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# A Posteriori Error Analysis and Adaptive Construction of Surrogate Models for Probabilities

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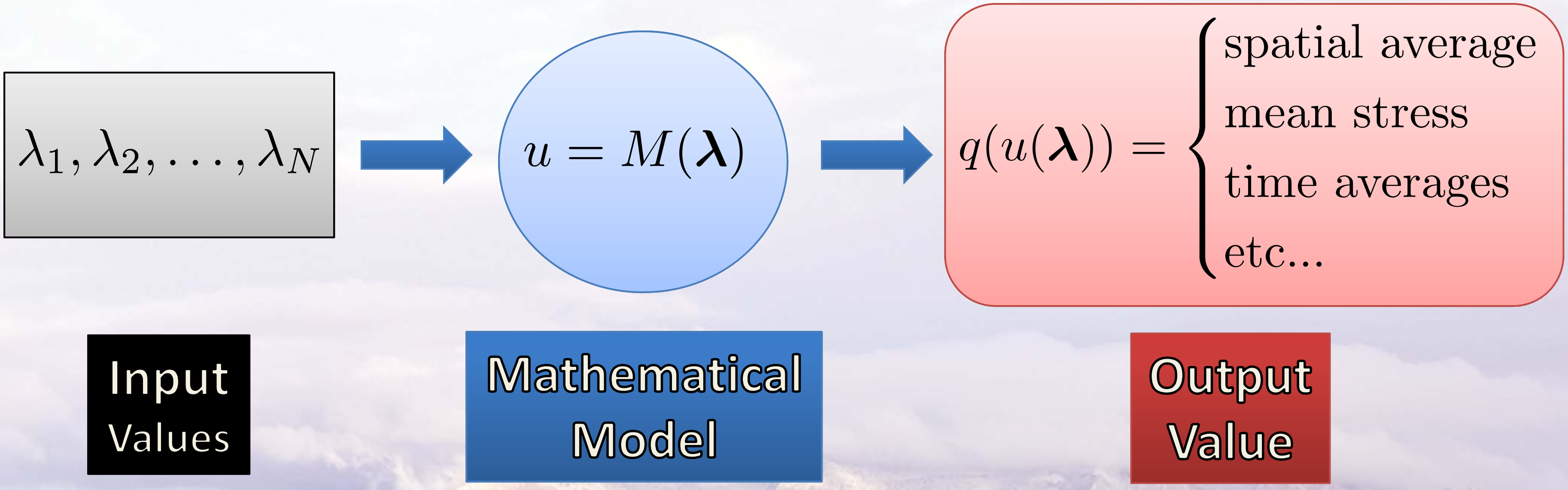
# Motivation

# Surrogate Models, UQ and Error

Ideally, we have:



$\lambda_1, \lambda_2, \ldots, \lambda_N$

$u = M(\boldsymbol{\lambda})$

$$q(u(\boldsymbol{\lambda})) = \begin{cases} \text{spatial average} \\ \text{mean stress} \\ \text{time averages} \\ \text{etc...} \end{cases}$$

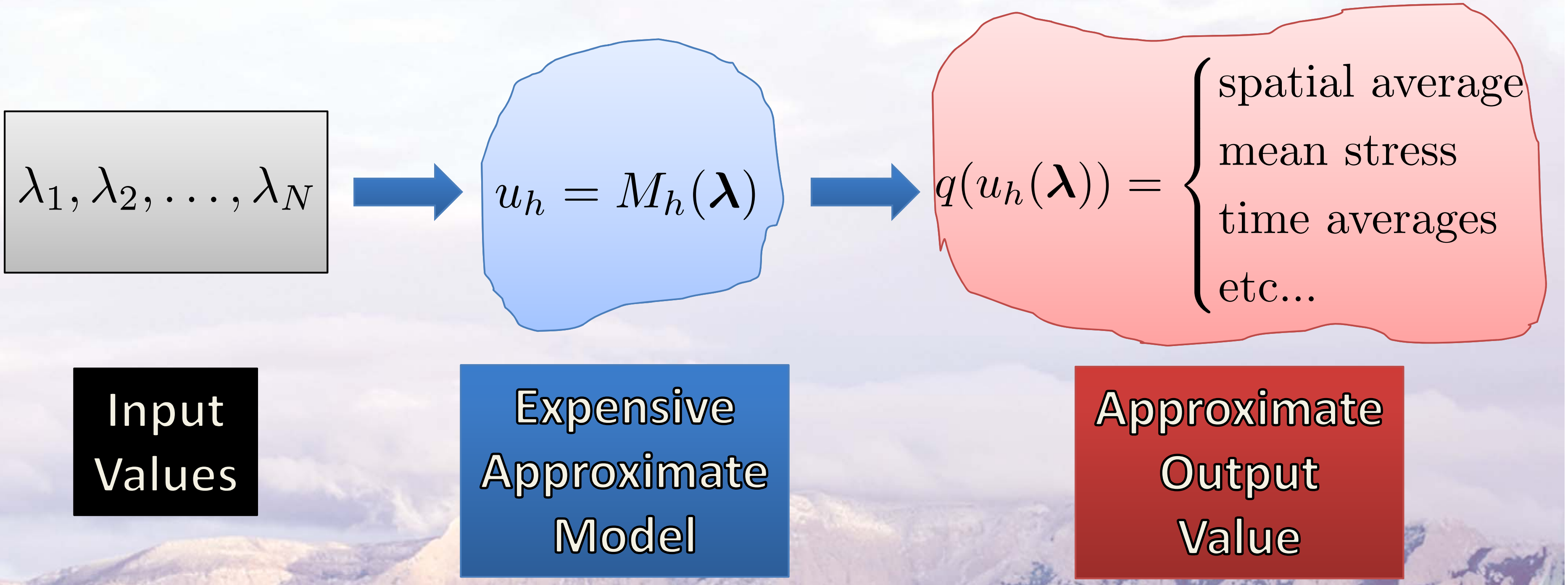
**Input**
Values

**Mathematical**
**Model**

**Output**
**Value**

# Surrogate Models, UQ and Error

Typically, we have:



$\lambda_1, \lambda_2, \ldots, \lambda_N$

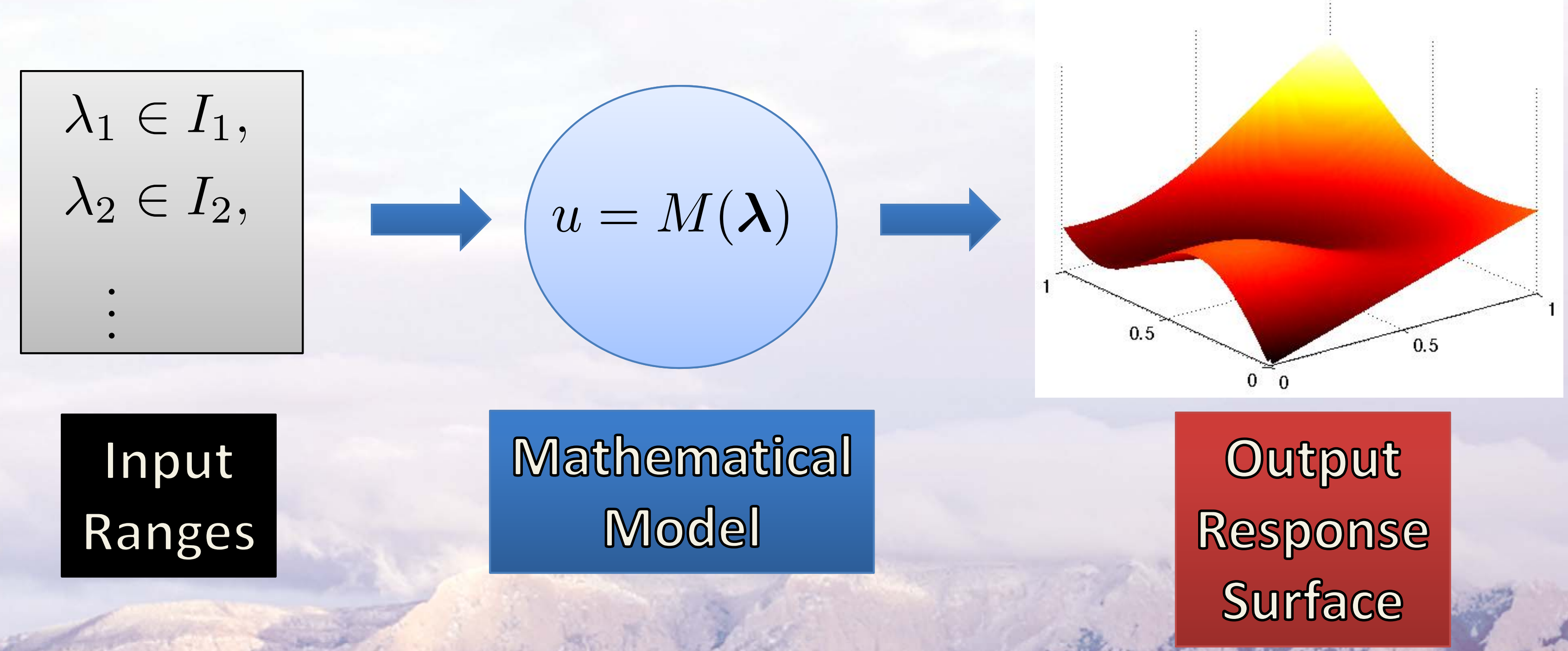
$u_h = M_h(\boldsymbol{\lambda})$

$$q(u_h(\boldsymbol{\lambda})) = \begin{cases} \text{spatial average} \\ \text{mean stress} \\ \text{time averages} \\ \text{etc...} \end{cases}$$

Fortunately, adjoint-based *a posteriori* error estimation helps us assess the accuracy in $q(u_h(\boldsymbol{\lambda}))$.

# Surrogate Models, UQ and Error

Generalizing …



$$\lambda_1 \in I_1, \quad \lambda_2 \in I_2, \quad \vdots$$

$$u = M(\boldsymbol{\lambda})$$

**Input Ranges**

**Mathematical Model**

**Output Response Surface**

At this point, everything is deterministic …

# Surrogate Models, UQ and Error

If we assume the parameters are random variables with known distributions,

$(\Omega, \mathcal{F}, P)$

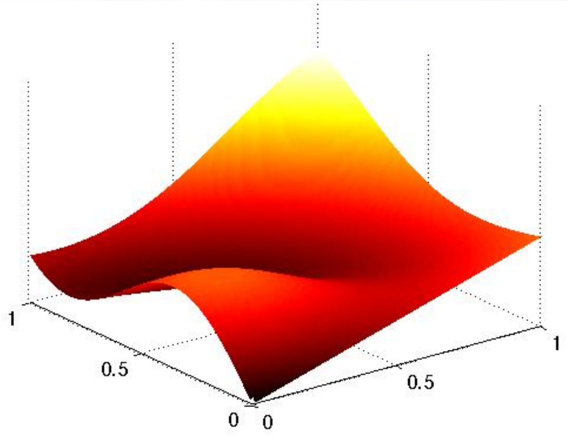
$\boldsymbol{\lambda} : \Omega \rightarrow \Pi_{i=1}^{N} I_i$

$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

→

$u = M(\boldsymbol{\lambda})$

→



**Input Random Variables**

**Mathematical Model**

**Output Response Surface**

then we can investigate statistics of the response (mean, variance, distribution, probabilities).

# Surrogate Models, UQ and Error

We sample the parameters according to the distribution, propagate these samples through the model,

$(\Omega, \mathcal{F}, P)$

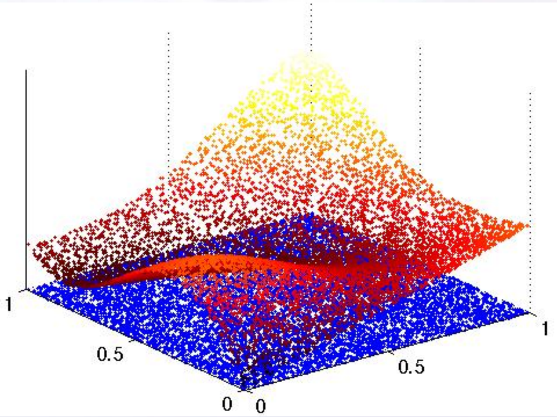
$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$

$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

**Input Random Variables**

$u = M(\boldsymbol{\lambda})$

**Mathematical Model**



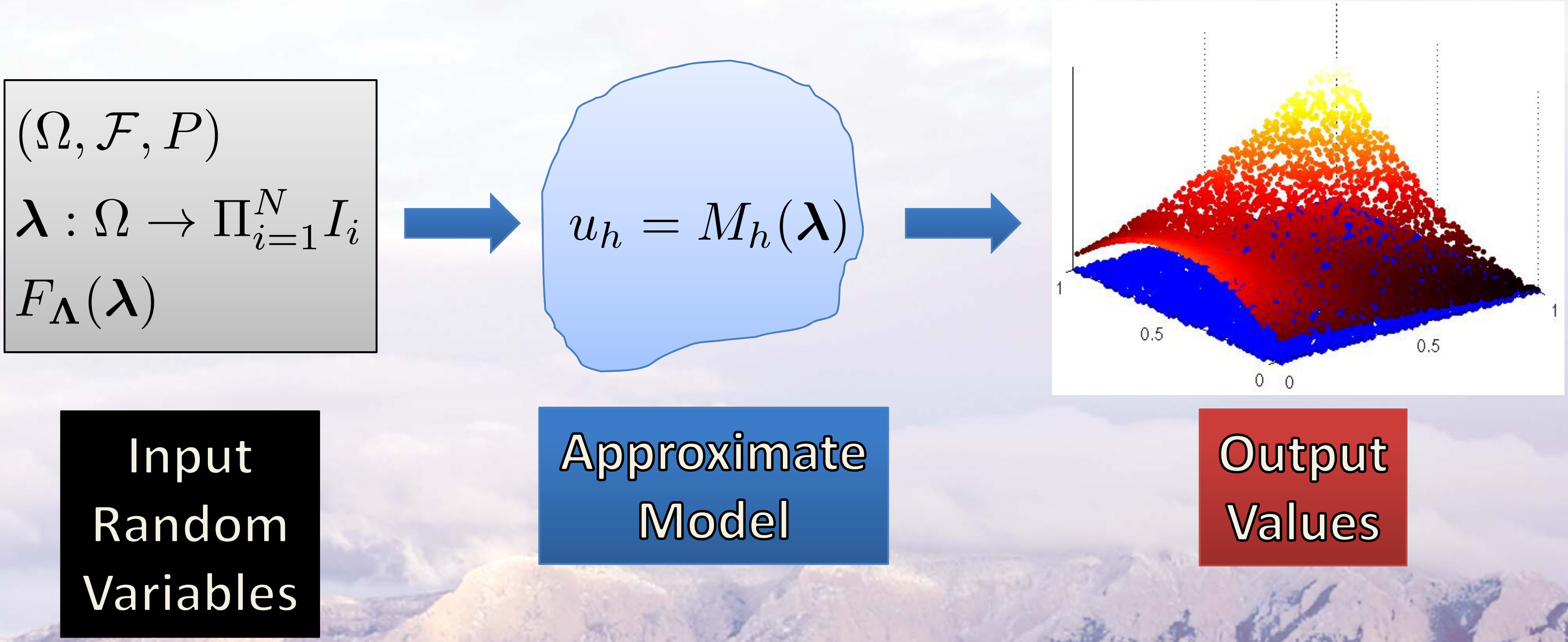
**Output Values**

and calculate the desired statistics from the response.

Unfortunately ...

# Surrogate Models, UQ and Error

We only have an approximate model.



$(\Omega, \mathcal{F}, P)$

$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$

$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

$u_h = M_h(\boldsymbol{\lambda})$

Input Random Variables

Approximate Model

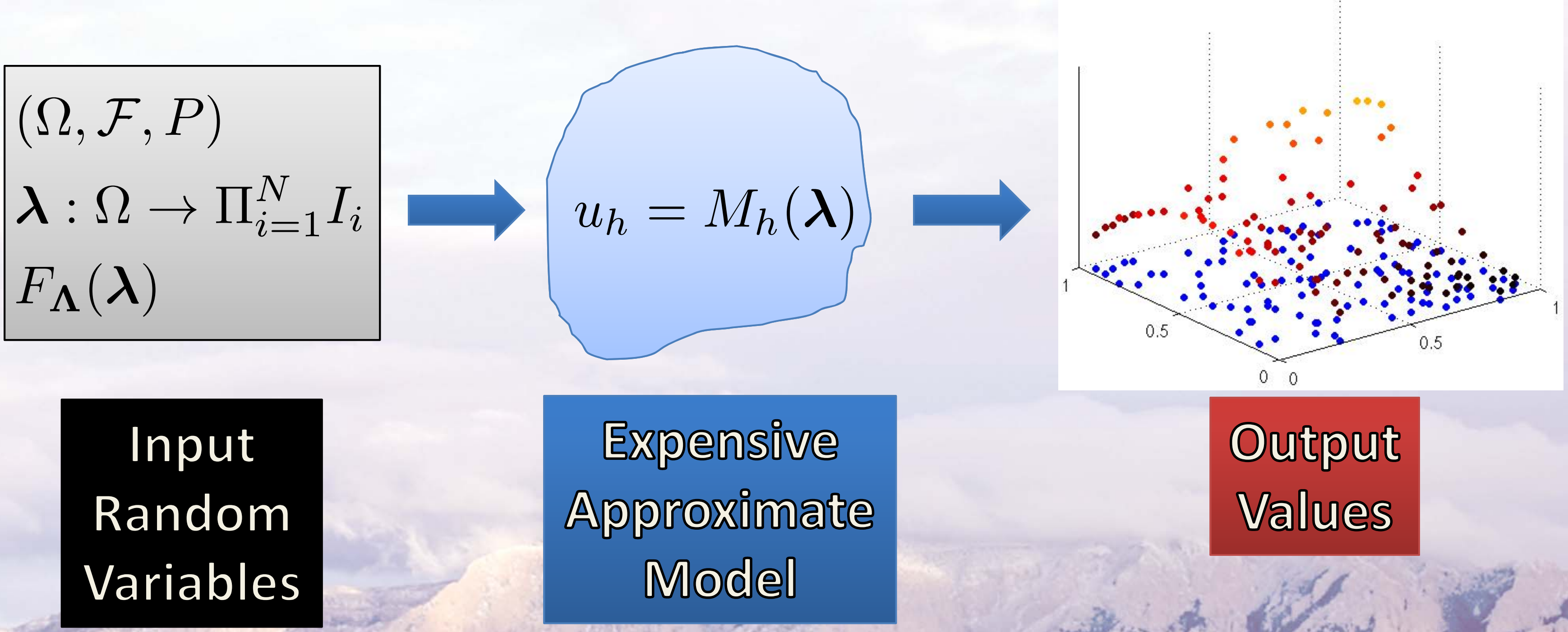
Output Values

There is error in the statistics due to the error in each sample.

Worse still ...

# Surrogate Models, UQ and Error

The approximate model is expensive to evaluate, which limits the number of samples.



$(\Omega, \mathcal{F}, P)$

$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$

$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

$u_h = M_h(\boldsymbol{\lambda})$

Input Random Variables

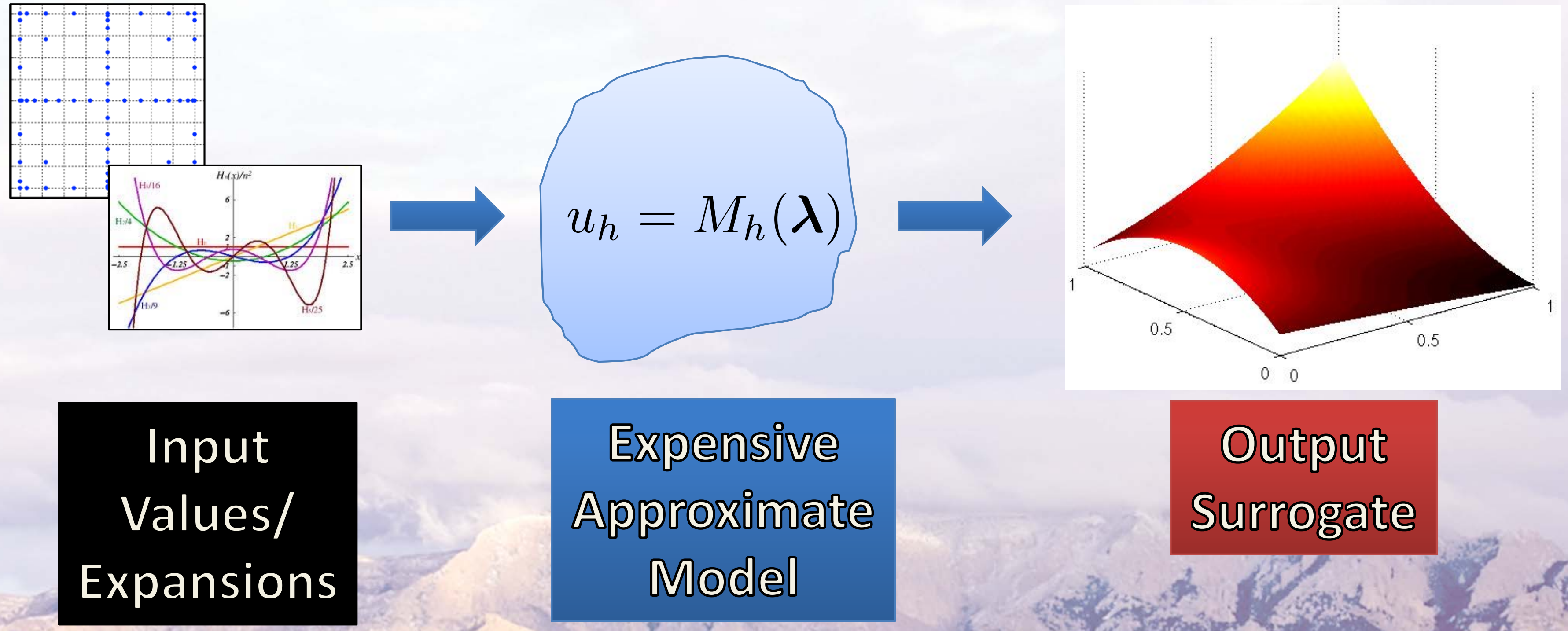
Expensive Approximate Model

Output Values

There is error in the statistics due to the error in each sample and due to the sampling error from the small number of samples.

# Surrogate Models, UQ and Error

Alternatively, we can use the expensive approximate model to construct a surrogate model



Input Values/ Expansions

$u_h = M_h(\boldsymbol{\lambda})$

Expensive Approximate Model

Output Surrogate

Examples include polynomial chaos, stochastic collocation, pseudospectral projection, Gaussian processes, etc.

# Surrogate Models, UQ and Error

Some methods provide analytic approximation of mean and variance.

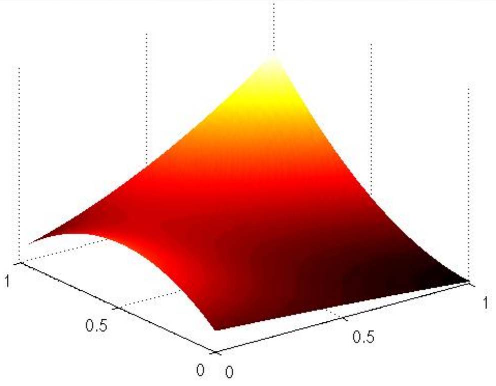
Otherwise, we sample the surrogate to estimate the statistics.

$(\Omega, \mathcal{F}, P)$

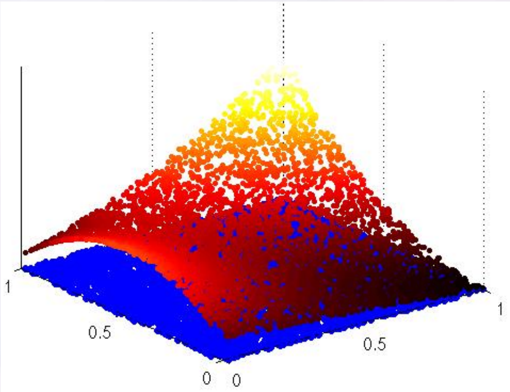
$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$

$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

Input Random Variables



Surrogate Model



Output Values

We have eliminated the statistical sampling error.

However, the error in each sample may be much greater.

# Surrogate Models and Sampling

*Spectral Methods for Uncertainty Quantification.* O. P. Le Maitre and O. M. Knio, pgs. 39-40:

> ... the statistics of the random variable can be estimated by means of sampling strategies ... evaluation of the PC series at the sample points. We shall rely heavily on such sampling procedure to estimate densities, cumulative density functions, probabilities, etc.

"Stochastic spectral methods for efficient Bayesian solution of inverse problems". Y. Marzouk, H. Najm, and L. Rahn. Journal of Comp. Phys. 224 (2007) 560-586:

> Indeed, the per-sample cost is three orders of magnitude smaller for PC evaluations than for direct evaluations...

"Evaluation of failure probability via surrogate models". J. Li and D. Xiu. Journal of Comp. Phys., 229 (2010) 8966-8980:

> ... the straightforward sampling of a surrogate model can lead to erroneous results, no matter how accurate the surrogate model is.

# A Posteriori Error Estimates for Samples of a Surrogate

# Adjoint-Based Error Estimation

Consider the linear algebraic equation: $Ax = b$.

Let $X \approx x$ and define $e = x - X$ and $R = b - AX$.

Let $\phi$ solve the *adjoint problem*: $A^T \phi = \psi$.

Error representation:

$$\underset{\substack{\uparrow \\ \text{Not computable}}}{(e, \psi)} = (e, A^T \phi) = (Ae, \phi) = \underset{\substack{\uparrow \\ \text{Computable}}}{(R, \phi)}.$$

# Parameterized Linear Systems

Let $x(s) \in \mathbb{R}^n$ solve the parameterized linear system,

$$A(s)x(s) = b(s), \quad s \in \Omega,$$

for a given $A(s) \in \mathbb{R}^n \times \mathbb{R}^n$ and $b(s) \in \mathbb{R}^n$.

Let $x_N$ be a surrogate approximation and define, $e(s) = x(s) - x_N(s)$.

We assume the following point-wise error estimate holds,

$$\|e(s)\|_{L^\infty(\Omega;l^2(\mathbb{R}^n))} \leq C\epsilon_1(N)$$

for some $\epsilon_1(N) \geq 0$.

# Error Analysis

Let $\phi(s)$ solve the adjoint problem,

$$A^T(s)\phi(s) = \psi, \quad \forall s \in \Omega.$$

At each $\hat{s} \in \Omega$ we derive the error representation:

$$\begin{aligned} \langle \psi, e(\hat{s}) \rangle &= \langle R(\hat{s}), \phi(\hat{s}) \rangle \\ &= \langle R(\hat{s}), \phi_M(\hat{s}) \rangle + \langle R(\hat{s}), \phi(\hat{s}) - \phi_M(\hat{s}) \rangle \end{aligned}$$

where $\phi_M(s)$ is some approximation of $\phi(s)$.

$\langle R(\hat{s}), \phi_M(\hat{s}) \rangle$ represents a computable estimate of the error.

May be used as a bound or for adaptivity.

Or, to define an *improved linear functional*:

$$g(x_N(s), \phi_M(s)) = \langle \psi, x_N(s) \rangle + \langle R(s), \phi_M(s) \rangle .$$

# An Improved Linear Functional

If the pointwise error in the adjoint solution satisfies,

$$\|\phi(s) - \phi_M(s)\|_{L^\infty(\Omega;l^2(\mathbb{R}^n))} \leq \epsilon_2(M),$$

then the pointwise error in the improved linear functional is bounded by,

$$\| \langle \psi, x(s) \rangle - g(x_N(s), \phi_M(s))\|_{L^\infty(\Omega)} \leq C\epsilon_1(N)\epsilon_2(M),$$

where $C > 0$ depends only on $A(s)$.

Sandia National Laboratories

# Example: Smooth Solution

Parameterized linear system:

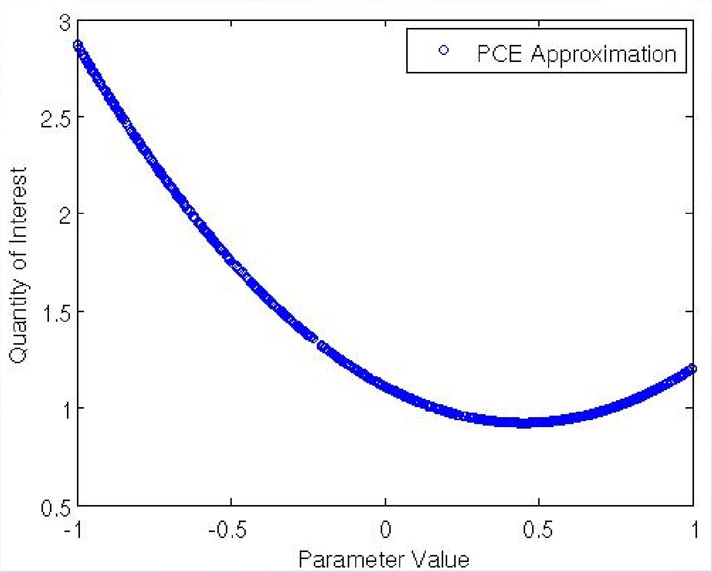
$$\begin{bmatrix} 1+\epsilon & s \\ s & 1 \end{bmatrix} \begin{bmatrix} x_1(s) \\ x_2(s) \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

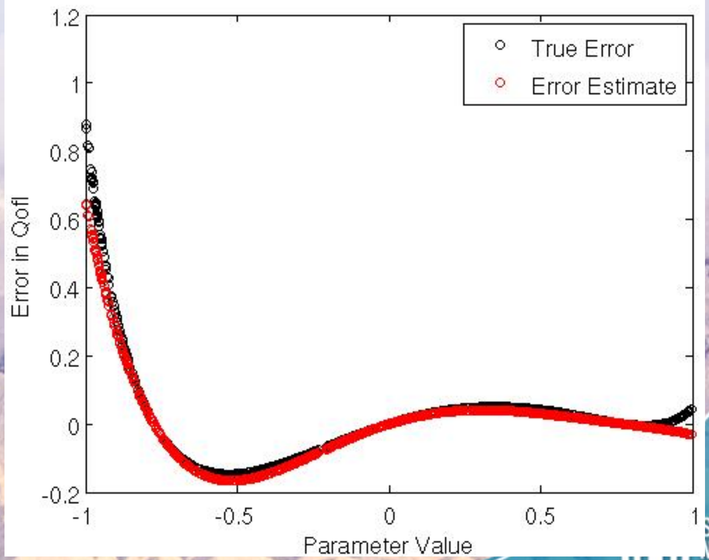
with $s \in [-1, 1]$ and $\epsilon = 0.8$.

Quantity of interest is $x_1(s)$.

Parameterized adjoint system:

$$\begin{bmatrix} 1+\epsilon & s \\ s & 1 \end{bmatrix} \begin{bmatrix} \phi_1(s) \\ \phi_2(s) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$





# Example: Discontinuous Solution

Parameterized linear system:

$$\begin{bmatrix} 2 & -s_1 \\ -s_2 & 1 \end{bmatrix} \begin{bmatrix} x_1(s) \\ x_2(s) \end{bmatrix} = \begin{bmatrix} 1 \\ \lceil s_3 - 1/3 \rceil \end{bmatrix}$$

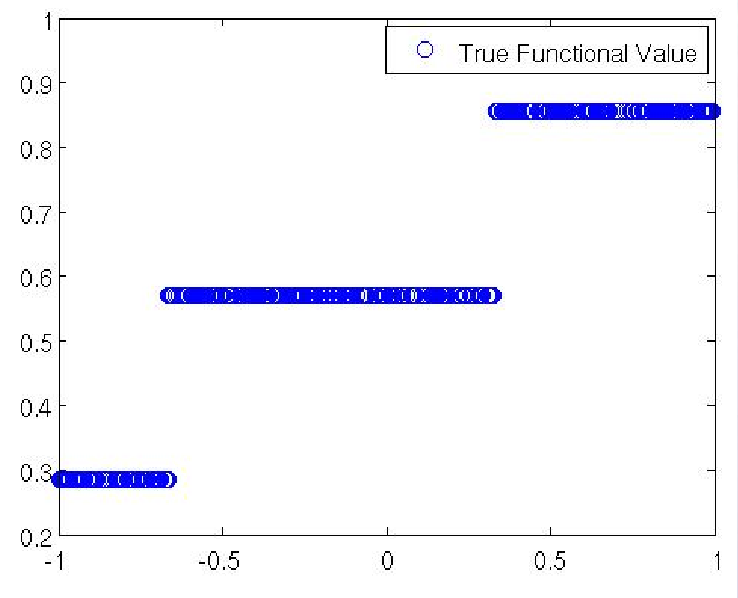
where $\lceil \cdot \rceil$ is the ceiling operator and $s_i \in [-1, 1]$.

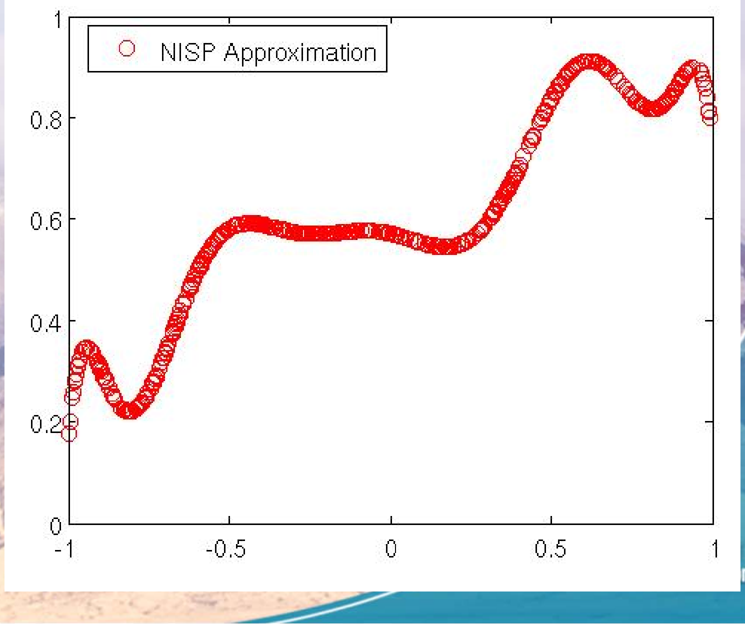
Discontinuity at $s_3 = -2/3, 1/3$

Quantity of interest is $x_1(s)$.

Parameterized adjoint system:

$$\begin{bmatrix} 2 & -s_2 \\ -s_1 & 1 \end{bmatrix} \begin{bmatrix} \phi_1(s) \\ \phi_2(s) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$





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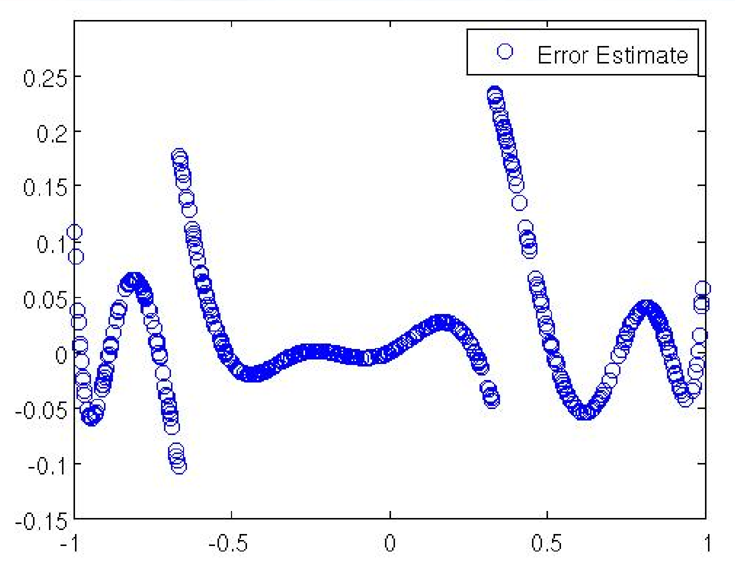

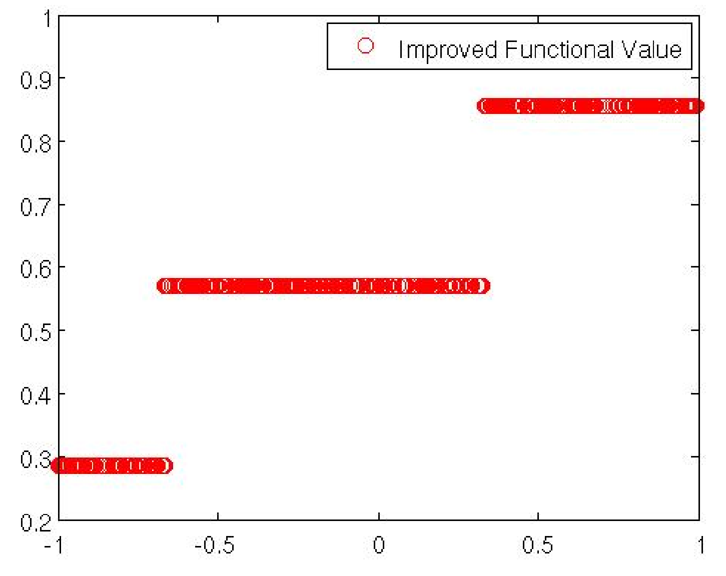

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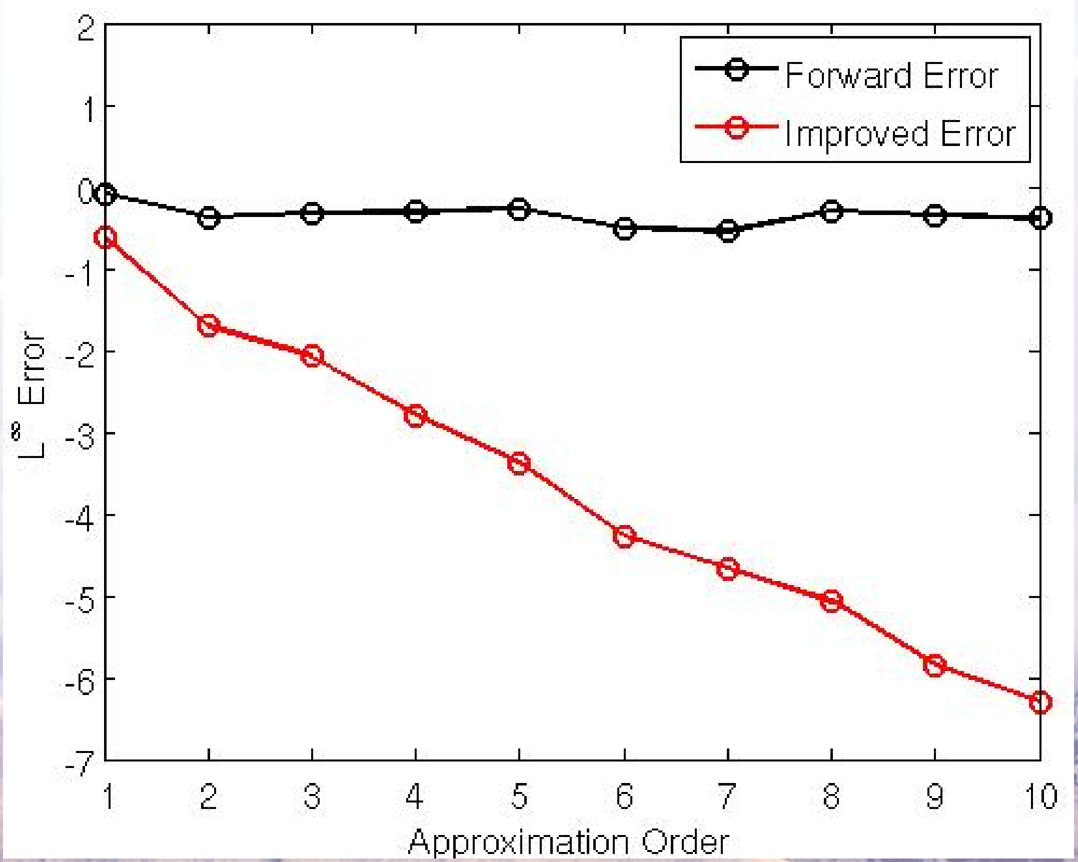

# Partial Differential Equations

Model for nonlinear stochastic diffusive transport:

$$\begin{cases} \frac{\partial u}{\partial t} - \nabla \cdot (A(x,t,\lambda)\nabla u) + g(x,t;u) = f(x,t,\lambda), & x \in S, 0 < t \leq T, \\ A\nabla u \cdot \boldsymbol{n} = 0, & x \in \partial S, 0 < t \leq T, \\ u(x,0) = 0, & x \in S, \end{cases}$$

where $S$ is a convex polygonal domain.

Let $(\cdot,\cdot)_S$ denote the $\mathrm{L}^2$ inner product.

Variational formulation for a fixed $\lambda$: Find $u \in L^2([0,T];H^1(S))$ s.t.

$$\int_0^T \left[(\partial u/\partial t, v)_S + (A(x,t,\lambda)\nabla u, \nabla v)_S + (g(x,t;u),v)_S\right]\, dt \\ = \int_0^T (f(x,t,\lambda),v)_S \, dt$$

for all $v \in L^2([0,T];H^1(S))$ with $v(x,0) = 0$.

# Polynomial Chaos Expansions

Let $\{\Omega, \mathcal{F}, P\}$ be a probability space.

Let $Z(\omega)$ be a random variable and let $\{\Phi_i(Z)\}_{i=1}^{\infty}$ be a set of polynomials orthogonal w.r.t density of $Z$.

Model parameter as a random variable $\lambda = \Lambda(\omega)$ with finite variance,

$$\Lambda(\omega) = \sum_{i=0}^{\infty} \lambda_i \Phi_i(Z(w)), \qquad \text{where } \lambda_i = \frac{\langle \Lambda, \Phi_i \rangle}{\langle \Phi_i, \Phi_i \rangle}.$$

Truncate expansion at order $p$, giving the total number of terms,

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

# Variational Formulation

Seek $u = \sum_{k=0}^{P} u_k(x,t)\Phi_k(Z)$, such that for $k = 0, 1, \ldots, P$,

$$\int_0^T (\partial u_k/\partial t, v)_S \; dt$$

$$+ \frac{1}{\|\Phi_k\|^2} \int_0^T \left( \left\langle A\left(x, t; \sum_{i=0}^{P} \lambda_i \Phi_i(Z)\right) \sum_{j=0}^{P} \nabla u_j \Phi_j(Z), \Phi_k \right\rangle, \nabla v \right)_S \; dt$$

$$+ \frac{1}{\|\Phi_k\|^2} \int_0^T \left( \left\langle g\left(x, t; \sum_{j=0}^{P} u_j \Phi_j \right), \Phi_k \right\rangle, v \right)_S \; dt$$

$$= \int_0^T (f_k(x,t), v)_S \; dt$$

for all $v \in L^2([0,T]; H^1(S))$.

# Discretization

Let

- $\mathcal{T}_h$ be a quasiuniform triangulation of $S$,
- $0 = t_0 < t_i < \cdots < t_N = T$ discretize $[0, T]$ with intervals $I_n = (t_{n-1}, t_n)$.
- $V_h$ denote the space of continuous piecewise linear polynomials on $\mathcal{T}_h$.
- $W_n^{(q)} = V_h \times \mathbb{P}^{(q)}(I_n)$ where $\mathbb{P}^{(q)}(I_n)$ is the space of polynomials of degree $q$ on $I_n$.

We compute $U_k \in W_n^{(q)}$ for $n = 1, 2, \ldots$ such that the variational formulation holds for all $v \in W_n^{(q)}$.

We have our PC finite element approximation, but what is the error in samples of the quantity of interest?

# The Adjoint Operator

The strong from of the adjoint to the nonlinear stochastic diffusion transport problem is,

$$\begin{cases} -\frac{\partial \phi}{\partial t} - \nabla \cdot \left( A^T(x,t,\lambda) \nabla \phi \right) + \overline{g(u,U;\lambda)}^T \phi = 0, & x \in S, T > t \geq 0, \\ A^T \nabla \phi \cdot \boldsymbol{n} = 0, & x \in \partial S, T > t \geq 0, \\ \phi(x,T) = \psi, & x \in S, \end{cases}$$

where $\overline{g(u,U;\lambda)} = \int_0^1 \partial_u g(x,t;su + (1-s)U)\, ds.$

The adjoint data, $\psi$, depends on the quantity of interest.

We approximate $\phi$ using a PC expansion:

$$\phi(x,t;\lambda) \approx \sum_{i=0}^{P} \phi_i(x,t) \Phi_i(Z(\omega)).$$

# The Error Representation

We follow standard steps (substitutions, integration-by-parts, etc.) to derive the error representation:

$$\begin{aligned}(e(x,T;\lambda),\psi)_S = & (e(x,0;\lambda),\phi(x,0;\lambda))_S \\ & - \sum_{n=1}^{N}\int_{I_n} (\partial U(x,t;\lambda)/\partial t, \phi(x,t;\lambda))_S \; dt \\ & + \sum_{n=2}^{N} \left([U(x,t;\lambda)], \phi(x,t;\lambda)\right)_S + \sum_{n=1}^{N}\int_{I_n} (f,\phi(x,t;\lambda))_S \; dt \\ & - \sum_{n=1}^{N}\int_{I_n} (A(x,t;\lambda)\nabla U(x,t;\lambda), \nabla\phi(x,t;\lambda))_S \; dt \\ & - \sum_{n=1}^{N}\int_{I_n} (g(x,t;U),\phi(x,t;\lambda))_S \; dt\end{aligned}$$

# Problem Description

Consider the contaminant source problem[2]:

$$\frac{\partial u}{\partial t} - \nabla \cdot \nabla u = \frac{s}{2\pi\sigma^2} \exp\left(-\frac{|\lambda - x|^2}{2\sigma^2}\right)(1 - H(t - 0.05))$$

with $S = [0,1]^2$, $T = 0.21$, $u(x,0) = 0$, $s = 10$ and $\sigma = 0.1$.

Random variable $\lambda$ uniformly distributed on $[0,1]^2$.

Quantities of interest: Concentration at $t = 0.05$ and $t = 0.15$ at 9 measurement locations.

Discretization: $h = 0.1$, $\Delta t = 0.005$ and $6^{\text{th}}$−order PC expansion.

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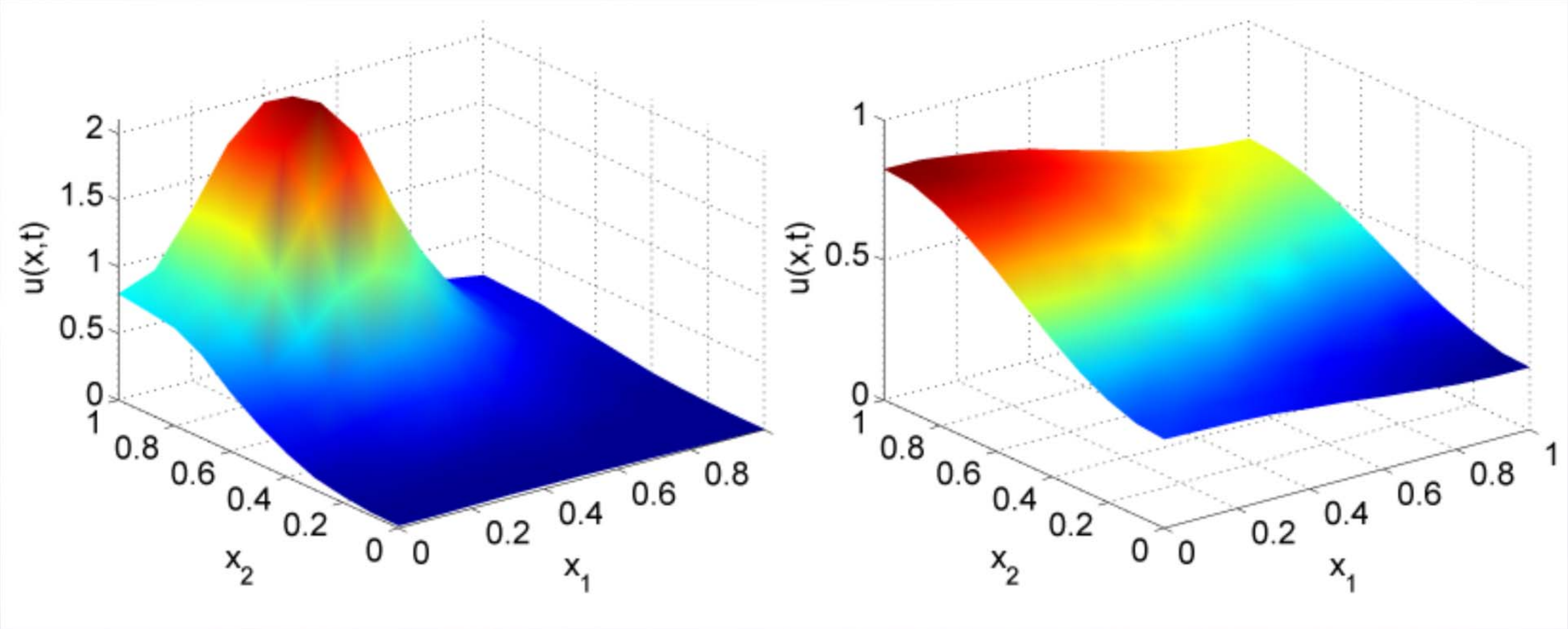
[2] See "Stochastic spectral methods for efficient Bayesian solution of inverse problems". Y. Marzouk, H. Najm and L. Rahn. 2007.

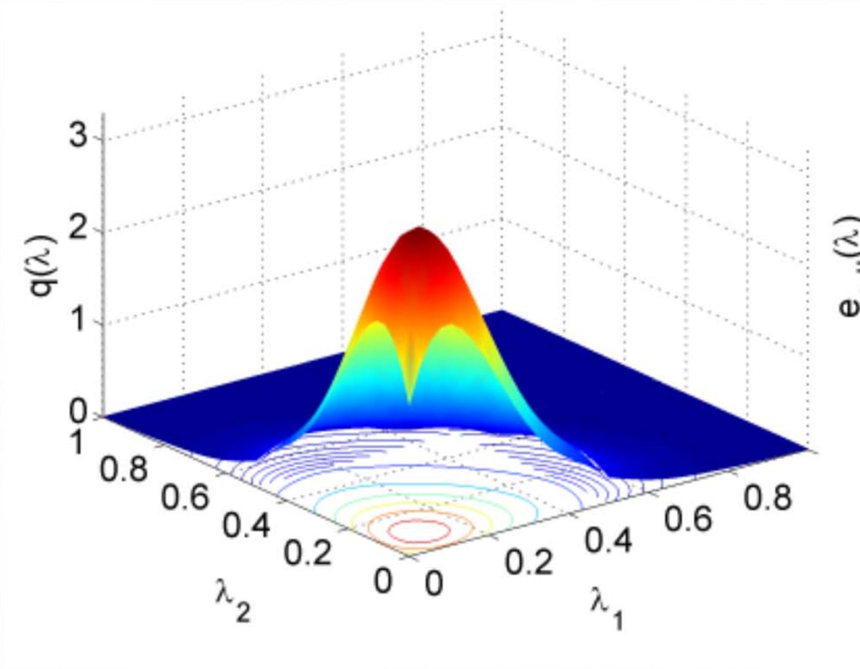
# Contaminant Approximation: λ = (0.4,0.8)



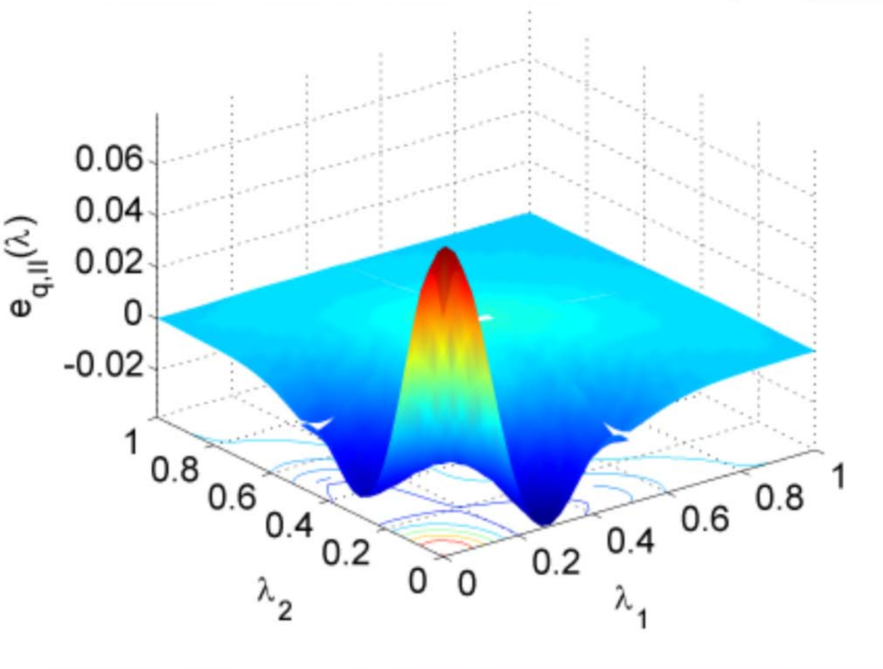
$t = 0.05$

$t = 0.15$

# First Quantity of Interest at t = 0.05

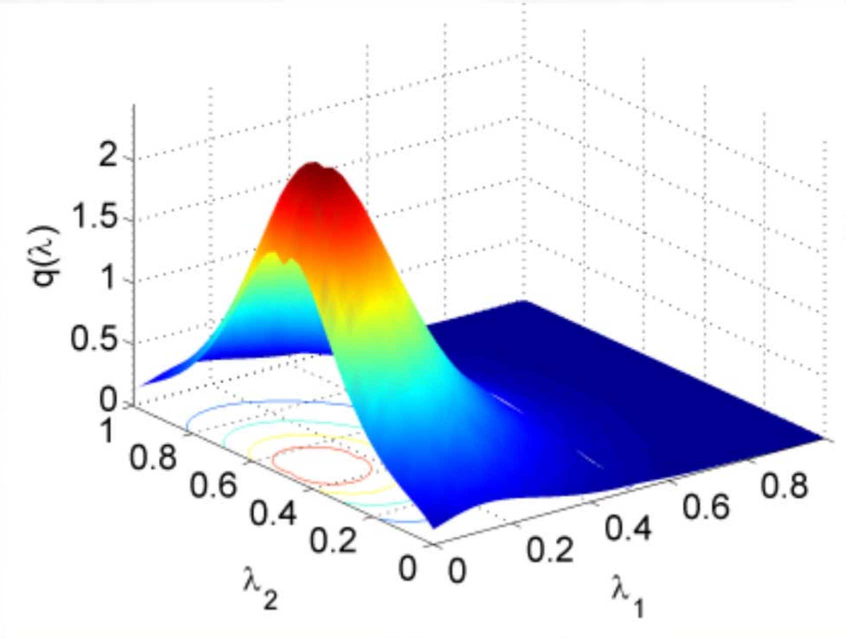


PC approximation

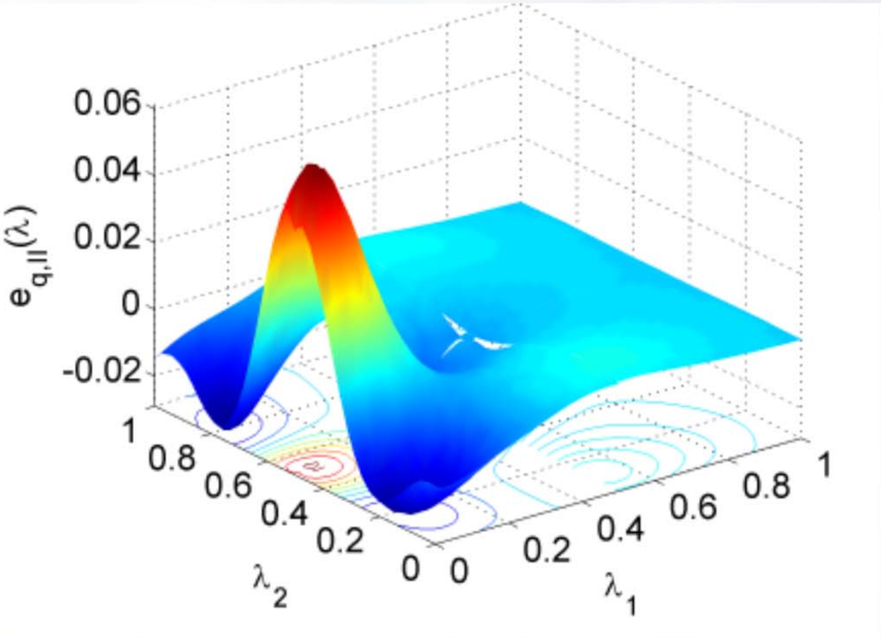


A posteriori error estimate

# Fourth Quantity of Interest at t = 0.05

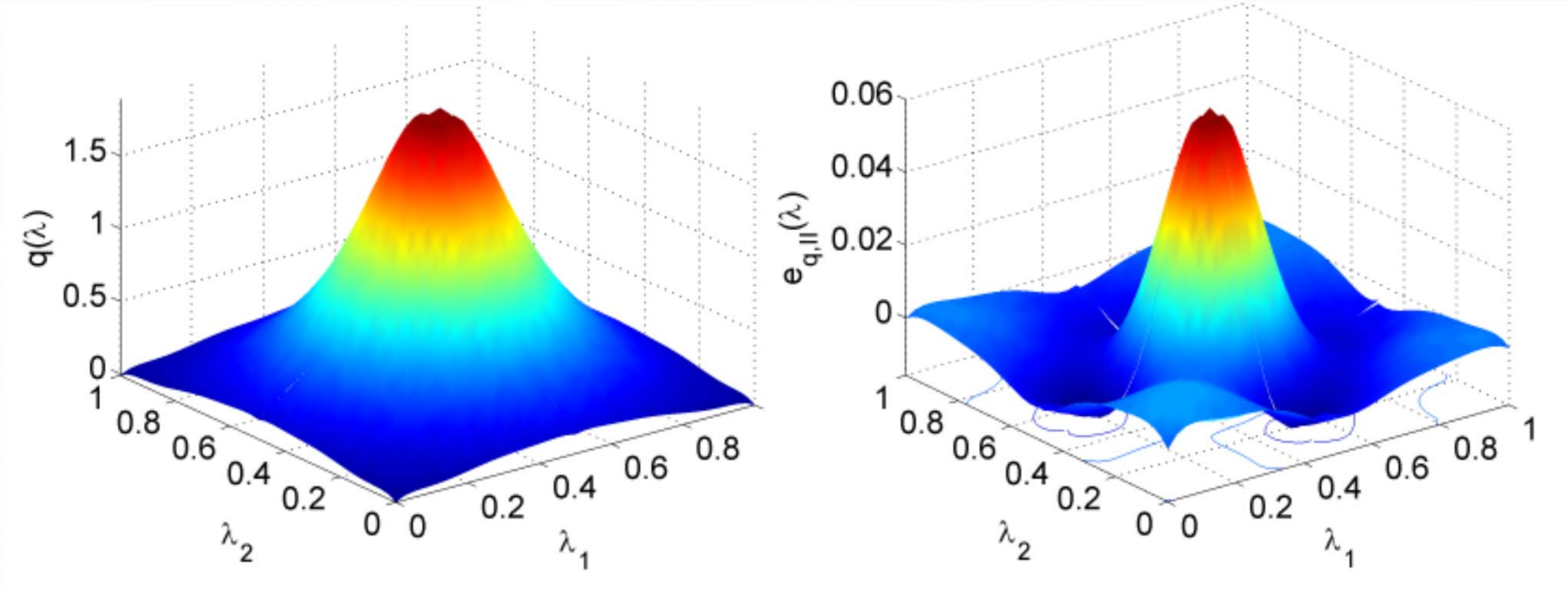


PC approximation



A posteriori error estimate

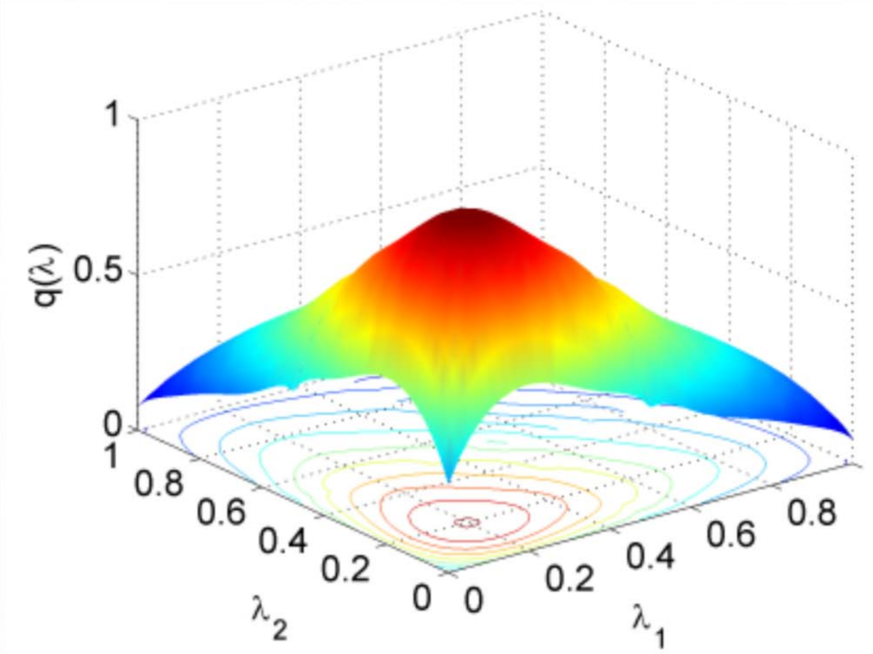
# Fifth Quantity of Interest at t = 0.05



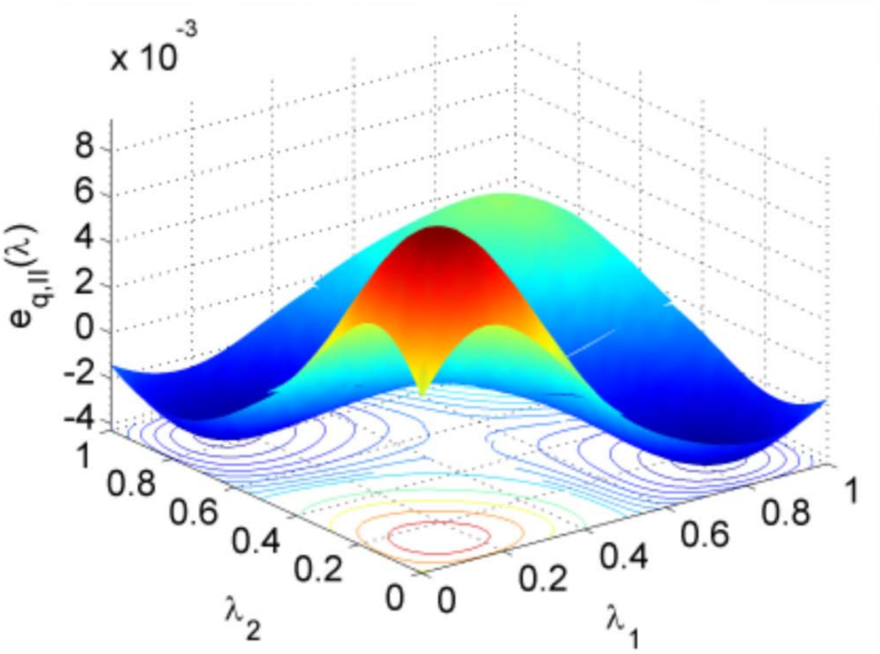
PC approximation

A posteriori error estimate

# First Quantity of Interest at t = 0.15

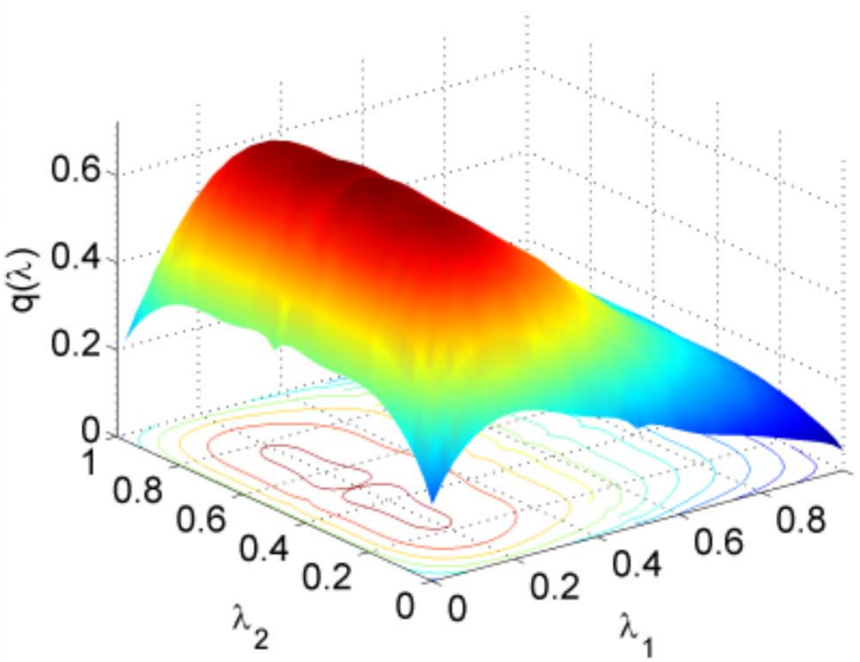


PC approximation

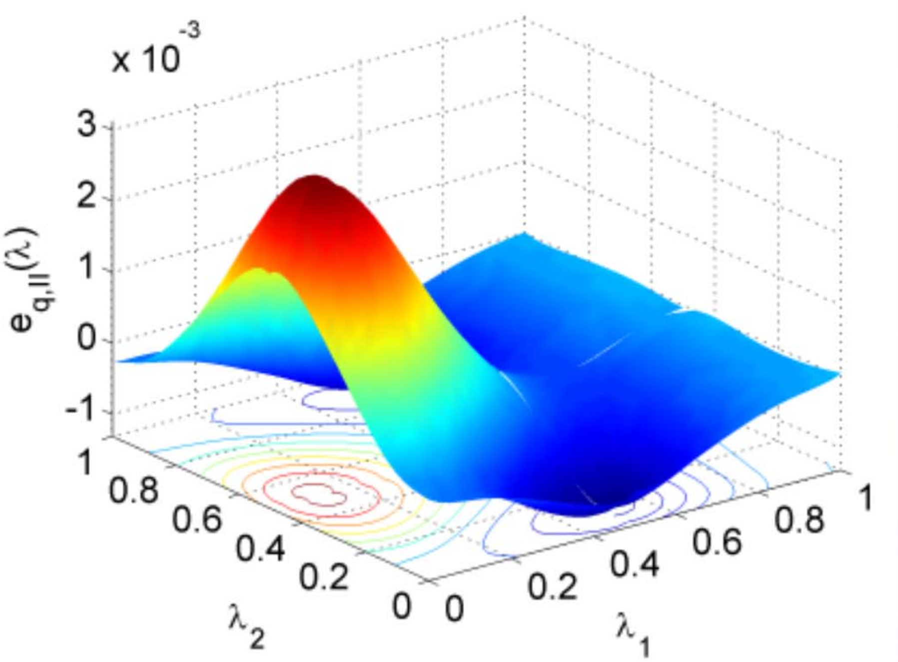


A posteriori error estimate

# Fourth Quantity of Interest at t = 0.15

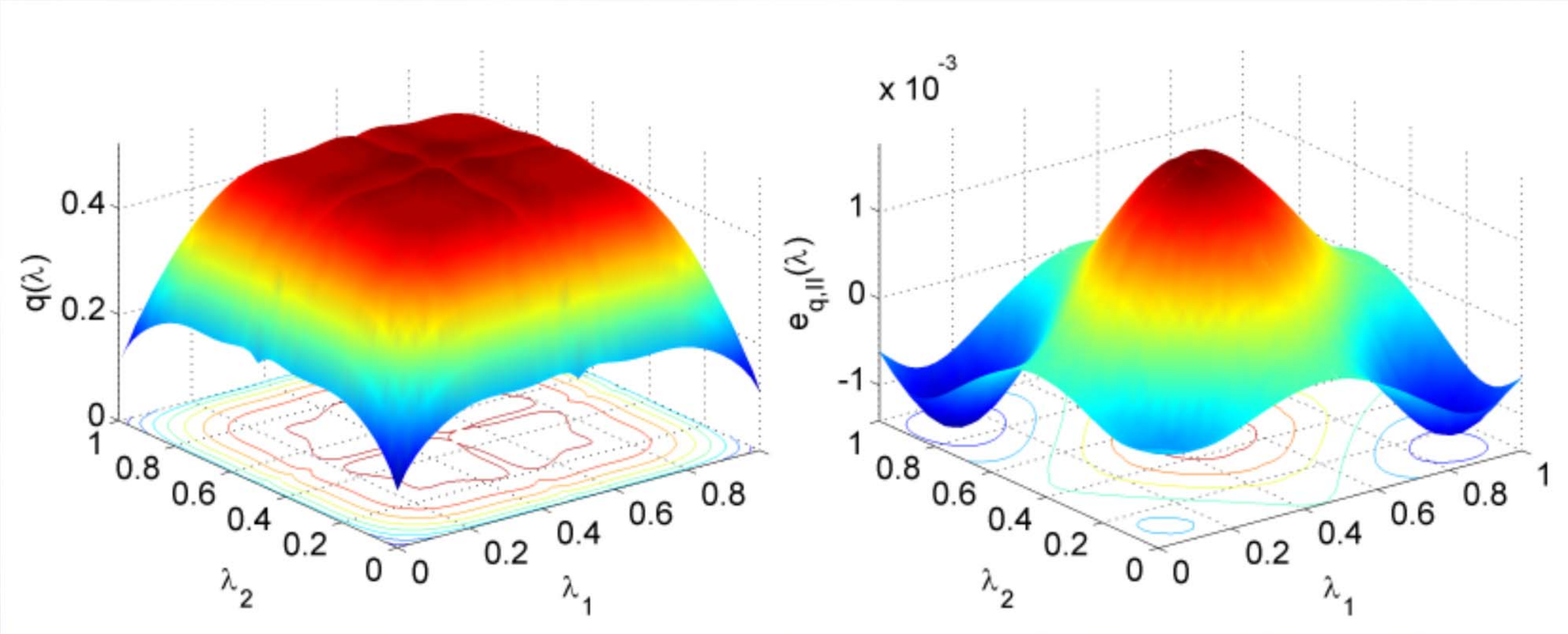


PC approximation



A posteriori error estimate

# Fifth Quantity of Interest at t = 0.15



PC approximation

A posteriori error estimate

# Effectivity of Error Estimate

| Time | $\lambda$ | Std Err Est $u(x^{\{1\}}, t)$ | PC Err Est $u(x^{\{1\}}, t)$ | Ratio |
|---|---|---|---|---|
| 0.05 | $(0.25, 0.25)$ | $-1.094E-02$ | $-1.207E-02$ | 1.103 |
| 0.05 | $(0.75, 0.25)$ | $2.142E-03$ | $2.144E-03$ | 1.001 |
| 0.05 | $(0.25, 0.75)$ | $2.347E-03$ | $2.348E-03$ | 1.001 |
| 0.05 | $(0.75, 0.75)$ | $1.439E-03$ | $1.466E-03$ | 1.019 |
| 0.05 | $(0.4, 0.375)$ | $4.273E-03$ | $4.508E-03$ | 1.055 |
| 0.15 | $(0.25, 0.25)$ | $5.754E-03$ | $5.812E-03$ | 1.010 |
| 0.15 | $(0.75, 0.25)$ | $-3.637E-03$ | $-3.670E-03$ | 1.009 |
| 0.15 | $(0.25, 0.75)$ | $-3.511E-03$ | $-3.553E-03$ | 1.012 |
| 0.15 | $(0.75, 0.75)$ | $1.444E-03$ | $1.4376E-03$ | 0.996 |
| 0.15 | $(0.4, 0.375)$ | $7.686E-05$ | $9.389E-05$ | 1.222 |

# Effectivity of Error Estimate

| Time | $\lambda$ | Std Err Est $u(x^{\{4\}}, t)$ | PC Err Est $u(x^{\{4\}}, t)$ | Ratio |
|---|---|---|---|---|
| 0.05 | $(0.25, 0.25)$ | $-5.477E-03$ | $-5.936E-03$ | 1.084 |
| 0.05 | $(0.75, 0.25)$ | $2.352E-03$ | $2.352E-03$ | 1.000 |
| 0.05 | $(0.25, 0.75)$ | $-1.211E-03$ | $-1.833E-03$ | 1.513 |
| 0.05 | $(0.75, 0.75)$ | $1.953E-03$ | $1.943E-03$ | 0.995 |
| 0.05 | $(0.4, 0.375)$ | $-3.628E-03$ | $-3.883E-03$ | 1.070 |
| 0.15 | $(0.25, 0.25)$ | $4.951E-04$ | $5.018E-04$ | 1.013 |
| 0.15 | $(0.75, 0.25)$ | $-5.848E-04$ | $-5.959E-04$ | 1.019 |
| 0.15 | $(0.25, 0.75)$ | $6.266E-04$ | $6.301E-04$ | 1.006 |
| 0.15 | $(0.75, 0.75)$ | $-5.766E-04$ | $-5.778E-04$ | 1.002 |
| 0.15 | $(0.4, 0.375)$ | $4.516E-04$ | $4.447E-04$ | 0.985 |

# Effectivity of Error Estimate

| Time | $\lambda$ | Std Err Est $u(x^{\{5\}}, t)$ | PC Err Est $u(x^{\{5\}}, t)$ | Ratio |
|---|---|---|---|---|
| 0.05 | $(0.25, 0.25)$ | $2.387E - 03$ | $2.238E - 03$ | 0.938 |
| 0.05 | $(0.75, 0.25)$ | $-8.675E - 03$ | $-8.803E - 03$ | 1.015 |
| 0.05 | $(0.25, 0.75)$ | $-8.377E - 03$ | $-8.383E - 03$ | 1.051 |
| 0.05 | $(0.75, 0.75)$ | $-1.499E - 03$ | $-1.707E - 03$ | 1.139 |
| 0.05 | $(0.4, 0.375)$ | $1.918E - 02$ | $1.860E - 02$ | 0.970 |
| 0.15 | $(0.25, 0.25)$ | $2.782E - 04$ | $2.815E - 04$ | 1.012 |
| 0.15 | $(0.75, 0.25)$ | $-2.299E - 04$ | $-2.286E - 04$ | 0.994 |
| 0.15 | $(0.25, 0.75)$ | $-3.882E - 04$ | $-3.893E - 04$ | 1.003 |
| 0.15 | $(0.75, 0.75)$ | $3.887E - 04$ | $3.935E - 04$ | 1.012 |
| 0.15 | $(0.4, 0.375)$ | $1.439E - 03$ | $1.439E - 03$ | 1.000 |

# Problem Description

Consider the contaminant source problem:

$$\frac{\partial u}{\partial t} - \nabla \cdot A(x,t;\lambda)\nabla u = \frac{s}{2\pi\sigma^2} \exp\left(-\frac{|\overline{x}-x|^2}{2\sigma^2}\right)(1 - H(t-0.05))$$

with $S = [0,1]^2$, $T = 0.21$, $u(x,0) = 0$, $s = 10$ and $\sigma = 0.1$.

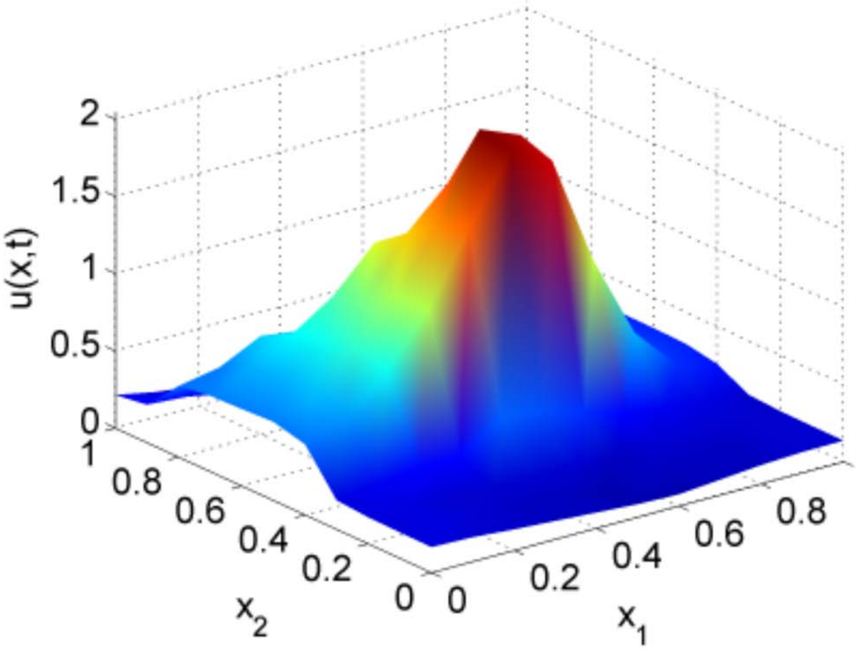
$$A(x,t;\lambda) = \begin{pmatrix} \lambda \exp(2\sin(2\pi x)\cos(4\pi y) & 0 \\ 0 & \exp(2\sin(4\pi y) + 2\cos(2\pi x) \end{pmatrix}$$

Random variable $\lambda$ uniformly distributed on $[0.5, 1.5]$.

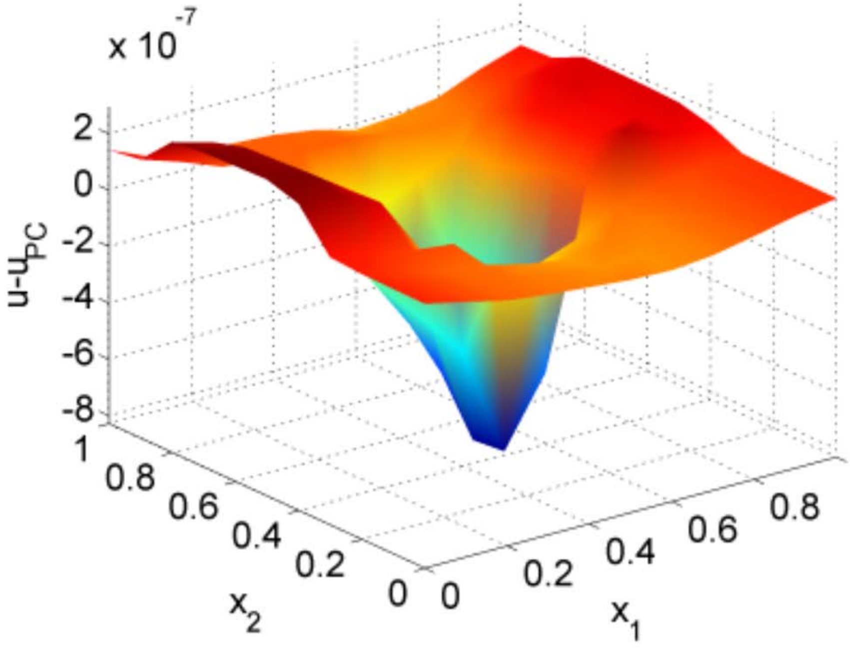
Quantities of interest: Concentration at $t = 0.05$ and $t = 0.15$
at 9 measurement locations.

Discretization: $h = 0.1$, $\Delta t = 0.005$ and $6^{\text{th}}-$order PC expansion.

# Approximation and PC Error at λ = 1

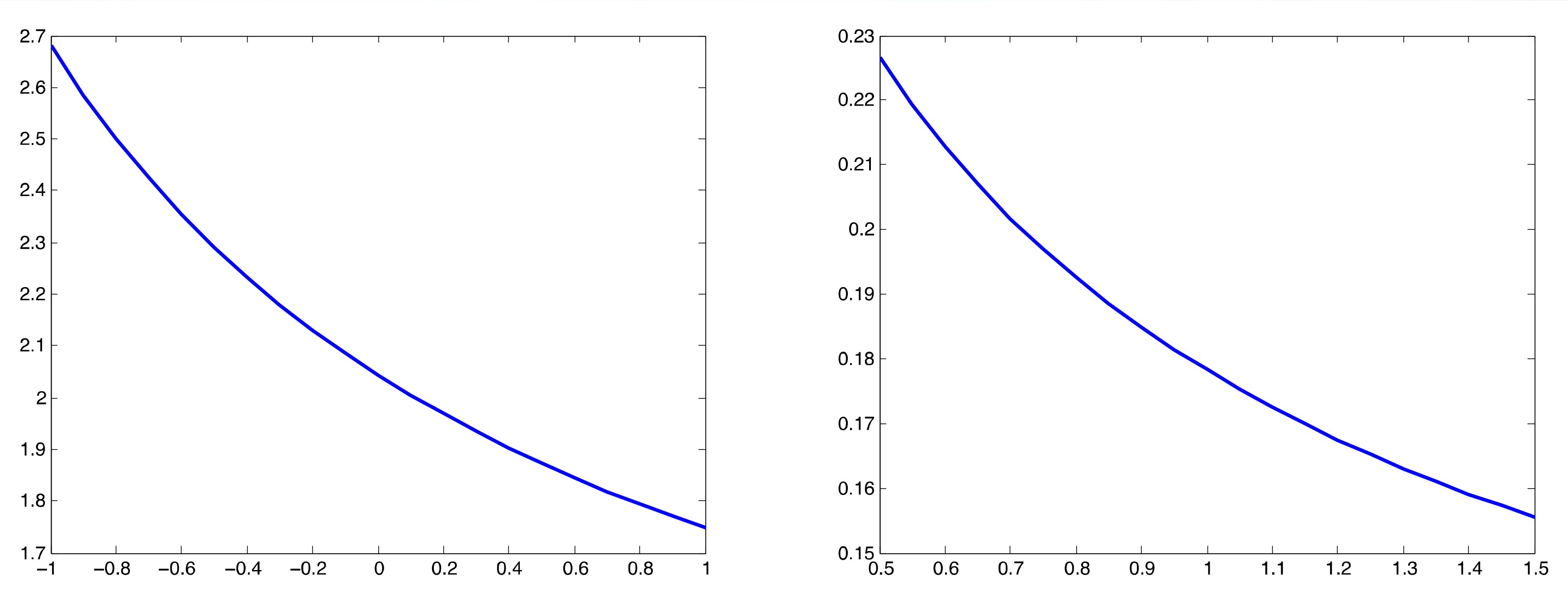


PC approximation



PC truncation error

# Fifth Quantity of Interest at t = 0.05



PC approximation

A posteriori error estimate

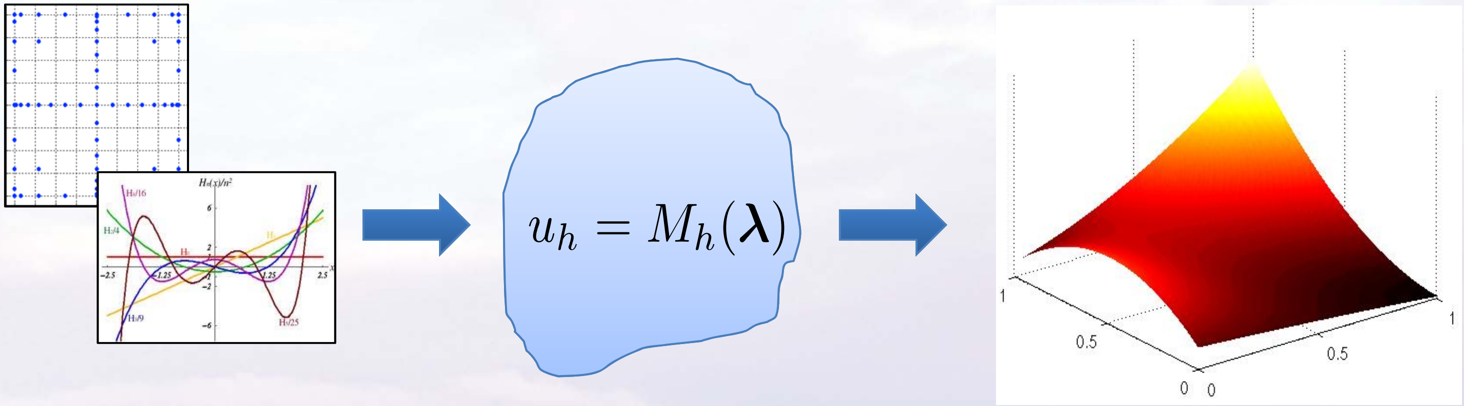
# Effectivity of Error Estimate

| $\lambda$ | Std Err Est $u(x^{\{5\}}, t)$ | PC Err Est $u(x^{\{5\}}, t)$ | Ratio |
|---|---|---|---|
| 0.50 | 0.22660 | 0.22667 | 1.00032 |
| 0.75 | 0.19693 | 0.19694 | 1.00006 |
| 1.00 | 0.17823 | 0.17823 | 1.00000 |
| 1.25 | 0.16520 | 0.16519 | 0.99996 |
| 1.50 | 0.15550 | 0.15548 | 0.99983 |

# Adaptive Construction of Surrogate Models

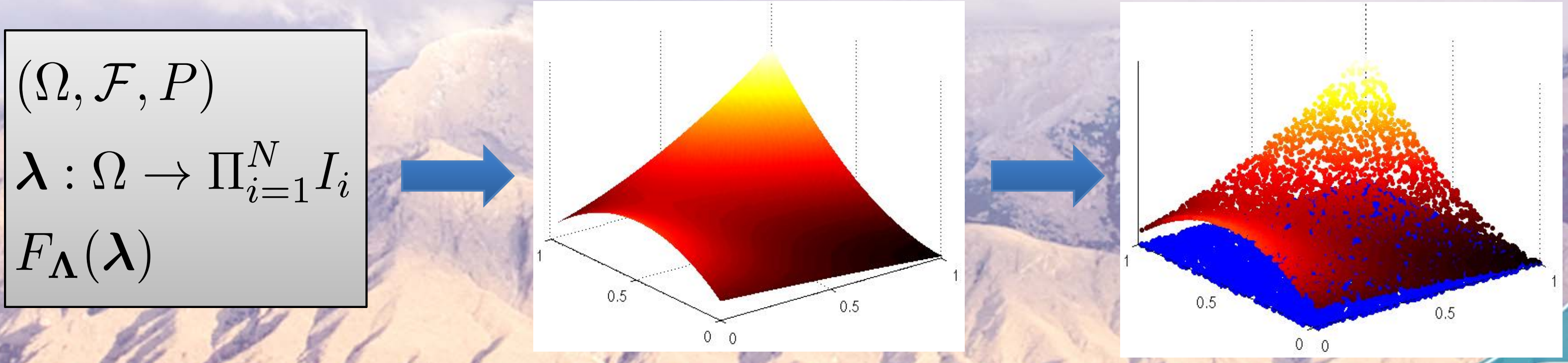
# Estimation of Probabilities

Recall that first we build the surrogate ...



$u_h = M_h(\boldsymbol{\lambda})$

... then we estimate the statistics by sampling the surrogate.



$(\Omega, \mathcal{F}, P)$

$\boldsymbol{\lambda} : \Omega \rightarrow \Pi_{i=1}^{N} I_i$

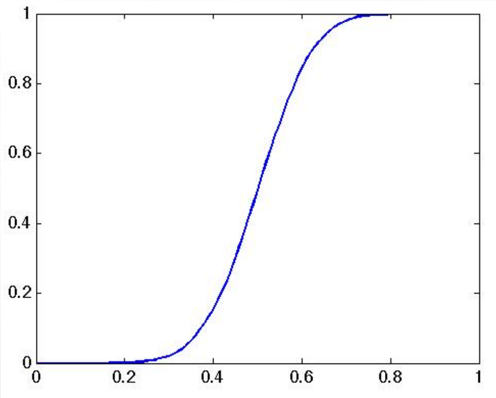
$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$

# Estimation of Probabilities

Moments and distributions require global accuracy.

$$E[q] = \int_\Omega q(\lambda)\ d\mu$$

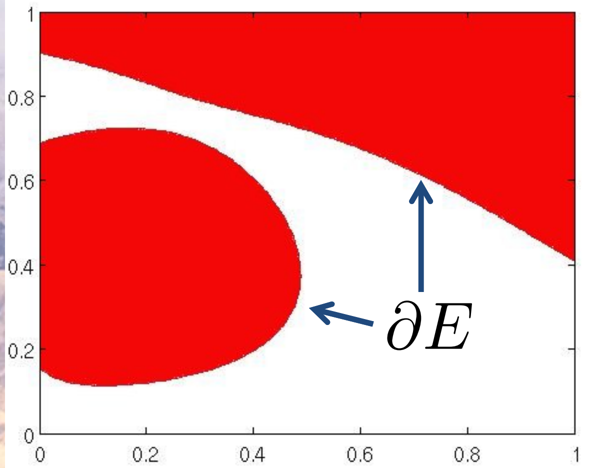
$$\mathrm{Var}[q] = \int_\Omega (E[q] - q(\lambda))^2\ d\mu$$



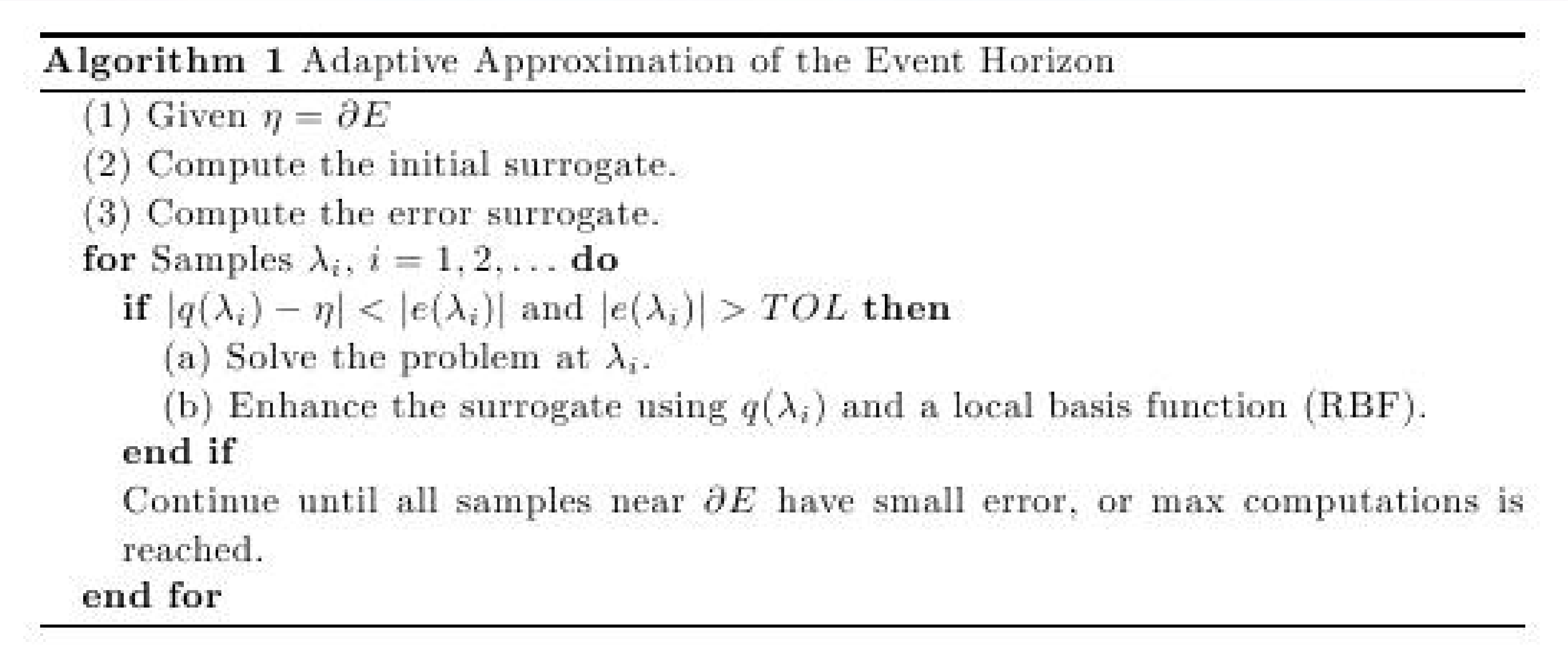
Probabilities require only local accuracy.

$$P[q \in E] = \int_\Omega \mathcal{X}_E\ d\mu$$

$$\partial E = \begin{cases} \text{limit state surface} \\ \text{event horizon} \end{cases}$$



# An Adaptive Algorithm



```
Algorithm 1 Adaptive Approximation of the Event Horizon
  (1) Given $\eta = \partial E$
  (2) Compute the initial surrogate.
  (3) Compute the error surrogate.
  for Samples $\lambda_i$, $i = 1, 2, \ldots$ do
    if $|q(\lambda_i) - \eta| < |e(\lambda_i)|$ and $|e(\lambda_i)| > TOL$ then
      (a) Solve the problem at $\lambda_i$.
      (b) Enhance the surrogate using $q(\lambda_i)$ and a local basis function (RBF).
    end if
    Continue until all samples near $\partial E$ have small error, or max computations is reached.
  end for
```

# Example

Model for convection/diffusion:

$$\begin{cases} -\nabla \cdot (\boldsymbol{K}\nabla u) + \boldsymbol{b}(\boldsymbol{\lambda}) \cdot \nabla u = f, & x \in S, \\ u = 0, & x \in \partial S, \end{cases}$$

where $S = (0,1) \times (0,1)$.

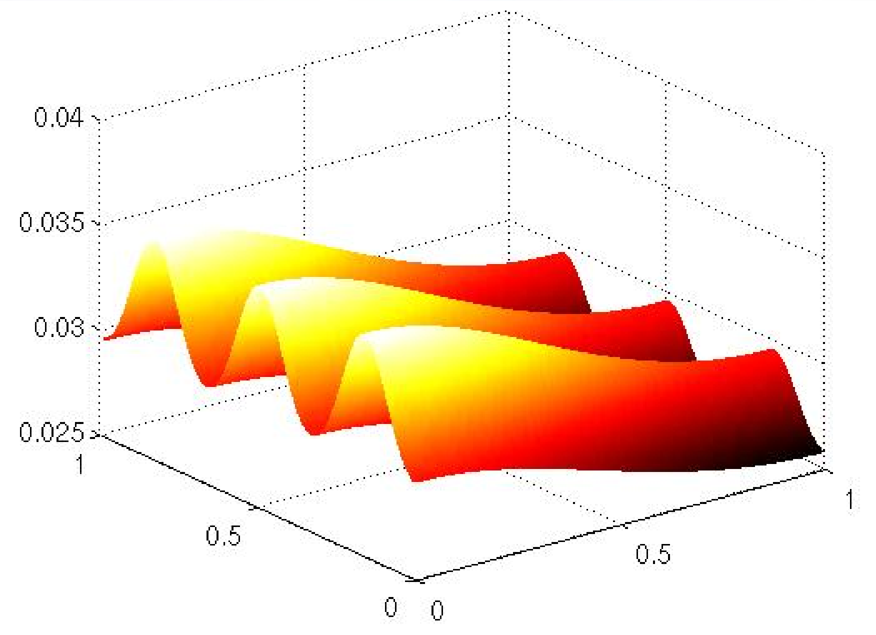
Quantity of interest is $u(0.5, 0.5)$.

Forward and adjoint solutions approximated using finite elements and pseudospectral projection.

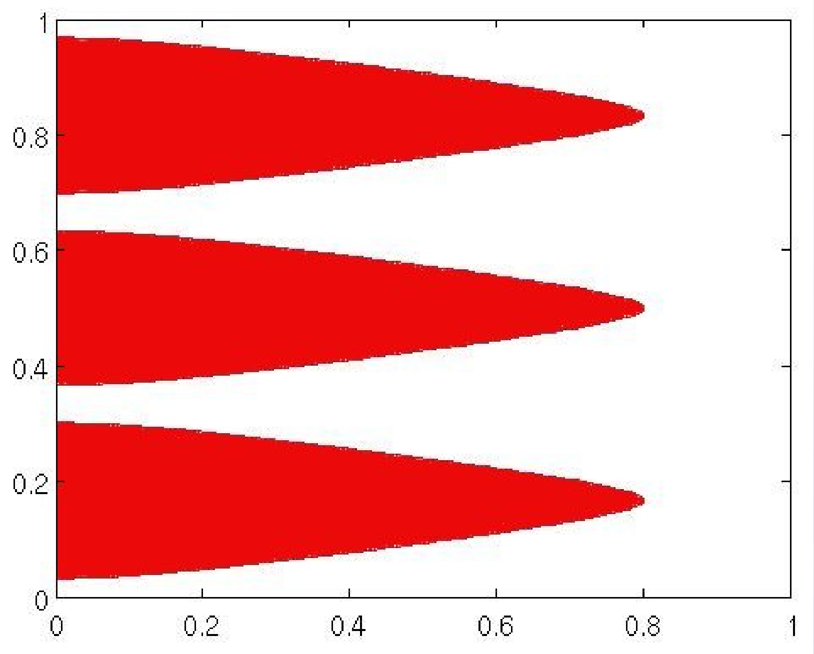
Discretization error at each evaluation point is $\mathcal{O}(10^{-5})$.

We are interested in $P[q(\lambda) > 0.03]$.

# Example

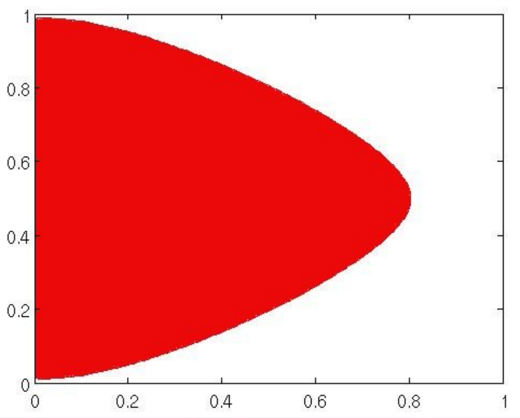


Quantity of Interest

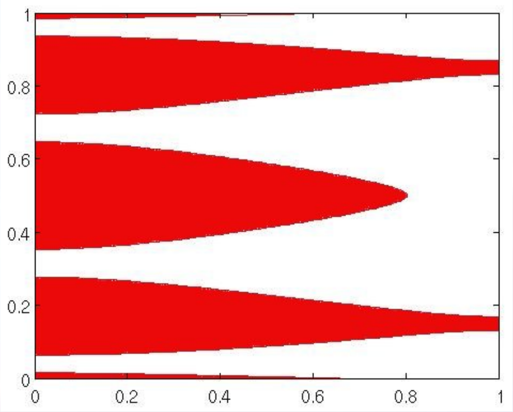


Region where $q(u(\boldsymbol{\lambda})) > 0.3$

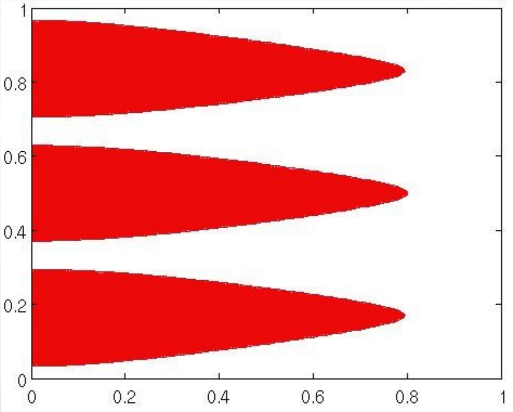
# Example



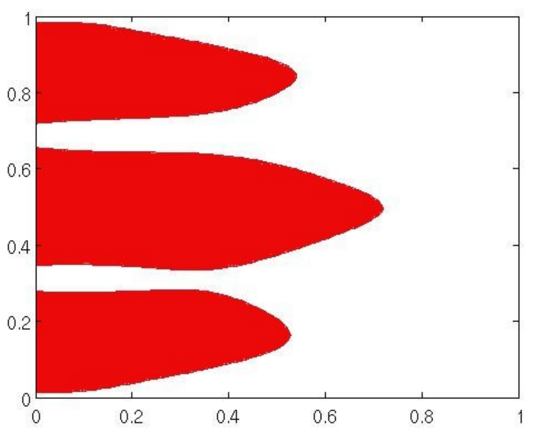
PCE-4



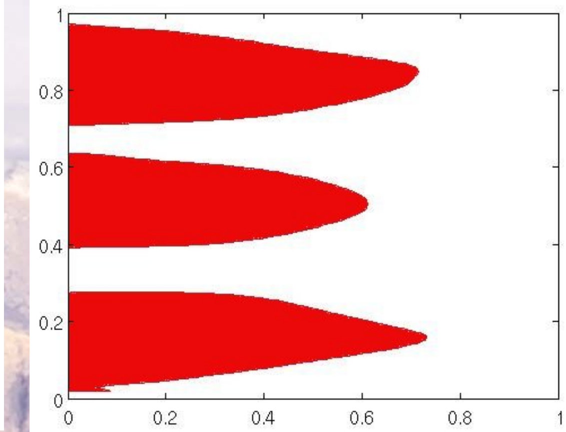
PCE-8



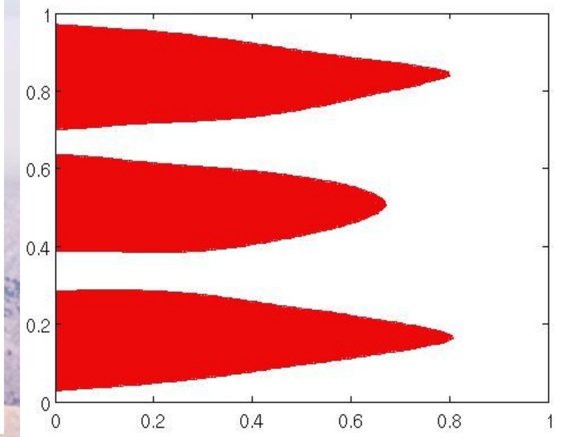
PCE-12



PCE-4 + 10 RBF’s



PCE-4 + 50 RBF’s



PCE-4 + 100 RBF’s

# Conclusions

# Conclusions

- Surrogate models typically have errors due to:
  - spatial and temporal discretizations
  - truncated stochastic expansions or quadrature
- All statistics of the surrogate model are affected by error in the surrogate.
- We can produce a posteriori error estimates for samples of a quantity of interest obtained from a surrogate model.
- Can be used for error estimates, error bounds, defining improved quantities of interest, and adaptivity.

## Thank you for your attention!
## Questions?

Sandia
National
Laboratories