Utilizing Adjoint-Based Techniques to Improve the Accuracy and Reliability in Uncertainty Quantification

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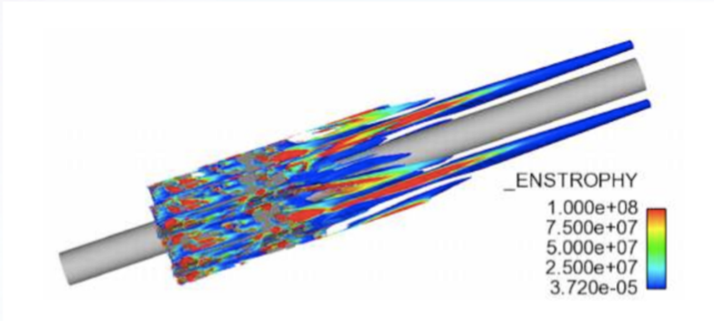
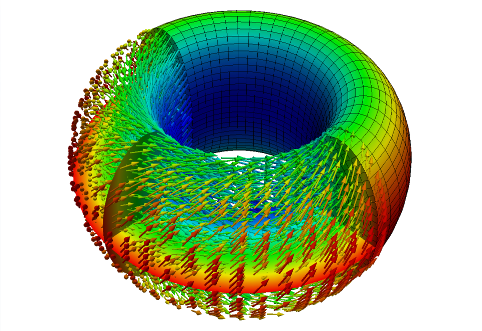
Motivation

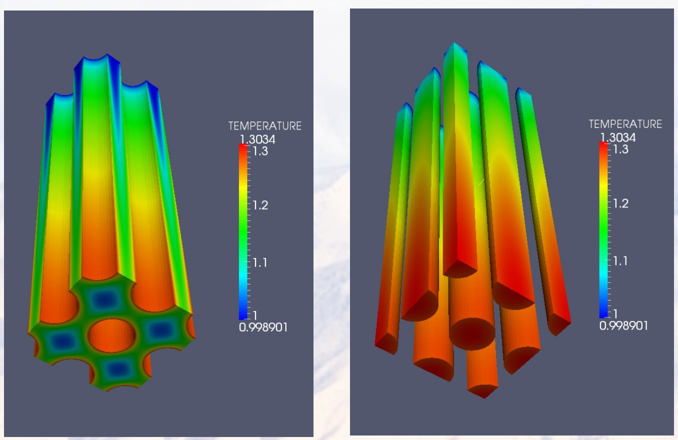
Large Scale Nonlinear Multi-Physics Simulations



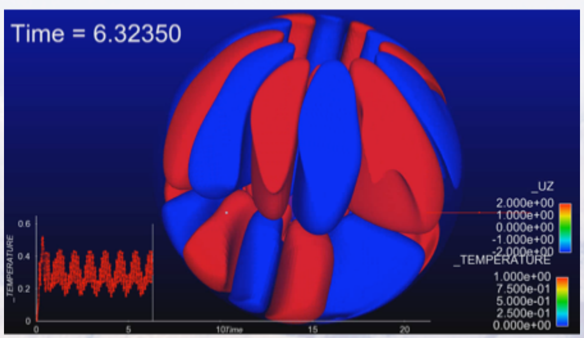
Flow in Nuclear Reactor (Turbulent CFD)


Tokamak Equilibrium (MHD)

1. **PDE constrained optimization with large number of design parameters**
2. **Understand the accuracy in quantities of interest**



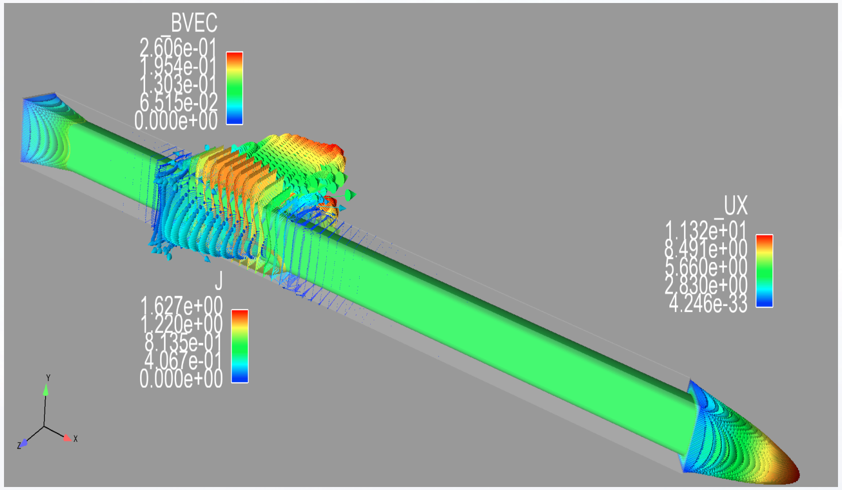
Fully-coupled conjugate heat transfer



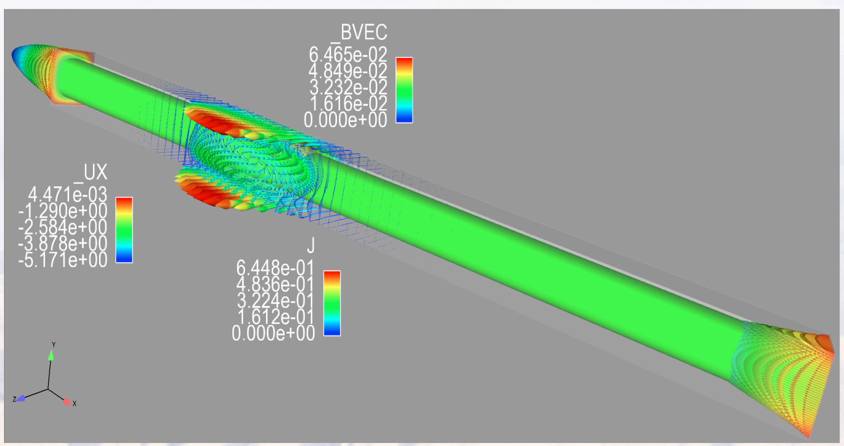
Geodynamo (MHD)

Drekar Resistive MHD Adjoint Test Problems

MHD Generator (Re ~ 2500, Re_m ~ 10, Ha = 5)



Forward Solution



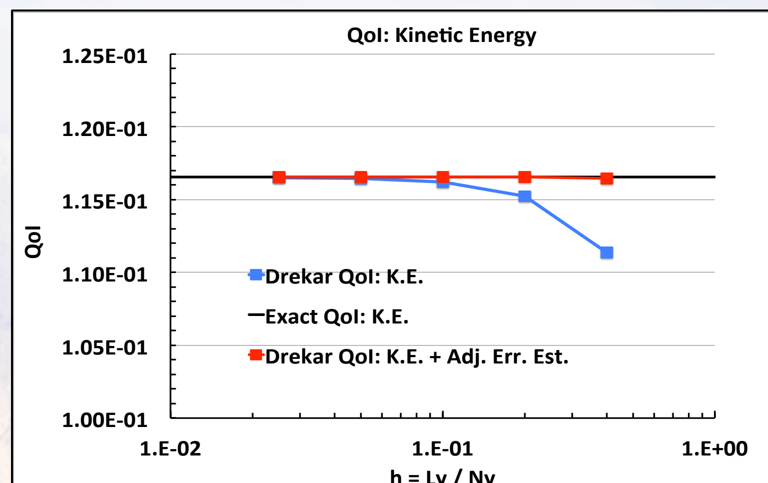
Adjoint Solution

Hartmann Flow

Accuracy in derivatives:

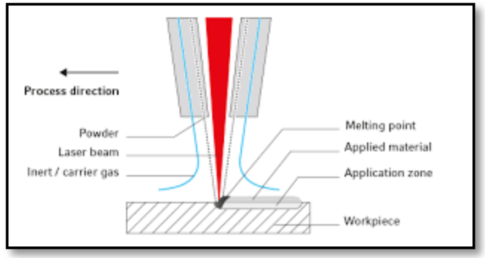
Physical Parameter	Analytic	Drekar /Adjoint	Rel. Err.
Pressure Gradient	-20.9318	-20.9753	0.21%
Dynamic Viscosity	-3972.97	-3979.72	0.17%
Resistivity	778.574	779.988	0.18%

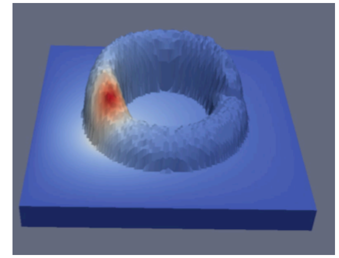
Accuracy in error estimates:

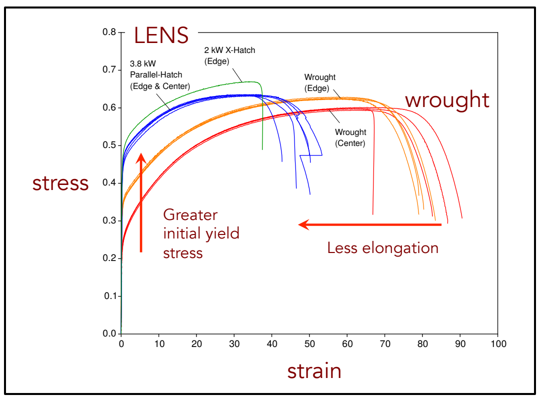


Predict/Control Performance of Additive Manufacturing of Materials and Components with Quantified Uncertainty

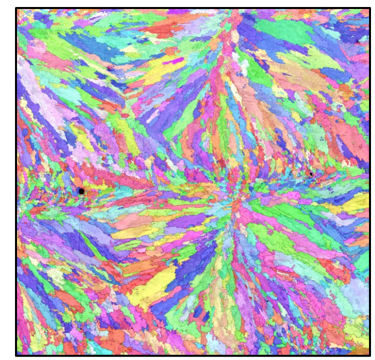
AM Process Modeling



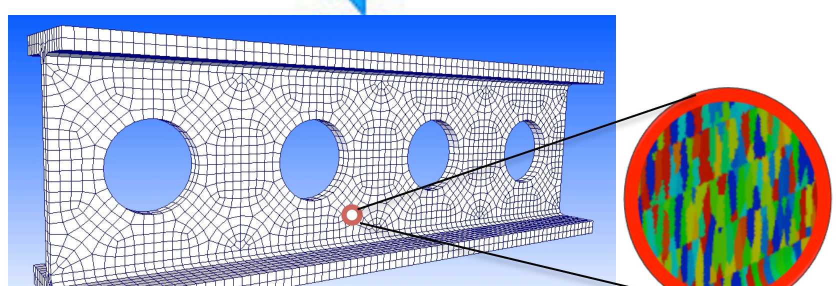




Component performance assessment
- J. Carroll (SNL)



Material characterization with quantified uncertainty
- J. Michael and D. Adams (SNL)



Multi-scale Modeling

Emerging Concepts in PDE-Constrained Optimization Under Uncertainty

Goal: Develop *efficient* methods to determine *resilient* optimal controls & designs that *mitigate high-consequence rare events*.

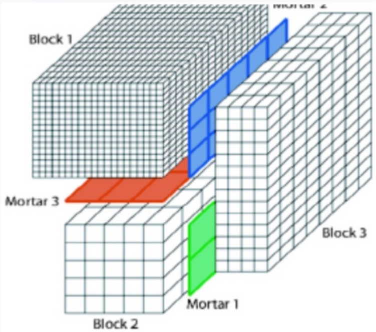
Minimize **risk** *subject to* **probabilistic** *constraints:*

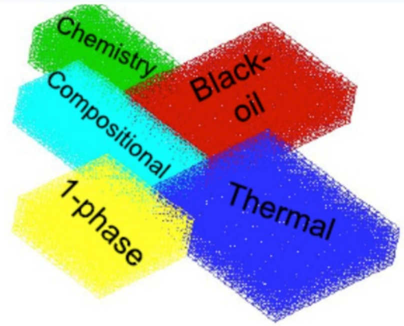
$$\min_{z\in\mathcal{Z}} \mathcal{R}(J(U(z),z)) \quad \text{subject to} \quad p_\tau(U(z)) \le p_0.$$

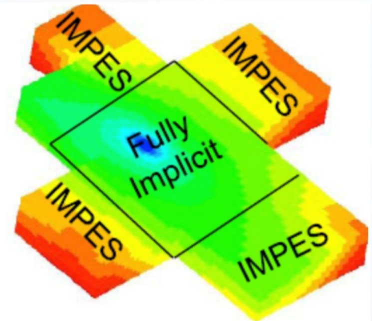
Solving these problems requires addressing significant challenges (high-dimensional spaces, rare-event detection, non-smooth objective functions, etc.) and is the subject of active research.

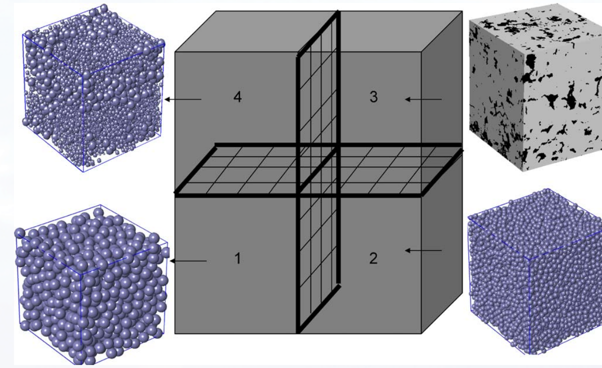
D. Kouri, D. Ridzal, B. van Bloemen Waanders (SNL); W. Aquino (Duke);
S. Uryasev, R,Rockafellar (U-Florida); A. Shapiro (GA-Tech)

Multi-scale Modeling with Mortar Methods





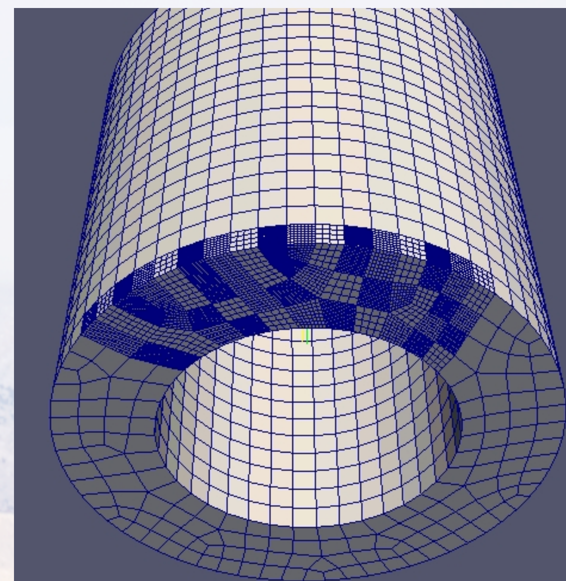




M. Balhoff (UT-Austin)

Benefits of Multi-scale Mortar Approach

- Solid mathematical foundation *[Arbogast et al 2007]*
- Enables different discretizations, physics, and/or numerical methods *[Pencheva et al 2013, Girault et al 2008, Tavener, W. 2013]*
- Easily incorporates non-PDE based models *[Balhoff, Wheeler 2008]*
- No upscaling/homogenization of parameters *[Peszyńska et al 2002]*
- Provides a concurrent multi-scale formulation
- Hierarchical structure easily extended to finer or coarser levels
- Related to hybridizable discontinuous Galerkin
- Provides new opportunities for embedded V&V/UQ
- **Straightforward to define continuous/discrete adjoints** ***[Tavener, W. 2013]***



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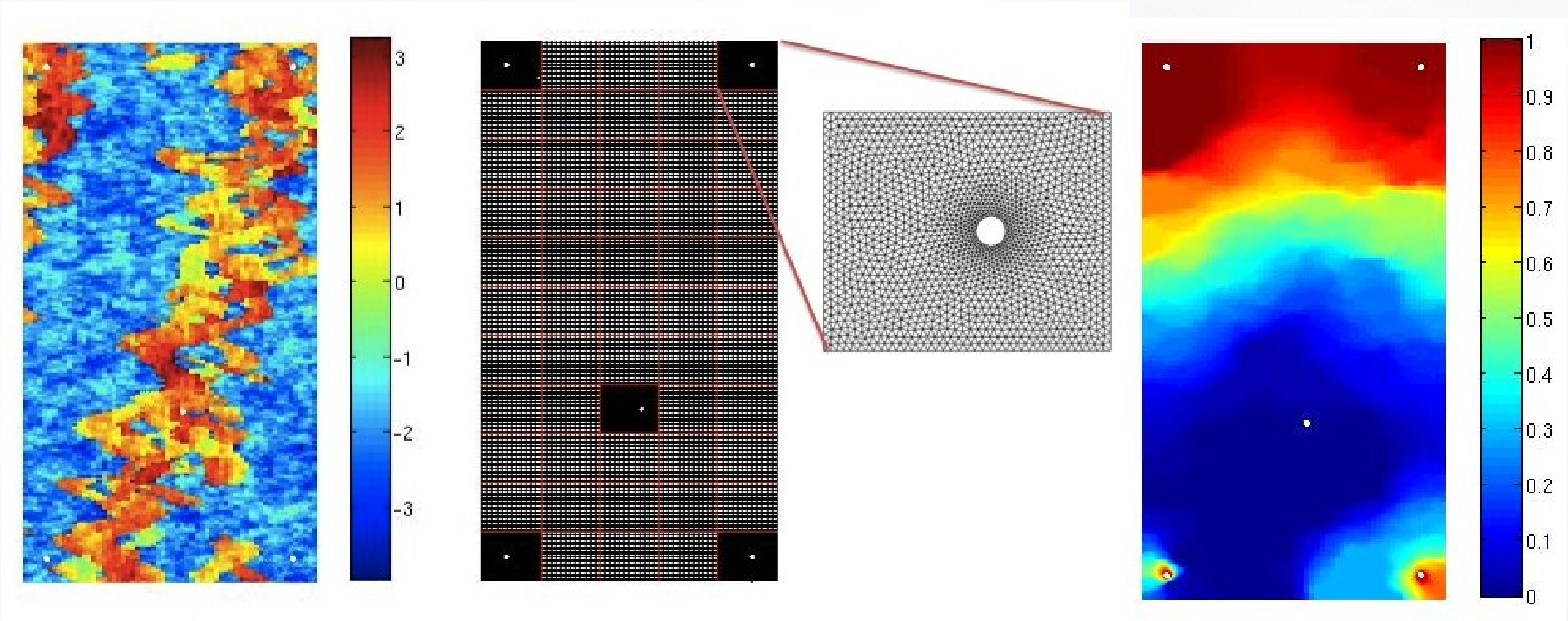
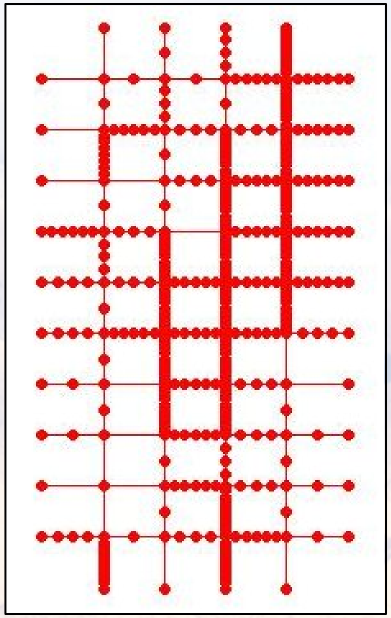
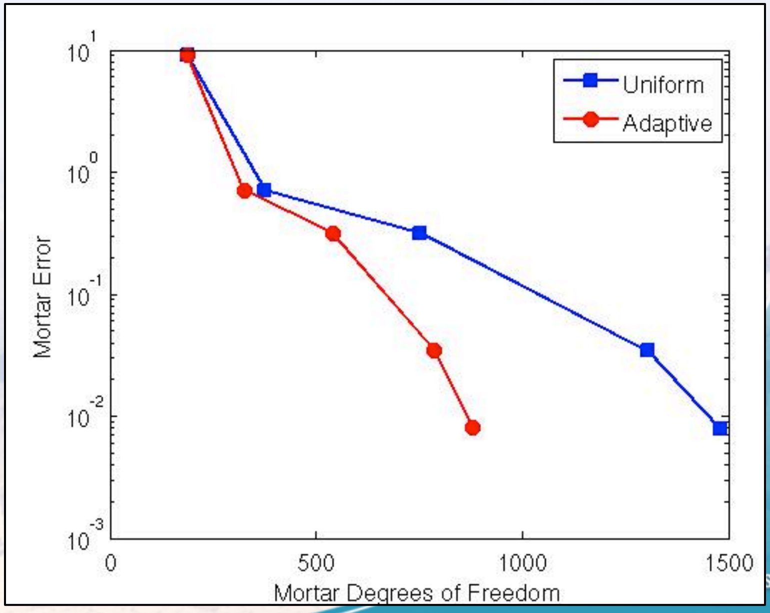
Adjoint-Based Error Estimation and Adaptivity

[Tavener, W. SISC 2013]



- SPE10 permeability field (layer 75)
- 4 injection wells, 1 production well
- Subdomains with wells use DG with grids adapted to wells
- Other subdomains use CCFV
- QoI is the pressure at production well
- Subdomain grids are fixed
- **Error estimate provides separate indicators for coarse and fine scale**
- Goal is to **adaptively refine coarse scale** to accuracy of fine scale

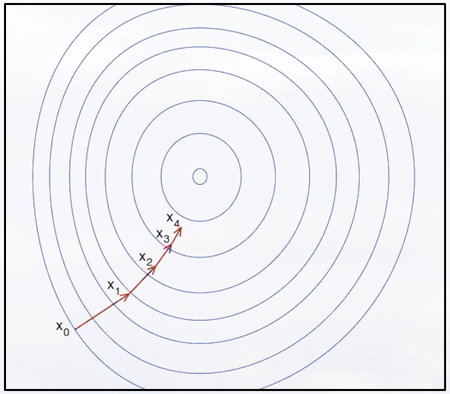


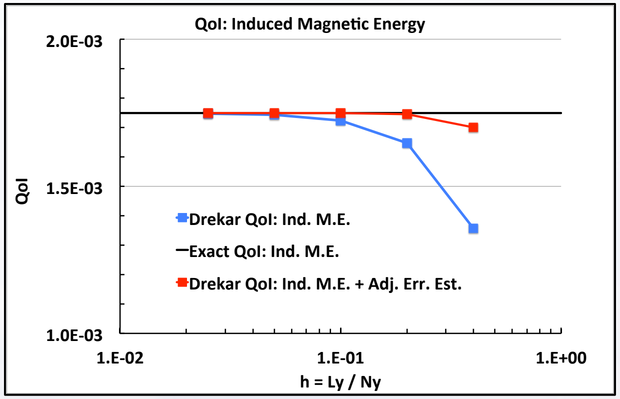


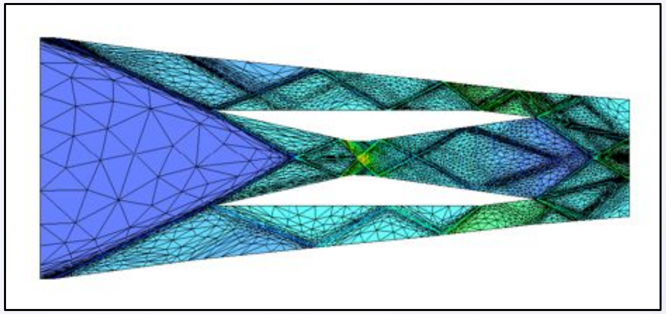
Leveraging Adjoint Capabilities

Motivations for Adjoint Development

- Accurate and efficient gradients for large-scale PDE constrained optimization
- Accurate goal-oriented error estimates
- Goal-oriented adaptive mesh refinement







Source: *Belme et al, JCP 2012*

Can we leverage these capabilities for UQ?

- Multi-physics problems have numerous sources of uncertainty
- High computational cost for single simulation -> limits number of runs
- Often interested in low-probability (rare), high consequence events
- Quantities of interest may have discontinuities

Uncertainty Quantification, Error Estimates, and Response Surface Approximations

UQ, Response Surfaces and Error

We are often faced with:

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_N \end{bmatrix} \;\Rightarrow\; u = M(\boldsymbol{\lambda}) \;\Rightarrow\; q(u(\boldsymbol{\lambda})) = \begin{cases} \text{spatial average} \\ \text{mean stress} \\ \text{time averages} \\ \text{etc...} \end{cases}$$

UQ, Response Surfaces and Error

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

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

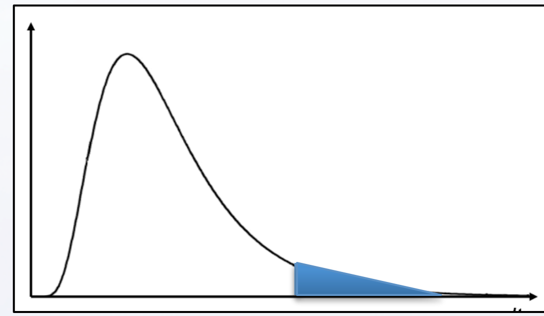
$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$

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

→

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

→



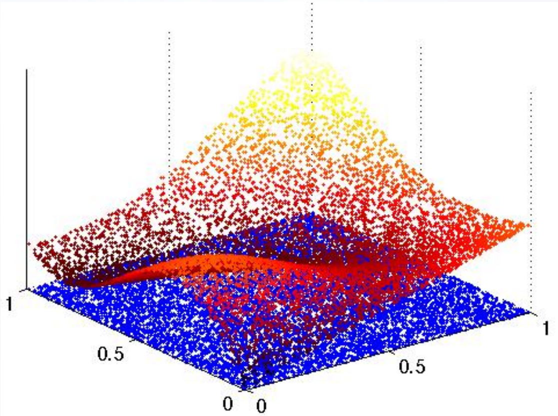
then we can investigate statistics of the response (mean, variance, distribution, probabilities).

UQ, Response Surfaces and Error

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

$$(\Omega, \mathcal{F}, P)$$
$$\boldsymbol{\lambda} : \Omega \to \Pi_{i=1}^{N} I_i$$
$$F_{\boldsymbol{\Lambda}}(\boldsymbol{\lambda})$$

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



and calculate the desired statistics from the response.

Unfortunately ...

UQ, Response Surfaces and Error

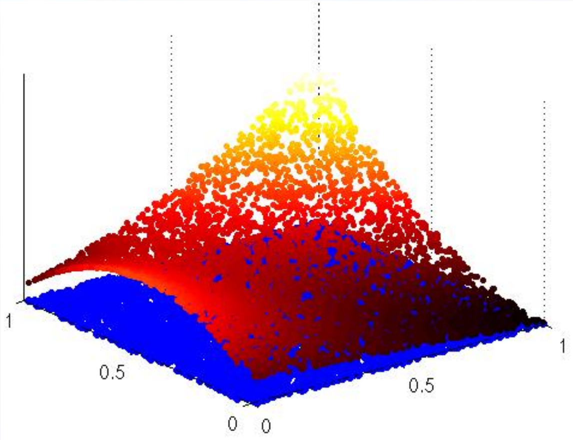
We only have an approximate model.

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

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

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

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



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

Worse still ...

UQ, Response Surfaces and Error

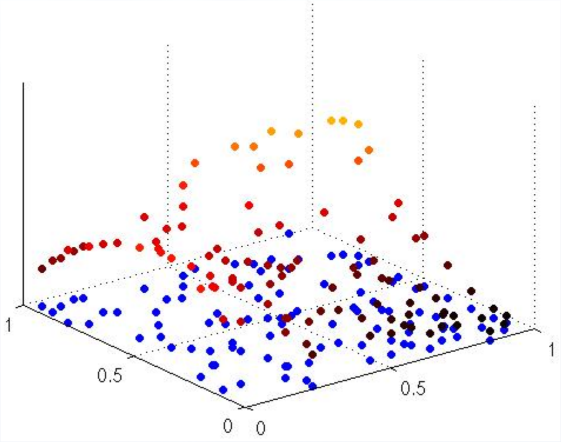
The approximate model is expensive to evaluate, which limits the number of samples.

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

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

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

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



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

Do you trust the results?

Monte Carlo


François GRIMALDI
" MALIZIA "
1297 - 1997


François GRIMALDI
" MALIZIA "
1297 - 1997

Monte Carlo

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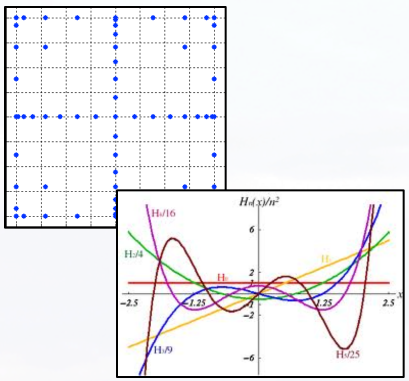
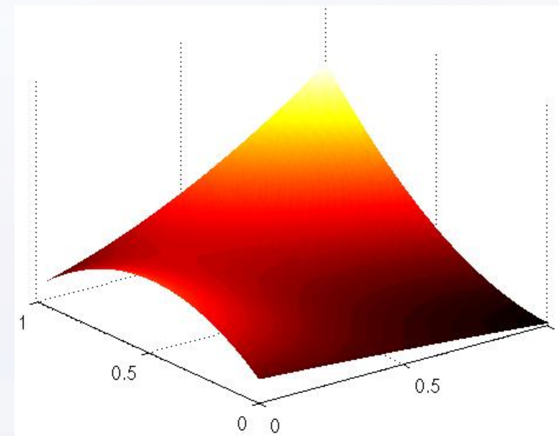
UQ, Response Surfaces and Error

Alternatively, we can use a small number of evaluations to approximate the response surface.



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



Examples include polynomial chaos, stochastic collocation, regression, etc.

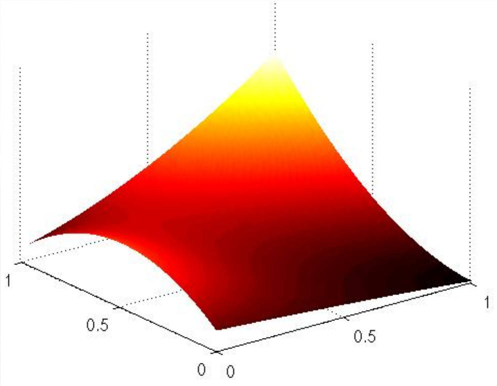
UQ, Response Surfaces and Error

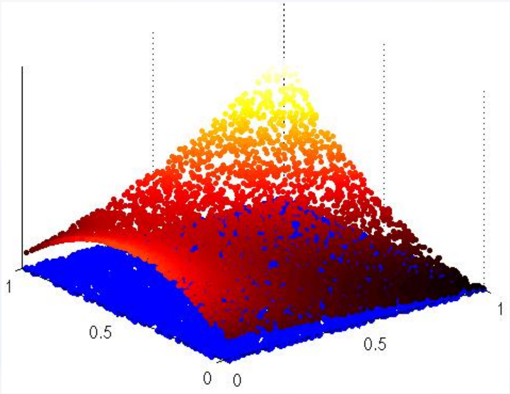
We can estimate the statistics using samples of the response surface approximation.

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

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

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



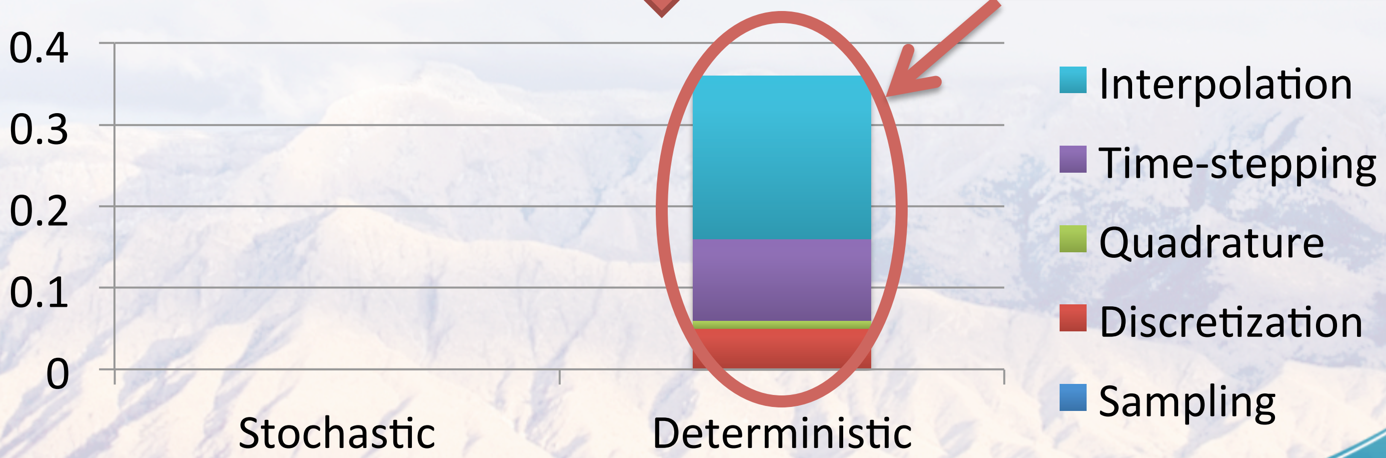


We have reduced the statistical sampling error.

Is the prediction more accurate?

UQ, Response Surfaces and Error

Can we estimate or correct these deterministic errors?



Error Estimates for Samples of a Response Surface Approximation

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Standard Adjoint-Based Error Estimate for Systems of Partial Differential Equations

Consider the following system of partial differential equations,

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{A}(\boldsymbol{\lambda}; \boldsymbol{u}) = \boldsymbol{0}, \quad \boldsymbol{u}(\boldsymbol{\lambda}; 0, \boldsymbol{x}) = \boldsymbol{u}_0$$

for $\boldsymbol{x} \in D \subset \mathbb{R}^n$ with suitable boundary conditions.

$\boldsymbol{\lambda} \in \boldsymbol{\Lambda} \subset \mathbb{R}^d$ represents the uncertain parameters.

For now, assume $\boldsymbol{\lambda}$ is fixed.

Let $\boldsymbol{u}_h$ be some discrete approximation of $\boldsymbol{u}$.

We want to estimate the error in a *quantity of interest*:

$$J(\boldsymbol{\lambda}; \boldsymbol{u}) - J(\boldsymbol{\lambda}; \boldsymbol{u}_h)$$

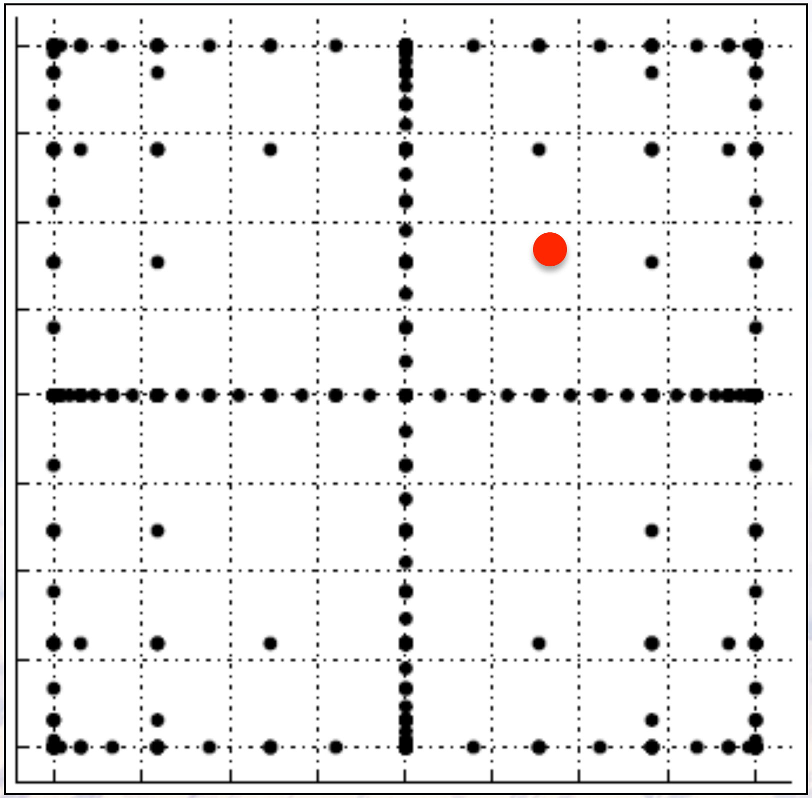
Standard adjoint-based error estimate:

$$J(\boldsymbol{\lambda}; \boldsymbol{u}) - J(\boldsymbol{\lambda}; \boldsymbol{u}_h) \approx \epsilon(\boldsymbol{\lambda}; \boldsymbol{u}_h, \boldsymbol{\phi})$$

A Computable Error Estimate

Given an arbitrary point in the parameter space, we need to estimate the error in the response surface at that point.

Example: isotropic sparse grid



- Points where we evaluate the model
- Point where we evaluate the sparse grid approximation

A Computable Error Estimate

We use sparse grid approximations of the forward and adjoint solutions ($\boldsymbol{u}_{h,n}$ and $\boldsymbol{\phi}_{h,n}$) to estimate the error:

$$J(\boldsymbol{\lambda};\boldsymbol{u}) - J(\boldsymbol{\lambda};\boldsymbol{u}_h) \approx \epsilon(\boldsymbol{\lambda};\boldsymbol{u}_{h,n},\boldsymbol{\phi}_{h,n})$$

Theorem *[Jakeman, W., JCP 2015]*

For sufficiently smooth functions $\boldsymbol{u}$ and $\boldsymbol{\phi}$ discretized using space-time finite elements and isotropic Smolyak formula based on Clenshaw-Curtis abscissa, the error estimate satisfies:

$$\|\epsilon(\boldsymbol{\lambda};\boldsymbol{u}_h,\boldsymbol{\phi}) - \epsilon(\boldsymbol{\lambda};\boldsymbol{u}_{h,n},\boldsymbol{\phi}_{h,n})\|_{L^\infty(\Gamma_{\boldsymbol{\xi}})} \leq \left(C_1(\sigma_1)n^{-\mu_1} + \hat{C}_1(\boldsymbol{u})\left(h^{s_1} + \Delta t^{\beta_1}\right)\right) \times \left(C_2(\sigma_2)n^{-\mu_2} + \hat{C}_2(\boldsymbol{\phi})\left(h^{s_2} + \Delta t^{\beta_2}\right)\right)$$

A Computable Error Estimate

We use sparse grid approximations of the forward and adjoint solutions ($\boldsymbol{u}_{h,n}$ and $\boldsymbol{\phi}_{h,n}$) to estimate the error:

$$J(\boldsymbol{\lambda}; \boldsymbol{u}) - J(\boldsymbol{\lambda}; \boldsymbol{u}_h) \approx \epsilon(\boldsymbol{\lambda}; \boldsymbol{u}_{h,n}, \boldsymbol{\phi}_{h,n})$$

Theorem *[Jakeman, W., JCP 2015]*

For sufficiently smooth functions $\boldsymbol{u}$ and $\boldsymbol{\phi}$ discretized using space-time finite elements and isotropic Smolyak formula based on Clenshaw-Curtis abscissa, the error estimate satisfies:

$$\begin{aligned} \text{Error in the error estimate} &\leq (\text{Error in forward}) \\ &\quad \times (\text{Error in adjoint}) \end{aligned}$$

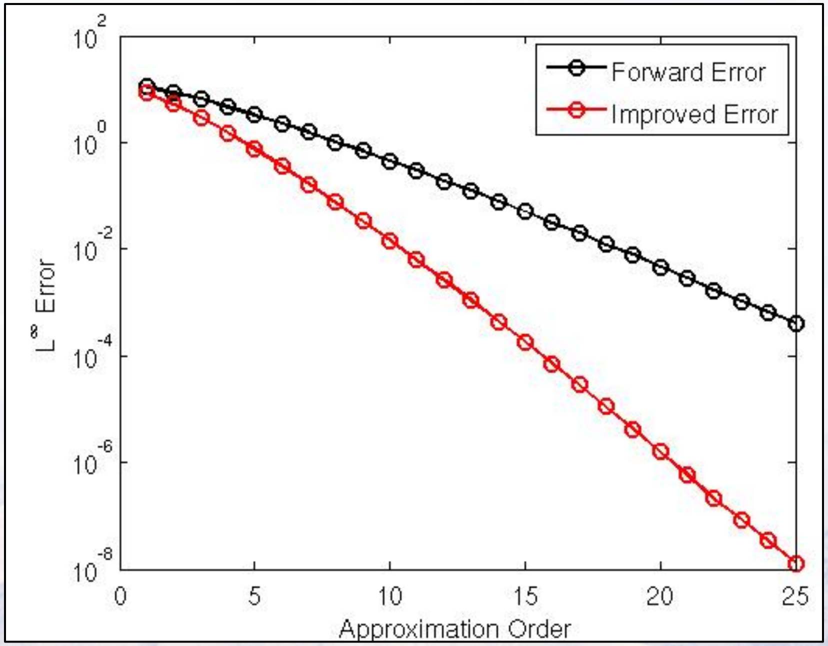
Similar results for spectral Galerkin for PDEs *[Butler, Dawson, W., SISC 2011, SJUQ 2013]* and parameterized linear systems *[Butler, Constantine, W., SIMAX 2012]*

Applications for Error Estimates in UQ

Applications for Error Estimates in UQ

1. To define an enhanced QoI with higher rate of convergence
   – Enhanced QoI = Response Surface + Error Estimate

$$J_{s+}(\lambda) = J_s(\lambda) + \epsilon(\lambda)$$



Pseudo-spectral approximation
of a parameterized linear system
[Butler, Constantine, W. SIMAX 2012]

25D Diffusion Problem

[Jakeman, W. JCP, 2015]

Consider the following diffusion problem:

$$-\nabla \cdot (K(\boldsymbol{x}, \boldsymbol{\lambda})\nabla z) = 0, \quad \boldsymbol{x} \in D = (0, 1),$$

with $z(0, \boldsymbol{\lambda}) = 1$ and $z(1, \boldsymbol{\lambda}) = 0$. Quantity of interest is $z(0, 5)$.

KL-expansion (set $d = 25$):

$$\log K(\boldsymbol{x}, \boldsymbol{\lambda}) = \overline{K} + \sigma_a \sum_{i=1}^{d} \sqrt{\eta_i}\xi_i(\boldsymbol{x})\lambda_i$$

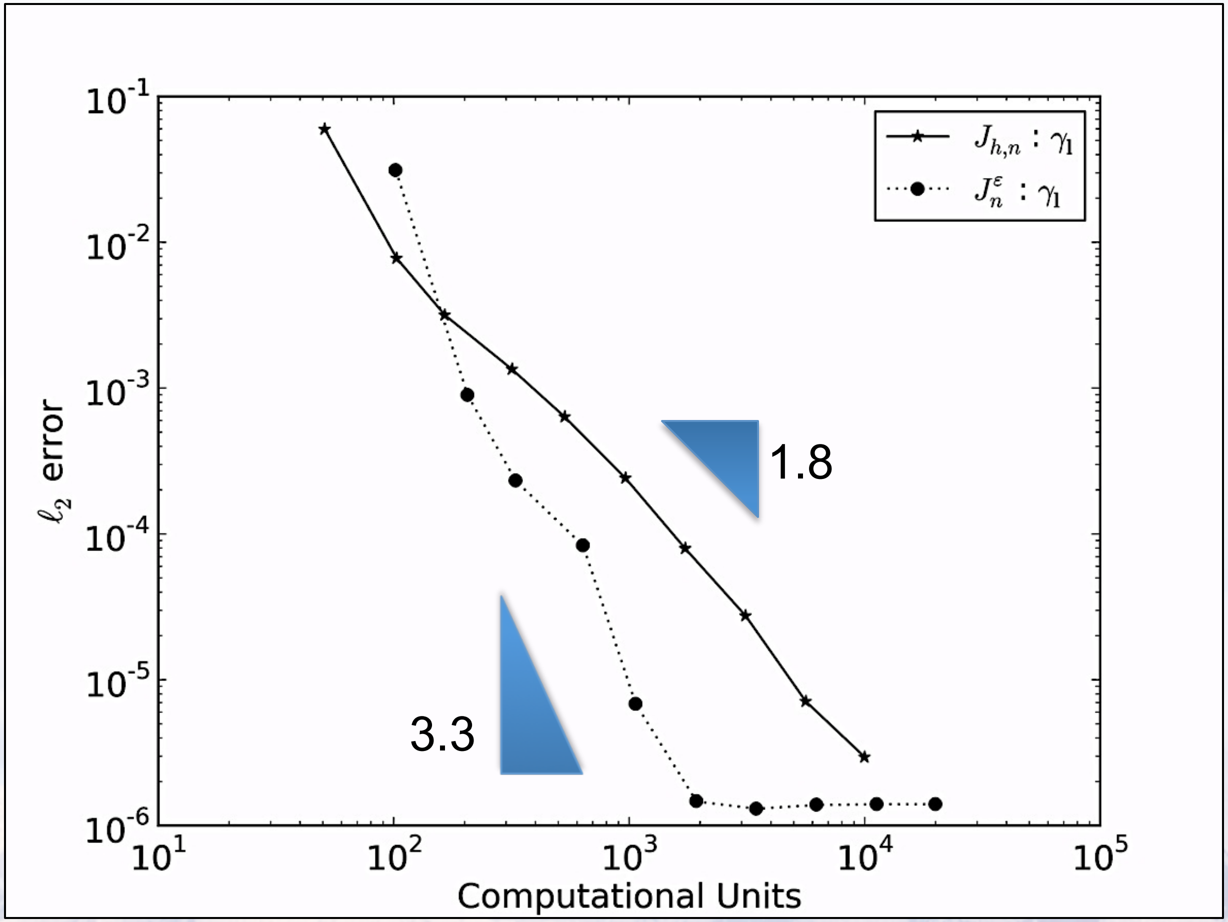
Spatial discretization: finite elements with $h = 1/100$.

Construct a dimension-adaptive sparse grid with Clenshaw-Curtis absissa.

Use a 100,000 Latin hypercube samples to compare.

25D Diffusion Problem

[Jakeman, W. JCP, 2015]



Error vs. computational cost for the quantity of interest and the enhanced quantity of interest.

Applications for Error Estimates in UQ

1. To define an enhanced QoI with higher rate of convergence
   – Enhanced QoI = Response Surface + Error Estimate

$$J_{s+}(\lambda) = J_s(\lambda) + \epsilon(\lambda)$$

2. To adaptively refine the response surface approximation and/or physical discretization for a global metric, e.g. variance.

Stochastic and Deterministic Adaptivity

We want accurate predictions ... without over-solving the problem.

Understanding the various contributions to the error is critical.

We might want to:

- Adaptively refine both physical and parametric discretizations.
- For a fixed physical discretization, resolve the parametric error to comparable accuracy.

Requires that we can split the error estimate into contributions from each discretization (nontrivial!).

$$J(\boldsymbol{z}(\boldsymbol{\lambda})) - J(\boldsymbol{z}_{h,N}(\boldsymbol{\lambda})) = \underbrace{J(\boldsymbol{z}(\boldsymbol{\lambda})) - J(\boldsymbol{z}_h(\boldsymbol{\lambda}))}_{\text{Physical discretization error}} + \underbrace{J(\boldsymbol{z}_h(\boldsymbol{\lambda})) - J(\boldsymbol{z}_{h,N}(\boldsymbol{\lambda}))}_{\text{Surrogate approximation error}}$$

Example: Steady Navier Stokes

[Bryant, Prudhomme, W., SJUQ 2015]

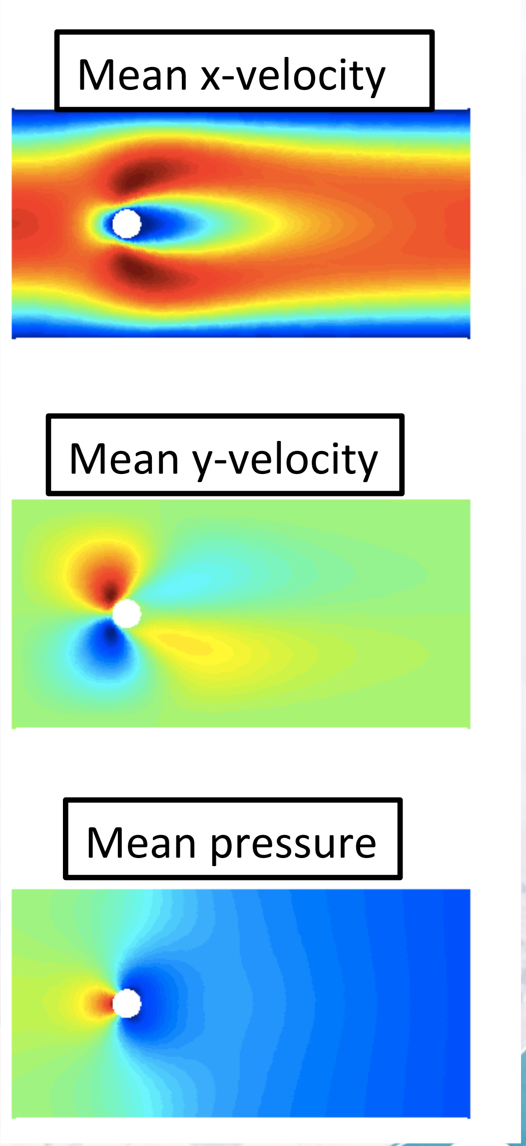
$$-\nu\Delta \boldsymbol{u} + \rho \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p = \mathbf{0},$$
$$\nabla\cdot\boldsymbol{u} = 0.$$

Random parameters:

- The viscocity, $\nu \in U(0.01, 0.1)$,
- The mean inflow velocity, $|\boldsymbol{u}_{in}| \in U(1,3)$

SUPG/PSPG stabilized Galerkin approx.

QoI: Value of x-velocity at point behind cylinder



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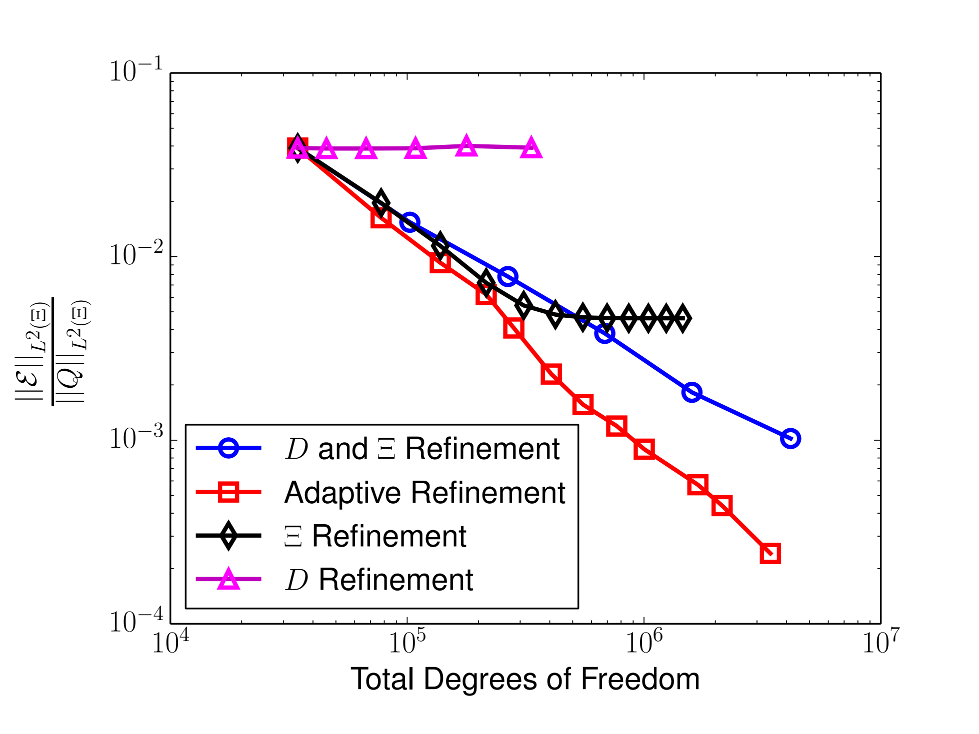
Example: Steady Navier Stokes

[Bryant, Prudhomme, W., SJUQ 2015]



- On the initial mesh, the parametric error dominates.
- Adapting in physical domain only is useless!
- Adapting in parametric domain eventually stagnates when physical error becomes dominant.
- Refining the discretization with the dominant contribution performs best!

Applications for Error Estimates in UQ

1. To define an enhanced QoI with higher rate of convergence
   – Enhanced QoI = Response Surface + Error Estimate

$$J_{s+}(\lambda) = J_s(\lambda) + \epsilon(\lambda)$$

2. To adaptively refine the response surface approximation and/or physical discretization for a global metric, e.g. variance.

3. To estimate bounds on, or to adaptively resolve, the probability of an event.

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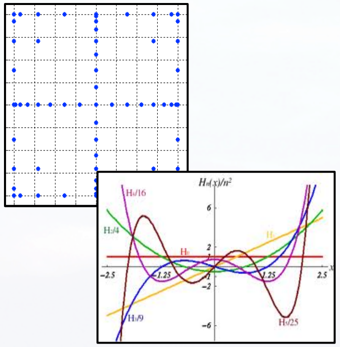
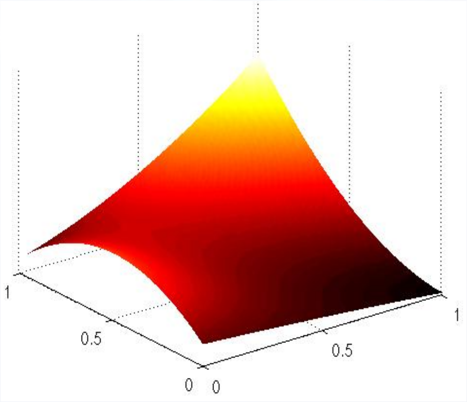
Estimation of Probabilities

Recall that first we build the surrogate ...



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

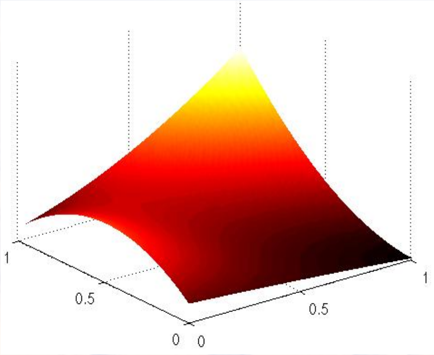


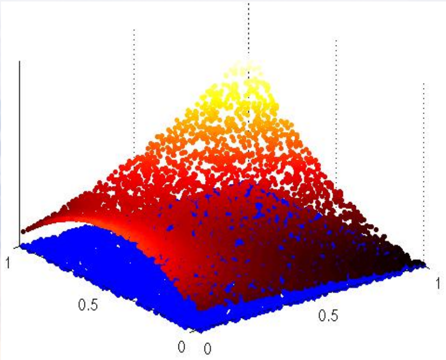
... then we estimate the statistics by sampling the surrogate.

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

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

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





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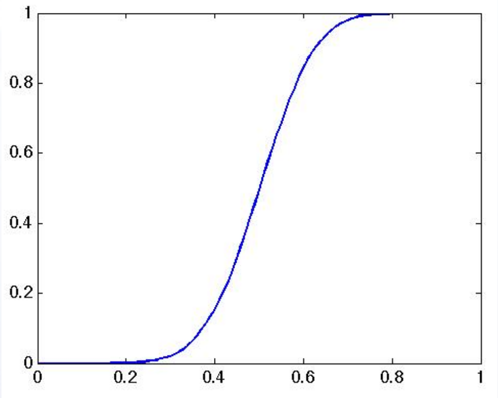
Estimation of Probabilities

Moments and distributions require global accuracy.

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

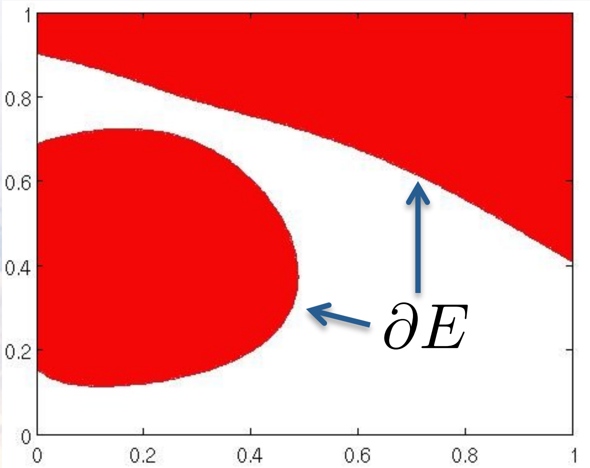
$$\mathrm{Var}[q] = \int_\Omega (E[q] - q(\lambda))^2\ d\mu$$



Probabilities require only local accuracy.

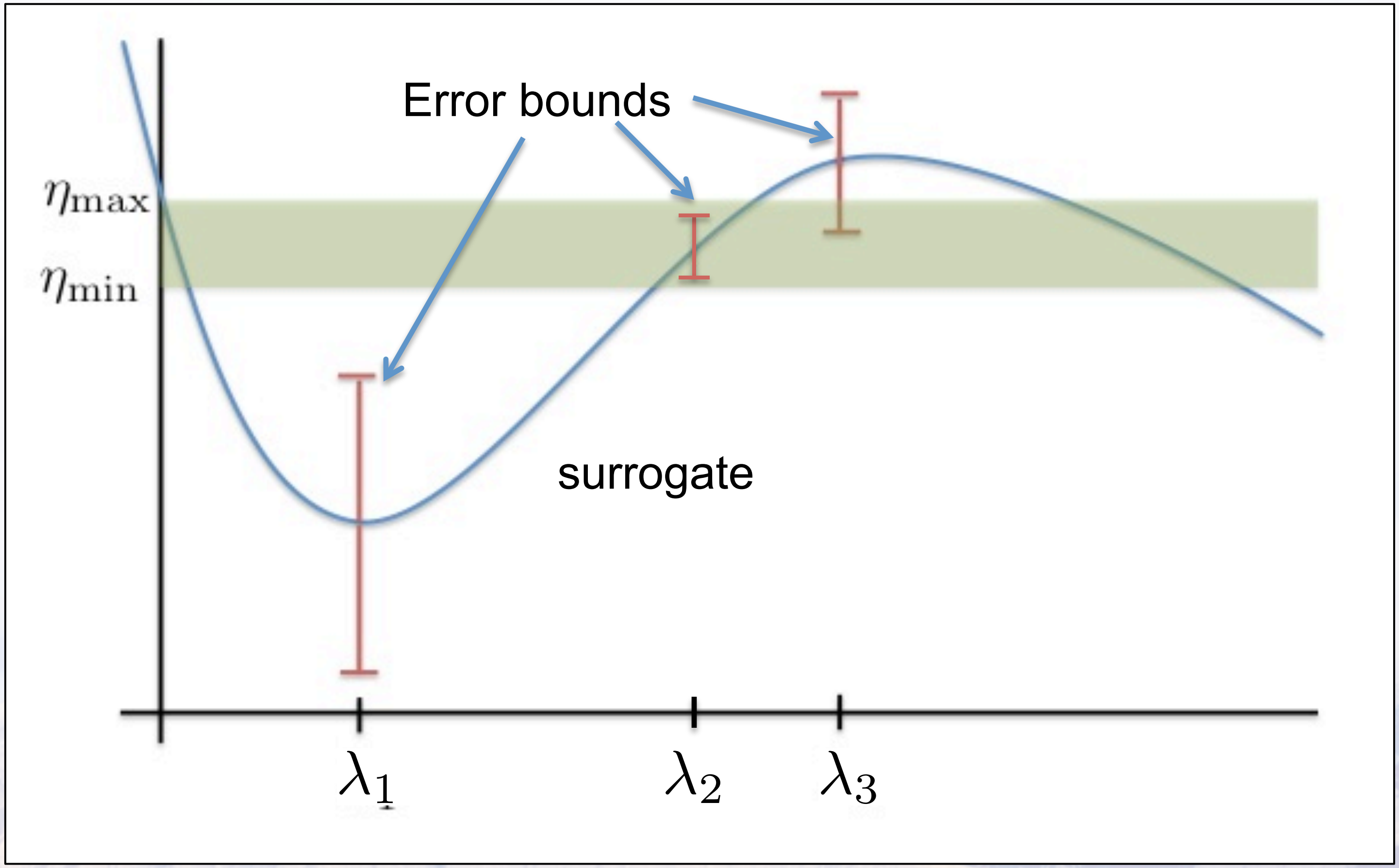
$$P[q \in E] = \int_\Omega \mathcal{X}_E\ d\mu$$

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



When can we *trust* a sample of a surrogate?

$$E = \{q \mid \eta_{\min} \leq q \leq \eta_{\max}\}$$



Only three cases: OUT, IN, NOT SURE

An Adaptive Approach

Algorithm 1: ADaptive Enhancement for Probabilities of EvenTs (ADEPT)

Given: ;

- An initial response surface approximation for the QoI, $J_s(\lambda)$;
- An approximation of the error, $\epsilon_s(\lambda)$;
- Threshold values for the event horizons: $\eta_{\min}$ and $\eta_{\max}$;
- A set of M samples from the input distribution;
- A safety factor, $C_s \geq 1$;

for $i = 1 : M$ **do**

  Evaluate $J_{s+}(\lambda_i)$ and $\epsilon_{s+}(\lambda_i)$;

  if $|J_{s+}(\lambda_i) - \eta_{min}| < C_s|\epsilon_{s+}(\lambda_i)|$ *or* $|J_{s+}(\lambda_i) - \eta_{max}| < C_s|\epsilon_{s+}(\lambda_i)|$ **then**

    Evaluate the model at λ_i;

    Use the new evaluation to update $\epsilon_k(\lambda)$ and $\xi_k(\lambda)$;

  end

end

Compute $\text{Prob}_{MC}[E_{s+}]$.

Update step: $$J_{s+}(\lambda) = \underbrace{J_s(\lambda)}_{\text{Initial surrogate}} + \underbrace{\epsilon_k(\lambda)}_{\text{Discrepancy model}}$$

We use a GP regression model in Dakota

Similar for the error update.

Accuracy of the Estimate of the Probability

Theorem *[Butler, W., Submitted to IJ4UQ 2016]*

If the error estimate satisfies

$$|J(\lambda_i) - J_{s+}(\lambda_i)| \leq C_s|\epsilon_{s+}(\lambda_i)|, \quad 1 \leq i \leq P,$$

then our approach will produce the same estimate of the probability of E as a direct sampling of the high-fidelity model.

Similar approach explored in *[Li, Xiu 2010]* and *[Li, Li, Xiu 2011]*

- We prove the accuracy of the estimate of the probability of the event.
- We use a provably higher-order a posteriori error estimate rather than a heuristic a priori error bound.
- We use each high-fidelity model evaluation to adaptively improve the response surface and the error estimate.

Accuracy of the Estimate of the Probability

Theorem *[Butler, W., Submitted to IJ4UQ 2016]*

If the error estimate satisfies

$$|J(\lambda_i) - J_{s+}(\lambda_i)| \leq C_s|\epsilon_{s+}(\lambda_i)|, \quad 1 \leq i \leq P,$$

then our approach will produce the same estimate of the probability of E as a direct sampling of the high-fidelity model.

- The constant, C_s, is called the safety factor.
- Required since we are using a higher-order error *estimate* as an error *bound*.
- For high-order response surface approximations, $C_s \approx 1$.
- In general, we use a combination of cross-validation and an *a priori* lower bound to estimate C_s.

Example: Bounds and Adaptivity

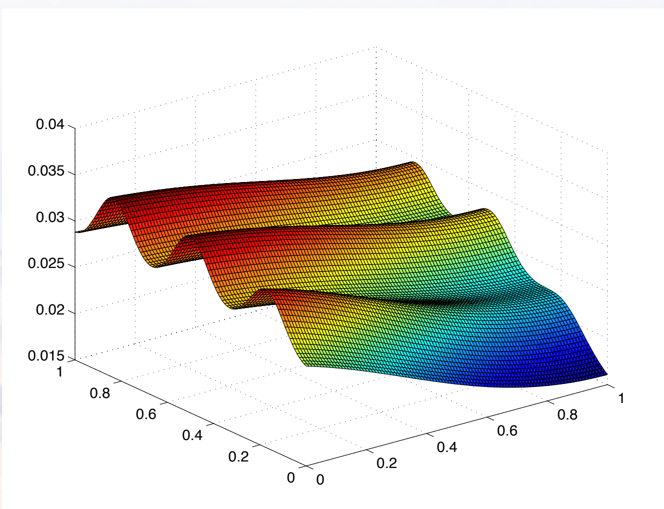
Model for convection/diffusion:

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

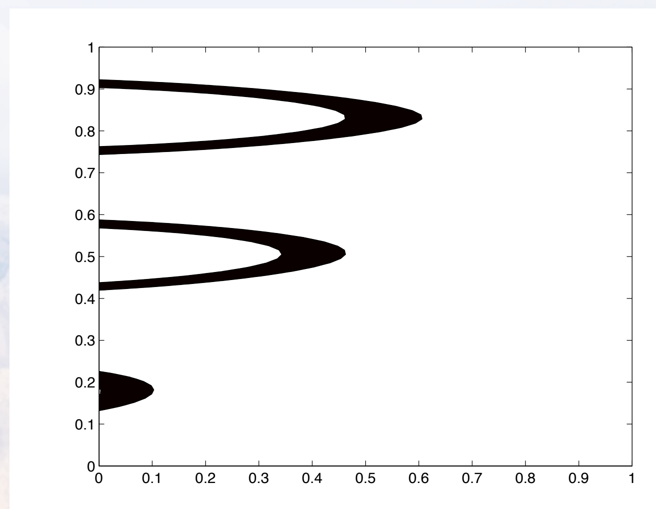
where $S = (0,1) \times (0,1)$. Quantity of interest is $u(0.5, 0.5)$.

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

$E = \{\lambda \, : \, 0.031 \leq J(\boldsymbol{\lambda}) \leq 0.032\}$



Response surface approximation



Approximation of *E*

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Example: Bounds and Adaptivity

Monte Carlo estimate of the probability of E using 1E6 samples: 5.9528E-2

	Polynomial Chaos Order					
	2	4	8	12	16	25
$\mathrm{Prob}_{MC}[E_s]$	1.18072E-1	8.6422E-2	6.2558E-2	6.1282E-2	5.9088E-2	5.9540E-2
Error	98.3%	45.2%	5.1%	2.9%	-0.7%	-0.02%
Safety Factor	4.9839	1.3133	1.0929	1.2223	1.0386	1.0010
Lower Bounds	3.0E-4	8.001E-3	1.727E-2	4.7226E-2	5.3215E-2	5.9047E-2
Upper Bounds	0.6629	0.427194	0.130729	7.5147E-2	6.5072E-2	6.0052E-2

Approximations of the probability of *E* using polynomial chaos surrogate models. Also, lower and upper bounds on the probability using the adjoint-based error estimate.

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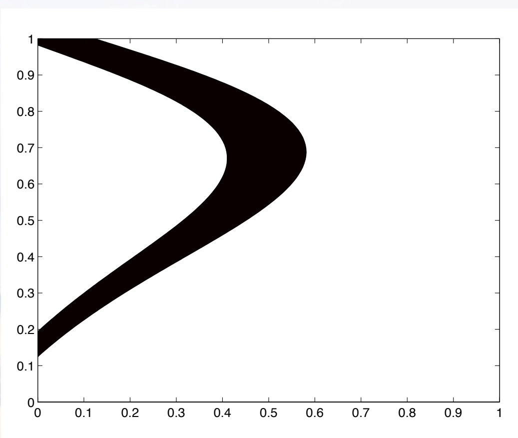
Example: Bounds and Adaptivity

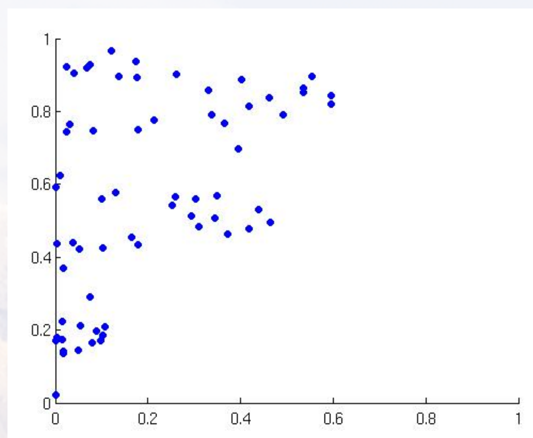
	Polynomial Chaos Order					
	2	4	8	12	16	25
Evaluations	135	99	87	57	57	38
$\mathrm{Prob}_{MC}[E_s]$	5.9528E-2	5.9528E-2	5.9528E-2	5.9529E-2	5.9528E-2	5.9528E-2
Safety Factor	7.4759	1.9699	1.6394	1.8289	1.5578	1.5015
Cost Ratio	6535.9	6289.3	3861.0	2469.1	1550.4	714.3

Approximations of the probability of the event.

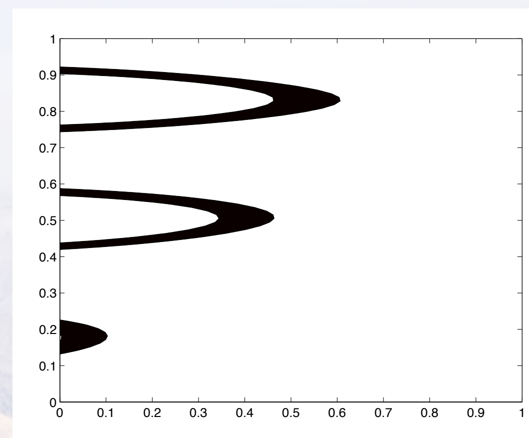
Cost ratio compares cost of our adaptive approach with cost of Monte Carlo.



Initial surrogate approximation of E

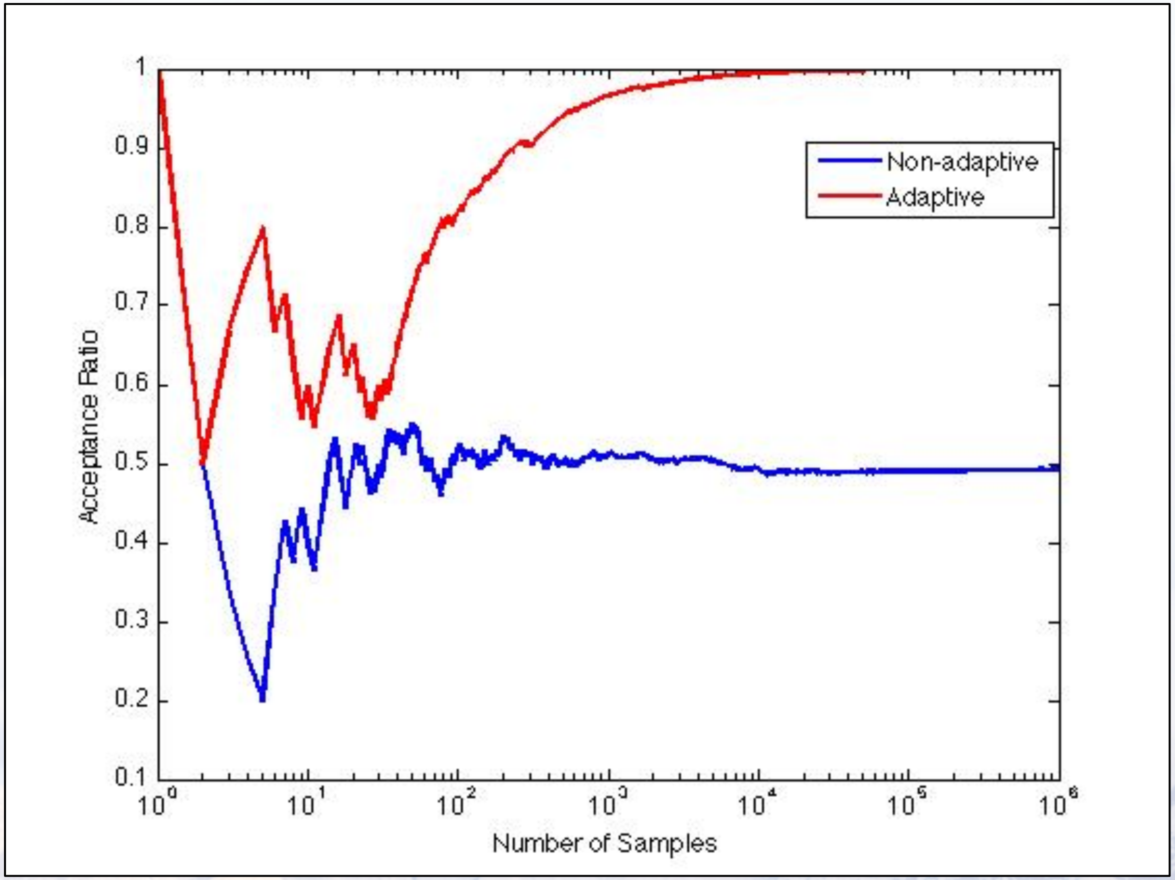


Points where we evaluate the high-fidelity model



Final surrogate approximation of E

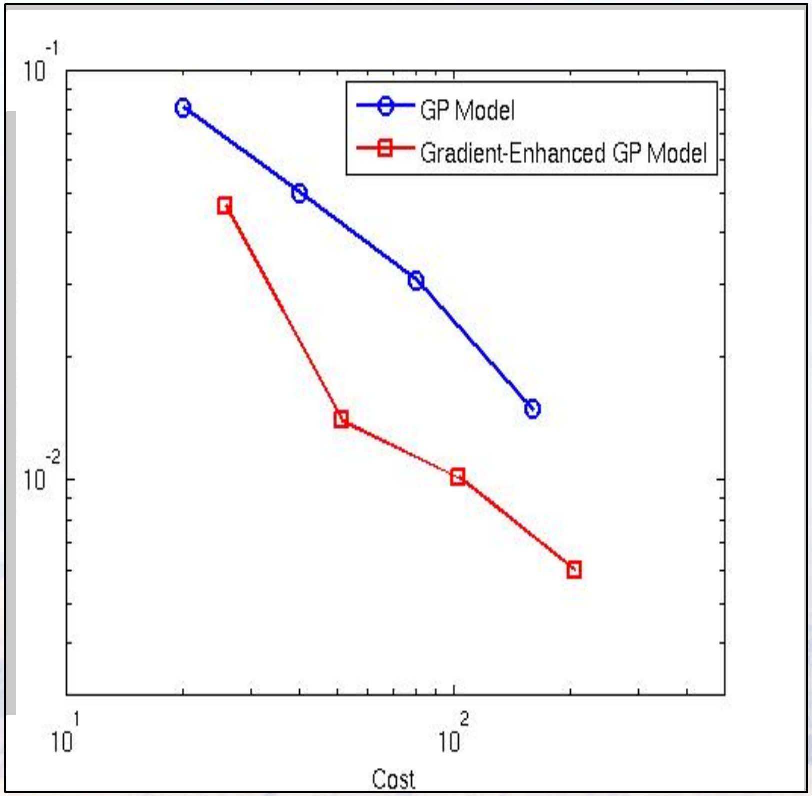
Does Adaptivity Help?



Acceptance ratio versus number of samples with and without adaptivity using a 4th order PCE as the initial response surface approximation.

Applications for Derivatives in UQ

1. To define a gradient-enhanced response surface approximation
   - Local linear models *[Estep, Neckels 2006; Marchuk, 1995]*
   - Gradient enhanced Kriging/Gaussian process models *[Lockwood et al 2010; Dalbey 2013]*
   - Gradient enhanced compressive sensing polynomial chaos



Convergence of a QoI from resistive MHD using Gaussian process regression in a 5D parameter space

Applications for Derivatives in UQ

1. To define a gradient-enhanced response surface approximation
   - Local linear models *[Estep, Neckels 2006; Marchuk, 1995]*
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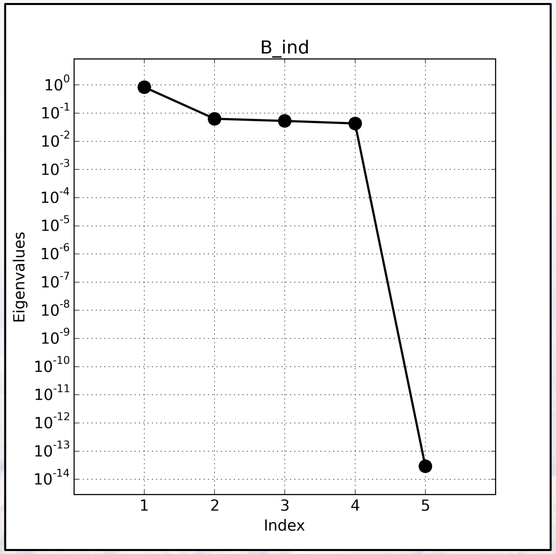
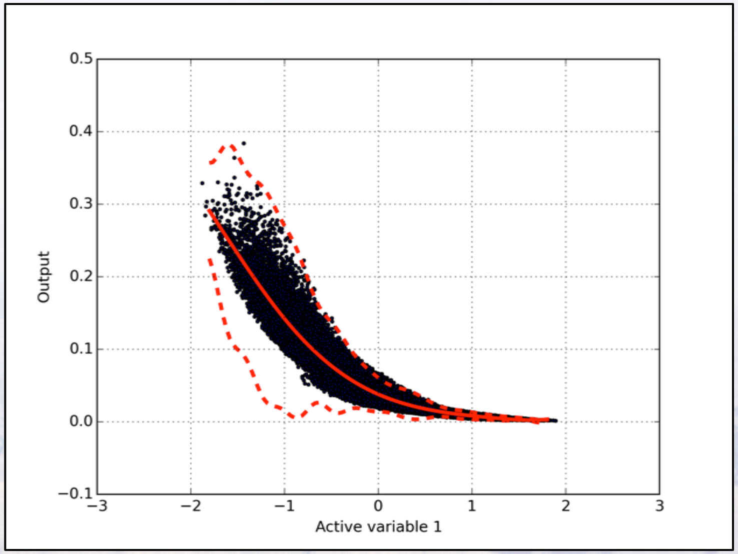
   - Gradient enhanced compressive sensing polynomial chaos
2. To perform dimension reduction using active subspace techniques *[Constantine 2014]*



Decay of eigenvalues from resistive MHD



Surrogate approximation in 1D active subspace with optimization-based bounds

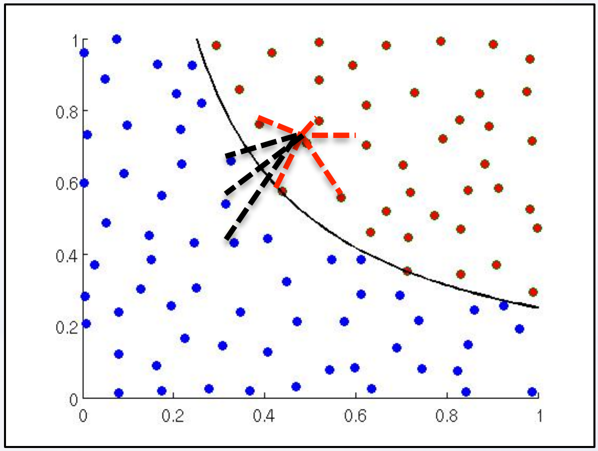
Applications for Derivatives in UQ

1. To define a gradient-enhanced response surface approximation
   - Local linear models *[Estep, Neckels 2006; Marchuk, 1995]*
   - Gradient enhanced Kriging/Gaussian process models *[Lockwood et al 2010; Dalbey 2013]*
   - Gradient enhanced compressive sensing polynomial chaos
2. To perform dimension reduction using active subspace techniques *[Constantine 2014]*
3. To detect a discontinuity and to enable us to account for our lack of knowledge regarding the location of the discontinuity.

Utilizing Adjoints to Enable Efficient UQ for Discontinuous Functions

- Numerous discontinuity detection algorithms exist:
  - Polynomial annihiliation *[Archibald et al 2009, Jakeman et al 2013]*
  - ENO/WENO smoothness indicators *[Barth 2011, Witteveen 2013]*
- Developed **adjoint-enhanced discontinuity detection**
  - Uses both point values and gradients
  - Leverages standard ENO/WENO smoothness indicators

$$\beta = \sum_{j=1}^{3} \Delta x^{2j-1} \int_{s=x_1}^{s=x_2} \left(\frac{\partial^j}{\partial s^j} p(s) \right)^2 \; ds,$$



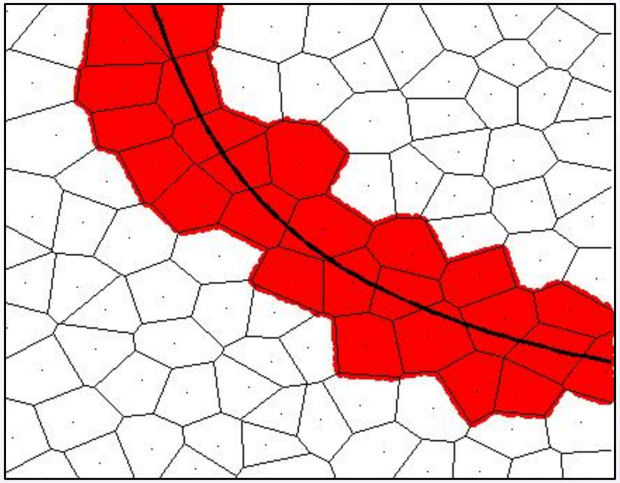
- Enables clustering of samples
- We use the Voronoi cells to define the subdomains
- **Gradient enhanced response surface approximations on each subdomain**
  - Gradient enhanced Kriging
  - Gradient enhanced PCE

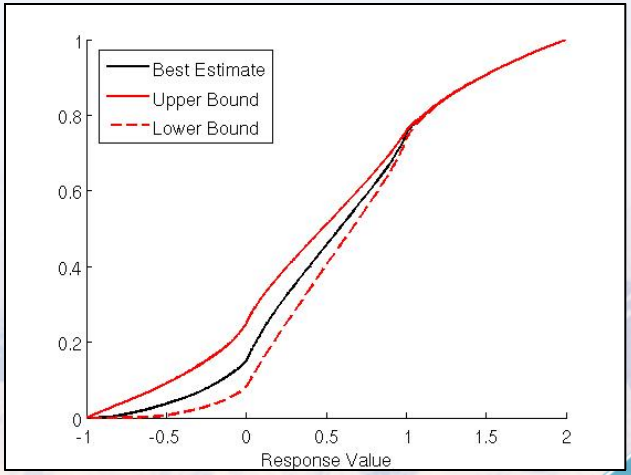
Utilizing Adjoints to Enable Efficient UQ for Discontinuous Functions

- We view the location of the discontinuity as an epistemic uncertainty
- Mark Voronoi cells near the discontinuity
- Samples in these cells may belong to one subdomain or the other
- We evaluate each response surface approximation at these samples
- We solve a discrete optimization problem, e.g.:

$$\max E[f] = \sum_{i=1}^{N} \frac{1}{N} \max\{\tilde{f}_j\}_{j=1}^{P}$$

- **Provides robust bounds on probabilistic quantities given our lack of knowledge regarding the precise location of the discontinuity.**





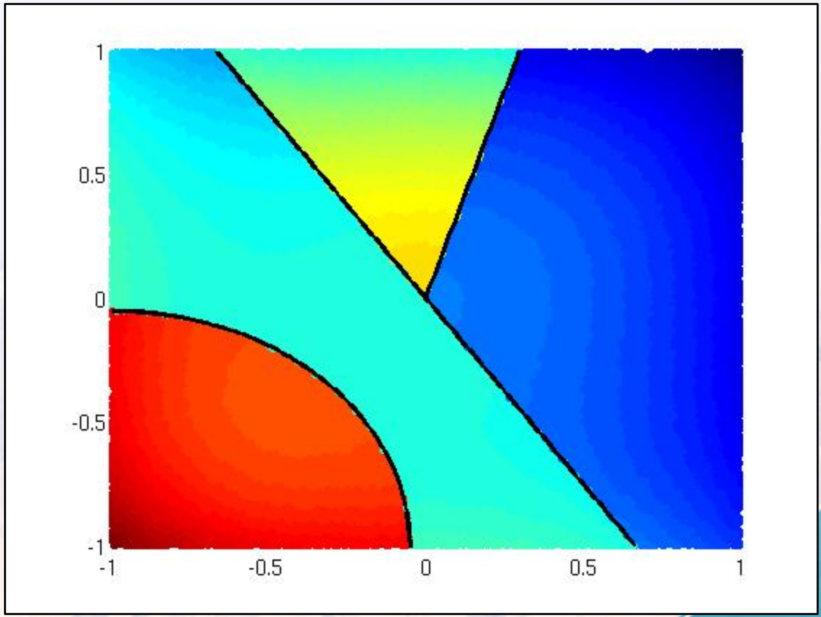
Example: Accounting for Discontinuities

- We consider the function introduced in *[Jakeman et al, 2013]*:

$$f_d^{\text{multi}}(x) = \begin{cases} f^1(x) - 2, & 3x_1 + 2x_2 \geqslant 0 \quad \text{and} \quad -x_1 + 0.3x_2 < 0, \\ 2f_d^2(x), & 3x_1 + 2x_2 \geqslant 0 \quad \text{and} \quad -x_1 + 0.3x_2 \geqslant 0, \\ 2f^1(x) + 4, & (x_1+1)^2 + (x_2+1)^2 < 0.95^2 \quad \text{and} \quad d = 2, \\ f^1(x), & \text{otherwise.} \end{cases}$$

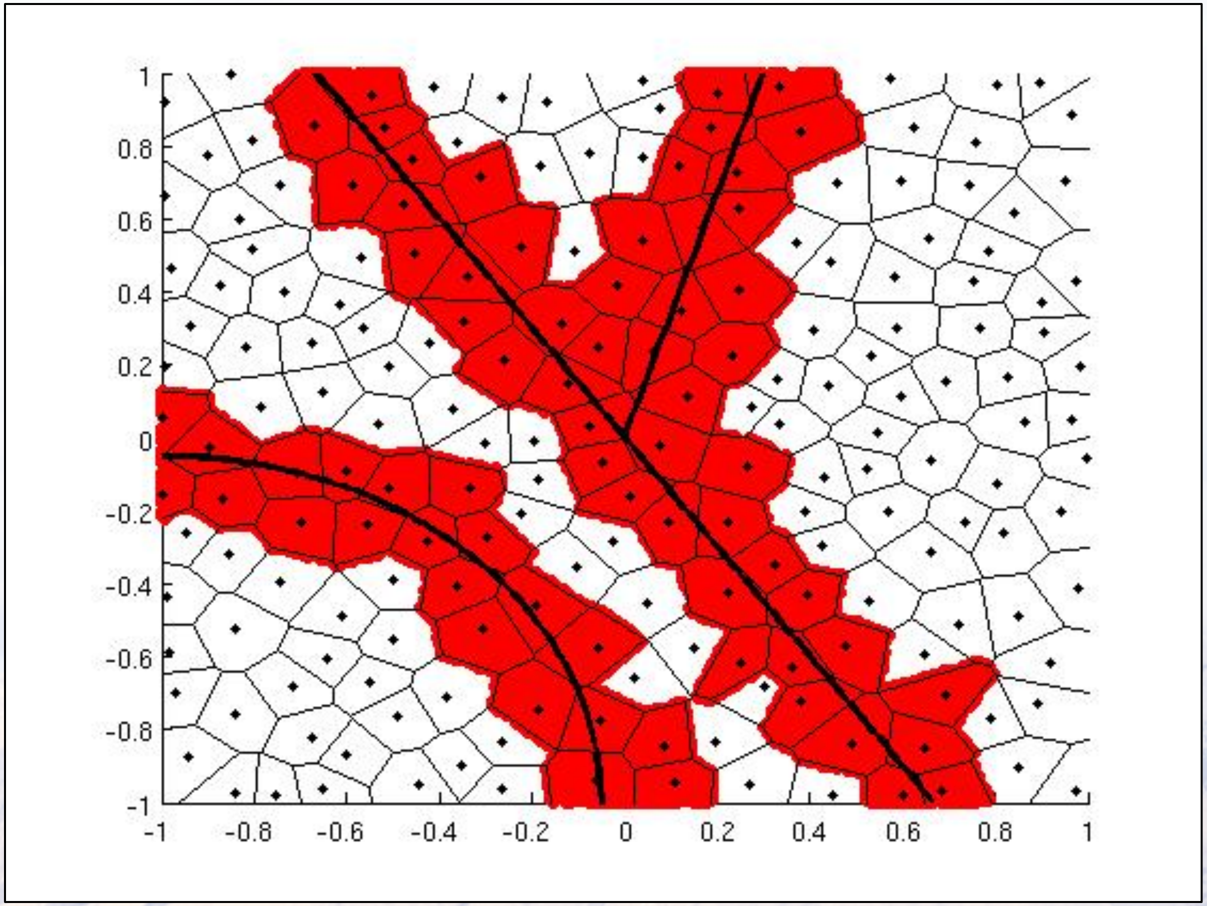
$$f^1(x) = \exp\left(-\sum_{i=1}^{2} x_i^2\right) - x_1^3 - x_2^3,$$

$$f_d^2(x) = 1 + f^1(x) + \frac{1}{4d}\sum_{i=2}^{d} x_i^2.$$



Example: Accounting for Discontinuities

- We start with 200 evaluations of the model and gradient



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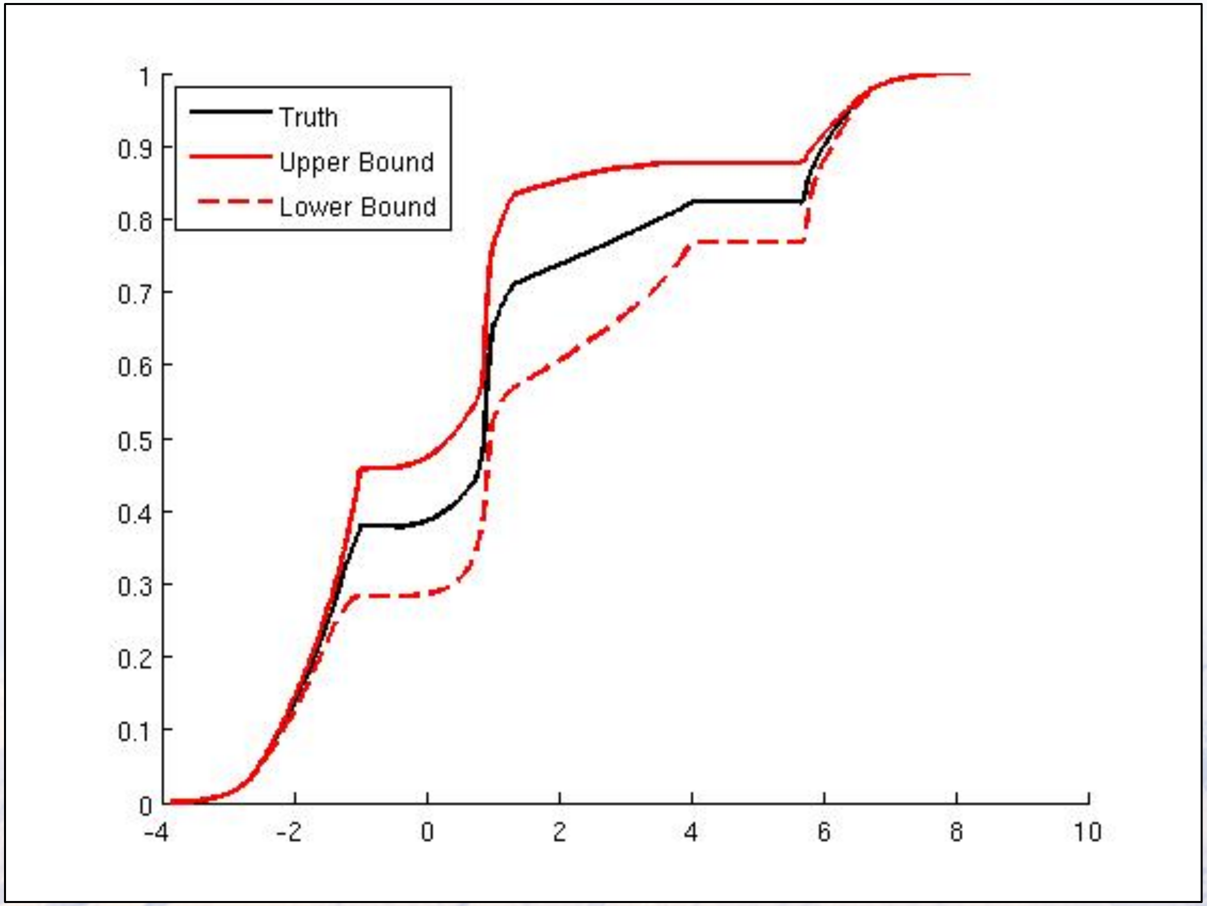
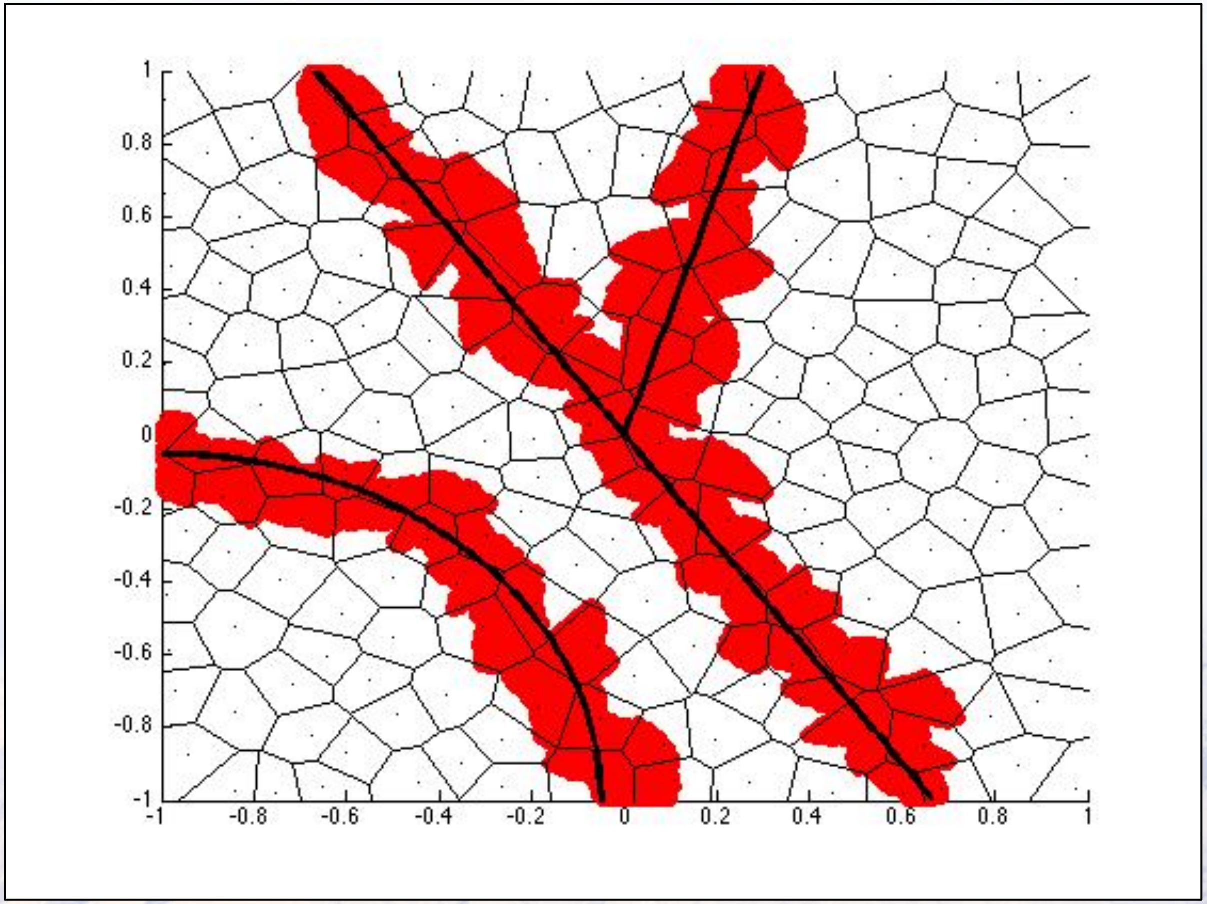


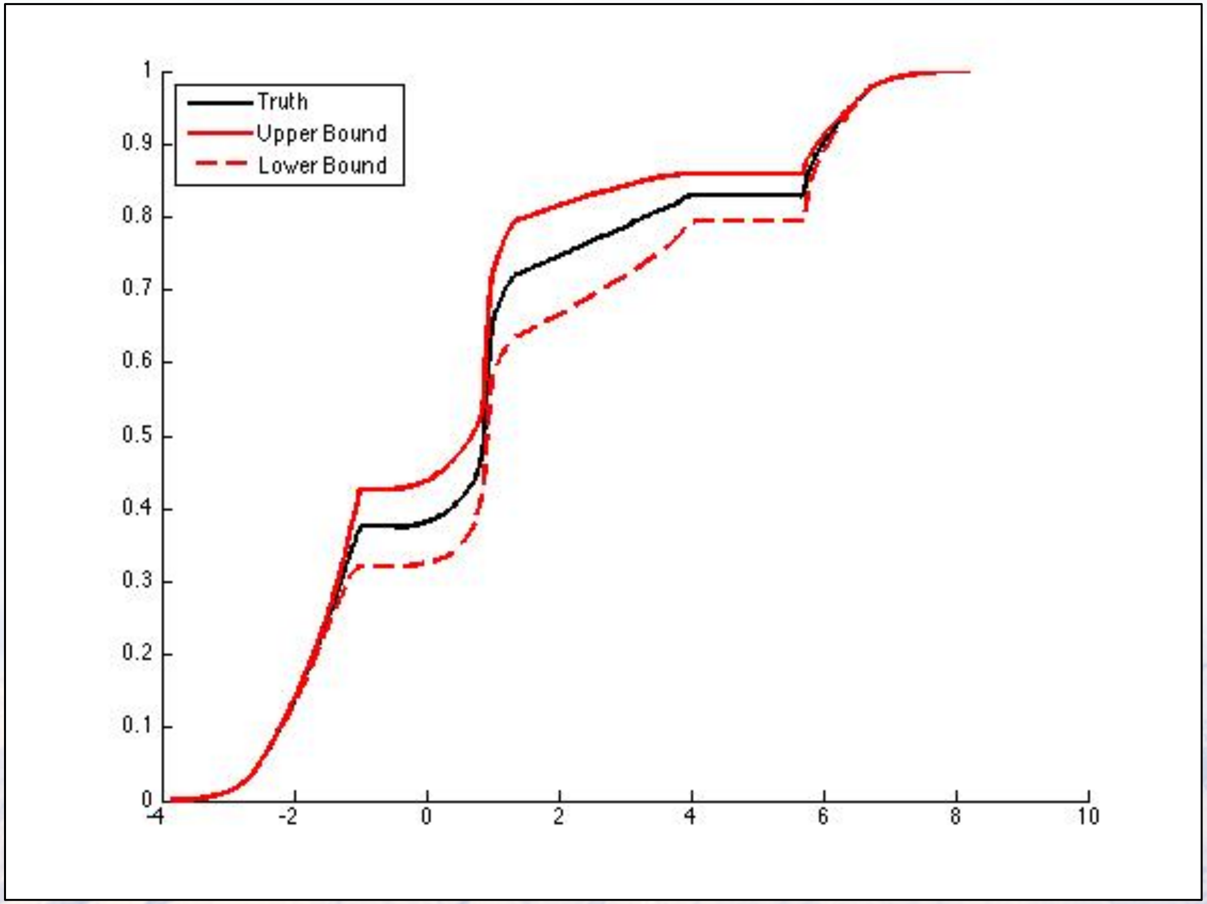
Example: Accounting for Discontinuities

- We do not need to use the Voronoi cells



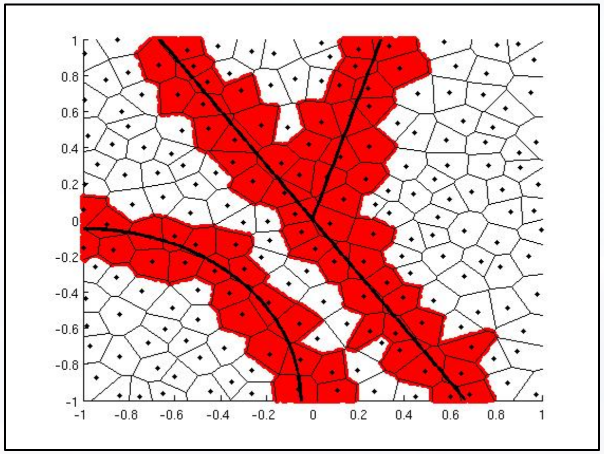
Example: Accounting for Discontinuities

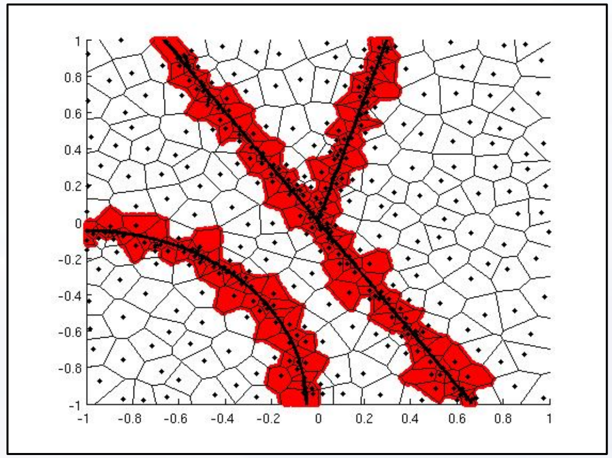
- Leads to tighter bounds, but perhaps less robust

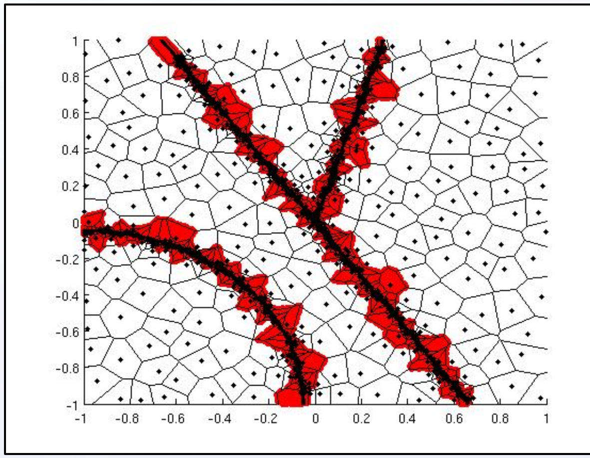


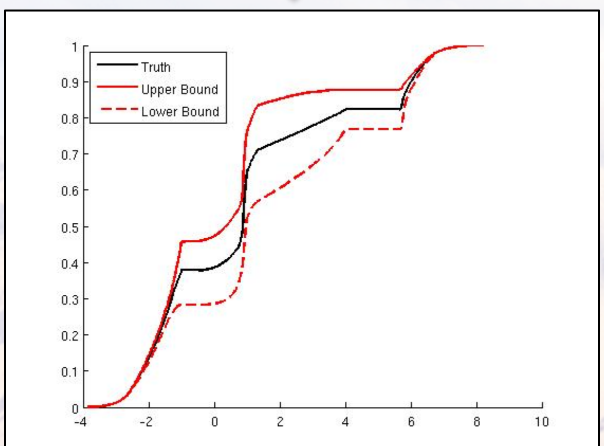
Example: Accounting for Discontinuities

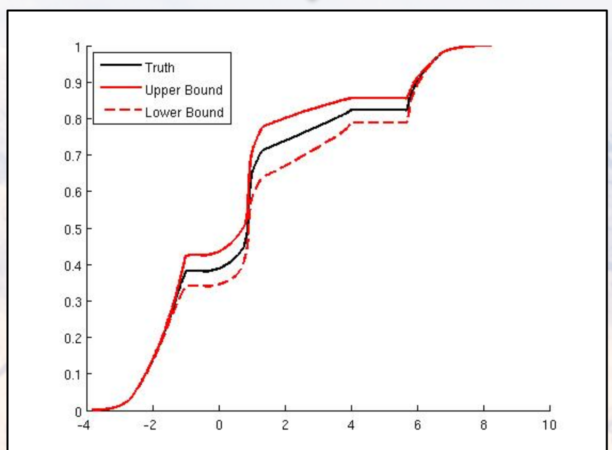
N = 200 **N = 391** **N = 982**

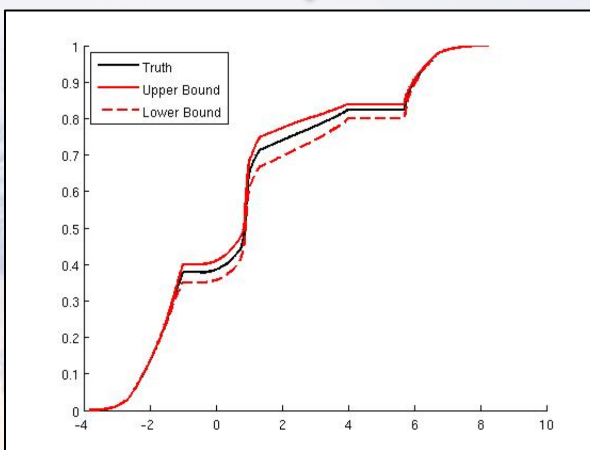












Conclusions

Conclusions

- Traditional uses for adjoints include optimization (gradients), verification (error estimates), and goal-oriented adaptivity.
- Adjoint-based techniques can also improve UQ
  - Define an enhanced response surface with higher rate of convergence
  - Adaptively resolve the physical and/or parametric discretization
  - Estimate bounds on probabilities of an event
  - Judiciously add samples of the high-fidelity model to adaptively resolve event horizons and accurately estimate probabilities of events
  - Identify and account for discontinuities in parameter space
- Only discussed forward UQ … how about inverse UQ?

Thank you for your attention!
Questions?

tmwilde@sandia.gov

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