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# A Posteriori Error Analysis of Stochastic Differential Equations Using Polynomial Chaos Expansions


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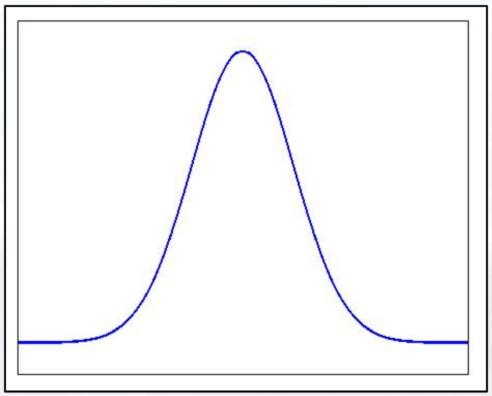
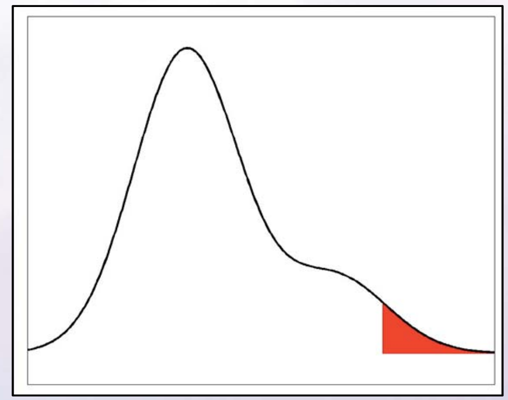
# Motivation

# Uncertainty Quantification



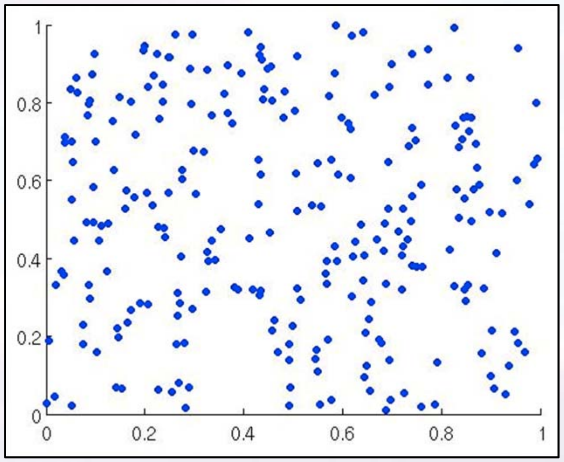
**Model:**
$u = M(\lambda)$



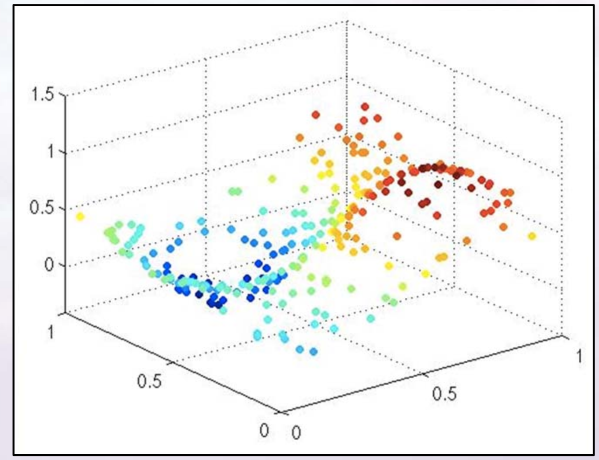
Given parameter(s) $\lambda$ with distribution(s). (Aleatoric)

Calculate probabilities on quantities of interest $q(u(\lambda))$.

# Monte Carlo Sampling (LHS, IS)




**Model:**
$u = M(\lambda)$




$$\mathrm{P}[q(u(\lambda)) > 1] = 0$$

Unfortunately, we oftentimes use approximate models,

$$U = M_{\Delta x, \Delta t}(\lambda)$$

Deterministic error analysis can estimate how these numerical errors propagate and accumulate to impact the quantity of interest for each sample.

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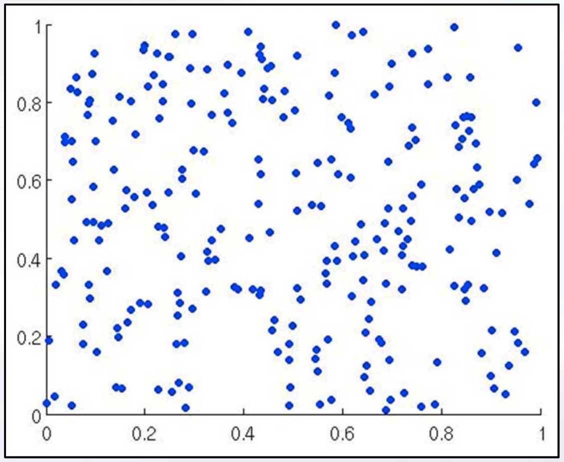
# Monte Carlo Sampling (LHS, IS)




**Model:**
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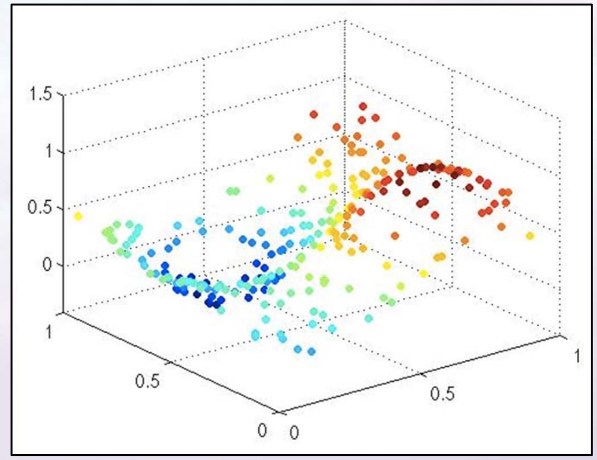



$$\mathrm{P}[q(u(\lambda)) > 1] = 0$$

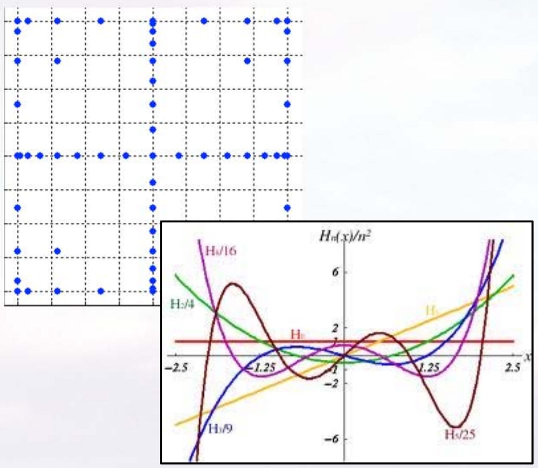
Do we trust Monte Carlo (LHS, IS) to compute probabilities of rare events given a small number of samples?[1]

[1] "Importance Sampling: Promises and Limitations". L. P. Swiler and N. J. West. 2010.

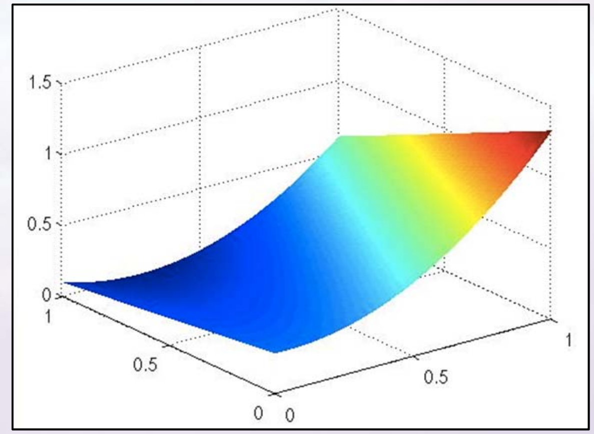
# Monte Carlo


# Monte Carlo


# Surrogate Models and Sampling




**Model:**
$u = M(\lambda)$




$$\mathrm{P}[q(u(\lambda)) > 1] = 0.035$$

We have potentially traded accuracy for a large number of samples.

Do we trust surrogate methods to compute probabilities of rare events given (virtually) unlimited samples?

See "Epistemic Uncertainty in the Quantification of Margins". L. Swiler, T. Paez, R. Mayes and M. Eldred. SAND Report 2008.

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# 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.

# Model Problem and Approximations

# Model Problem

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,

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

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

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

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# 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?

# A Posteriori Error Analysis for Polynomial Chaos Approximations

# 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:

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

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# The Error Representation

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

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

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# Numerical Results

# 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 $\sigma = 0.1$.

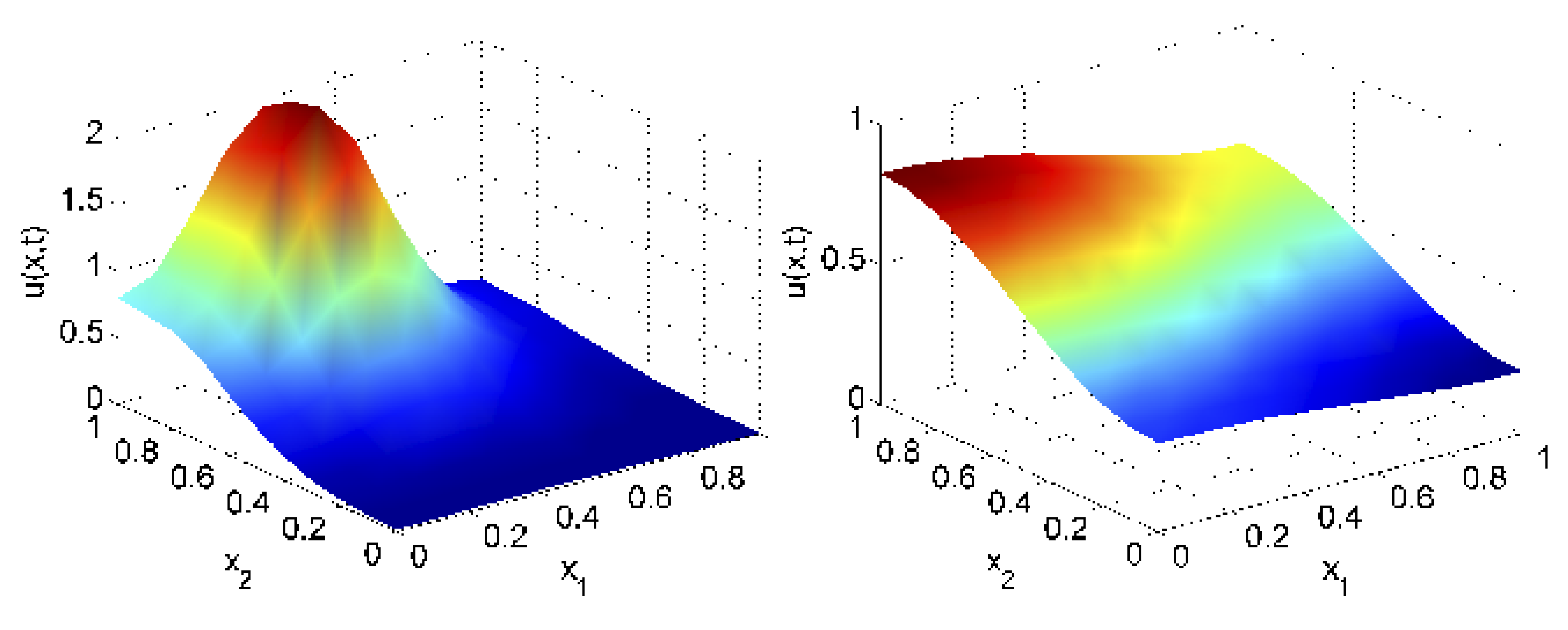
Random variable $\lambda$ uniformly distributed on $[0,1]^2$.

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.

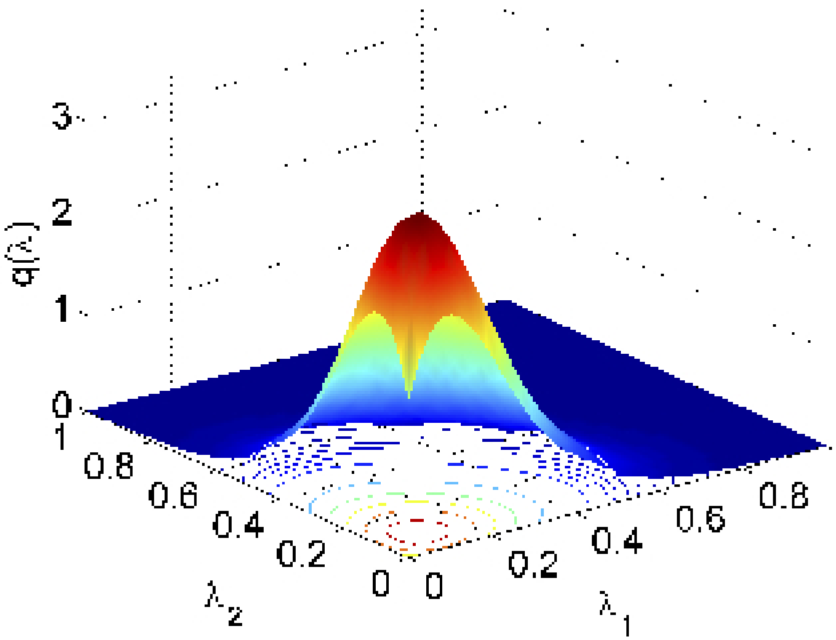
[2]See "Stochastic spectral methods for efficient Bayesian solution of inverse problems". Y. Marzouk, H. Najm and L. Rahn. 2007.

# Contaminant Approximation: λ = (0.4,0.8)

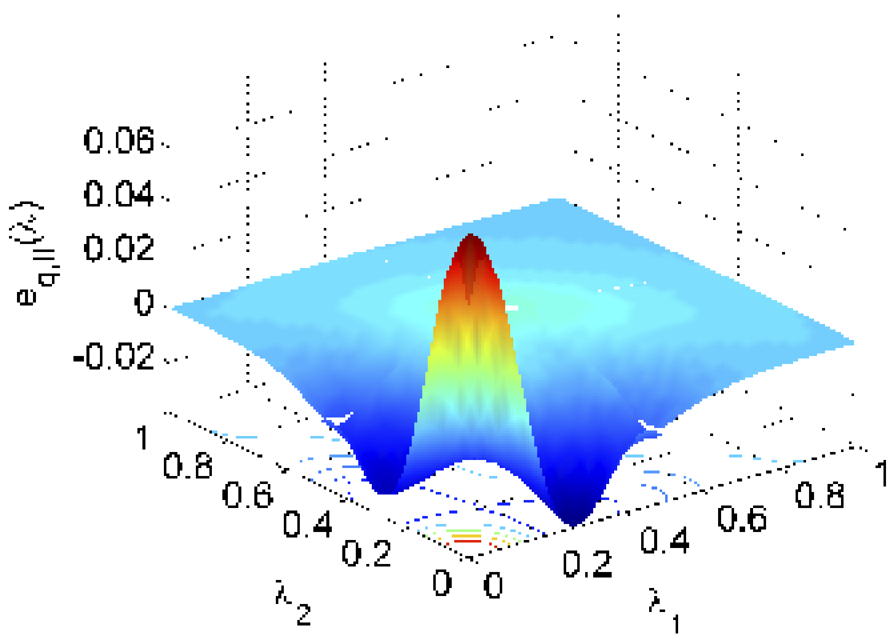



$t = 0.05$ $t = 0.15$

# First Quantity of Interest at t = 0.05

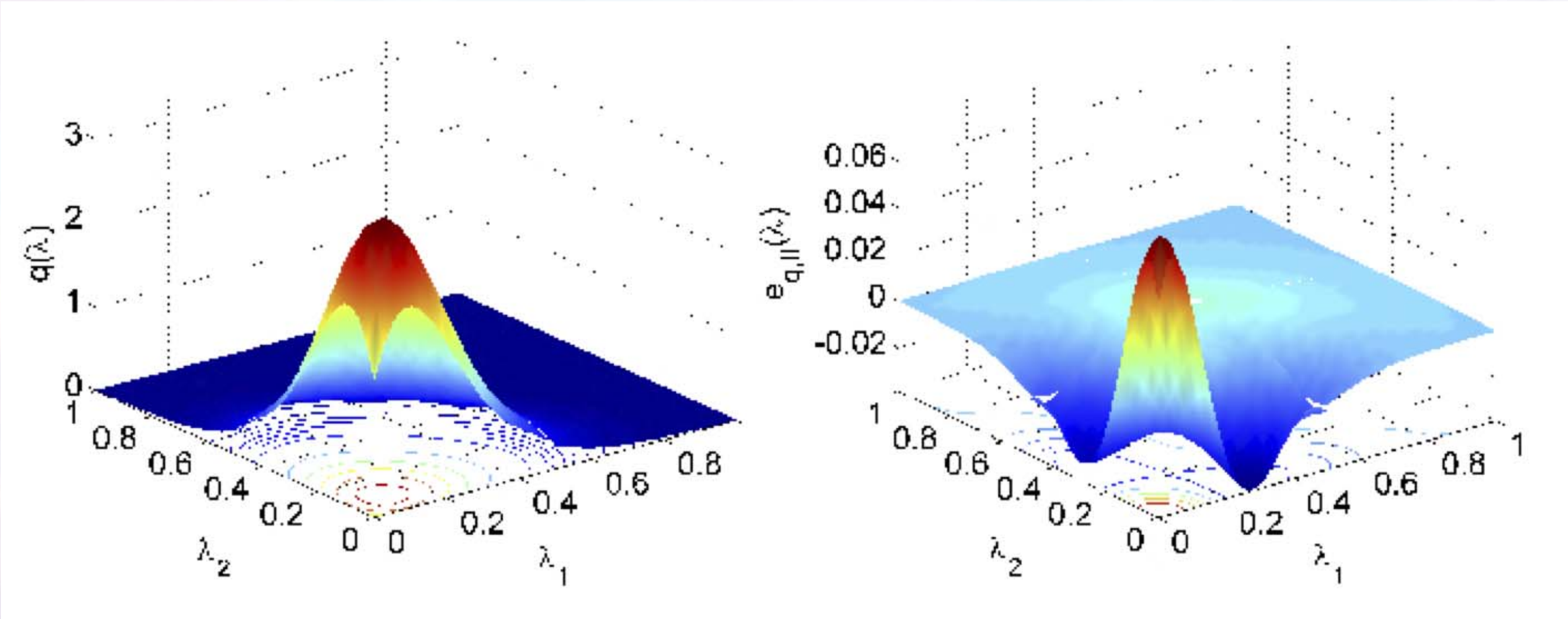



PC approximation



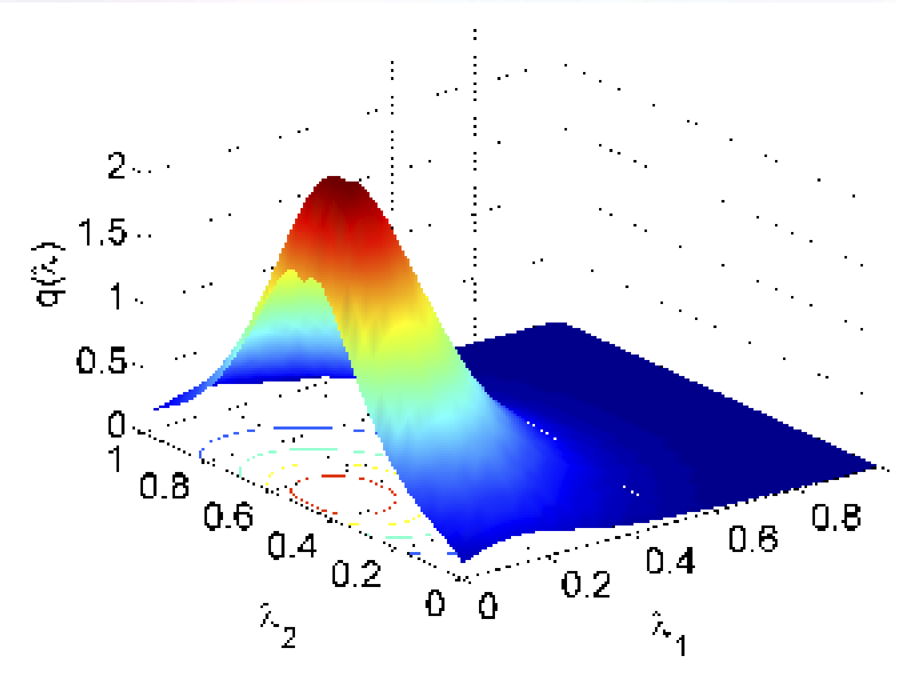

A posteriori error estimate

# First Quantity of Interest at t = 0.05

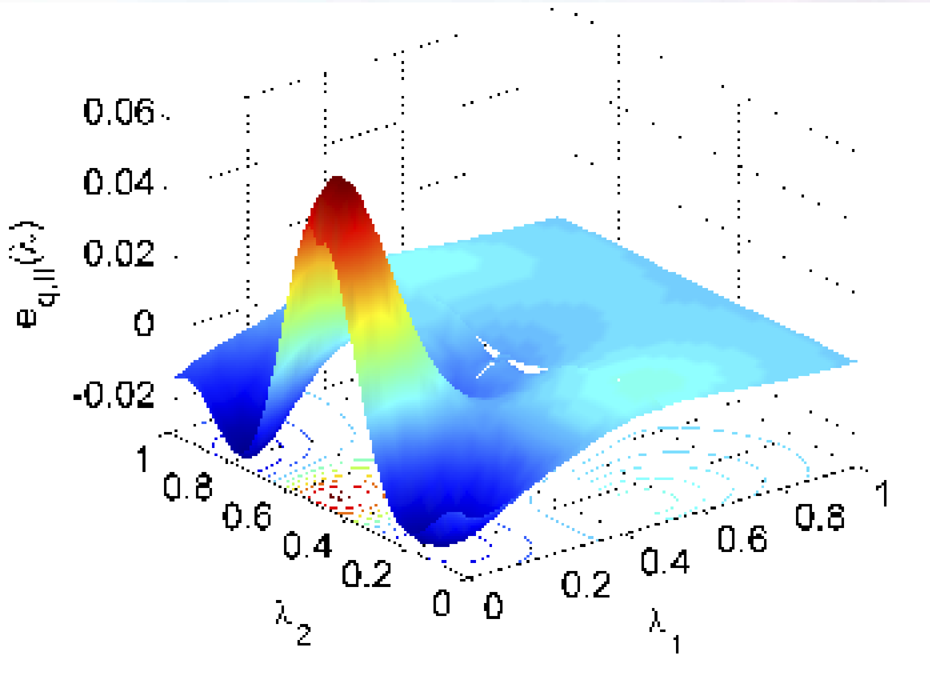



PC approximation A posteriori error estimate

# Fourth Quantity of Interest at t = 0.05

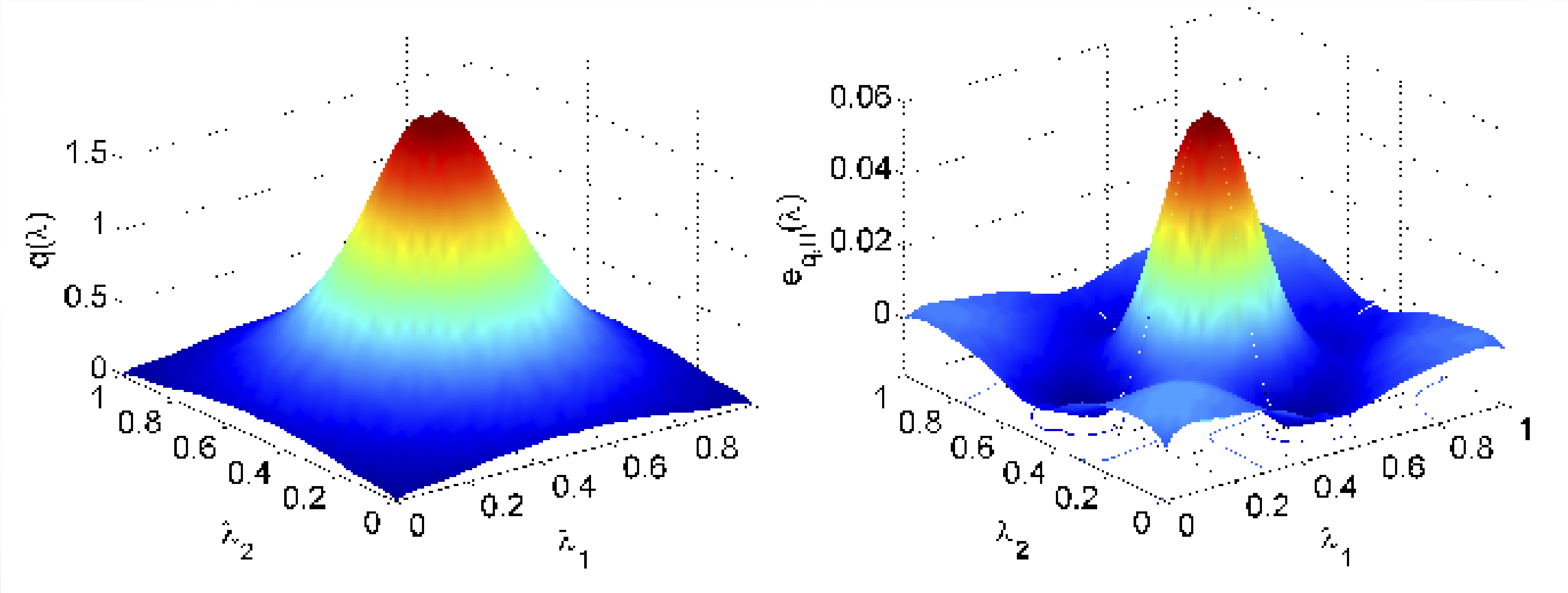



PC approximation



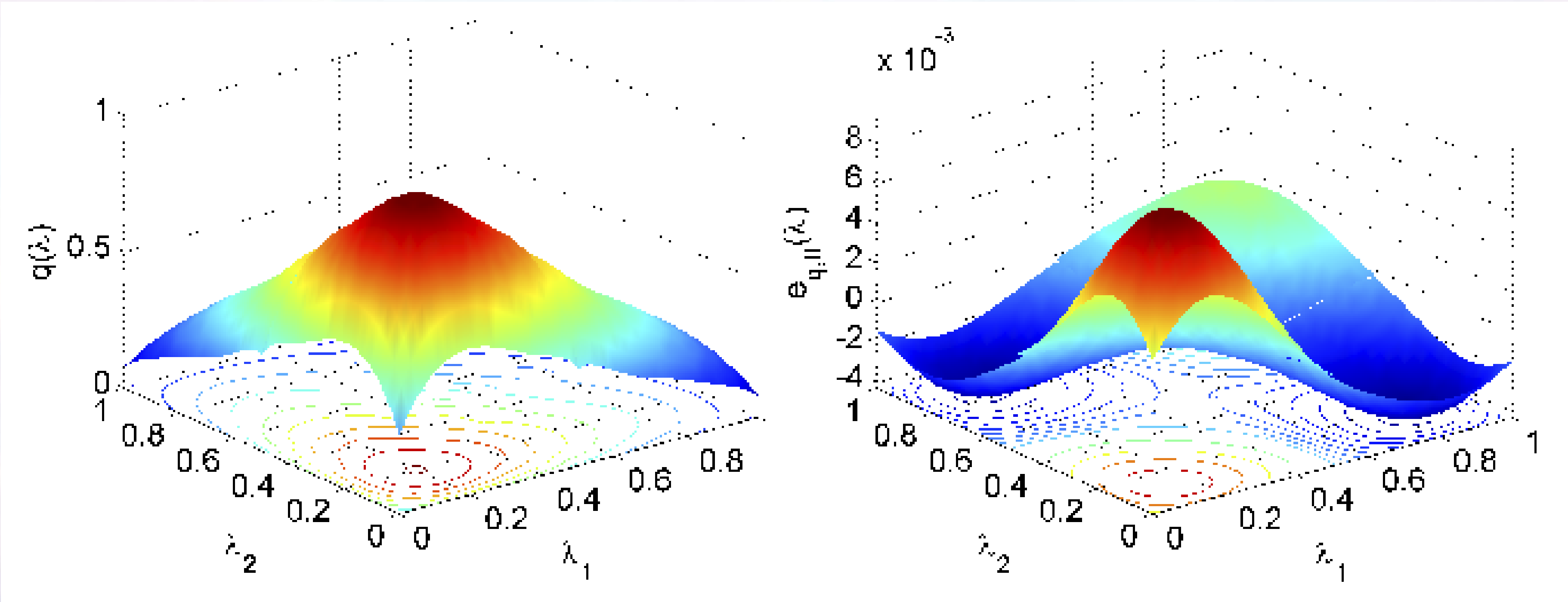

A posteriori error estimate

# Fifth Quantity of Interest at t = 0.05




PC approximation | A posteriori error estimate

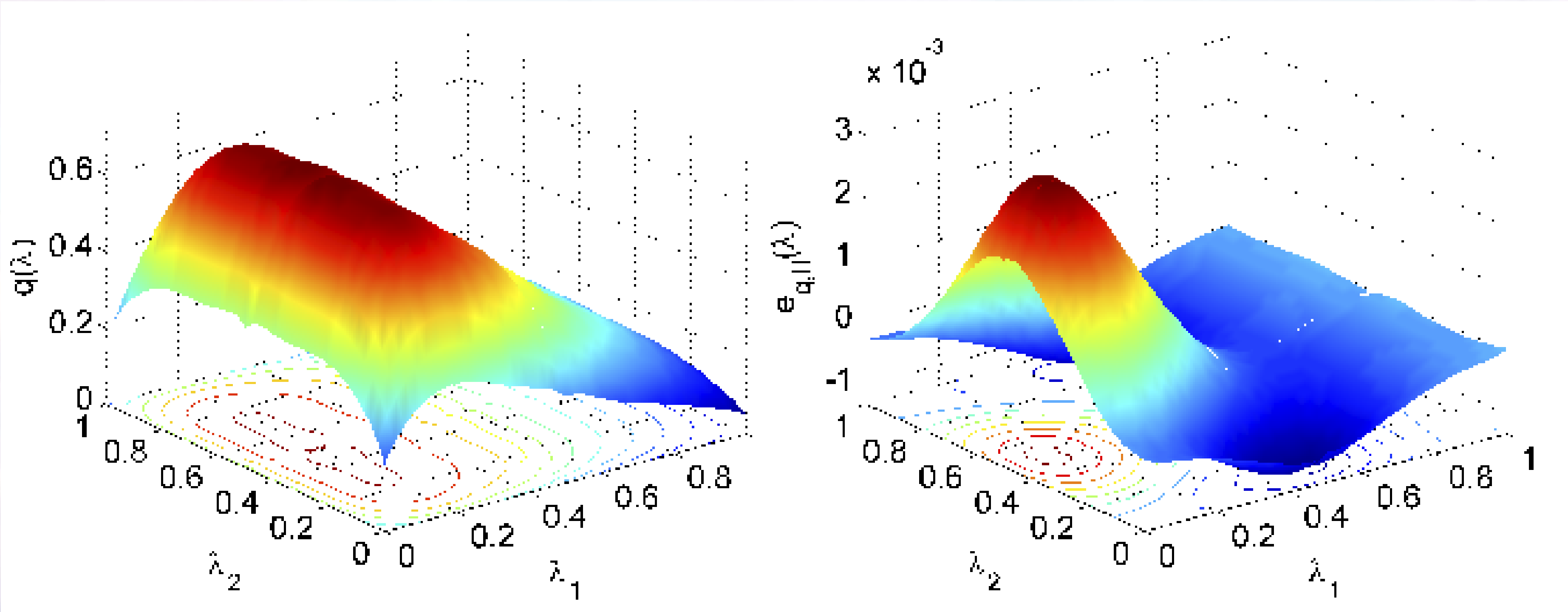
# First Quantity of Interest at t = 0.15




PC approximation

A posteriori error estimate

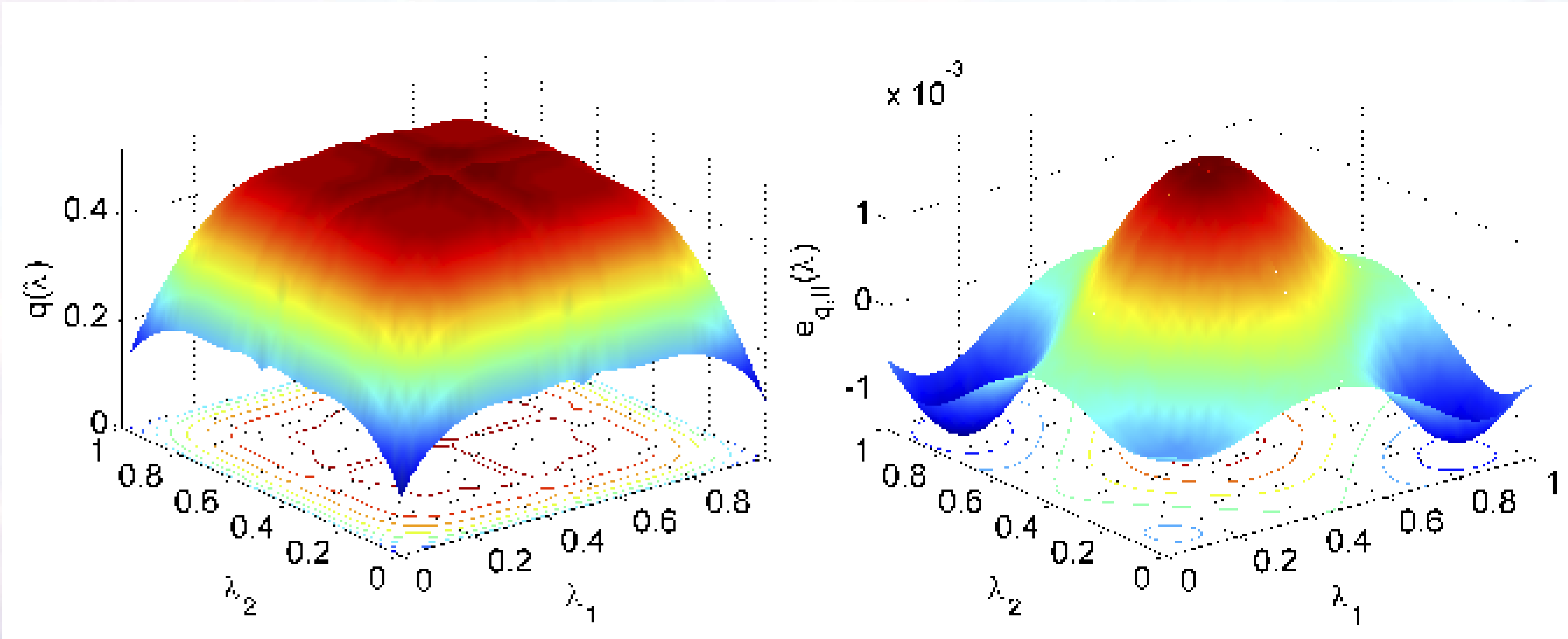
# Fourth Quantity of Interest at t = 0.15




PC approximation

A posteriori error estimate

# Fifth Quantity of Interest at t = 0.15




PC approximation    A posteriori error estimate

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# 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 |

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# 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 |

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# 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 $\sigma = 0.1$.

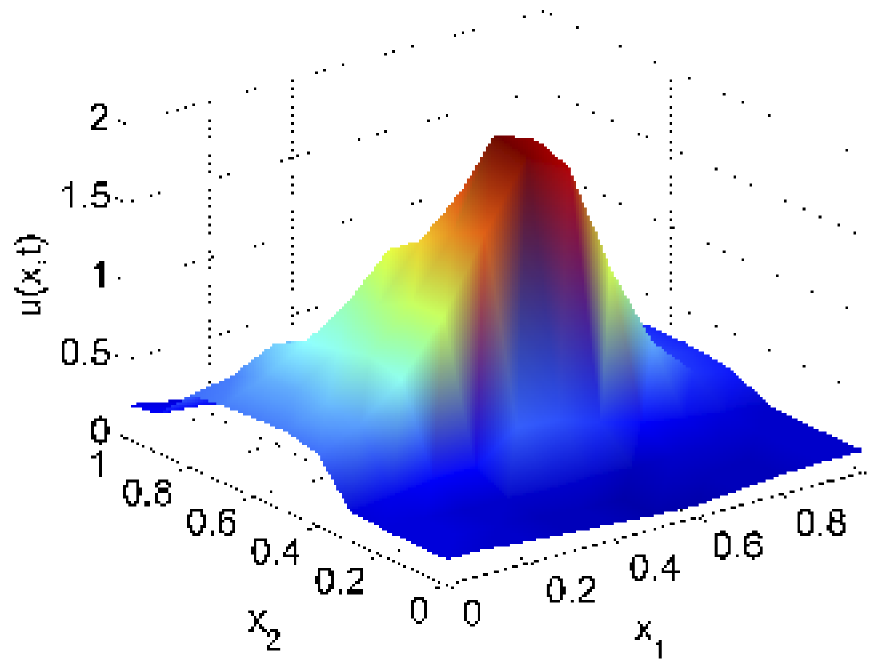
$$A(x,t;\lambda) = \begin{pmatrix} \lambda \exp(2\sin(2\pi x)\cos(4\pi y) & 0 \\ 0 & \exp(2\sin(4\pi y) + 2\cos(2\pi x) \end{pmatrix}$$

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

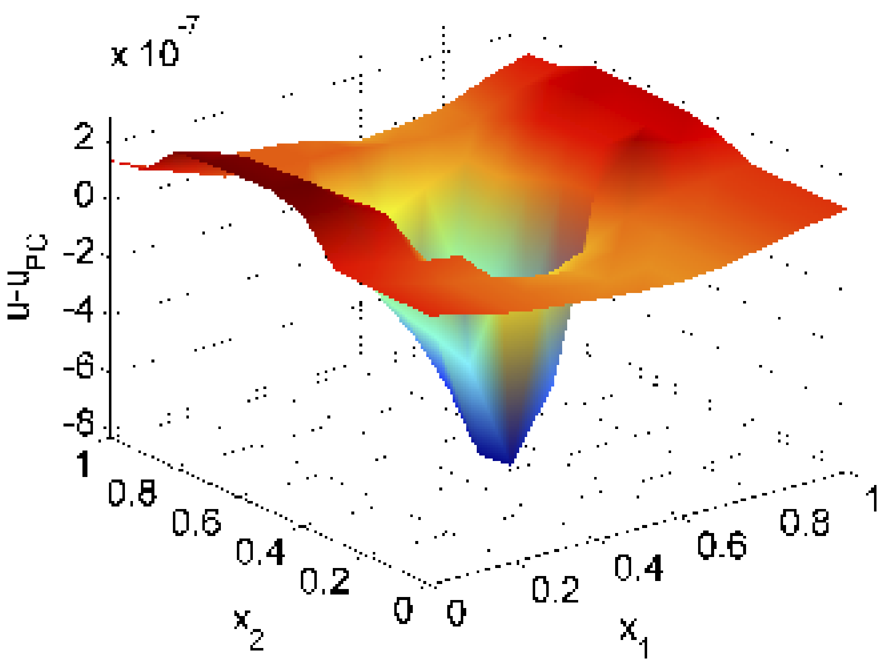
Quantities of interest: Concentration at $t = 0.05$ and $t = 0.15$ at 9 measurement locations.

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

# Approximation and PC Error at λ = 1

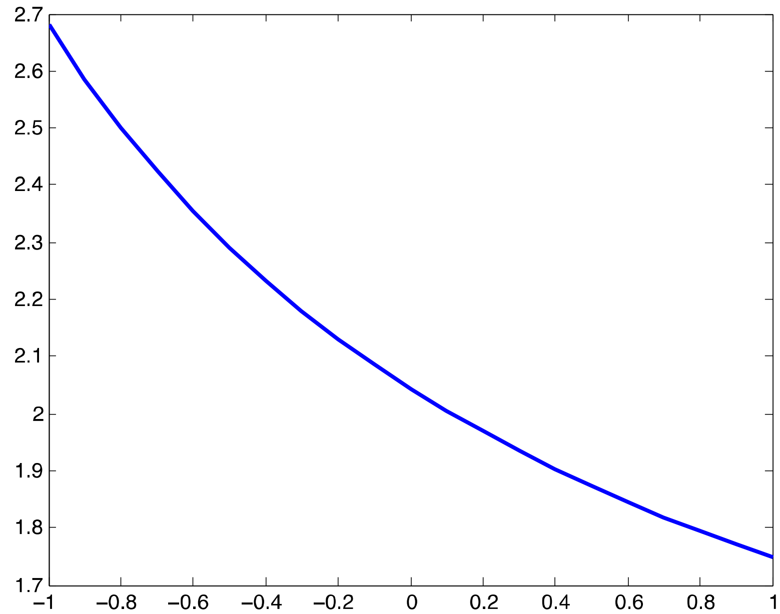



PC approximation

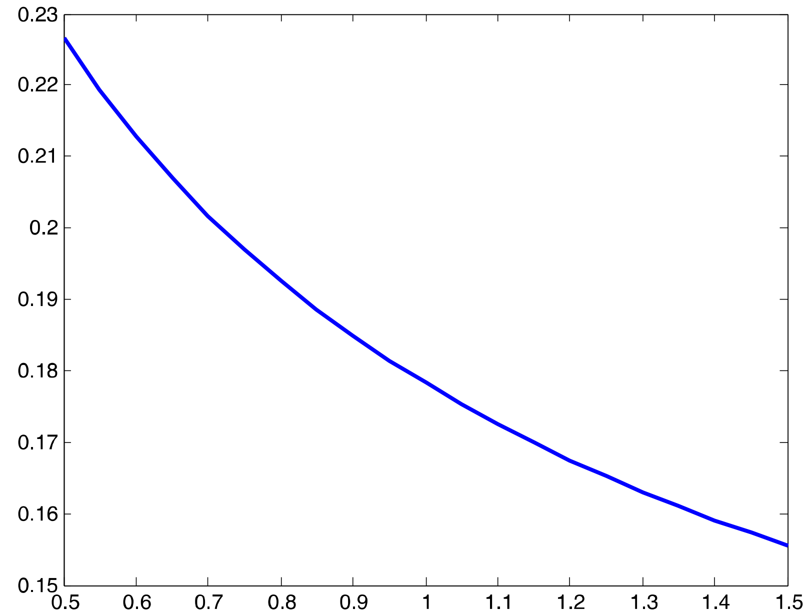



PC truncation error

# Fifth Quantity of Interest at t = 0.05




PC approximation




A posteriori error estimate

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# 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 |

# Conclusions and Future Work

# Conclusions and Future Work

- Surrogate models typically have errors due to:
  - spatial and temporal discretizations
  - truncated stochastic expansions or quadrature
- We can produce a posteriori error estimates for a quantity of interest obtained by sampling a surrogate model.
- Can be used for error estimates, error bounds, defining improved quantities of interest, and adaptivity.
- Future work will include:
  - Stochastic adaptivity,
  - Inverse problems.
  - Account for propagation of uncertainty in multiphysics and multi-scale problems.