel
- Cons: Tensor product rule for d dimensions requires N_q^d samples

Gauss quadrature rules are very efficient

$$\int u\Psi_k(\xi)w(\xi)d\xi = \sum_{i=1}^{N_q} q^i u(\xi^i)\Psi_k(\xi^i)$$

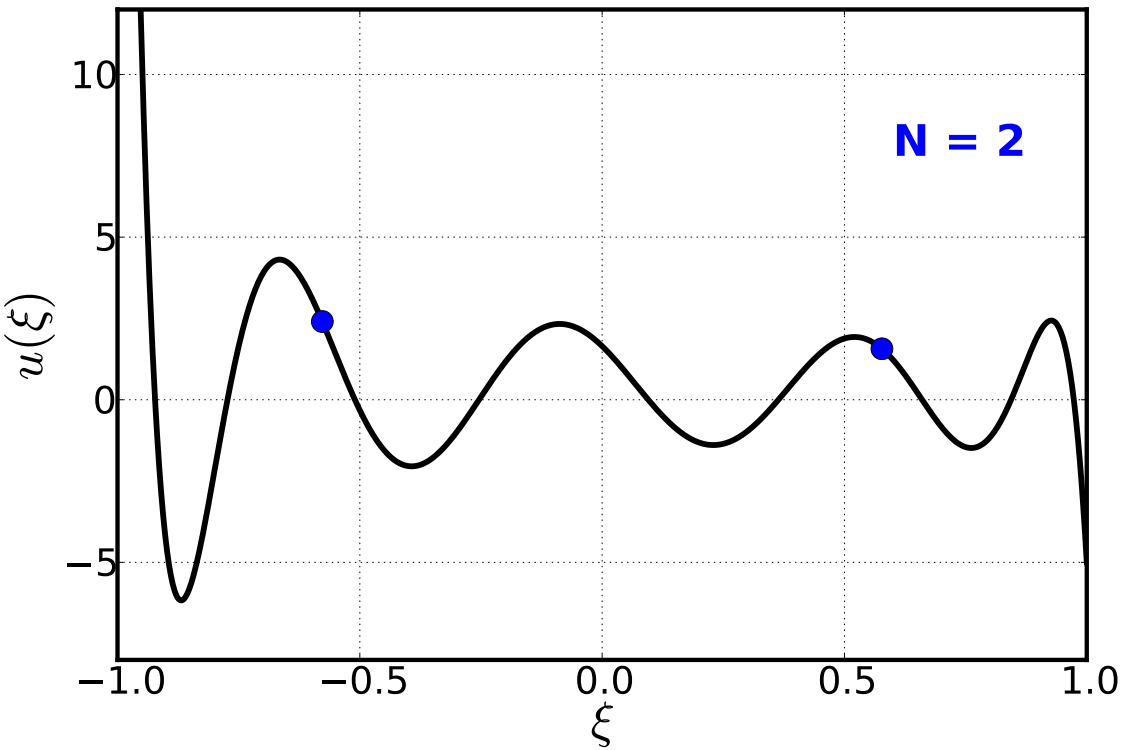
- N_q quadrature points can integrate polynomial of order $2N_q - 1$ exactly
- Gauss-Hermite and Gauss-Legendre quadrature tailored to specific choices of the weight function $w(\xi)$

Example quadrature integration of polynomial



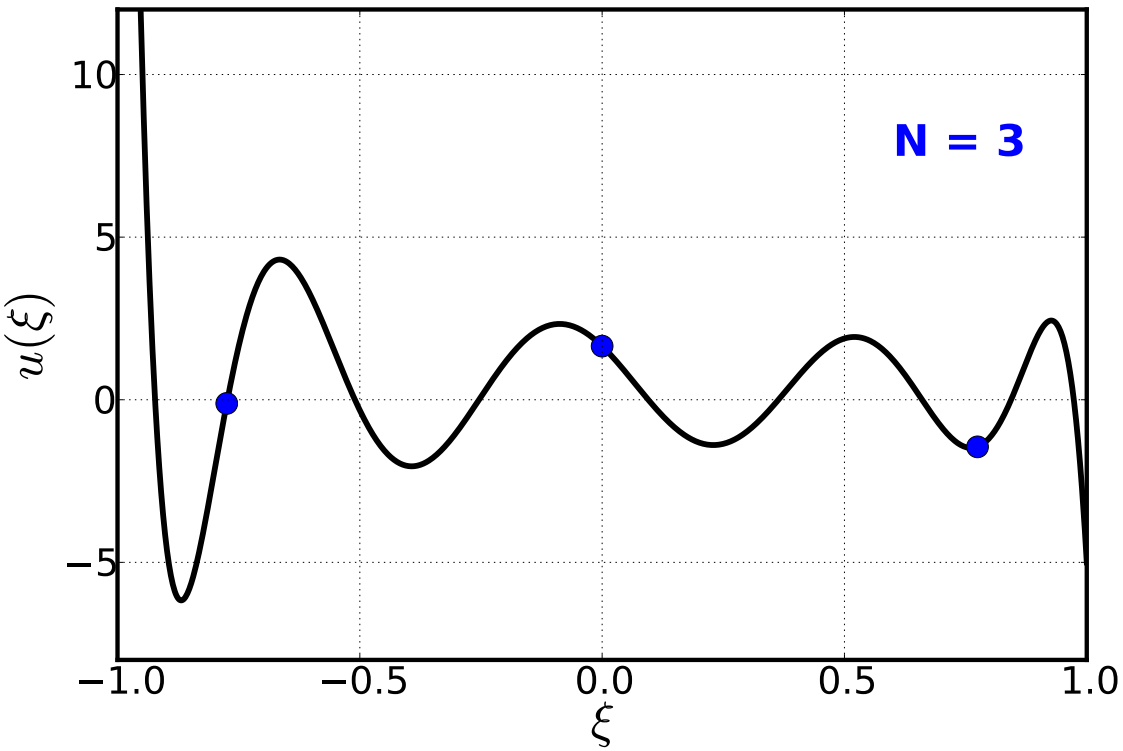
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 1 quadrature point gives integral = 1.65

Example quadrature integration of polynomial



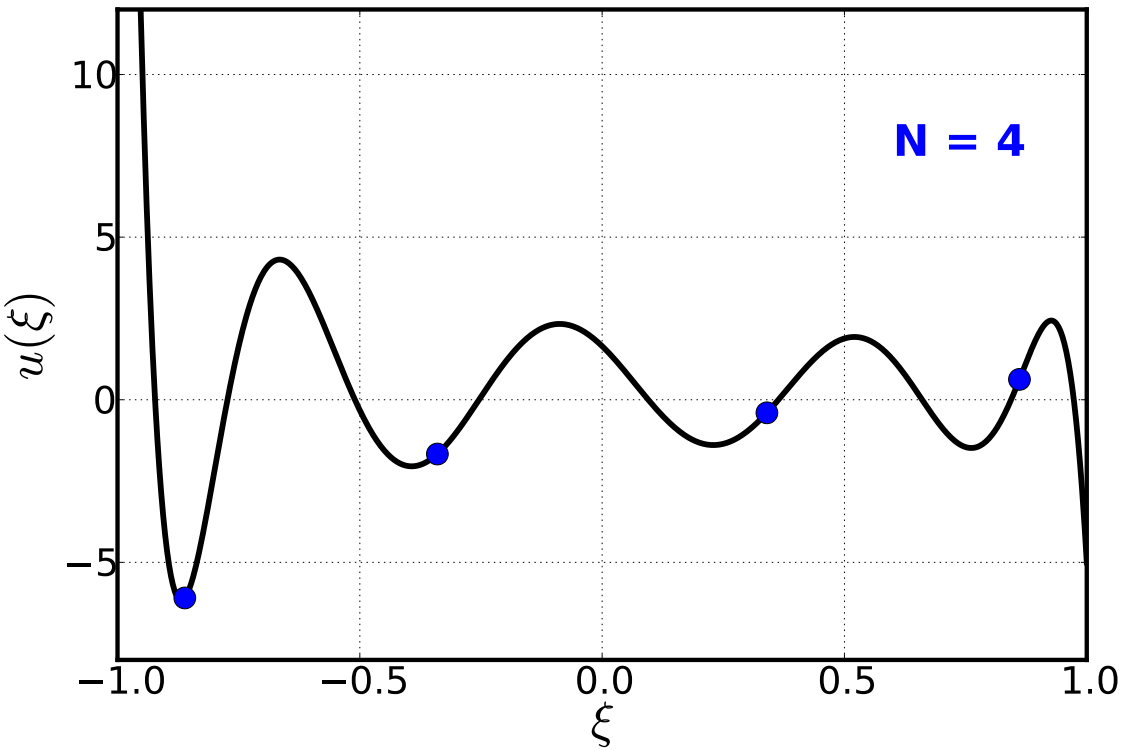
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 2 quadrature points gives integral = 1.99

Example quadrature integration of polynomial



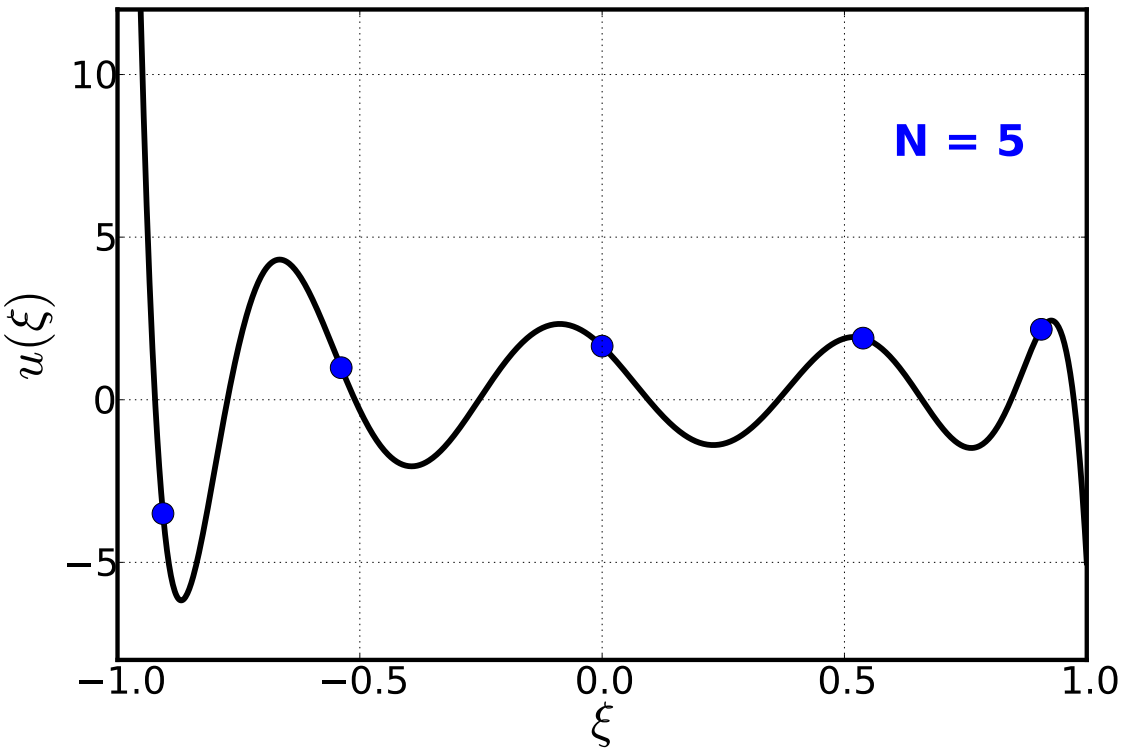
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 3 quadrature points gives integral = 0.30

Example quadrature integration of polynomial



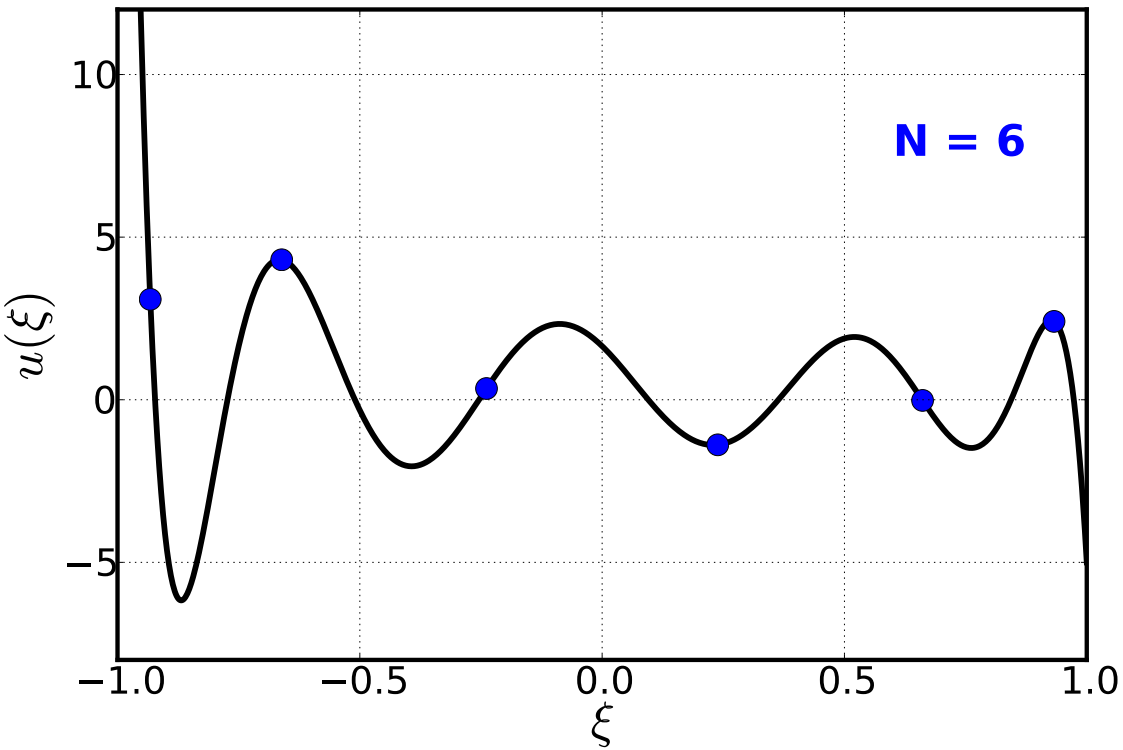
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 4 quadrature points gives integral = -1.63

Example quadrature integration of polynomial



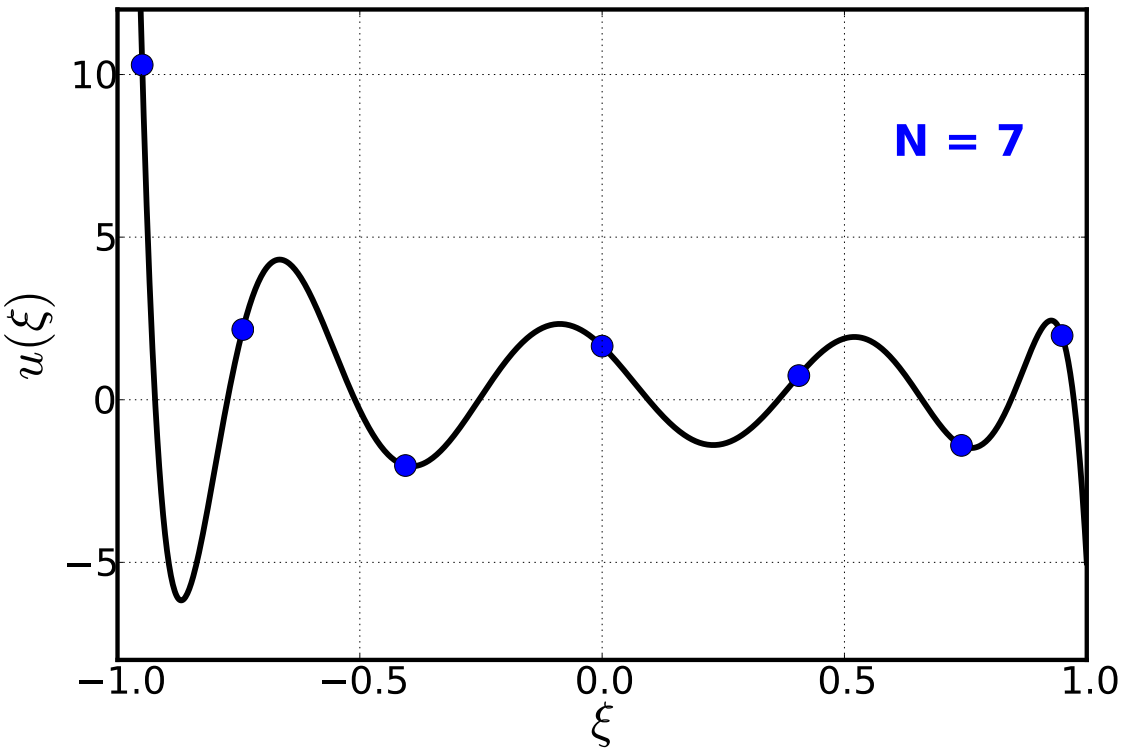
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 5 quadrature points gives integral = 1.00

Example quadrature integration of polynomial



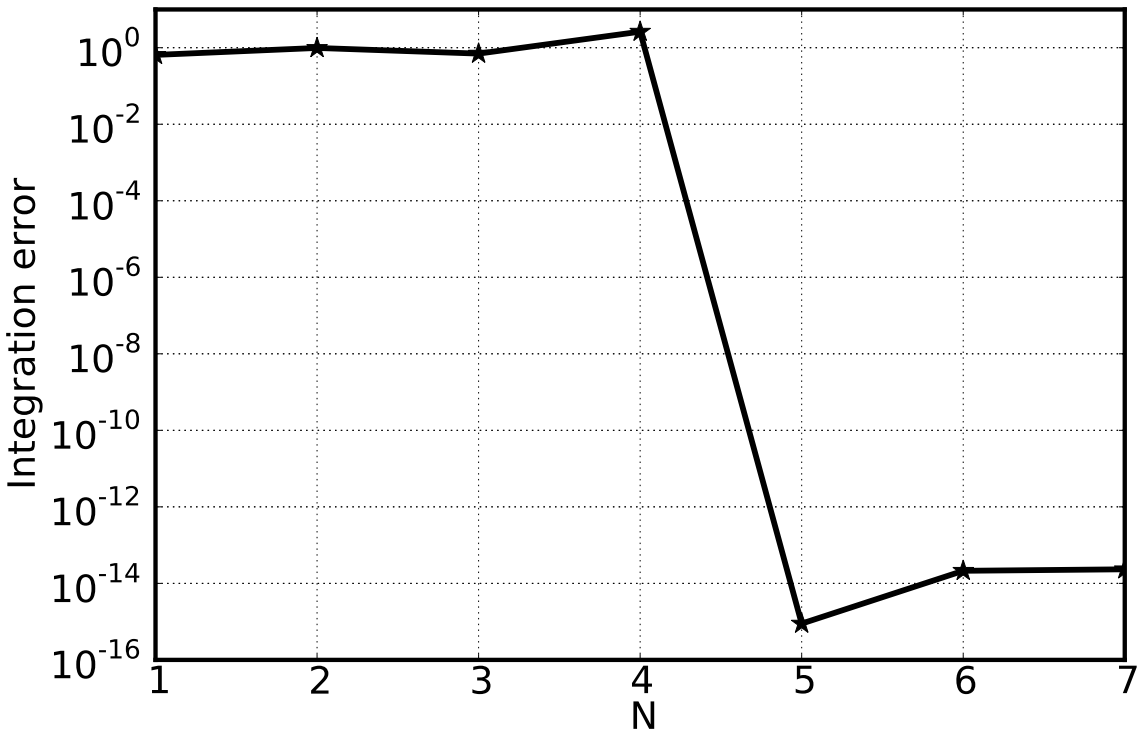
- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 6 quadrature points gives integral = 1.00

Example quadrature integration of polynomial



- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 7 quadrature points gives integral = 1.00

Example quadrature integration of polynomial



- Integral of 9^{th} order polynomial
- Gauss-Legendre quadrature with 5 or more points is exact

Minimum number of quadrature points for Galerkin projection

$$\int u\Psi_k(\xi)w(\xi)d\xi = \sum_{i=1}^{N_q} q^i u(\xi^i)\Psi_k(\xi^i)$$

- As a rule of thumb, $p+1$ quadrature points are needed for Galerkin projection of PCE of order p
  - If both u and Ψ_k are of order p, then integrand is of order $2p$
  - $2p \leq 2N_q - 1$ or $N_q \geq p + \frac{1}{2}$
  - Only exact if u is indeed a polynomial of order $\leq p$

Surface Reaction Model

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\end{aligned}$$

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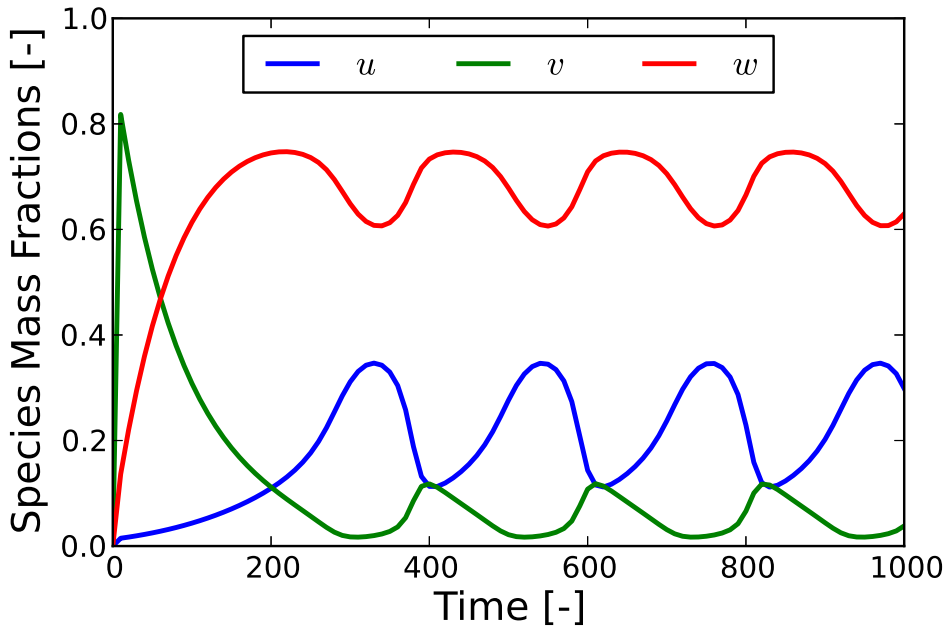

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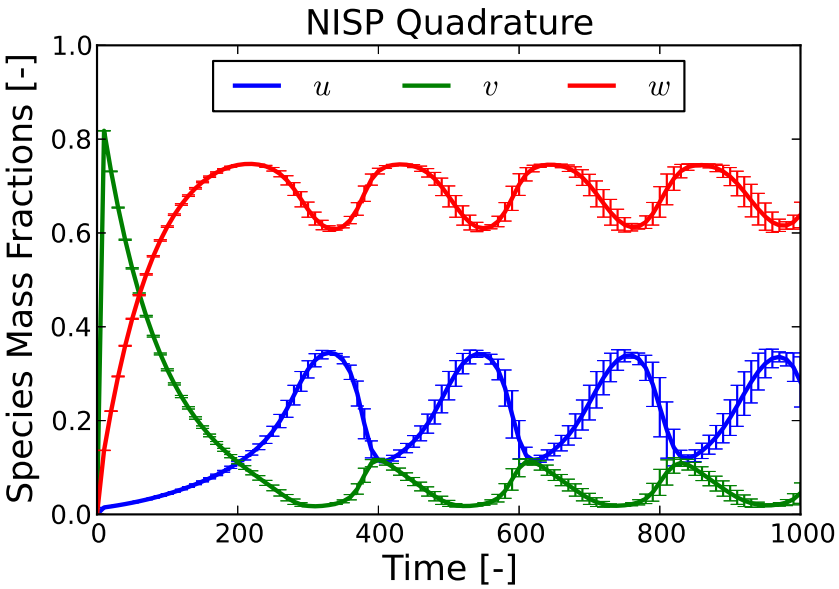
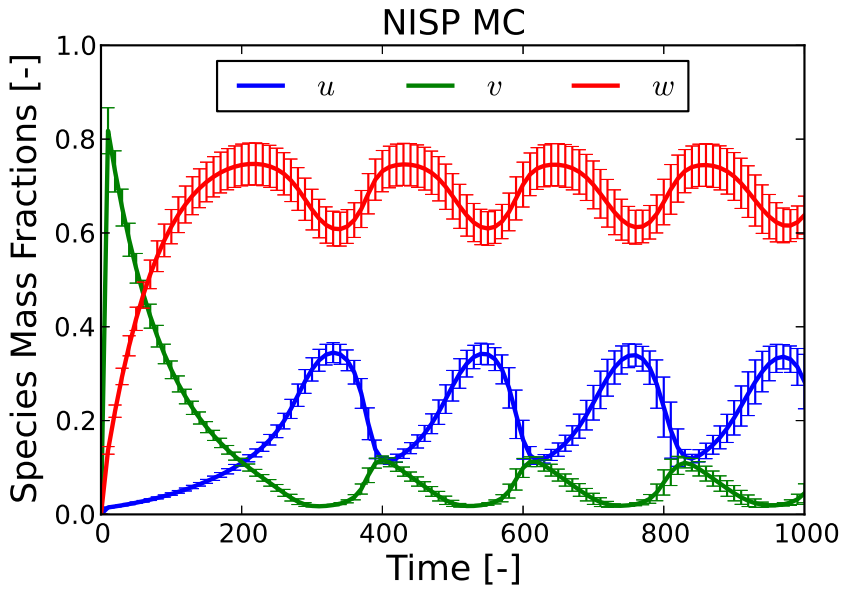
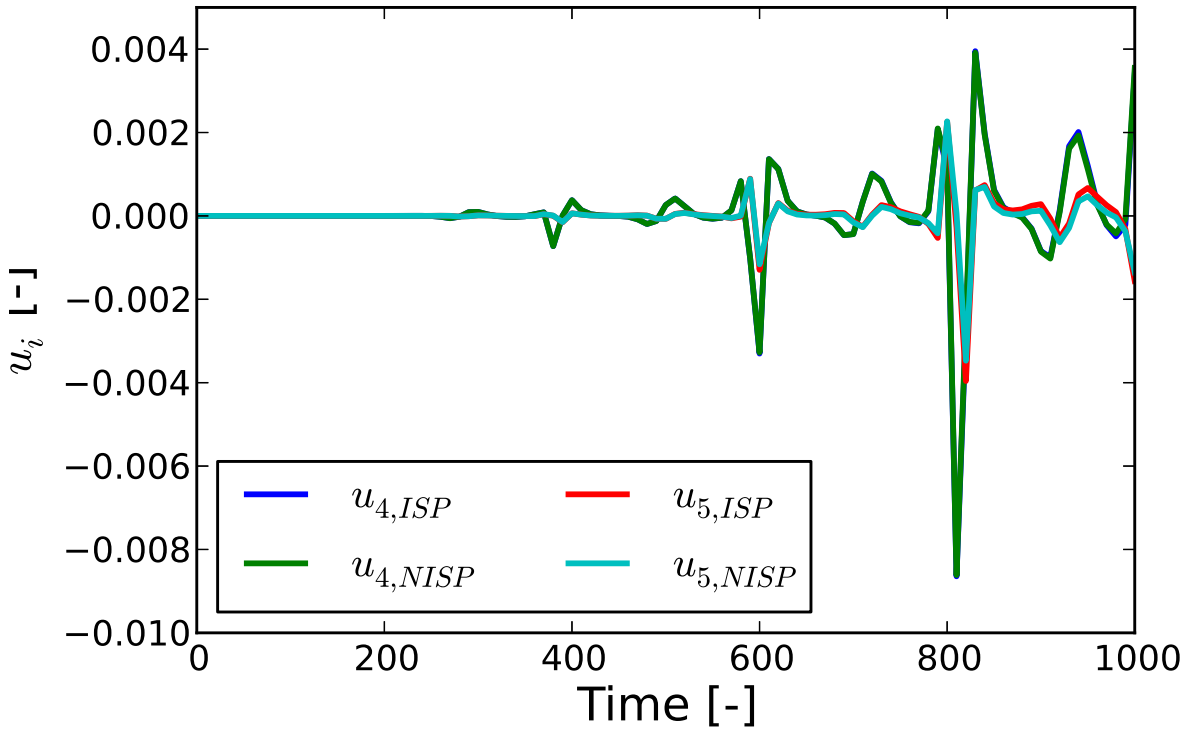
Surface Reaction Model: NISP results





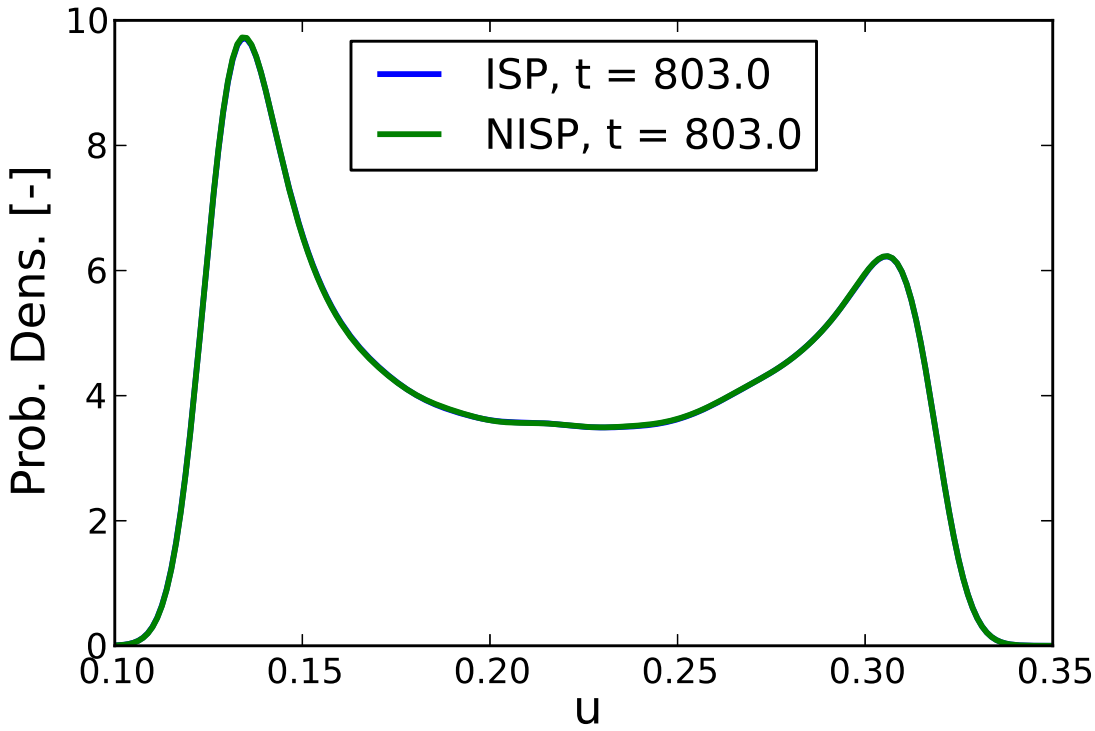
- Mean and standard deviation for u, v, and w
- Quadrature approach agrees well with ISP approach using 6 quadrature points
- Monte Carlo sampling approach converges slowly
  - With a 1000 samples, results are quite different from ISP and NISP

Surface Reaction Model: Comparison ISP and NISP



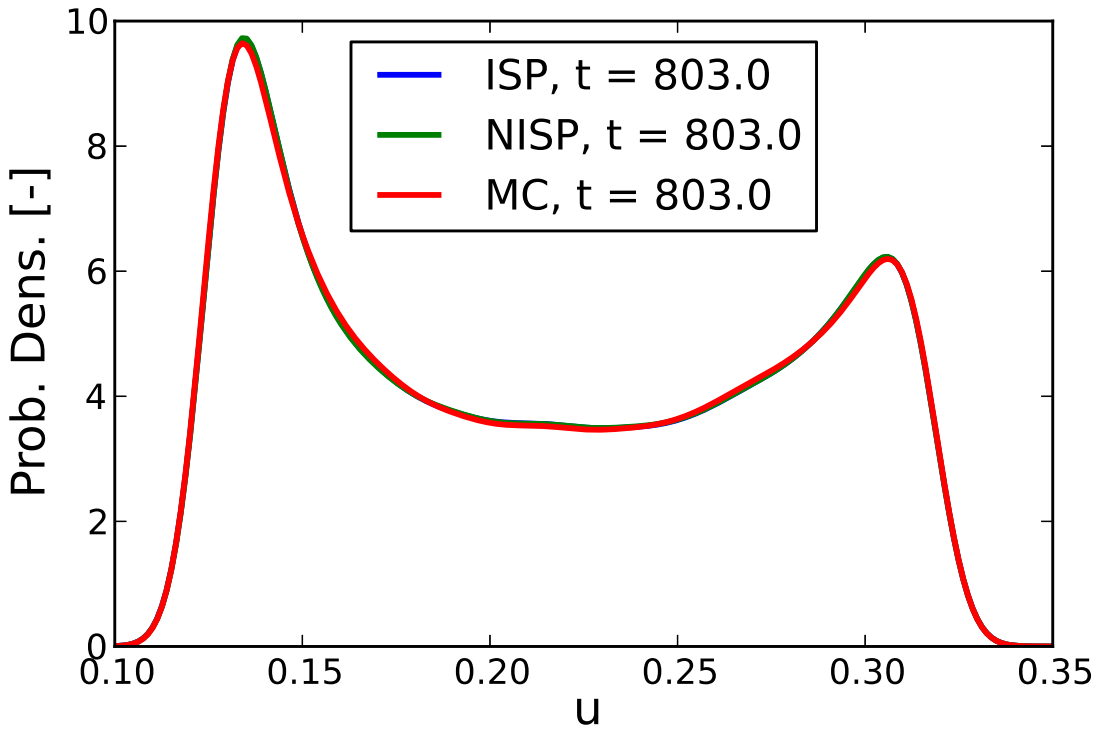
- Lower order modes agree perfectly
- Very small differences in higher order modes
  - Difference increases with time

Surface Reaction Model: Comparison ISP and NISP



- All pdf's based on 50K samples each and evaluated with Kernel Density Estimation (KDE)
- No difference in PDFs of sampled PCEs between NISP and ISP

Surface Reaction Model: Comparison ISP, NISP, and MC



- All pdf's based on 50K samples each and evaluated with Kernel Density Estimation (KDE)
- Good agreement between intrusive, non-intrusive projection, and Monte Carlo sampling

ISP pros and cons

- Pros:
  - Elegant
  - One time solution of system of equations for the PC coefficients fully characterizes uncertainty in all variables at all times
  - Tailored solvers can (potentially) take advantage of new hardware developments
- Cons:
  - Often requires re-write of the original code
  - Reformulated system is factor (P+1) larger than the original system and can be challenging to solve
  - Challenges with increasing time-horizon for ODEs
- Many efforts in the community to automate ISP

NISP pros and cons

- Pros:
  - Easy to use as wrappers around existing codes
  - Embarassingly parallel
  - Can be used even when there is no explicit equation for the observable
- Cons:
  - Most methods suffer from curse of dimensionality $N_q = n^{N_d}$
- Many development efforts for smarter sampling approaches and dimensionality reduction
  - (Adaptive) Sparse Quadrature approaches
  - Compressive Sensing
  - ...
- Sampling methods have found very wide spread use in the community

Software for intrusive and non-intrusive UQ

- DAKOTA: `http://dakota.sandia.gov/`
  - Wide variety of non-intrusive methods for uncertainty propagation, sensitivity analysis, *etc.*
  - Mature and well-supported
- UQ Toolkit (UQTk):
  `http://www.sandia.gov/UQToolkit/`
  - Intrusive and non-intrusive
  - Geared towards algorithm development and educational use
- Sundance:
  `http://www.math.ttu.edu/~klong/Sundance/html/`
  - UQ-enabled finite-element solution of PDEs
- Stokhos:
  `http://trilinos.sandia.gov/packages/stokhos/`
  - Package for intrusive Galerkin based UQ
- ...

Uncertainty Quantification Toolkit (UQTk)

- A library of C++ and Python functions for propagation of uncertainty through computational models
- Mainly relies on Polynomial Chaos Expansions (PCEs) for representing random variables and stochastic processes
- Target usage:
  - Rapid prototyping
  - Algorithmic research
  - Tutorials / educational
- Version 2.1 released under the GNU Lesser General Public License
  - C++ Tools for intrusive and non-intrusive UQ
  - Bayesian inference tools
  - Bayesian compressed sensing
  - Python postprocessing and analysis tools
- Available at `http://www.sandia.gov/UQToolkit/`

Outline

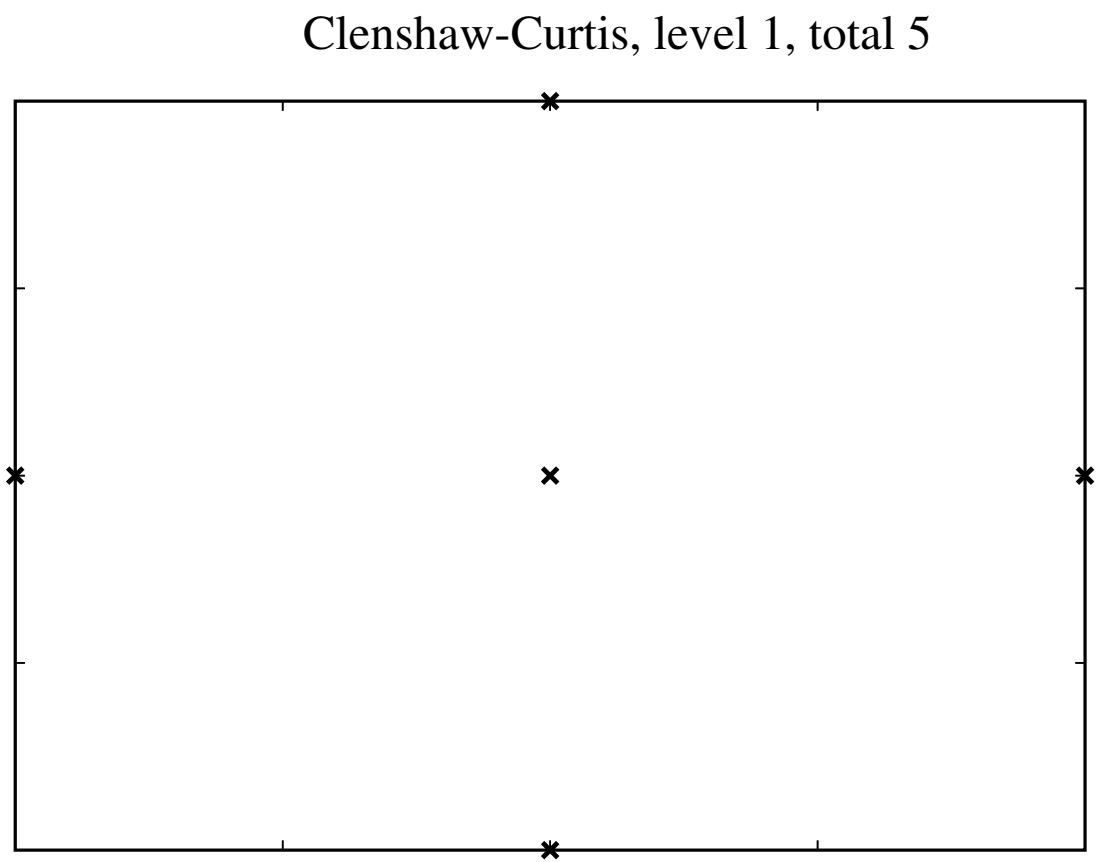
Sparse Quadrature Approaches for High-Dimensional Systems

- Need for sparse quadrature
- Sparse quadrature grids
- Application to heat transfer example

Full product quadrature is wasteful in high-dimensional systems

- Define the **precision** as the highest order of a polynomial that is integrated *exactly* by the quadrature rule
- Gaussian quadratures are optimal in 1d
  - N points achieve the highest possible precision of $2N - 1$
- In multi-d, full product quadrature is wasteful:
  - A 5 ppd (point per dimension) rule is of precision $P = 9$, but it integrates a polynomial $x^9 y^9$ exactly
- Sparse quadratures are built to achieve maximal precision with as few points as possible
  - *E.g.* Smolyak construction

Clenshaw-Curtis nested quadrature rules allow reuse of function evalutions



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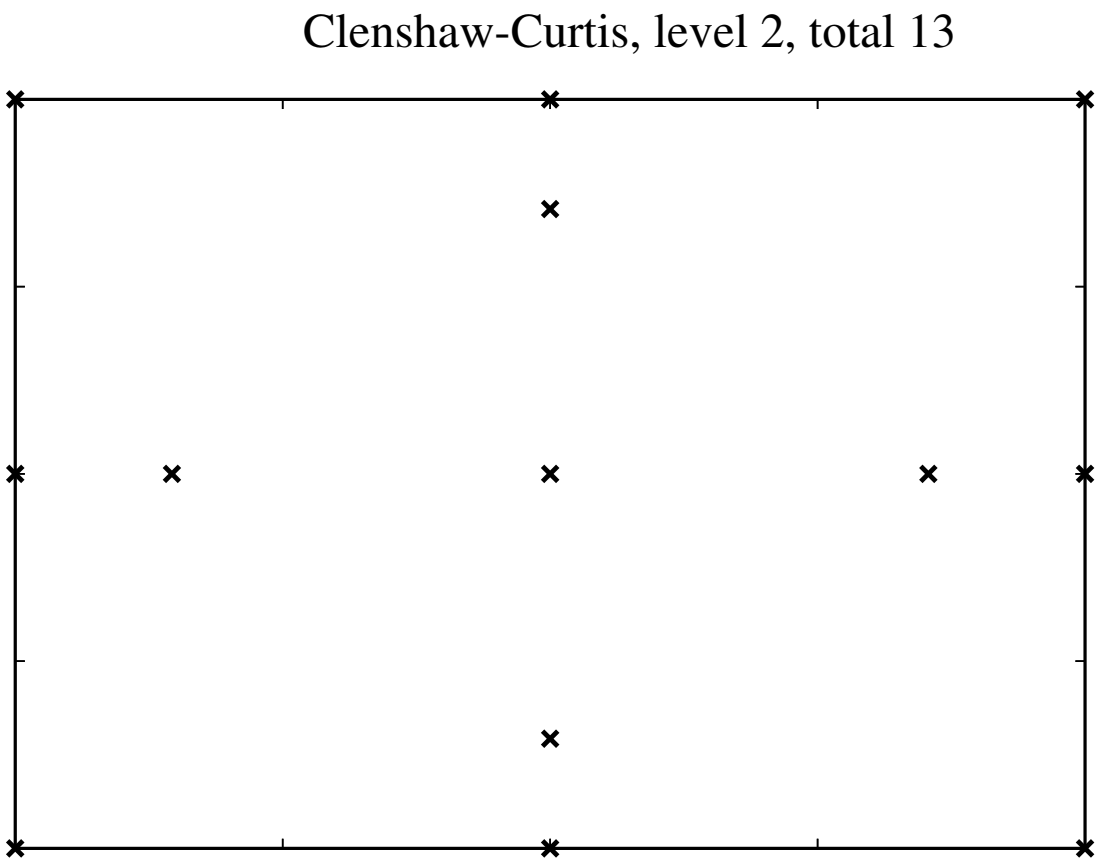

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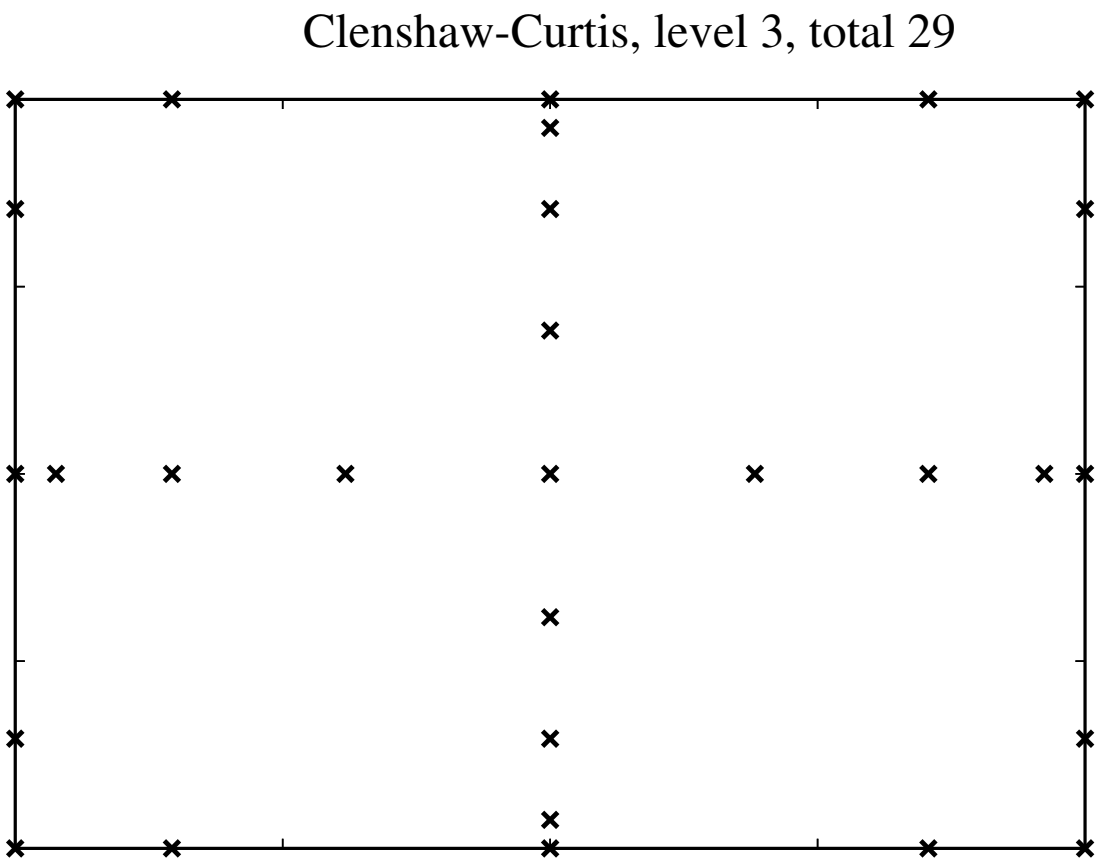

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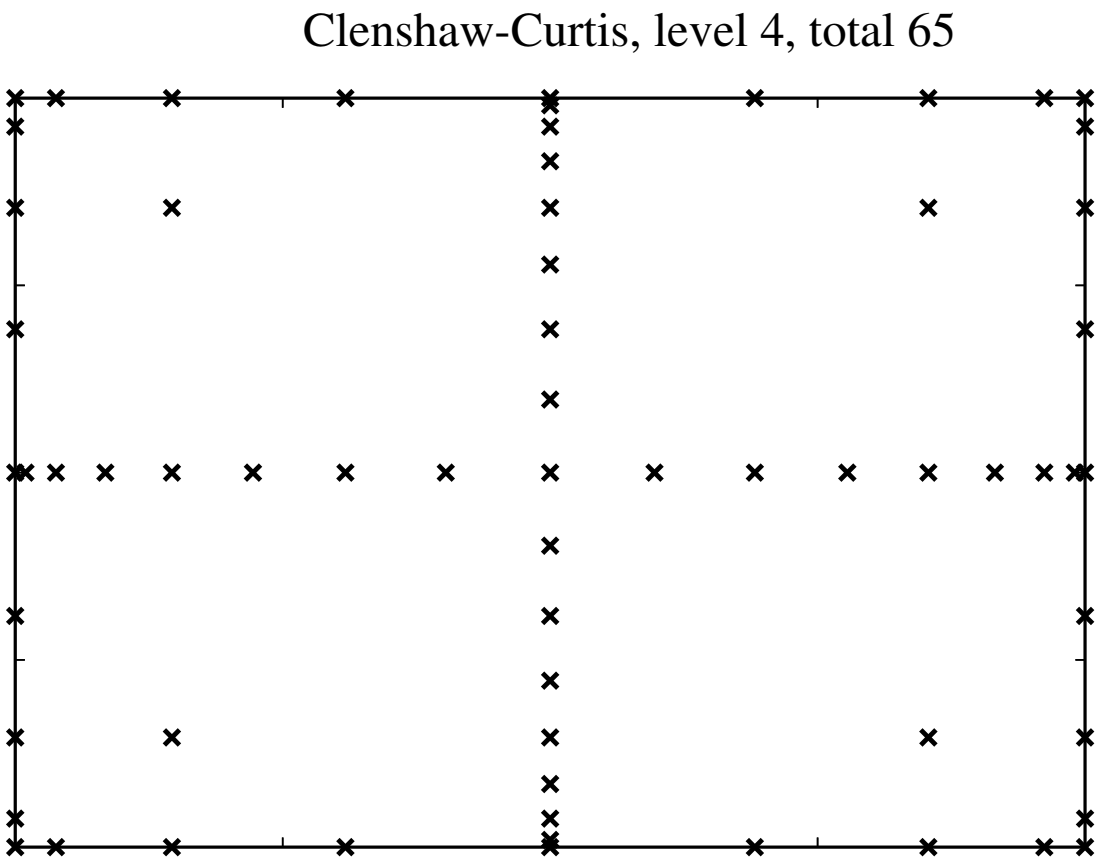

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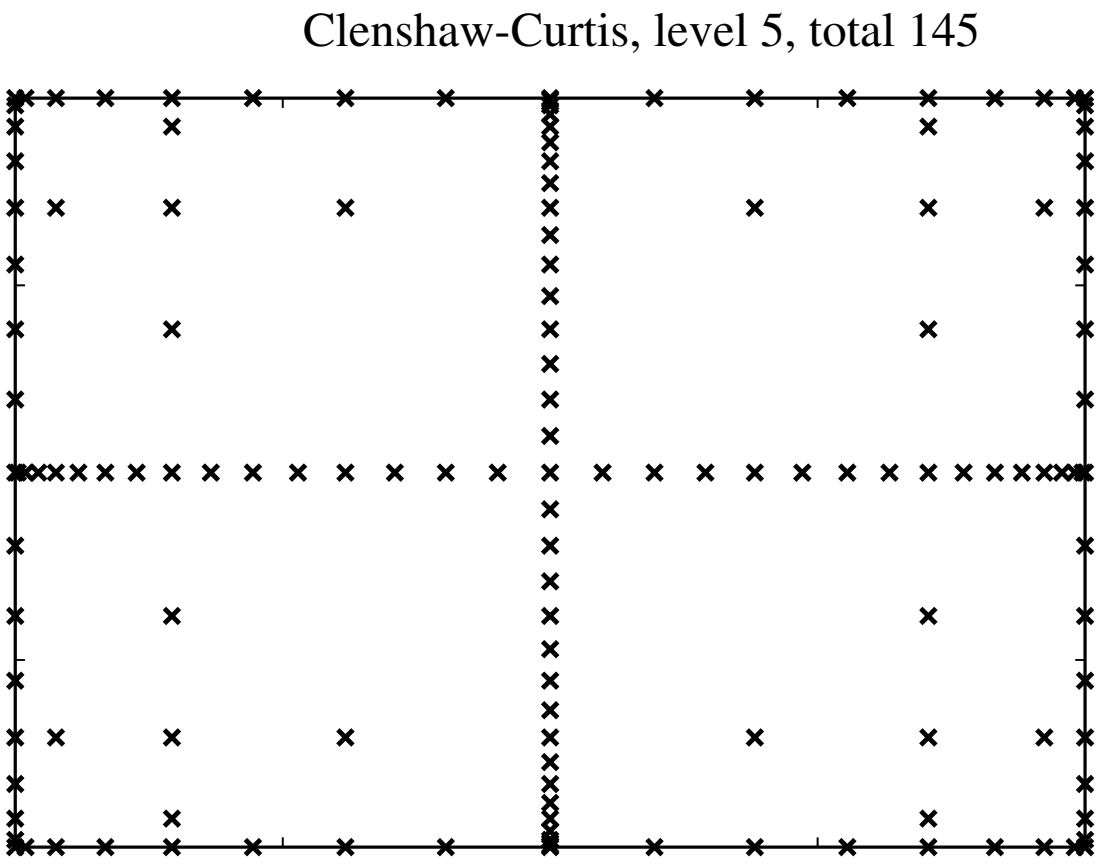
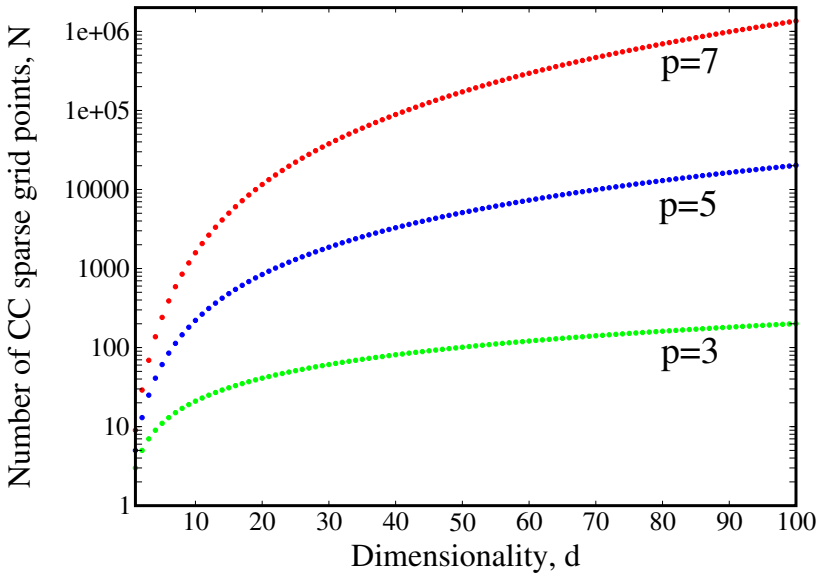


The number of function evaluations is drastically reduced compared to full quadrature

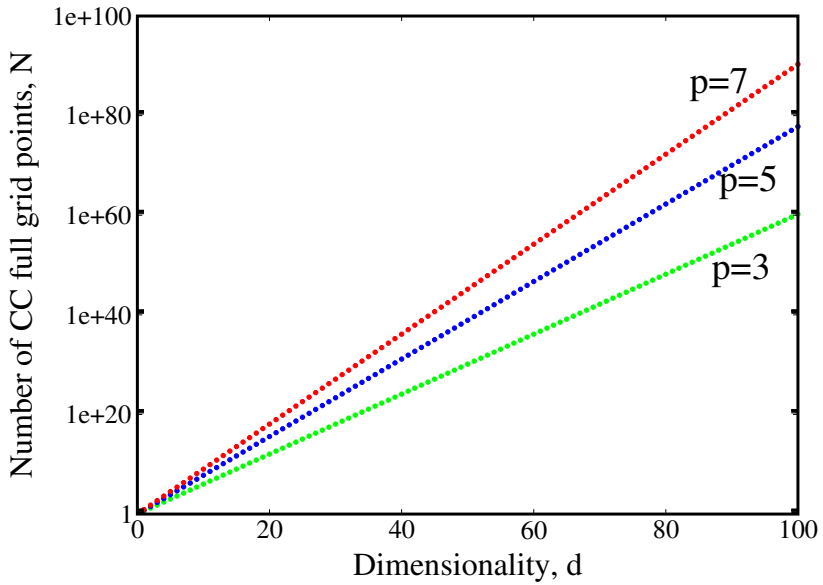
Table : The number of Clenshaw-Curtis sparse grid quadrature points for various levels and dimensionalities.

Level L	Precision $p = 2L - 1$	N $(d = 2)$	N $(d = 5)$	N $(d = 10)$	$N(d)$ General
1	1	1	1	1	1
2	3	5	11	21	$1 + 2d$
3	5	13	61	221	$1 + 2d + 2d^2$
4	7	29	241	1581	$1 + \frac{14}{3}d + 2d^2 + \frac{4}{3}d^3$
5	9	65	801	8801	$1 + \frac{20}{3}d + \frac{22}{3}d^2 + \frac{4}{3}d^3 + \frac{2}{3}d^4$
6	11	145	2433	41265	$\cdots$
7	13	321	6993	171425	$\cdots$
8	15	705	19313	652065	$\cdots$
9	17	1537	51713	2320385	$\cdots$

The number of function evaluations is drastically reduced compared to full quadrature

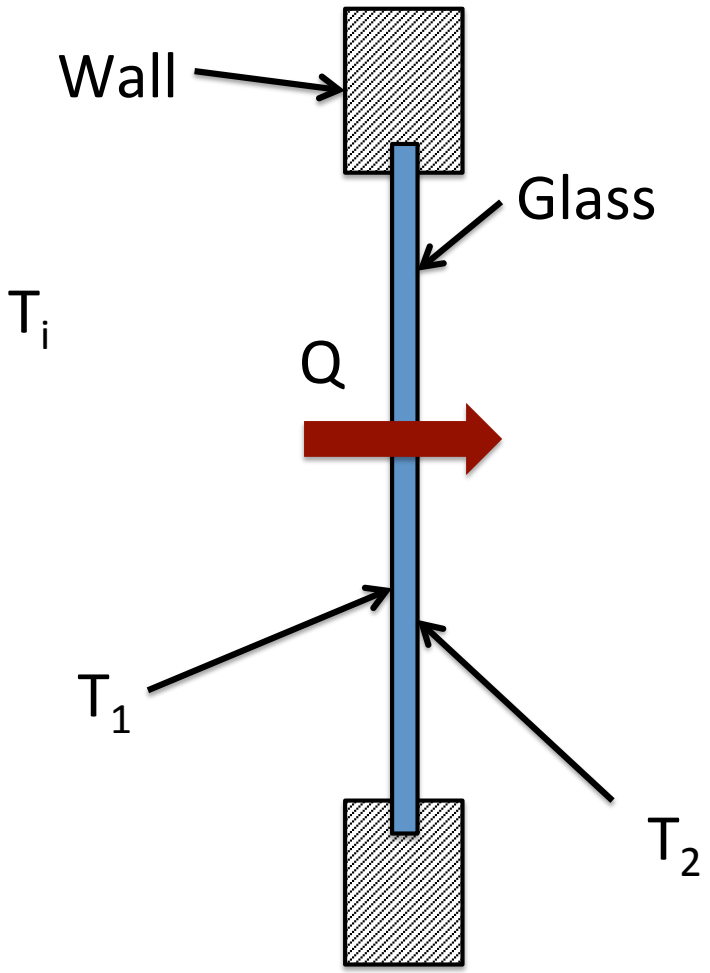


Sparse grid: polynomial growth, $\mathcal{O}(d^{\frac{p-1}{2}})$



Full grid: exponential growth, $(p+1)^d$

Heat Transfer through a Window



$$h_i(T_i - T_1) = k_w \frac{(T_1 - T_2)}{d_w}$$

$$k_w \frac{(T_1 - T_2)}{d_w} = h_o(T_2 - T_o)$$

6 Uncertain, Gaussian parameters

$$T_i = 293\mathrm{K}, \sigma = 0.5\%$$
$$T_o = 273\mathrm{K}, \sigma = 0.5\%$$
$$d_w = 0.01\mathrm{m}, \sigma = 1\%$$
$$k_w = 1\mathrm{W/mK}, \sigma = 5\%$$
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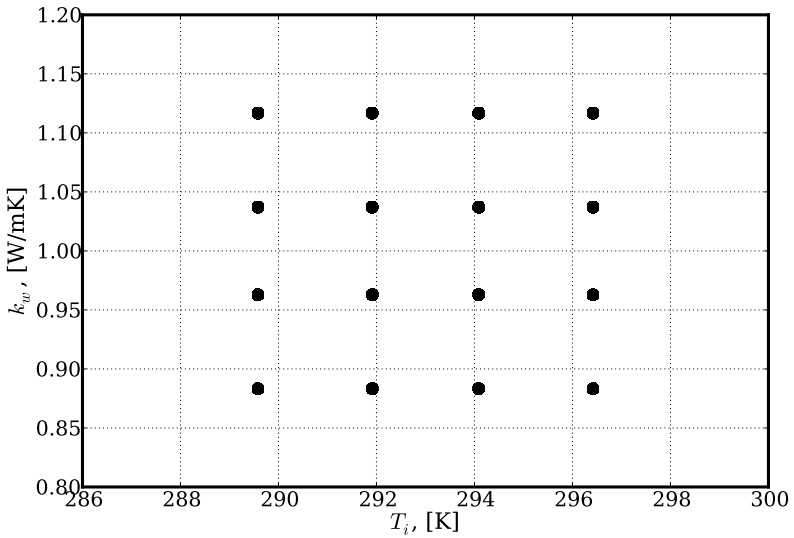
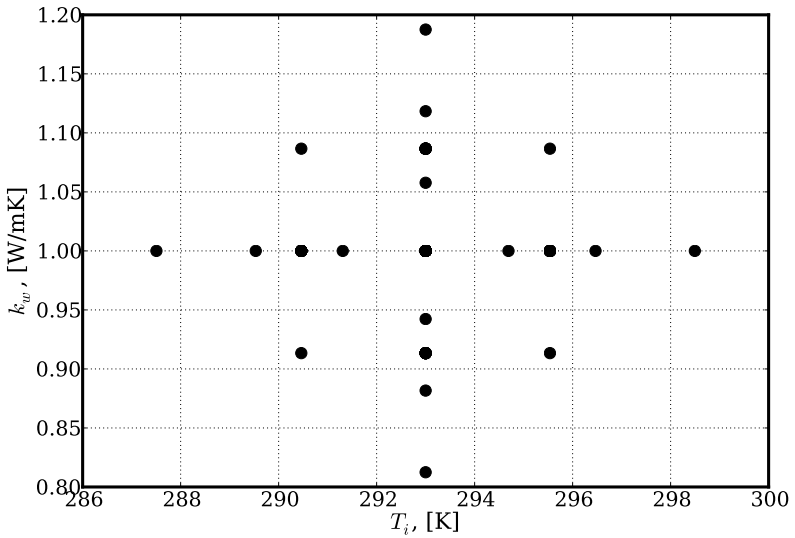
$$h_o = 6\mathrm{W/m^2K}, \sigma = 15\%$$

Sparse quadrature grid uses much fewer points than full tensor product



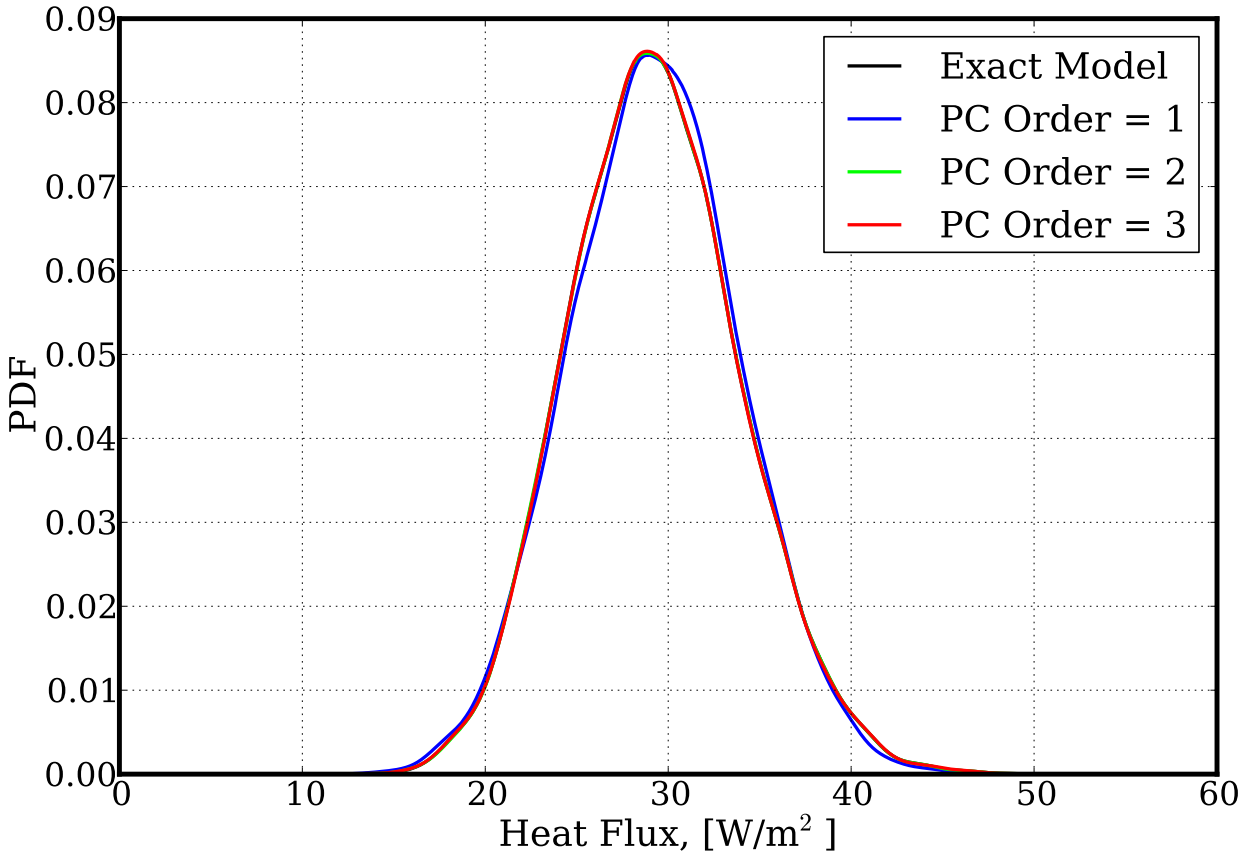
Full tensor product in 6D:
$N = 4^6 = 4096$



Level 2 sparse rule in 6D:
$N = 109$

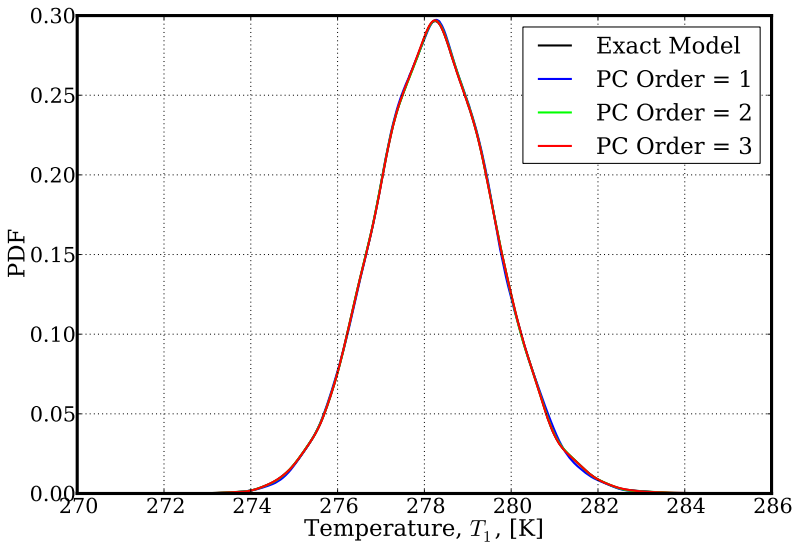
- Wiener-Hermite base rule in both cases
- Constructed for exact 3^{rd} order Galerkin projection

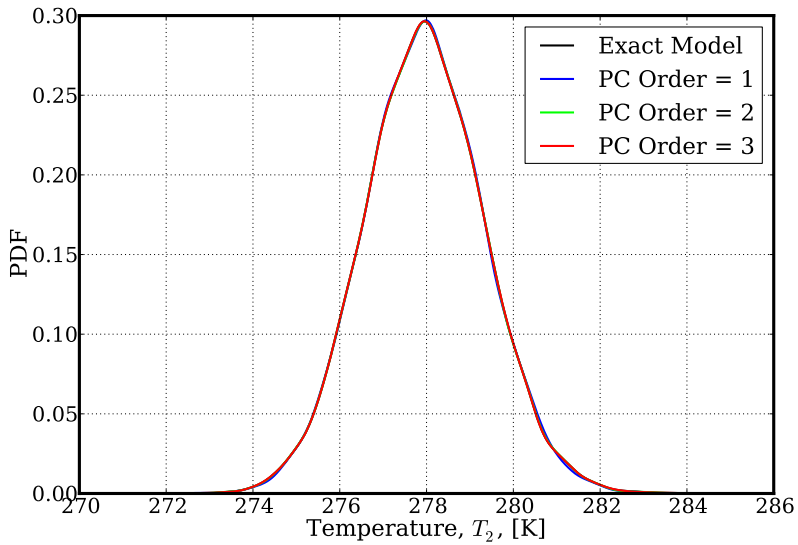
Second order PC is sufficient for forward propagation



- Second and third order PCE results coincide

Second order PC is sufficient for forward propagation





- Not much nonlinearity in temperatures
- Temperature drop across glass is small

Advantages and caveats of sparse quadrature approaches

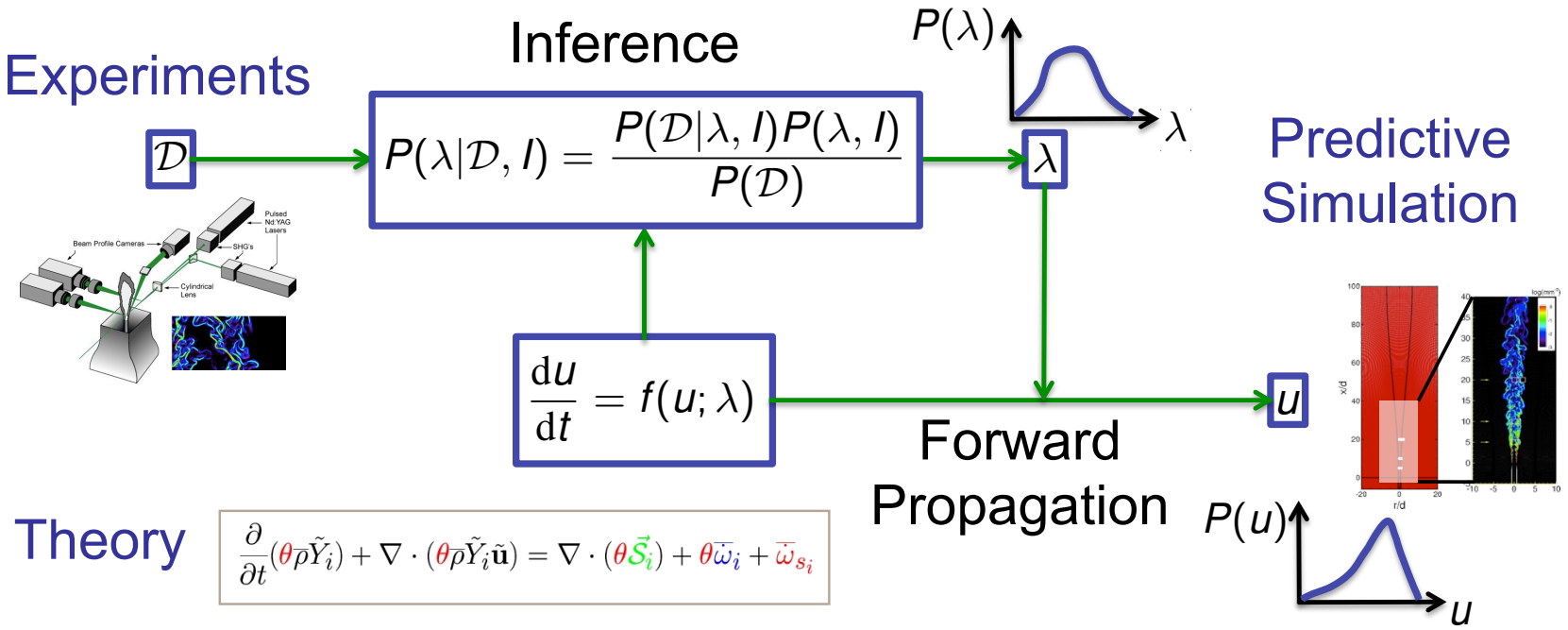
- Pro: number of required samples scales much more gracefully with number of dimensions than full tensor product quadrature rule
- Caveats:
  - Function to be integrated needs to be smooth
  - Due to negative quadrature weights, integrating a noisy positive function can give a negative answer
  - For very high dimensions, even sparse quadrature is too expensive

Taking Advantage of Sparsity in the System

- For really high dimensional systems, even sparse quadrature requires too many function evaluations
  - For 80-dimensional climate land model, $L = 4$ requires $\approx 10^6$ points
- Such systems can only be tackled with dimensionality reduction and/or adaptive order
  - Sensitivity analysis
  - High Dimensional Model Representation (HDMR)
  - Adaptive sparse quadrature approaches
- More generally, use only the basis terms needed to represent the physics / information in the system / data
  - (Bayesian) Compressive Sensing (CS) approaches
- If information content is sparse, it can be represented at reasonable cost
  - If not, you need to pay the price

Outline

Sensitivity analysis gives insight into key sources of uncertainty



- Obtaining global sensitivity analysis from PCEs
  - Identify dominant sources of uncertainty
  - Attribution

PC postprocessing: global sensitivity information is readily obtained from PCE

$$g(\xi_1, \ldots, \xi_d) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

- Global sensitivity analysis $\equiv$ Variance decomposition
- Total variance

$$Var[g(\boldsymbol{\xi})] = \sum_{k>0} c_k^2 ||\Psi_k||^2$$

PC postprocessing: global sensitivity information is readily obtained from PCE

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i)]}{Var[g(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

  $\mathbb{I}_i$ is the set of bases with only ξ_i involved. S_i is the uncertainty contribution that is due to i-th parameter only.

- Joint sensitivity indices

$$S_{ij} = \frac{Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i,\xi_j)]}{Var[g(\boldsymbol{\xi})]} - S_i - S_j = \frac{\sum_{k\in\mathbb{I}_{ij}} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

  $\mathbb{I}_{ij}$ is the set of bases with only ξ_i and ξ_j involved. S_{ij} is the uncertainty contribution that is due to (i,j) parameter pair.

PC postprocessing: sampling-based approaches

$$g(\xi_1, \ldots, \xi_d) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

- In some cases, need to resort to Monte-Carlo estimation, e.g.
  - Piecewise-PC with irregular subdomains
  - Output transformations, e.g. build PC for $\log g(\boldsymbol{\xi})$, but inquire sensitivity with respect to $g(\boldsymbol{\xi})$
- A brute-force sampling of $Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i)]$ is extremely inefficient.

PC postprocessing: sampling-based approaches

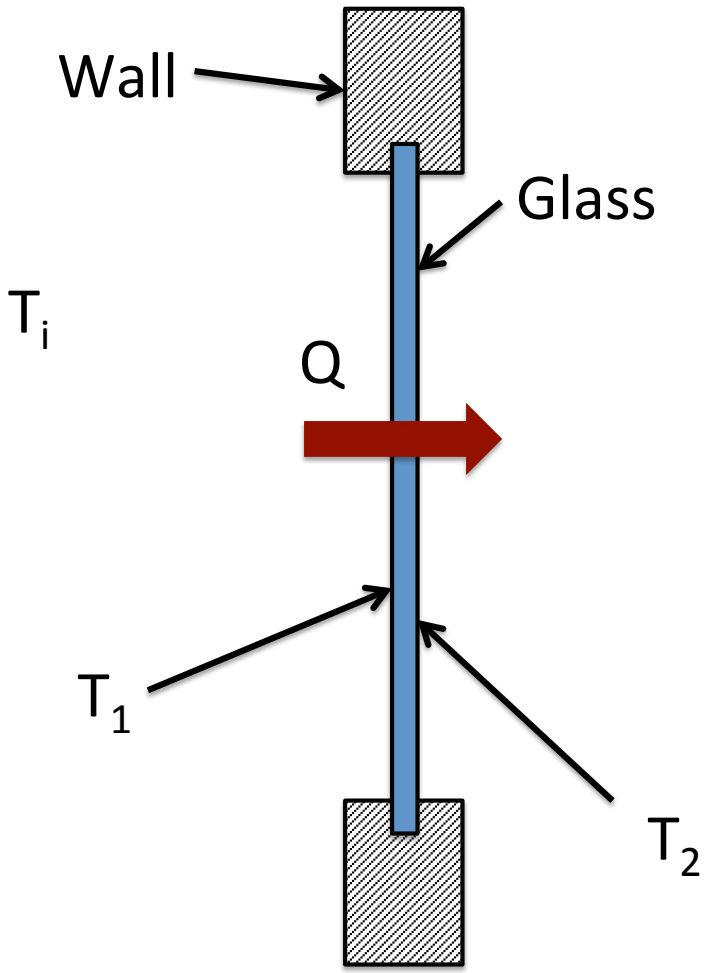
- Tricks are available, given a single set of sampled input [Saltelli, 2002]. E.g., use

$$\mathbb{E}[g(\boldsymbol{\xi}|\xi_i)^2] = \mathbb{E}[g(\boldsymbol{\xi}|\xi_i)g(\boldsymbol{\xi}'|\xi_i)] = \frac{1}{N-1}\sum_{r=1}^{N} g(\boldsymbol{\xi}^{(r)})g(\tilde{\boldsymbol{\xi}}^{(r)}),$$

  where $\tilde{\boldsymbol{\xi}}$ is $\boldsymbol{\xi}'$ with i-th element replaced by ξ_i.
- Similar formulae available for joint sensitivity indices.

- Con: as all Monte-Carlo algorithms, converges slowly.
- Pro: sampling is cheap.

Heat Transfer through a Window



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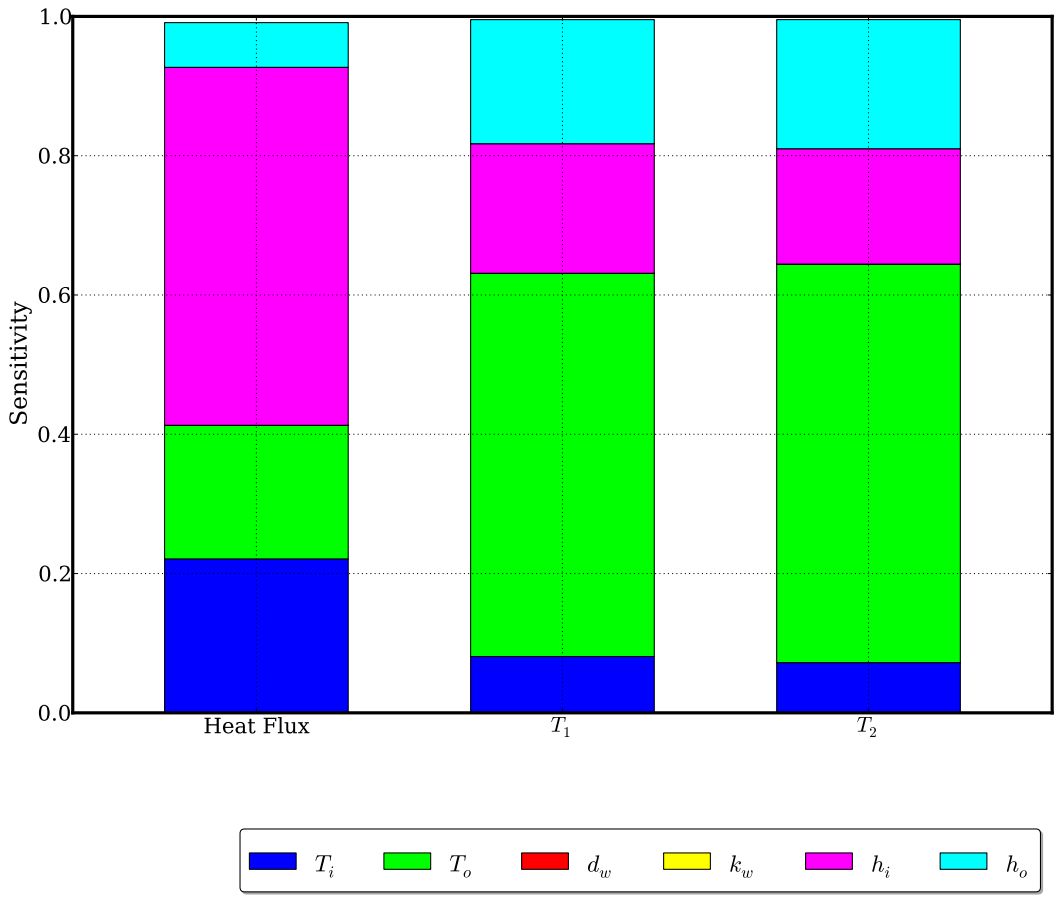
Outputs are most sensitive to ambient temperatures and convective heat transfer coefficients

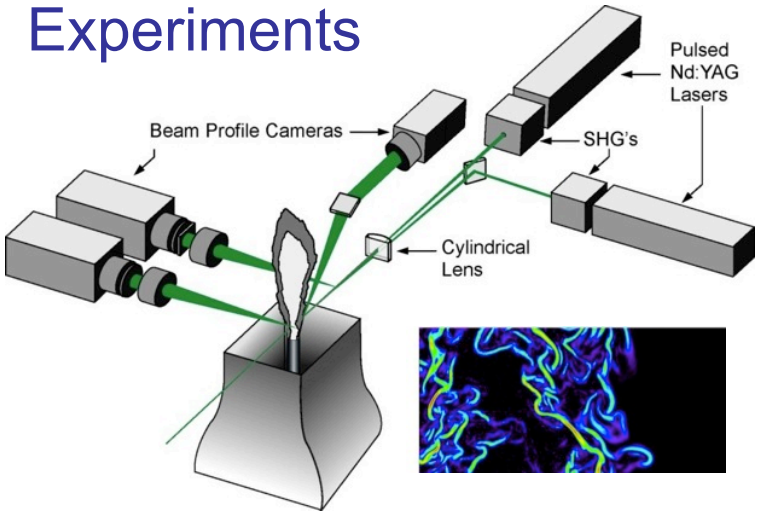


- Main effect sensitivities
  - Sum to 1 only if coupling terms do not matter
- k_w has minimal contribution due to its low uncertainty

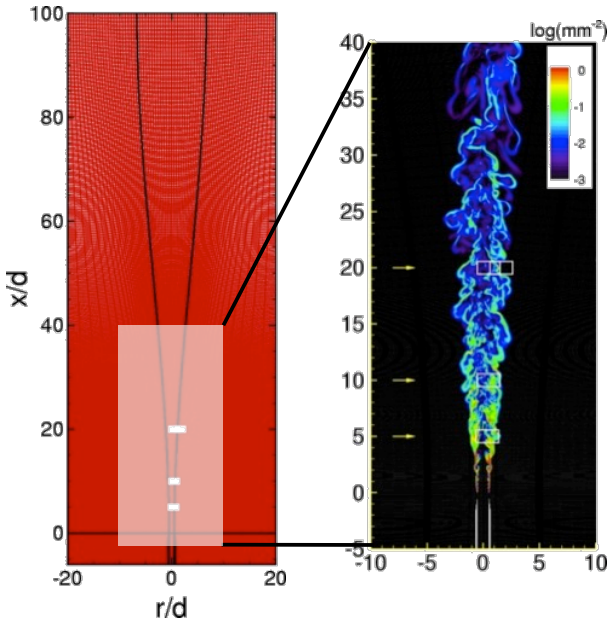
Outline

Experimental data is used to calibrate models

Experiments



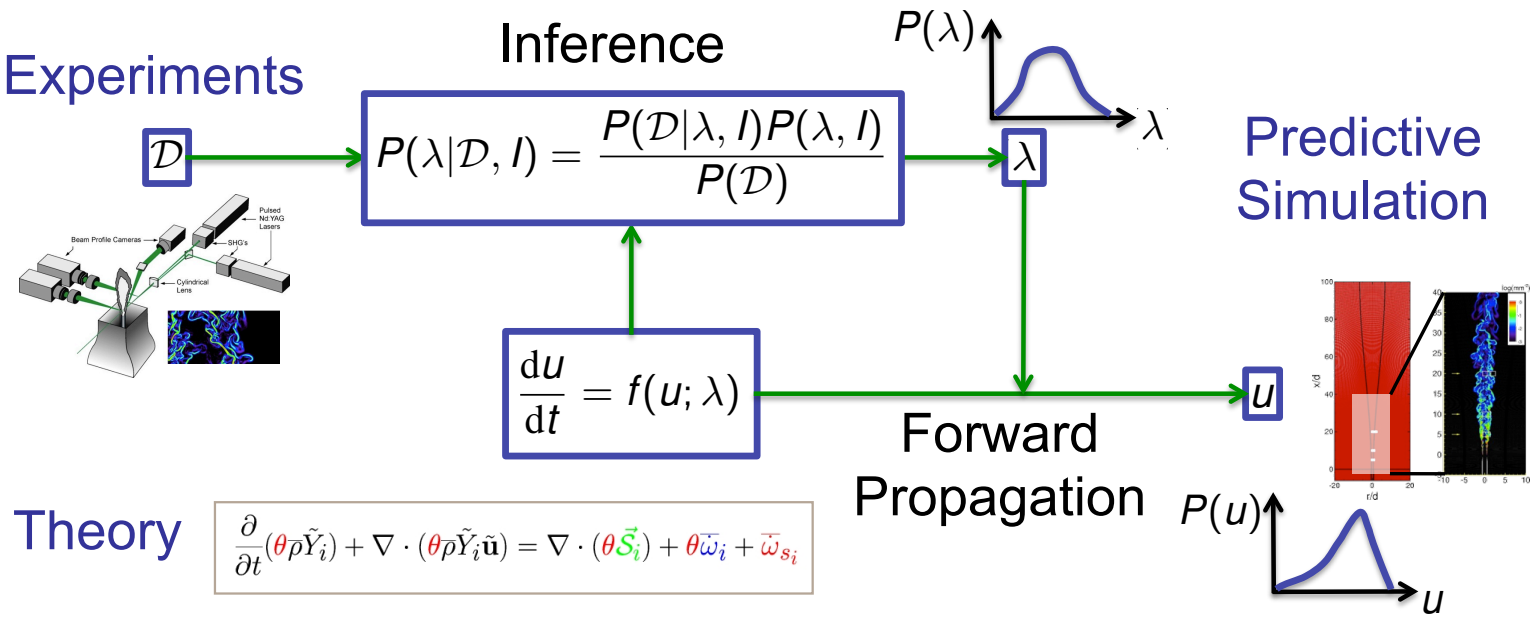
Predictive Simulation



$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\mathcal{S}}_i) + \theta\overline{\dot{\omega}}_i + \overline{\dot{\omega}}_{s_i}$$

Theory

Bayesian inference



- Bayesian inference can handle various sources of data
- Probabilistic formulation readily accommodates various sources of uncertainty

Bayes' rule updates prior belief with information extracted from data

- Bayes' formula

$$\overbrace{P(\boldsymbol{c}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{P(\mathcal{D}|\boldsymbol{c})}^{\text{Likelihood}} \overbrace{P(\boldsymbol{c})}^{\text{Prior}}$$

- Update prior distribution/knowledge about parameter $\boldsymbol{c}$ to posterior distribution given data $\mathcal{D}$, using likelihood function $\mathcal{L}(\boldsymbol{c}) \equiv P(\mathcal{D}|\boldsymbol{c})$
- Data $\mathcal{D} = \{d_i\}_{i=1}^{N}$ - measurements of *some* quantities of interest (QoIs)
- Prior distribution $P(\boldsymbol{c})$ is based on expert opinion/previous literature

Bayes' rule updates prior belief with information extracted from data

- Bayes' formula

$$\overbrace{P(\boldsymbol{c}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{P(\mathcal{D}|\boldsymbol{c})}^{\text{Likelihood}} \overbrace{P(\boldsymbol{c})}^{\text{Prior}}$$

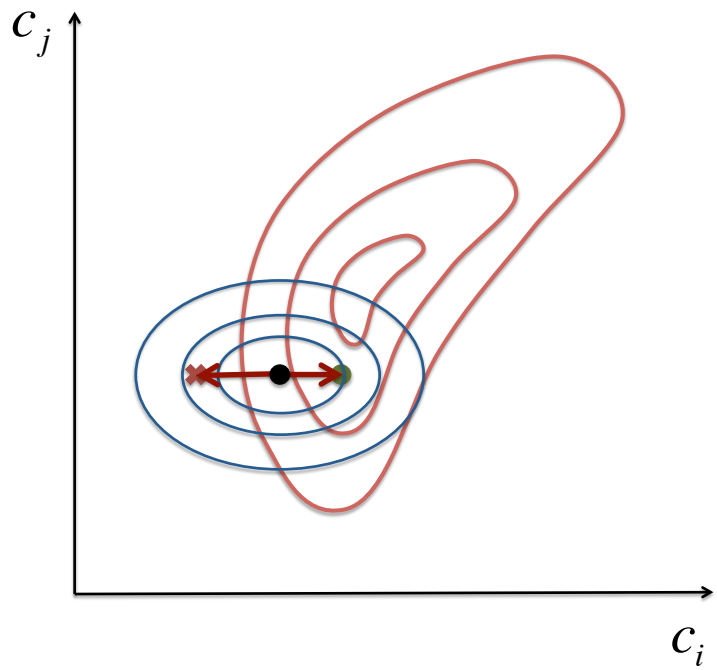
- Likelihood function measures goodness-of-fit and is the key component that connects the model inputs to measured QoIs, e.g.

$$\mathcal{L}(\boldsymbol{c}) = P(\mathcal{D}|\boldsymbol{c}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\sum_{i=1}^{N} \frac{(d_i - f_i(\boldsymbol{c}))^2}{2\sigma^2} \right)$$

- Input parameter $\rightarrow$ output QoI functions $f_i(\cdot)$ could be expensive or not even available
- Posterior distribution generally not analytically tractable: resort to Markov Chain Monte Carlo

Markov Chain Monte Carlo: Single Site

- Set current chain state $\boldsymbol{c}$ at *initial chain state* $\boldsymbol{c}^{(0)}$,
- Repeat for a predefined number (N_{MCMC}) of times,
  - For $k = 1, \ldots, K$,
    - generate a single-site proposal c'_k from a Gaussian distribution centered at the current chain state value of site c_k with *proposal width* σ_k,
    - compute $\alpha = \min\{1, P(\boldsymbol{c}'|D)/P(\boldsymbol{c}|D)\}$,
    - update the current chain state's k-th element $c_k = c'_k$ with probability α,
  - End
- End



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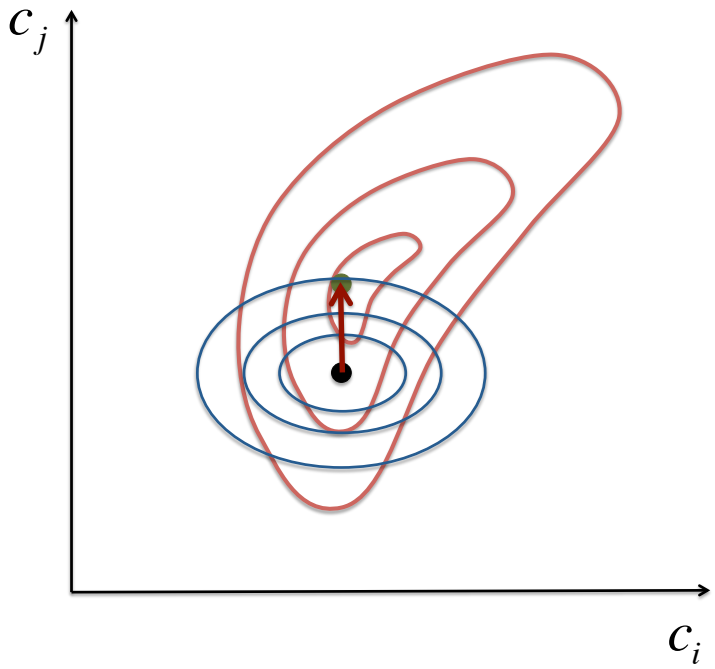
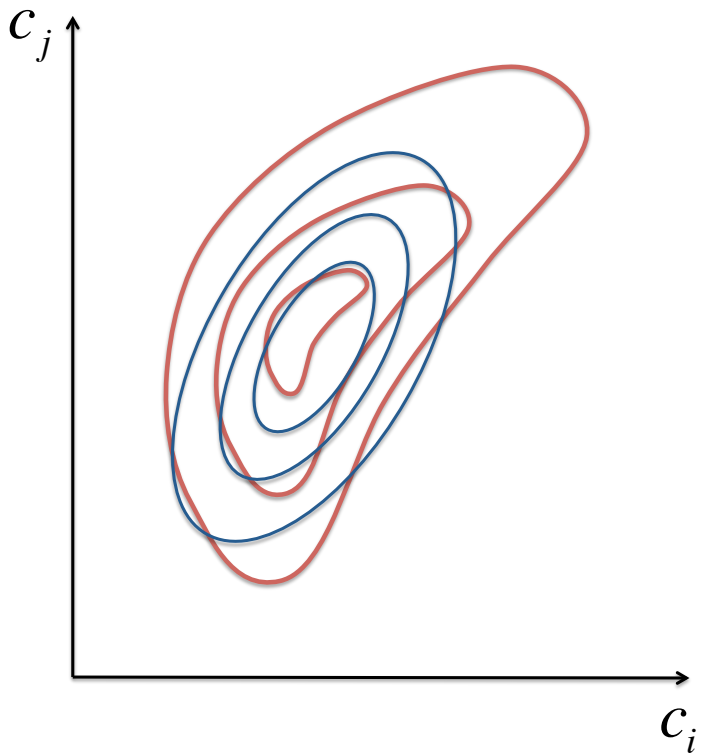


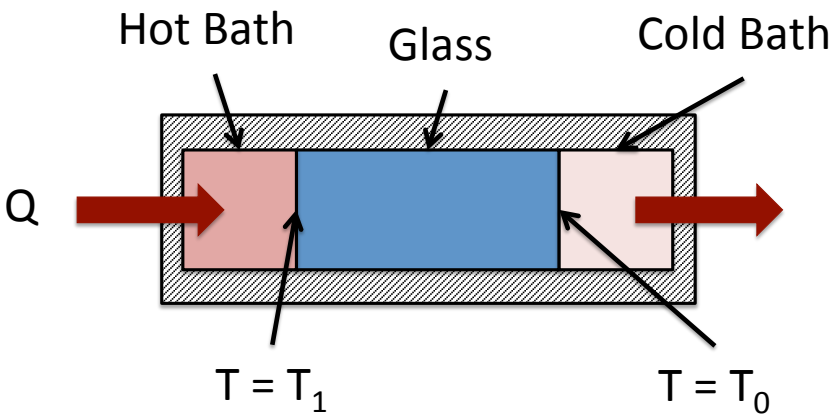
Markov Chain Monte Carlo: Adaptive

- Set current chain state $\boldsymbol{c}$ at *initial chain state* $\boldsymbol{c}^{(0)}$,
- Repeat for a predefined number (N_{MCMC}) of times,
  - generate a proposal $\boldsymbol{c}'$ from a multivariate Gaussian distribution centered at the current chain state value $\boldsymbol{c}$ with *proposal covariance* that is learnt from previous chain states,
  - compute $\alpha = \min\{1, P(\boldsymbol{c}'|D)/P(\boldsymbol{c}|D)\}$,
  - update the current chain state $\boldsymbol{c} = \boldsymbol{c}'$ with probability α,
- End



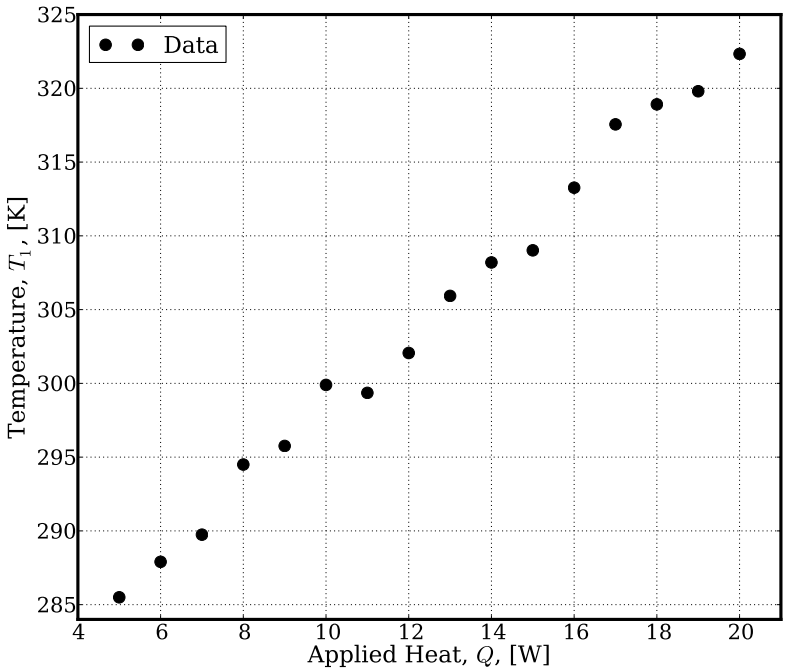
[Haario,2002]

Inference of Conductive Heat Transfer Coefficient



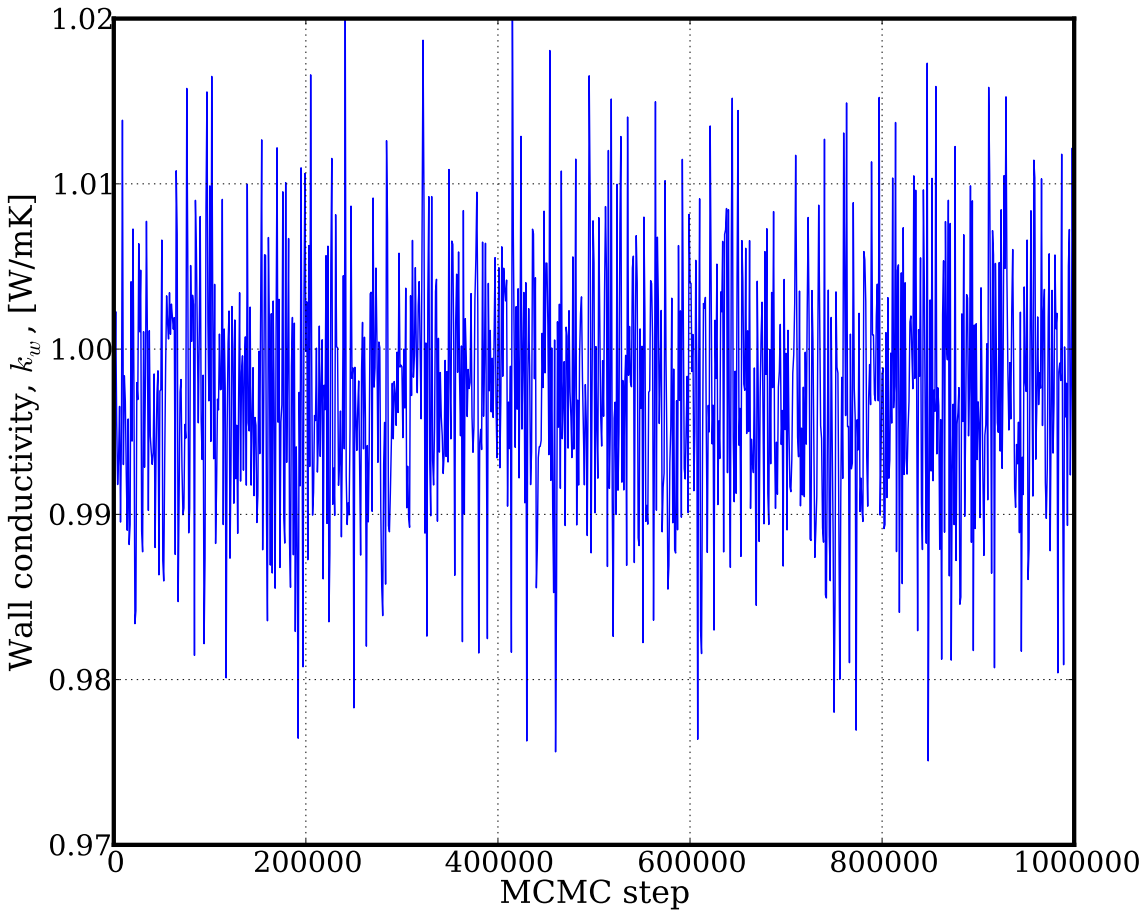
$$Q = k_w A_w \frac{(T_1 - T_0)}{d_w}$$

$$T_0 = 273 \text{ K}, A_w = 0.04 \text{ m}^2$$



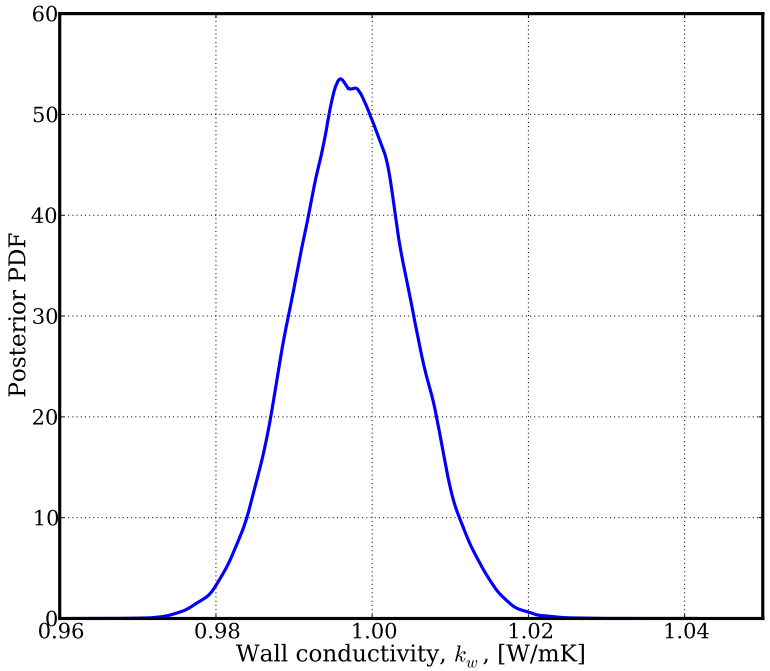
- Piece of glass between two isothermal baths
- Measure T_1 for various applied heat loads Q
- Assume Gaussian measurement noise with $\sigma = 1$ K
- Uniform prior on k_w between 0 and 5 W/mK

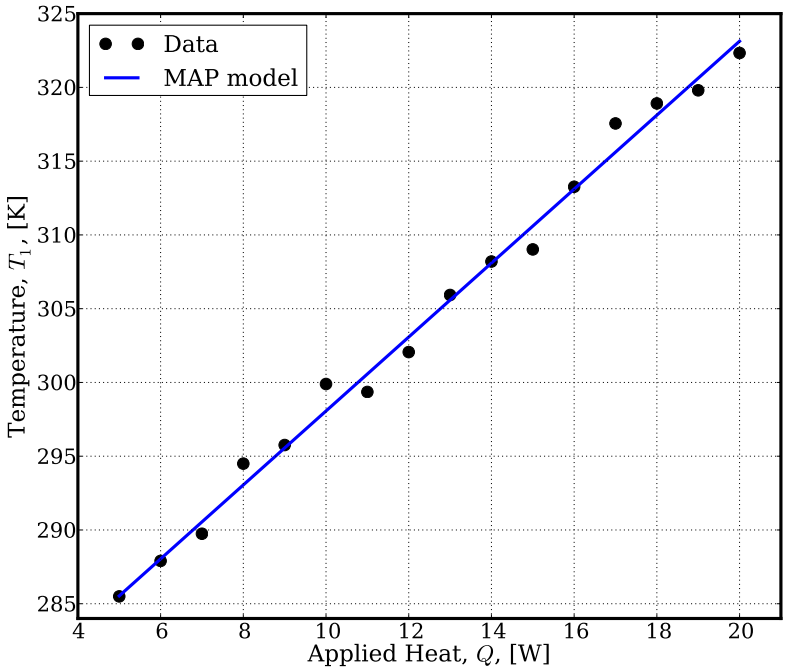
MCMC chain is well mixed



- Used adaptive MCMC with $\gamma = 1$

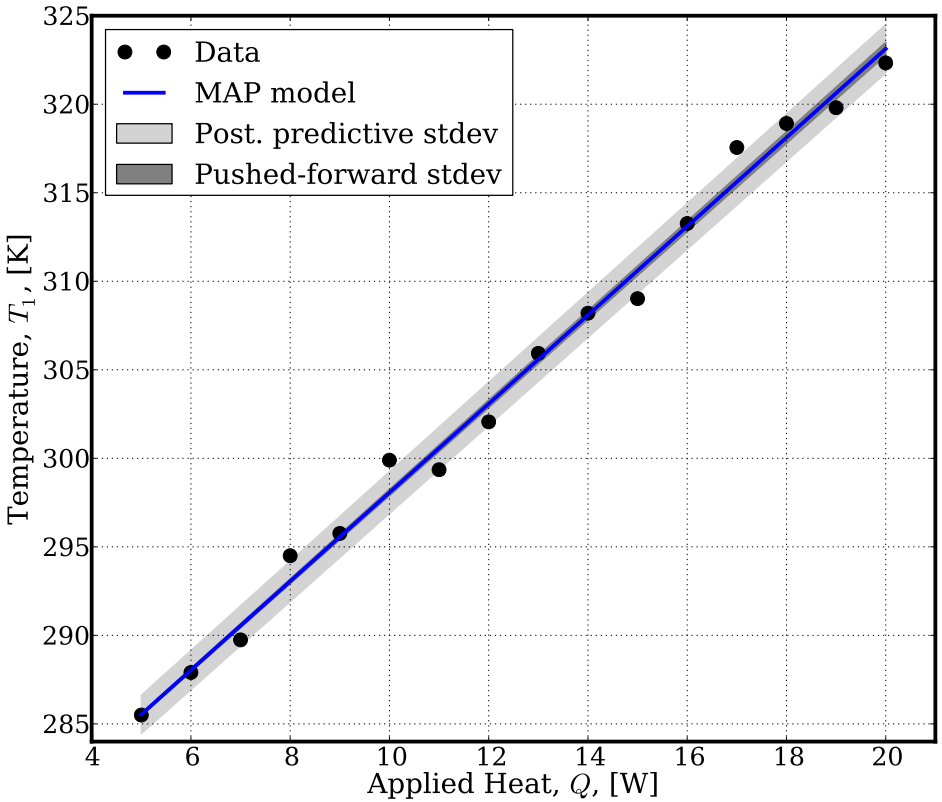
Posterior Distribution and MAP Fit





- Small amount of uncertainty around exact value $k_w = 1$ W/mK
- Maximum A Posteriori (MAP) value for k_w produces good fit to data

Posterior predictive distribution covers original data set



- Pushed forward posterior distribution produces small amount of uncertainty around MAP fit
- Posterior predictive distribution combines posterior uncertainty and measurement noise

Further Reading

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Extra Material on Forward Propagation

- Intrusive operations on PCEs
- Simple ODE example
- Intrusive UQ of incompressible flow
- Uncertainty Quantification Toolkit (UQTk) implementation of intrusive and non-intrusive UQ in surface reaction example (3 ODE system)

Intrusive Galerkin projection reformulates original equations

- Assume $v = f(u; a, \lambda)$, with
  - a deterministic parameter(s)
  - λ uncertain parameter(s)
  - u, v variables of interest (deterministic or uncertain)
- Represent uncertain variables with PCEs

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \qquad v = \sum_{k=0}^{P} v_k \Psi_k(\xi)$$

- Apply Galerkin projection to get PC coefficients of v

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle f(u; a, \lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

- Results in larger, but deterministic set of equations

Projection of linear operations: $v = \gamma + \lambda$

- Assume $v = \gamma + \lambda$, with $\gamma = \sum_{k=0}^{P} \gamma_k \Psi_k$, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (\gamma + \lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned} \langle (\gamma + \lambda) \Psi_k \rangle &= \left\langle \sum_{j=0}^{P} \gamma_j \Psi_j \Psi_k \right\rangle + \left\langle \sum_{j=0}^{P} \lambda_j \Psi_j \Psi_k \right\rangle \\ &= \sum_{j=0}^{P} \gamma_j \langle \Psi_j \Psi_k \rangle + \sum_{j=0}^{P} \lambda_j \langle \Psi_j \Psi_k \rangle \\ &= \gamma_k \langle \Psi_k^2 \rangle + \lambda_k \langle \Psi_k^2 \rangle \end{aligned}$$

- $\Rightarrow \quad v_k = \gamma_k + \lambda_k$

Projection of linear operations: $v = a + \lambda$

- Special case of $v = \gamma + \lambda$, with
  - $\gamma = a\,\Psi_0 = a$
  - $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$
  - $v = \sum_{k=0}^{P} v_k \Psi_k$
- Resulting in
  - $v_0 = a + \lambda_0, \quad v_{k>0} = \lambda_k$
- Deterministic parameter is a special case of a PCE with 0^{th} term only
- Adding a deterministic value to a PCE just shifts its mean

Projection of linear operations: $v = a + \lambda$

- Assume $v = a + \lambda$, with
  a deterministic, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (a+\lambda)\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned} \langle (a+\lambda)\Psi_k \rangle &= \langle a\Psi_k \rangle + \left\langle \sum_{j=0}^{P} \lambda_j \Psi_j \Psi_k \right\rangle \\ &= a \langle \Psi_k \rangle + \sum_{j=0}^{P} \lambda_j \langle \Psi_j \Psi_k \rangle \\ &= a\, \delta_{0k} + \lambda_k \langle \Psi_k^2 \rangle \end{aligned}$$

- $\Rightarrow \quad v_0 = a + \lambda_0, \quad v_{k>0} = \lambda_k$

Projection of linear operations: $v = a\,\lambda$

- Assume $v = a\,\lambda$, with
  a deterministic, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (a\,\lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned} \langle (a\,\lambda) \Psi_k \rangle &= \left\langle a \sum_{j=0}^{P} \lambda_j \Psi_j \Psi_k \right\rangle \\ &= \sum_{j=0}^{P} a\,\lambda_j \langle \Psi_j \Psi_k \rangle \\ &= a\,\lambda_k \langle \Psi_k^2 \rangle \end{aligned}$$

- $\Rightarrow \quad v_k = a\,\lambda_k$

Projection of product: $v = \gamma\ \lambda$

- Assume $v = \gamma\ \lambda$, with $\gamma = \sum_{k=0}^{P} \gamma_k \Psi_k$, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (\gamma\ \lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned}
\langle (\gamma\ \lambda) \Psi_k \rangle &= \left\langle \left(\sum_{i=0}^{P} \gamma_i \Psi_i \sum_{j=0}^{P} \lambda_j \Psi_j \right) \Psi_k \right\rangle \\
&= \left\langle \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_i \lambda_j \Psi_i \Psi_j \Psi_k \right\rangle \\
&= \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_i \lambda_j \langle \Psi_i \Psi_j \Psi_k \rangle
\end{aligned}$$

Projection of product: $v = \gamma\,\lambda$

$$\Rightarrow v_k = \sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_i\lambda_j\frac{\langle\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle} = \sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_i\lambda_j C_{ijk}$$

- $C_{ijk} = \frac{\langle\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle}$
- The C_{ijk} tensor can be computed up front for any given PC order and dimension and stored for use whenever two RVs are multiplied
- This tensor is sparse, *i.e.* many of its elements are zero

1D 4^{th}-Order C_{ijk} Example : Hermite polynomials

$\langle \Psi_i \Psi_j \Psi_k \rangle$	value
$\langle \Psi_0 \Psi_0 \Psi_0 \rangle$	1
$\langle \Psi_0 \Psi_1 \Psi_1 \rangle$	1
$\langle \Psi_0 \Psi_2 \Psi_2 \rangle$	2
$\langle \Psi_0 \Psi_3 \Psi_3 \rangle$	6
$\langle \Psi_0 \Psi_4 \Psi_4 \rangle$	24
$\langle \Psi_1 \Psi_1 \Psi_2 \rangle$	2
$\langle \Psi_1 \Psi_2 \Psi_3 \rangle$	6
$\langle \Psi_1 \Psi_3 \Psi_4 \rangle$	24
$\langle \Psi_2 \Psi_2 \Psi_2 \rangle$	8
$\langle \Psi_2 \Psi_2 \Psi_4 \rangle$	24
$\langle \Psi_2 \Psi_3 \Psi_3 \rangle$	36
$\langle \Psi_2 \Psi_4 \Psi_4 \rangle$	192
$\langle \Psi_3 \Psi_3 \Psi_4 \rangle$	216
$\langle \Psi_4 \Psi_4 \Psi_4 \rangle$	1728

k	$\langle \Psi_k^2 \rangle$
0	1
1	1
2	2
3	6
4	24

- $C_{ijk} = \langle \Psi_i \Psi_j \Psi_k \rangle \, / \, \langle \Psi_k^2 \rangle$
- and,

$$\begin{aligned} \langle \Psi_i \Psi_j \Psi_k \rangle &= \langle \Psi_i \Psi_k \Psi_j \rangle = \\ \langle \Psi_j \Psi_i \Psi_k \rangle &= \langle \Psi_j \Psi_k \Psi_i \rangle = \\ \langle \Psi_k \Psi_i \Psi_j \rangle &= \langle \Psi_k \Psi_j \Psi_i \rangle \end{aligned}$$

- with other not-reported $\langle \Psi_i \Psi_j \Psi_k \rangle$ zero

1D 4^{th}-Order C_{ijk} Example : Legendre polynomials

$\langle \Psi_i \Psi_j \Psi_k \rangle$	value
$\langle \Psi_0 \Psi_0 \Psi_0 \rangle$	1
$\langle \Psi_0 \Psi_1 \Psi_1 \rangle$	1/3
$\langle \Psi_0 \Psi_2 \Psi_2 \rangle$	1/5
$\langle \Psi_0 \Psi_3 \Psi_3 \rangle$	1/7
$\langle \Psi_0 \Psi_4 \Psi_4 \rangle$	1/9
$\langle \Psi_1 \Psi_1 \Psi_2 \rangle$	2/15
$\langle \Psi_1 \Psi_2 \Psi_3 \rangle$	3/35
$\langle \Psi_1 \Psi_3 \Psi_4 \rangle$	4/63
$\langle \Psi_2 \Psi_2 \Psi_2 \rangle$	2/35
$\langle \Psi_2 \Psi_2 \Psi_4 \rangle$	2/35
$\langle \Psi_2 \Psi_3 \Psi_3 \rangle$	4/105
$\langle \Psi_2 \Psi_4 \Psi_4 \rangle$	$\approx$0.029
$\langle \Psi_3 \Psi_3 \Psi_4 \rangle$	$\approx$0.026
$\langle \Psi_4 \Psi_4 \Psi_4 \rangle$	$\approx$0.018

k	$\langle \Psi_k^2 \rangle$
0	1
1	1/3
2	1/5
3	1/7
4	1/9

- $C_{ijk} = \langle \Psi_i \Psi_j \Psi_k \rangle \, / \, \langle \Psi_k^2 \rangle$
- and,

$$\begin{aligned} \langle \Psi_i \Psi_j \Psi_k \rangle &= \langle \Psi_i \Psi_k \Psi_j \rangle = \\ \langle \Psi_j \Psi_i \Psi_k \rangle &= \langle \Psi_j \Psi_k \Psi_i \rangle = \\ \langle \Psi_k \Psi_i \Psi_j \rangle &= \langle \Psi_k \Psi_j \Psi_i \rangle \end{aligned}$$

- with other not-reported $\langle \Psi_i \Psi_j \Psi_k \rangle$ zero

Projection of triple product: $v = \gamma\ \lambda\ u$

- Assume $v = \gamma\ \lambda\ u$, with $\gamma = \sum_{k=0}^{P} \gamma_k \Psi_k$, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, $u = \sum_{k=0}^{P} u_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (\gamma\ \lambda\ u) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned}
\langle (\gamma\ \lambda\ u) \Psi_k \rangle &= \left\langle \left(\sum_{l=0}^{P} \gamma_l \Psi_l \sum_{i=0}^{P} \lambda_i \Psi_i \sum_{j=0}^{P} u_j \Psi_j \right) \Psi_k \right\rangle \\
&= \left\langle \sum_{l=0}^{P} \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_l \lambda_i u_j \Psi_l \Psi_i \Psi_j \Psi_k \right\rangle \\
&= \sum_{l=0}^{P} \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_l \lambda_i u_j \langle \Psi_l \Psi_i \Psi_j \Psi_k \rangle
\end{aligned}$$

Projection of triple product: $v = \gamma\ \lambda\ u$

$$\Rightarrow v_k = \sum_{l=0}^{P}\sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_l\lambda_i u_j \frac{\langle\Psi_l\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle} = \sum_{l=0}^{P}\sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_l\lambda_i u_j D_{lijk}$$

- $D_{lijk} = \frac{\langle\Psi_l\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle}$
- The D_{lijk} tensor can also be computed up front for any given PC order and dimension and stored for use whenever three RVs are multiplied
- While this tensor is sparse, it can be expensive to compute and store
- This fully spectral formulation is even less practical for higher order products

Pseudo-spectral triple product: $v = \gamma\ \lambda\ u$

- Assume $v = \gamma\ \lambda$, with $\gamma = \sum_{k=0}^{P} \gamma_k \Psi_k$, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, $u = \sum_{k=0}^{P} u_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Perform product in sub-steps

$$\begin{aligned} v = \gamma\ \lambda\ u &= ((\gamma\ \lambda)u) \\ &= \tilde{v}u \end{aligned}$$

- Each sub-step can be performed with regular binary product formula

$$\begin{aligned} \tilde{v} &= \gamma\ \lambda \\ v &= \tilde{v}u \end{aligned}$$

Pseudo-spectral product readily generalizes to higher order products

- Decompose higher order products or powers in sequences of binary products
  - Equivalent to successive multiplication (accounting for terms up to order $2p$) and projecting back to order p
- Efficient and convenient
- Can lead to aliasing errors due to loss of information in higher order modes
- See also [Debusschere *et al.*, *S*IAM J. Sci. Comp, 2004]

Intrusive propagation through non-polynomial functions

Addition, subtraction, and product allow (pseudo-)spectral evaluation of all polynomial functions

How to propagate PC expansions ($\{u_k\} \Rightarrow \{v_k\}$) through transcendental functions

$$v = \frac{1}{u}, \quad v = \ln u, \quad \text{or} \quad v = e^u$$

- Use local polynomial approximations, *e.g.* Taylor series
- Rework operation into a system of equations
- Integration approach
- Borchardt-Gauss Algorithm: Arithmetic-Geometric Mean (AGM) series

[Debusschere *et al.*, SISC 2004; McKale, Texas Tech, M.S. Thesis, 2011]

Taylor series allows computation of many transcendental functions

- Provides local polynomial approximation
  - *E.g.* $e^u = 1 + \frac{u}{1!} + \frac{u^2}{2!} + \frac{u^3}{3!} + \ldots$
- Expanding the series for $f(u)$ around u_0 speeds up convergence
- Works well in most cases, especially for small uncertainties
- Not very robust for larger uncertainties
  - Series can take too long to converge
  - High-order PC multiplications lead to aliasing
  - Instabilities if Taylor series range of convergence exceeded; *e.g.* $\log(u)$ expanded around u_0 only converges for $|u - u_0| < 1$

Inversion and division can be computed through a system of equations

- Assume three uncertain variables u, v, and w

$$w = \frac{u}{v} \Rightarrow \qquad v\ w = u$$

- Mode k of the stochastic product

$$\sum_{i=0}^{P}\sum_{j=0}^{P} C_{ijk}\, v_i\ w_j = u_k$$

- System of $P+1$ linear equations in w_j with known u_k and v_i,

$$V_{kj} = \sum_{i=0}^{P} C_{ijk}\, v_i \quad \Rightarrow \quad \mathbf{Vw} = \mathbf{u}$$

- More robust than Taylor series expansion for $1/u$

Integration approach for non-polynomial functions

- Consider the ODE $\frac{\mathrm{d}v}{\mathrm{d}u} = v$, with solution $v = e^u$ $\Rightarrow f(u) = e^u$ can be obtained from

$$\mathrm{d}v = v\,\mathrm{d}u \qquad \Rightarrow \qquad e^u - e^{u_o} = \int_{u_o}^{u} v\,\mathrm{d}u$$

- Similarly for e^{-u^2}, and $\ln(u)$

$$e^{-u^2} - e^{-u_o^2} = \int_{u_o}^{u} -2uv\,\mathrm{d}u, \qquad \ln(u) - \ln(u_o) = \int_{u_o}^{u} \frac{\mathrm{d}u}{u}$$

- Accurate if PC order is high enough to properly capture the random variable $v = f(u)$

More general formulation of integration approach for irrational functions

- To evaluate $v(u)$, $u = \sum_{k=0}^{P} u_k \Psi_k$, $v = \sum_{k=0}^{P} v_k \Psi_k$,
  - Use a deterministic IC u_a such that $v(u_a)$ is known
  - Express $\dot{v} = \mathrm{d}v/\mathrm{d}u = f(v, u)$;
    ... **require**: f is a rational function
    ... ensures that $(\dot{v})_k$ are found from v_k and u_k coeffs
  - Evaluate the integral:

$$v_k(u_b) - v_k(u_a) = \sum_{j=0}^{P} \int_{(u_a)_j}^{(u_b)_j} \sum_{i=0}^{P} C_{ijk} (\dot{v})_i \, \mathrm{d}u_j$$

- ok for e^u, e^{u^2}, and $\ln(u)$, with $\dot{v} = v$, $2uv$, and $1/u$ resp.
  - but not for $e^{\sin u}$, with $\dot{v} = v \cos u$
- More robust than Taylor series, but CPU-intensive

Overloading of operations

- Construction allows for a general representation using pseudo-spectral (PS) overloaded operations.
  - *E.g.* multiplication operation '$*$'

$$w = \lambda * u * u * v$$

    - Each deterministic function multiplication is transformed into a corresponding PC product
- Potential meta-code: take a general deterministic code function $F(u)$, produce a pseudo-spectral stochastic function $\tilde{F}(\tilde{u})$
  - Possibility of transforming legacy deterministic code into corresponding pseudo-spectral stochastic code.
  - UQToolkit: contains library of utilities for operations on random variables represented with PCEs

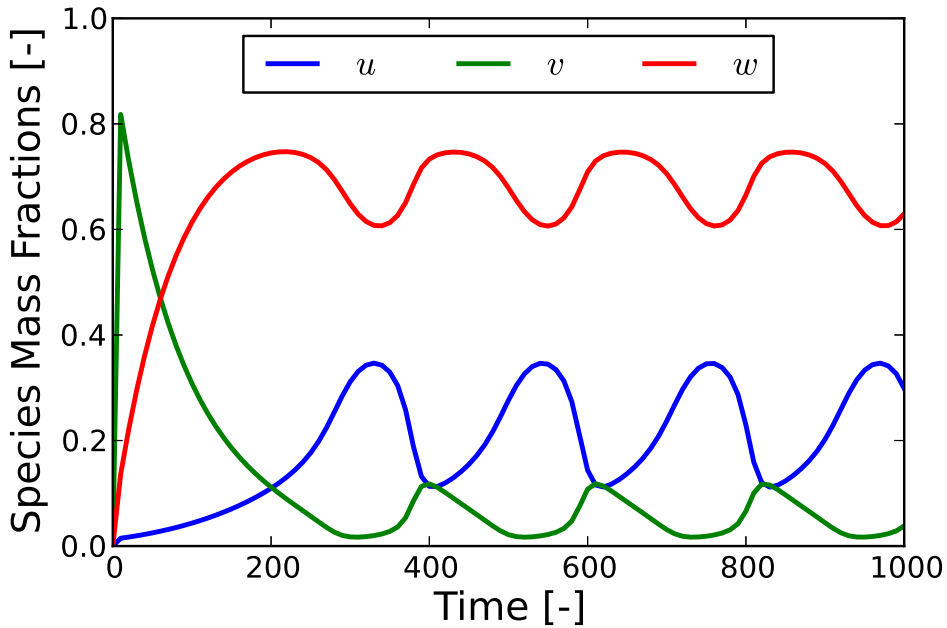
Surface Reaction Model

3 ODEs for a monomer (u), dimer (v), and inert species (w) adsorbing onto a surface out of gas phase.

$$\begin{aligned}
\frac{\mathrm{d}u}{\mathrm{d}t} &= az - cu - 4duv \\
\frac{\mathrm{d}v}{\mathrm{d}t} &= 2bz^2 - 4duv \\
\frac{\mathrm{d}w}{\mathrm{d}t} &= ez - fw \\
z &= 1 - u - v - w
\end{aligned}$$

$$u(0) = v(0) = w(0) = 0.0$$

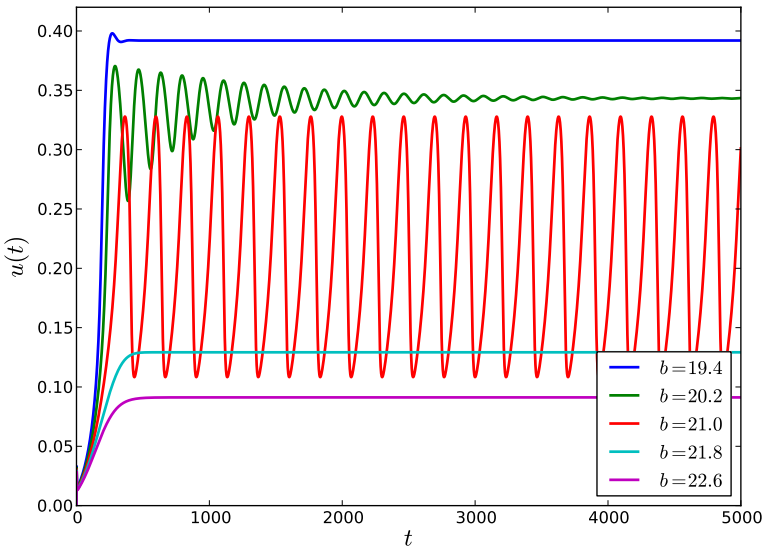
$$\begin{aligned}
a &= 1.6 \quad b = 20.75 \quad c = 0.04 \\
d &= 1.0 \quad e = 0.36 \quad f = 0.016
\end{aligned}$$

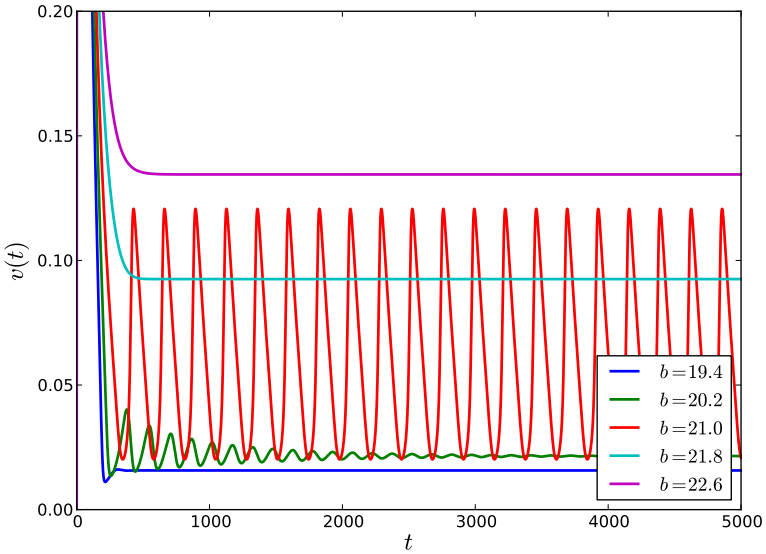


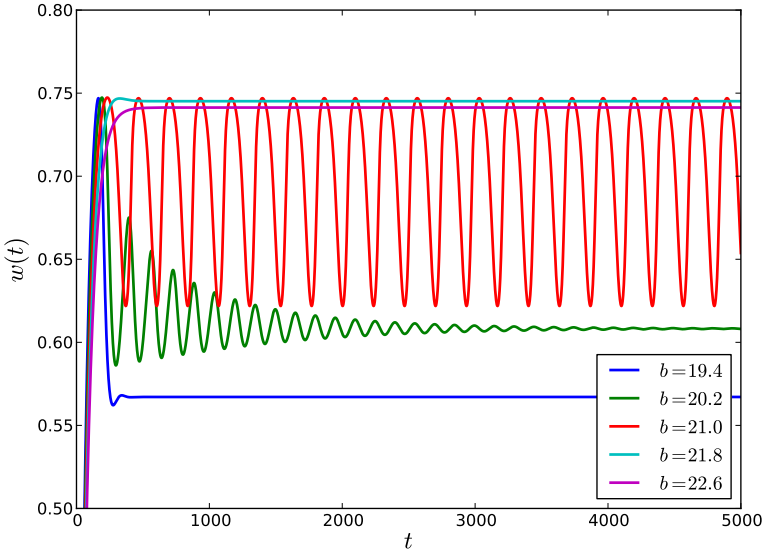
Oscillatory behavior for $b \in [20.2, 21.2]$

[Vigil *et al.*, Phys. Rev. E., 1996; Makeev *et al.*, J. Chem. Phys., 2002]

Surface reaction model shows wide range of dynamics







$$a = 1.6 \quad b = [19.4 \ldots 22.6]$$
$$c = 0.04 \quad d = 1.0$$
$$e = 0.36 \quad f = 0.016$$

Surface Reaction Model: Intrusive Spectral Propagation (ISP) of Uncertainty

- Assume PCE for uncertain parameter b and for the output variables, u, v, w
- Substitute PCEs into the governing equations
- Project the governing equations onto the PC basis functions
  - Multiply with Ψ_k and take the expectation
- Apply pseudo-spectral approximations where necessary

Surface Reaction Model: Specify PCEs for inputs and outputs

Represent uncertain inputs with PCEs with known coefficients:

$$b = \sum_{i=0}^{P} b_i \Psi_i(\xi)$$

Represent all uncertain variables with PCEs with unknown coefficients:

$$u(t) = \sum_{i=0}^{P} u_i(t)\Psi_i(\xi) \qquad v(t) = \sum_{i=0}^{P} v_i(t)\Psi_i(\xi)$$

$$w(t) = \sum_{i=0}^{P} w_i(t)\Psi_i(\xi) \qquad z(t) = \sum_{i=0}^{P} z_i(t)\Psi_i(\xi)$$

Surface Reaction Model: Substitute PCEs into governing equations and project onto basis functions

$$
\begin{aligned}
\frac{\mathrm{d}u}{\mathrm{d}t} &= az - cu - 4duv \\
\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} u_i\Psi_i &= a\sum_{i=0}^{P} z_i\Psi_i - c\sum_{i=0}^{P} u_i\Psi_i - 4d\sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j \\
\left\langle \Psi_k \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} u_i\Psi_i \right\rangle &= \left\langle a\Psi_k \sum_{i=0}^{P} z_i\Psi_i \right\rangle - \left\langle c\Psi_k \sum_{i=0}^{P} u_i\Psi_i \right\rangle \\
&- \left\langle 4d\Psi_k \sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j \right\rangle
\end{aligned}
$$

Surface Reaction Model: Reorganize terms

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k \left\langle \Psi_k^2 \right\rangle = a z_k \left\langle \Psi_k^2 \right\rangle - c u_k \left\langle \Psi_k^2 \right\rangle - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \left\langle \Psi_i \Psi_j \Psi_k \right\rangle$$

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k = a z_k - c u_k - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k = a z_k - c u_k - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j C_{ijk}$$

- Triple products $C_{ijk} = \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle}$ can be pre-computed and stored for repeated use

Surface Reaction Model: Substitute PCEs into governing equations and project onto basis functions

$$\frac{\mathrm{d}v}{\mathrm{d}t} = 2bz^2 - 4duv$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} v_i\Psi_i = 2\sum_{h=0}^{P} b_h\Psi_h \sum_{i=0}^{P} z_i\Psi_i \sum_{j=0}^{P} z_j\Psi_j - 4d\sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j$$

$$\left\langle \Psi_k \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{P} v_i\Psi_i \right\rangle = \left\langle 2\Psi_k \sum_{h=0}^{P} b_h\Psi_h \sum_{i=0}^{P} z_i\Psi_i \sum_{j=0}^{P} z_j\Psi_j \right\rangle$$

$$- \left\langle 4d\Psi_k \sum_{i=0}^{P} u_i\Psi_i \sum_{j=0}^{P} v_j\Psi_j \right\rangle$$

Surface Reaction Model: Reorganize terms

$$\frac{\mathrm{d}}{\mathrm{d}t} v_k \left\langle \Psi_k^2 \right\rangle = 2 \sum_{h=0}^{P} \sum_{i=0}^{P} \sum_{j=0}^{P} b_h z_i z_j \left\langle \Psi_h \Psi_i \Psi_j \Psi_k \right\rangle - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \left\langle \Psi_i \Psi_j \Psi_k \right\rangle$$

$$\frac{\mathrm{d}}{\mathrm{d}t} v_k = 2 \sum_{h=0}^{P} \sum_{i=0}^{P} \sum_{j=0}^{P} b_h z_i z_j \frac{\left\langle \Psi_h \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle} - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k^2 \right\rangle}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} v_k = 2 \sum_{h=0}^{P} \sum_{i=0}^{P} \sum_{j=0}^{P} b_h z_i z_j D_{hijk} - 4d \sum_{i=0}^{P} \sum_{j=0}^{P} u_i v_j C_{ijk}$$

- Pre-computing and storing the quad product D_{hijk} becomes cumbersome
- Use pseudo-spectral approach instead

Surface Reaction Model: Pseudo-Spectral approach for products

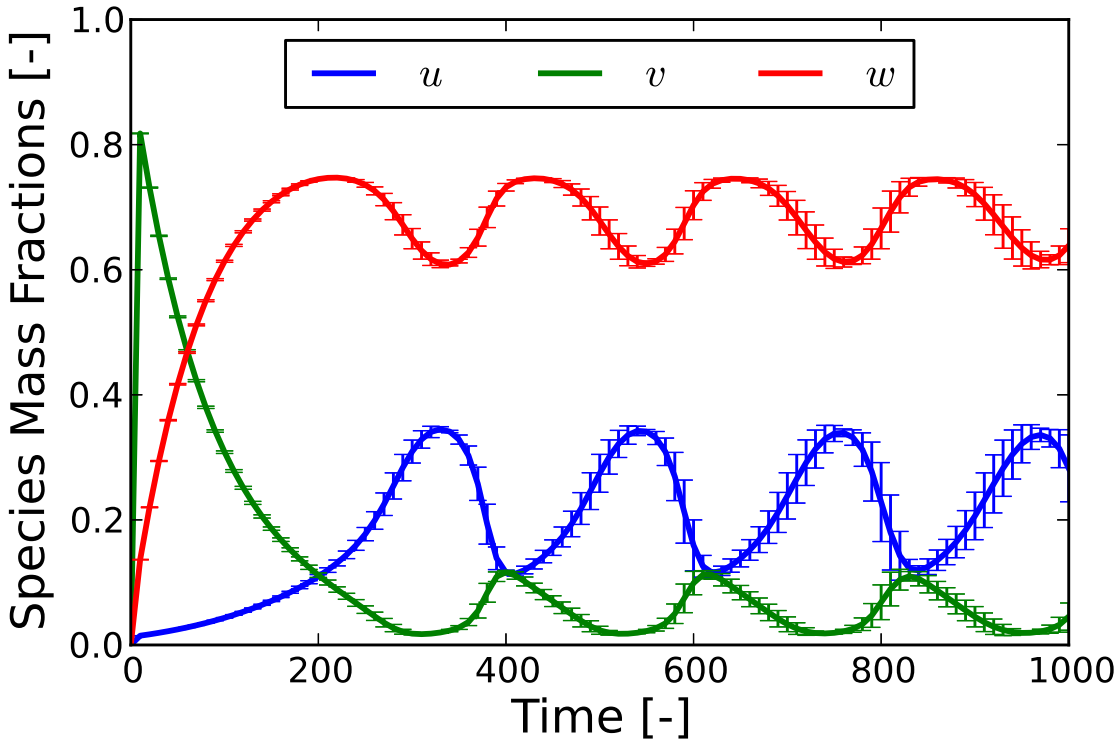
- Introduce auxiliary variable $g = z^2$

$$\begin{aligned} g &= z^2 \\ f = 2bz^2 &= 2bg \end{aligned}$$

$$\begin{aligned} g_k &= \sum_{i=0}^{P}\sum_{j=0}^{P} z_i z_j C_{ijk} \\ f_k &= 2\sum_{i=0}^{P}\sum_{j=0}^{P} b_i g_j C_{ijk} \end{aligned}$$

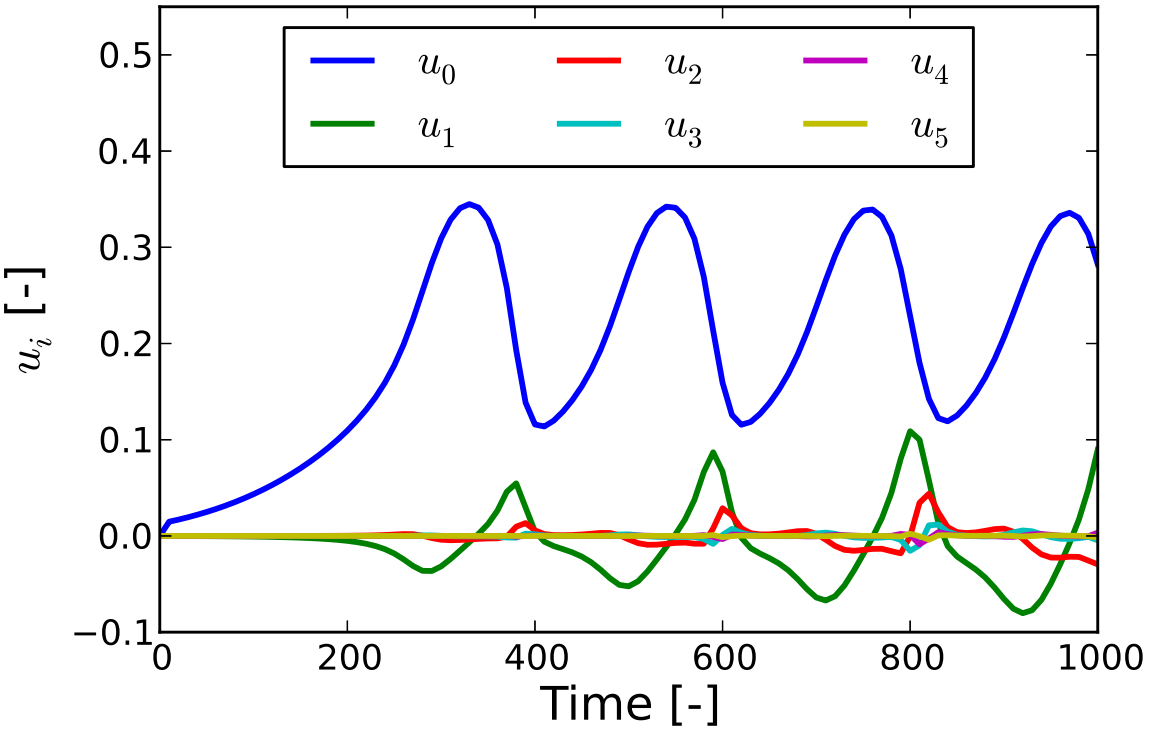
- Limits the complexity of computing product terms
  - Higher products can be computed by repeated use of the same binary product rule
- Does introduce errors if order of PCE is not large enough

Surface Reaction Model: ISP results



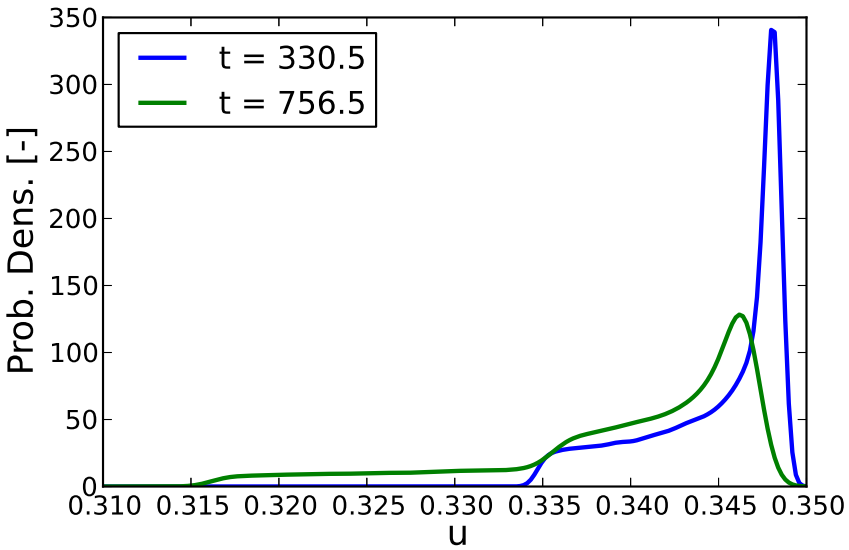
- Assume 0.5% uncertainty in b around nominal value
- Legendre-Uniform intrusive PC
- Mean and standard deviation for u, v, and w
- Uncertainty grows in time

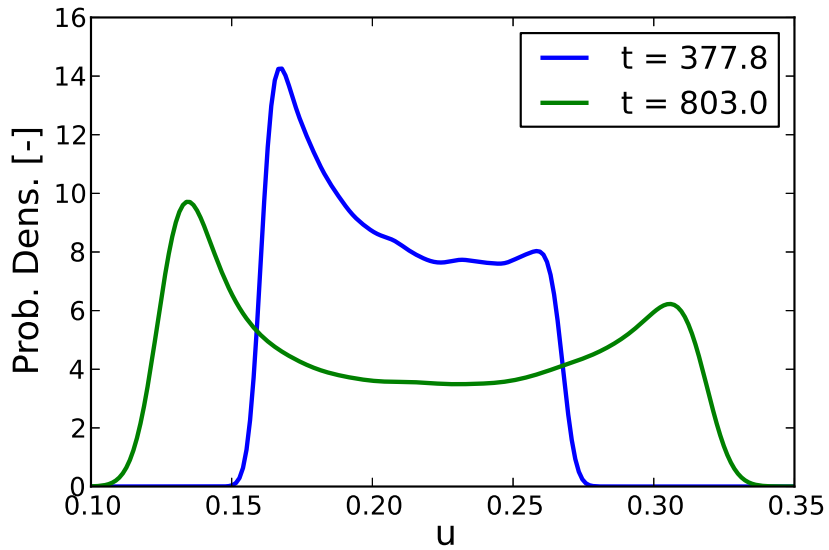
Surface Reaction Model: ISP results



- Modes of *u*
- Modes decay with higher order
- Amplitudes of oscillations of higher order modes grow in time

Surface Reaction Model: ISP results: PDFs





- Pdfs of u at maximum mean (left) and maximum standard deviation (right)
- Distributions get broader and multimodal as time increases
  - Effect of accumulating uncertainty in phase of oscillation

Extra Material on Forward Propagation

- Intrusive operations on PCEs
- Simple ODE example
- Intrusive UQ of incompressible flow
- Uncertainty Quantification Toolkit (UQTk) implementation of intrusive and non-intrusive UQ in surface reaction example (3 ODE system)

Intrusive Spectral Stochastic UQ Formulation: ODE Example

- Sample ODE with parameter λ:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \lambda u$$

- Let λ be uncertain; introduce $\xi \sim \mathcal{N}(0,1)$.
- Express λ and u using PCEs in ξ:

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \qquad u(t) = \sum_{k=0}^{P} u_k(t) \Psi_k(\xi)$$

- Substitute in ODE and apply a Galerkin projection on $\Psi_i(\xi)$,

Galerkin Projection on $\Psi_i(\xi)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{k=0}^{P} u_k(t)\Psi_k(\xi)\right) = \left(\sum_{p=0}^{P}\lambda_p\Psi_p(\xi)\right)\left(\sum_{q=0}^{P} u_q(t)\Psi_q(\xi)\right)$$

$$\sum_{k=0}^{P}\frac{\mathrm{d}u_k(t)}{\mathrm{d}t}\Psi_k(\xi) = \sum_{p=0}^{P}\sum_{q=0}^{P}\lambda_p u_q(t)\Psi_p(\xi)\Psi_q(\xi)$$

$$\left\langle\sum_{k=0}^{P}\frac{\mathrm{d}u_k(t)}{\mathrm{d}t}\Psi_k(\xi)\Psi_i(\xi)\right\rangle = \left\langle\sum_{p=0}^{P}\sum_{q=0}^{P}\lambda_p u_q(t)\Psi_p(\xi)\Psi_q(\xi)\Psi_i(\xi)\right\rangle$$

$$\sum_{k=0}^{P}\frac{\mathrm{d}u_k(t)}{\mathrm{d}t}\left\langle\Psi_k(\xi)\Psi_i(\xi)\right\rangle = \sum_{p=0}^{P}\sum_{q=0}^{P}\lambda_p u_q(t)\left\langle\Psi_p(\xi)\Psi_q(\xi)\Psi_i(\xi)\right\rangle$$

$$\frac{\mathrm{d}u_i}{\mathrm{d}t}\left\langle\Psi_i^2\right\rangle = \sum_{p=0}^{P}\sum_{q=0}^{P}\lambda_p u_q\left\langle\Psi_p\Psi_q\Psi_i\right\rangle$$

Resulting Spectral ODE system

- $(P+1)$-dimensional ODE system

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

  where $C_{pqi} = \langle \Psi_p \Psi_q \Psi_i \rangle / \langle \Psi_i^2 \rangle$
- The tensor C_{pqi} can be evaluated once and stored for any given PC order and dimension
- This tensor is sparse, i.e. many elements are zero

Pseudo-Spectral Construction–1

$$w = \lambda u^2 v, \qquad u = \sum_{k=0}^{P} u_k \Psi_k, \qquad \text{similarly for } \lambda \ \& \ v$$

Spectral:

$$\begin{aligned} w_i &= \left\langle \lambda u^2 v \right\rangle_i \\ &= \sum_{j=0}^{P} \sum_{k=0}^{P} \sum_{l=0}^{P} \sum_{m=0}^{P} \lambda_j u_k u_l v_m \left\langle \Psi_j \Psi_k \Psi_l \Psi_m \right\rangle_i , \quad i = 0, \ldots, P \end{aligned}$$

- The corresponding tensor of basis product expectations becomes too large to pre-compute and store

Pseudo-Spectral: Project each PC product onto a $(P+1)$-polynomial before proceeding further, thus:

Pseudo-Spectral Construction–2

$$\tilde{w} = uv \quad : \quad \tilde{w}_i = \langle uv \rangle_i = \sum_{j=0}^{P} \sum_{k=0}^{P} u_k v_j \langle \Psi_k \Psi_j \rangle_i , \quad i = 0, \ldots, P$$

$$\hat{w} = u\tilde{w} \quad : \quad \hat{w}_i = \langle u\tilde{w} \rangle_i = \sum_{j=0}^{P} \sum_{k=0}^{P} u_k \tilde{w}_j \langle \Psi_k \Psi_j \rangle_i , \quad i = 0, \ldots, P$$

$$w = \lambda\hat{w} \quad : \quad w_i = \langle \lambda\hat{w} \rangle_i = \sum_{j=0}^{P} \sum_{k=0}^{P} \lambda_k \hat{w}_j \langle \Psi_k \Psi_j \rangle_i , \quad i = 0, \ldots, P$$

- Aliasing errors
- Efficiency, and convenience

[Debusschere *et al.*, *SIAM J. Sci. Comp.*, 2004.]

Extra Material on Forward Propagation

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Spectral UQ: Incompressible Flow - Stochastic Projection Method

- $(P+1)$ Galerkin-Projected Mom./Cont. Eqns, $q = 0, \ldots, P$:

$$\begin{aligned} \frac{\partial \boldsymbol{v}_q}{\partial t} + \nabla \cdot \langle \boldsymbol{v}\boldsymbol{v} \rangle_q &= -\nabla p_q + \frac{1}{\mathrm{Re}} \nabla \cdot \left\langle \mu[(\nabla \boldsymbol{v}) + (\nabla \boldsymbol{v})^T] \right\rangle_q \\ \nabla \cdot \boldsymbol{v}_q &= 0 \end{aligned}$$

- Projection: for $q = 0, \ldots, P$:

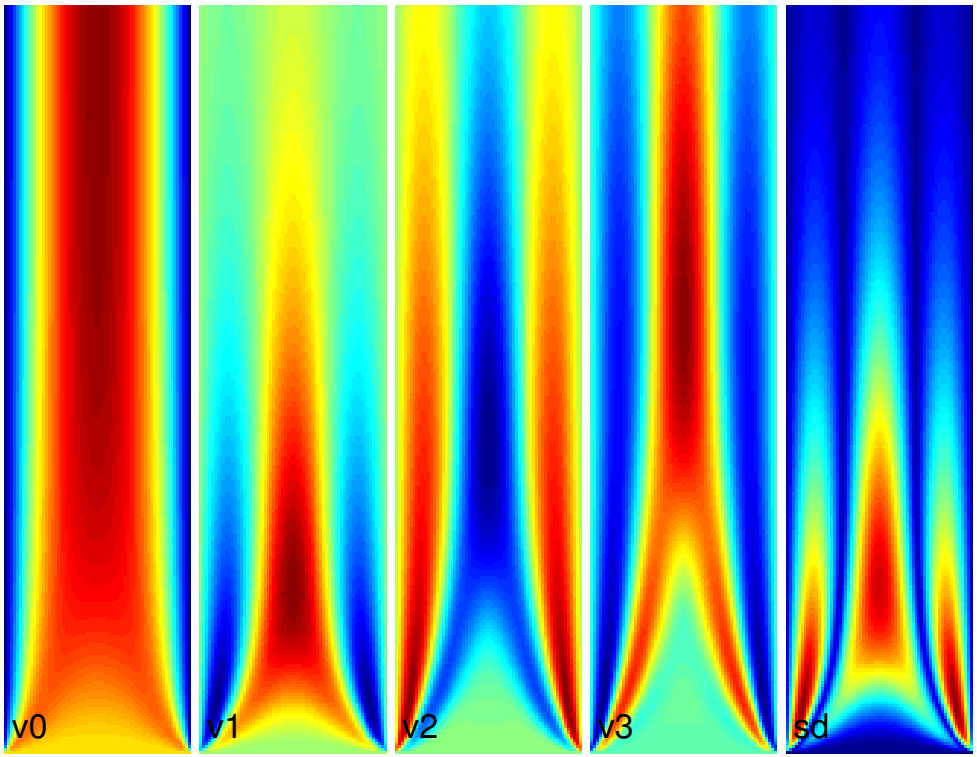
$$\begin{aligned} \frac{\tilde{\boldsymbol{v}}_q - \boldsymbol{v}_q^n}{\Delta t} &= C_q^n + D_q^n \\ \nabla^2 p_q &= -\frac{1}{\Delta t} \nabla \cdot \tilde{\boldsymbol{v}}_q \\ \frac{\boldsymbol{v}_q^{n+1} - \tilde{\boldsymbol{v}}_q}{\Delta t} &= -\nabla p_q \end{aligned}$$

- $P+1$ *decoupled* Poisson Eqns for the pressure modes

[Le Maître *et al.*, *J. Comp. Phys.*, 2001.]

Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Gaussian viscosity PDF
  - $\nu = \nu_0 + \nu_1 \xi$
- Streamwise velocity
  - $v = \sum_{i=0}^{P} v_i \Psi_i$
  - v_0: mean
  - v_i: i-th order mode
  - $\sigma^2 = \sum_{i=1}^{P} v_i^2 \left\langle \Psi_i^2 \right\rangle$



v_0 v_1 v_2 v_3 σ

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Uncertainty Quantification Toolkit (UQTk)

- A library of C++ and Matlab functions for propagation of uncertainty through computational models
- Mainly relies on Polynomial Chaos Expansions (PCEs) for representing random variables and stochastic processes
- Target usage:
  - Rapid prototyping
  - Algorithmic research
  - Tutorials / Educational
- Version 2.0 about to be released under the GNU Lesser General Public License
  - C++ Tools for intrusive and non-intrusive UQ
  - Matlab tools for intrusive and non-intrusive UQ
  - Karhunen-Loève decomposition
  - Bayesian inference tools
- Downloadable from

  `http://www.sandia.gov/UQToolkit/`

PCEs in the UQToolkit

```
// Initialize PC class
int ord = 5;   // Order of PCE
int dim = 1;   // Number of uncertain parameters
PCSet myPCSet("ISP",ord,dim,"LU"); // Legendre-Uniform PCEs
```

```
// Initialize PC class
int ord = 5;   // Order of PCE
int dim = 1;   // Number of uncertain parameters
PCSet myPCSet("NISP",ord,dim,"LU"); // Legendre-Uniform PCEs
```

- Currently support Wiener-Hermite, Legendre-Uniform, and Gamma-Laguerre (limited), Jacobi-Beta (development version)
- PCSet class initializes PC basis type and pre-computes information needed for working with PC expansions

Operations on PCEs in the UQToolkit

```
// PC coefficients in double*
double* a = new double[npc];
double* b = new double[npc];
double* c = new double[npc];

// Initialization
a[0] = 2.0;
a[1] = 0.1;
...
// Perform some arithmetic
myPCSet.Subtract(a,b,c);
myPCSet.Prod(a,b,c);
myPCSet.Exp(a,c);
myPCSet.Log(a,c);
```

```
// PC coefficients in Arrays
Array1D<double> aa(npc,0.e0);
Array1D<double> ab(npc,0.e0);
Array1D<double> ac(npc,0.e0);

// Initialization
aa(0) = 2.0;
aa(1) = 0.1;
...
// Perform arithmetic
myPCSet.Subtract(aa,ab,ac);
myPCSet.Prod(aa,ab,ac);
myPCSet.Exp(aa,ac);
myPCSet.Log(aa,ac);
```

- PC coefficients are either stored in `double*` vectors or in more advanced custom `Array1D<double>` classes
- Functions can take either data type as argument

Surface Reaction Model: UQTk implementation

```
// Build du/dt = a*z - c*u - 4.0*d*u*v
aPCSet.Multiply(z,a,dummy1);              // dummy1 = a*z
aPCSet.Multiply(u,c,dummy2);              // dummy2 = c*u
aPCSet.SubtractInPlace(dummy1,dummy2); // dummy1 = a*z - c*u
aPCSet.Prod(u,v,dummy2);                  // dummy2 = u*v
aPCSet.MultiplyInPlace(dummy2,4.e0*d); // dummy2 = 4.0*d*u*v
aPCSet.Subtract(dummy1,dummy2,dudt);   // dudt = a*z - c*u - 4.0*d*u
```

- All operations are replaced with their equivalent intrusive UQ counterparts
- Results in a set of coupled ODEs for the PC coefficients
  - u, v, w, z represent vector of PC coefficients
- This set of equations is integrated to get the evolution of the PC coefficients in time

Surface Reaction Model: Second equation implementation

```
// Build dv/dt = 2.0*b*z*z - 4.0*d*u*v
aPCSet.Prod(z,z,dummy1);                    // dummy1 = z*z
aPCSet.Prod(dummy1,b,dummy2);               // dummy2 = b*z*z
aPCSet.Multiply(dummy2,2.e0,dummy1);        // dummy1 = 2.0*b*z*z
aPCSet.Prod(u,v,dummy2);                    // dummy2 = u*v
aPCSet.MultiplyInPlace(dummy2,4.e0*d);      // dummy2 = 4.0*d*u*v
aPCSet.Subtract(dummy1,dummy2,dvdt);        // dvdt = 2.0*b*z*z - 4.0*d*u

// Build dw/dt = e*z - f*w
aPCSet.Multiply(z,e,dummy1);                // dummy1 = e*z
aPCSet.Multiply(w,f,dummy2);                // dummy2 = f*w
aPCSet.Subtract(dummy1,dummy2,dwdt);        // dwdt = e*z - f*w
```

- Dummy variables used where needed to build the terms in the equations
- Data structure is currently being enhanced to provide the operation result as the function return value
  - Will allow more elegant inline replacement of operators with their stochastic counterparts

Surface Reaction Model: NISP implementation in UQTk

Quadrature:

```
// Get the quadrature points
int nQdpts=myPCSet.GetNQuadPoints();
double* qdpts=new double[nQdpts];
myPCSet.GetQuadPoints(qdpts);
...
// Evaluate parameter at quad pts
for(int i=0;i<nQdpts;i++){
  bval[i]=myPCSet.EvalPC(b,&qdpts[i]);
}
...
// Run model for all samples
for(int i=0;i<nQdpts;i++){
  u_val[i] = ...
}
// Spectral projection
myPCSet.GalerkProjection(u_val,u);
myPCSet.GalerkProjection(v_val,v);
myPCSet.GalerkProjection(w_val,w);
```

Monte-Carlo Sampling:

```
// Get the sample points
int nSamples=1000;
Array2D<double> samPts(nSamples,dim);
myPCSet.DrawSampleVar(samPts);
...
// Evaluate parameter at sample pts
for(int i=0;i<nSamples;i++){
  ... // select samPt from samPts
  bval[i]=myPCSet.EvalPC(b,&samPt)
}
...
// Run model for all samples
for(int i=0;i<nSamples;i++){
  u_val[i] = ...
}
// Spectral projection
myPCSet.GalerkProjectionMC(samPts,u_val,u);
myPCSet.GalerkProjectionMC(samPts,v_val,v);
myPCSet.GalerkProjectionMC(samPts,w_val,w);
```