Advanced Stochastic Collocation Methods for Polynomial Chaos in RAVEN

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Introduction

Goals in Nuclear R&D

Research and Development Motives in Nuclear Industry

- New commercial reactor designs
  - Generation IV
  - Small Modular Reactors
- Restarting retired reactors
- Extending existing reactor life
- Change operation parameters
  - Changes in Regulations
  - Increase fuel usage

Introduction

Simulations in Nuclear

Research and Development Methods in Nuclear Industry

- Physical experiments
  - Expensive to construct
  - Difficult to analyze
  - Often requires licensing
- Numerical Simulations
  - Relatively inexpensive
  - Rarely requires licensing
  - Often produce valuable insights

Introduction

Numerical Simulations

Challenges for Numerical Simulations in Nuclear

- Many coupled physics
  - Fuels Performance
  - Safety Analysis
  - Thermal Hydraulics
  - Neutronics
  - Core Design
  - Molecular Dynamics
- Widely-varying Time Scales
- Tightly-coupled feedback

Introduction

Safety Margins

Traditional simulation approach to Safety Margins

- Build excess conservatism into models
- Assume final calculations are sufficiently conservative

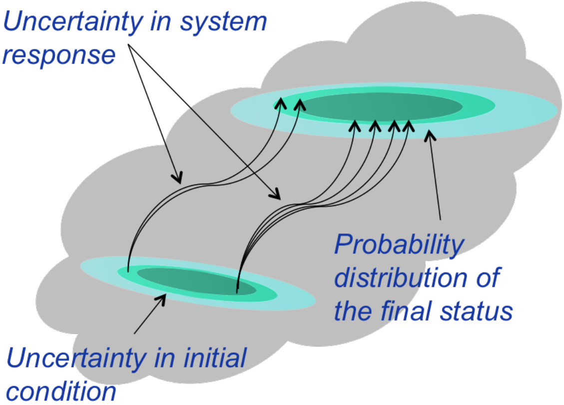
More advanced approach: Best Estimate Plus Uncertainty (BEPU)

- Analyze models as accurately as possible
- Propagate uncertainty to determine safety margins
- Example: RISMC

Introduction

Uncertainty Quantification

Uncertainty Quantification as explained by `RAVEN`



Introduction

Nomenclature

Consider a generic simulation

- Let $u(Y)$ be a response of interest
- Examples:
  - peak clad temperature for fuel performance
  - k-eigenvalue for neutronics
  - power peaking factors for core design
- $Y = (y_1, y_2, \ldots, y_N)$ are input parameters
  - Material properties
  - Boundary conditions
  - Initial conditions
  - Model tuning parameters
- General usage: provided inputs Y, obtain response $u(Y)$

Introduction

Nomenclature

More Definitions

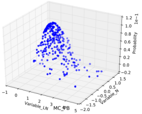
- $u(Y)$ is stochastic response
- Y is stochastic vector, $Y = (y_1, \ldots, y_N)$
- Probability space (Ω, σ, ρ)
- Each uncertain input y_n:
  - Probability space $(\Omega_n, \sigma_n, \rho_n)$
  - Probability Distribution is $\rho_n(Y)$
  - Realizations $y_n(\omega)$
- Full input realization $Y(\omega)$
- Response realization $u(Y(\omega))$

Introduction

Traditional Uncertainty Quantification Methods

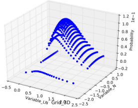
Monte Carlo

- Random sampling based on probability
- Strong, slow, dimension-agnostic



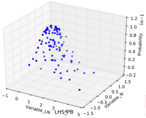
Grid

- Nodes equally spaced by probability
- Curse of dimensionality



Latin Hypercube

- Hybrid of MC and Grid
- Works for many models



Introduction

Dissertation Objective

Objectives of this work

- Explore advanced UQ sampling strategies
  - Stochastic Collocation for generalized Polynomial Chaos (SCgPC)
  - High-Dimensional Model Reduction (HDMR)
  - Adaptive SCgPC
  - Adaptive HDMR
- Advance adaptive methods
- Implement all methods in `RAVEN`

Outline

Discussion Points

Outline

SCgPC

Theory

Stochastic Collocation for generalized Polynomial Chaos (SCgPC)

1. Generalized Polynomial Chaos Expansion
2. Stochastic Collocation
3. Smolyak Sparse Grids

SCgPC

Generalized Polynomial Chaos

Expand model as sum of orthonormal polynomials

gPC Expansion

$$u(Y) \approx G[u](Y) = \sum_{k \in \Lambda(L)} u_k \Phi_k(Y)$$

- Λ: Chosen set of polynomial indices
- k: Multi-index of polynomial orders e.g. (2,1,3)
- u_k: Scalar expansions moments
- Φ_k: Multidimensional orthonormal polynomials

SCgPC

gPC: Polynomial Families

$$\Phi_k(Y) = \prod_{n=1}^{N} \phi_{k_n}^{(n)}(y_n)$$

Choice of polynomial family depends on distribution of y_n

Distribution	Polynomial Set
Uniform	Legendre
Normal	Hermite
Gamma	Laguerre
Beta	Jacobi
Arbitrary	Legendre

SCgPC

gPC: Useful Properties

gPC Expansion

$$u(Y) \approx G[u](Y) = \sum_{k \in \Lambda(L)} u_k \Phi_k(Y)$$

- Surrogate Model: Polynomials are fast to evaluate
- First two moments are very simple

$$\mathbb{E}[G[u](Y)] = u_{(0,\dots,0)}, \qquad \mathbb{E}[G[u](Y)^2] = \sum_{k \in \Lambda(L)} u_k^2$$

SCgPC

gPC: Polynomial Set Λ

gPC Expansion

$$u(Y) \approx G[u](Y) = \sum_{k\in\Lambda(L)} u_k \Phi_k(Y)$$

Choice of polynomial set: $\Lambda(L)$

- Tensor Product
- Total Degree
- Hyperbolic Cross

Truncated by limiting order L

SCgPC

gPC: Polynomial Set Λ

Tensor Product Index Set

$$\Lambda_{\text{TP}}(L) = \Big\{ k = (k_1, \cdots, k_N) : \max_{1 \le n \le N} k_n \le L \Big\}$$

Example: $N = 2, L = 3$

$$\Lambda_{TP}(3) = \begin{array}{|cccc|} \hline (3,0) & (3,1) & (3,2) & (3,3) \\ (2,0) & (2,1) & (2,2) & (2,3) \\ (1,0) & (1,1) & (1,2) & (1,3) \\ (0,0) & (0,1) & (0,2) & (0,3) \\ \hline \end{array}$$

SCgPC

gPC: Polynomial Set Λ

Total Degree Index Set

$$\Lambda_{\mathrm{TD}}(L) = \left\{ k = (k_1, \cdots, k_N) : \sum_{n=1}^{N} k_n \le L \right\}$$

Example: $N = 2, L = 3$

$$\Lambda_{TD}(3) = \boxed{\begin{array}{cccc} (3,0) & & & \\ (2,0) & (2,1) & & \\ (1,0) & (1,1) & (1,2) & \\ (0,0) & (0,1) & (0,2) & (0,3) \end{array}}$$

SCgPC

gPC: Polynomial Set Λ

Hyperbolic Cross Index Set

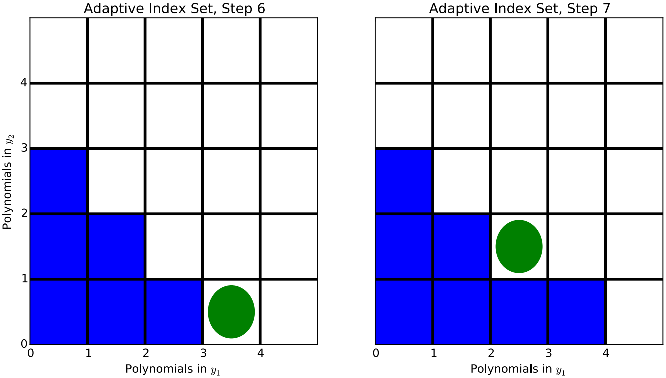
$$\Lambda_{\text{HC}}(L) = \left\{ k = (k_1, \ldots, k_N) : \prod_{n=1}^{N} (k_n + 1) \leq L + 1 \right\}$$

Example: $N = 2, L = 3$

$$\Lambda_{HC}(3) = \boxed{\begin{array}{llll} (3,0) & & & \\ (2,0) & & & \\ (1,0) & (1,1) & & \\ (0,0) & (0,1) & (0,2) & (0,3) \end{array}}$$

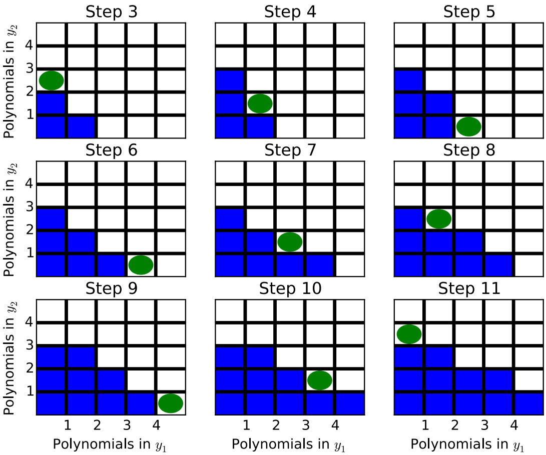
SCgPC
Adaptive SCgPC

Choose polynomials to add adaptively



SCgPC

Adaptive SCgPC



SCgPC

Adaptive SCgPC

Predictive Algorithm

- Use variance of previous polynomials to predict
- Converge on est. remaining variance
- Saves significant evaluations
- Assumption: monotonic variance decrease

SCgPC

gPC: Expansion Moments u_k

gPC Expansion

$$u(Y) \approx G[u](Y) = \sum_{k\in\Lambda(L)} u_k \Phi_k(Y)$$

Expansion moments u_k given through orthonormality of expansion polynomials

SCgPC

gPC: Expansion Moments u_k

Defining probability-weighted integration and orthonormality,

$$\int_\Omega (\cdot) dY \equiv \int_{a_1}^{b_1} \rho_1(y_1) \cdots \int_{a_N}^{b_N} \rho_N(y_N)(\cdot)\ dy_1 \cdots\ dy_N$$

$$\int_\Omega \Phi_j(Y)\Phi_k(Y)dY = \delta_{jk}$$

Expansion Moments

$$u_k = \int_\Omega u(Y)\Phi_k(Y)dY$$

SCgPC

gPC: Expansion Moments u_k

How to integrate

Expansion Moments

$$u_k = \int_\Omega u(Y)\Phi_k(Y)dY$$

- Analytic Integration
- Monte Carlo sampling
- Stochastic Collocation

SCgPC

Stochastic Collocation

Numerical Integration by Quadrature

$$
\begin{aligned}
\int_a^b f(y)\rho(y)\ dy &= \sum_{\ell=1}^{\infty} w_\ell f(y_\ell) \\
&\approx \sum_{\ell=1}^{p} w_\ell f(y_\ell) \\
&\equiv q^{(p)}[f(y)]
\end{aligned}
$$

SCgPC

Stochastic Collocation

Gauss quadrature

- Exact for polynomials order $2p - 1$
- Several quadratures for several weights
- Correspond to expansion polynomials

Distribution	Polynomial Set	Quadrature
Uniform	Legendre	Legendre
Normal	Hermite	Hermite
Gamma	Laguerre	Laguerre
Beta	Jacobi	Jacobi

SCgPC

Stochastic Collocation

Expansion Moments

$$u_k = \int_{\Omega} u(Y)\Phi_k(Y)dY$$

Integration Order and Quadrature Order Order of $u(Y)\Phi_k(Y)$

- Order of $\Phi_k(Y)$ is k
- Order of $u(Y)$ is unknown; assume $\mathcal{O}(G[u](Y))$
- Total order is $2k \rightarrow p_n = k_n + \frac{1}{2}$

Number of points should be $k_n + 1$ for each dimension n

SCgPC

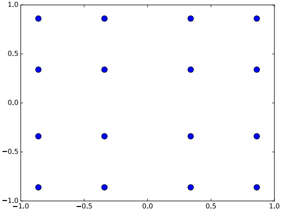
Stochastic Collocation

Multidimensional Numerical Integrals

Basic choice: tensor combination

$$\int_{a_1}^{b_1}\int_{a_2}^{b_2} f(Y)\rho(Y)\ dy_2\ dy_1 \approx Q^{(\vec{p})}[f(Y)]$$

$$Q^{(\vec{p})} = q^{(p_1)} \otimes q^{(p_2)} = \bigotimes_{n=1}^{N} q^{(p_n)}$$



SCgPC

Smolyak Sparse Grid

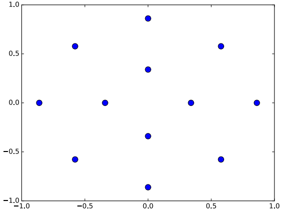
Tensor quadrature can be wasteful

$$\Lambda_{HC}(3) = \boxed{\begin{array}{llll} \color{red}{(3,0)} & & & \\ (2,0) & & & \\ (1,0) & \color{red}{(1,1)} & & \\ (0,0) & (0,1) & (0,2) & \color{red}{(0,3)} \end{array}}$$

Need fewer knots and weights

- 4th order in y_1
- 4th order in y_2
- 2nd $\times$ 2nd in (y_1, y_2)

Requires 12 instead of 16 points



SCgPC

Smolyak Sparse Grid

Smolyak Sparse Grid Quadrature

$$S^{(\vec{p})}_{\Lambda,N}[(\cdot)] = \sum_{k\in\Lambda(L)} c(k) \bigotimes_{n=1}^{N} q_n^{(p_n)}[(\cdot)]$$

$$c(k) = \sum_{\substack{j=\{0,1\}^N,\\ k+j\in\Lambda(L)}} (-1)^{|j|_1},$$

SCgPC

Smo...

Expansion Moments

$$u_k = \int_\Omega u(Y)\Phi_k(Y)dY$$

Calculate using Smolyak sparse grid

$$u_k \approx S^{(\vec{p})}_{\Lambda,N}[u(Y)\Phi_k(Y)]$$

gPC Expansion

$$u(Y) \approx G[u](Y) = \sum_{k\in\Lambda(L)} u_k\Phi_k(Y)$$

Outline

SCgPC Results

Introduction

Performed analysis on several analytic models

Considered impact of

- Changing regularity
- Changing dimensionality
- Different polynomial representations

Consider TP, TD, HC, and Adaptive SCgPC

SCgPC Results

Models

Analytic models used

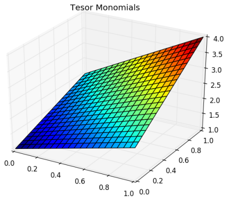
- Tensor Monomials
- Sudret Polynomial
- Attenuation
- Gauss Peak
- Ishigami
- Sobol G-Function

SCgPC Results

Tensor Monomials

Tensor Monomials

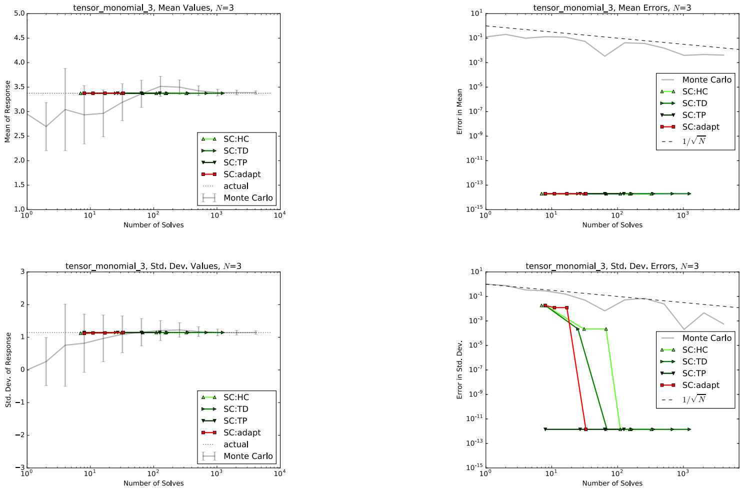
$$u(Y) = \prod_{n=1}^{N} (y_n + 1)$$



- Linear response
- All polynomial combinations

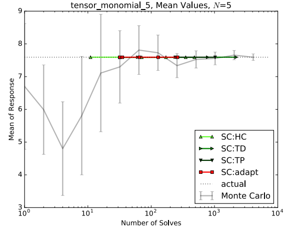
SCgPC Results

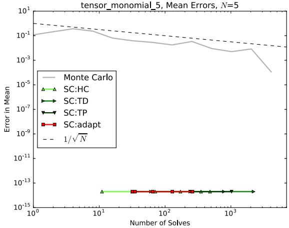
Tensor Monomials, $N = 3$

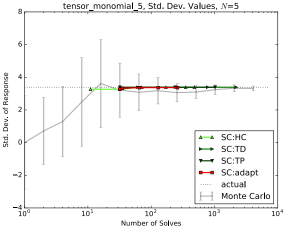


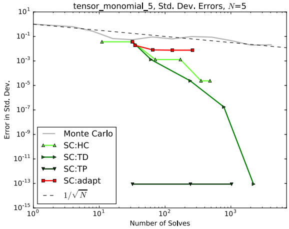
SCgPC Results

Tensor Monomials, $N = 5$



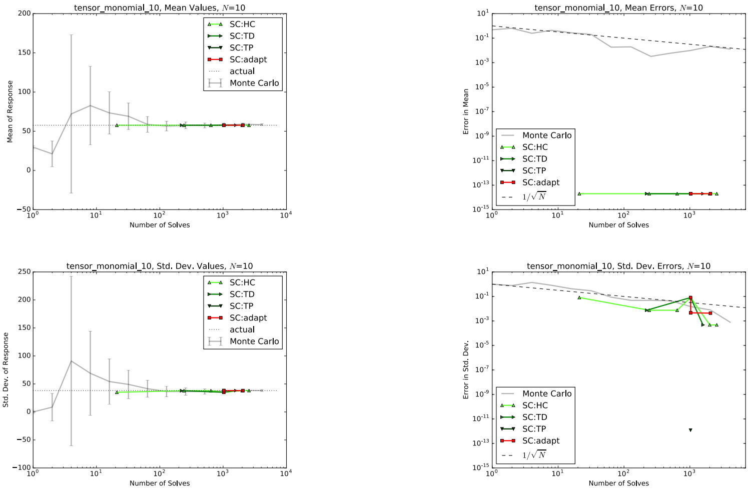






SCgPC Results

Tensor Monomials, $N = 10$

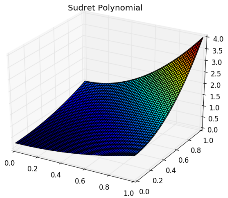


SCgPC Results

Sudret Polynomials

Sudret Polynomials

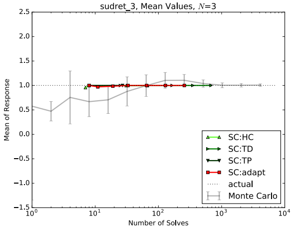
$$u(Y) = \frac{1}{2^N} \prod_{n=1}^{N} (3y_n^2 + 1)$$

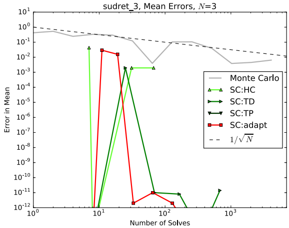


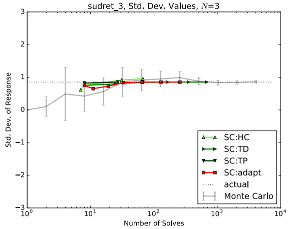
- Exclusively second-order interactions
- All second-order polynomial combinations

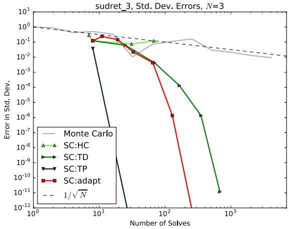
SCgPC Results

Sudret Polynomials, $N = 3$



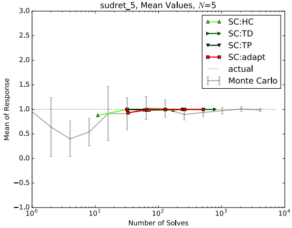


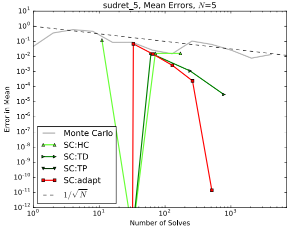


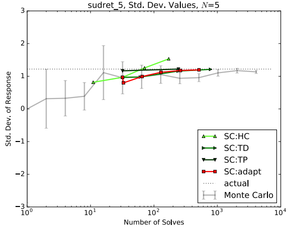


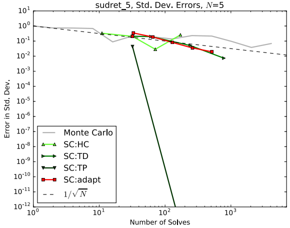
SCgPC Results

Sudret Polynomials, $N = 5$







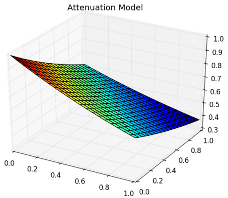


SCgPC Results

Attenuation

Attenuation

$$u(Y) = \prod_{n=1}^{N} \exp(-y_n/N)$$



- Tensor of decreasing-importance polynomials
- Combination terms over single-variable

SCgPC Results

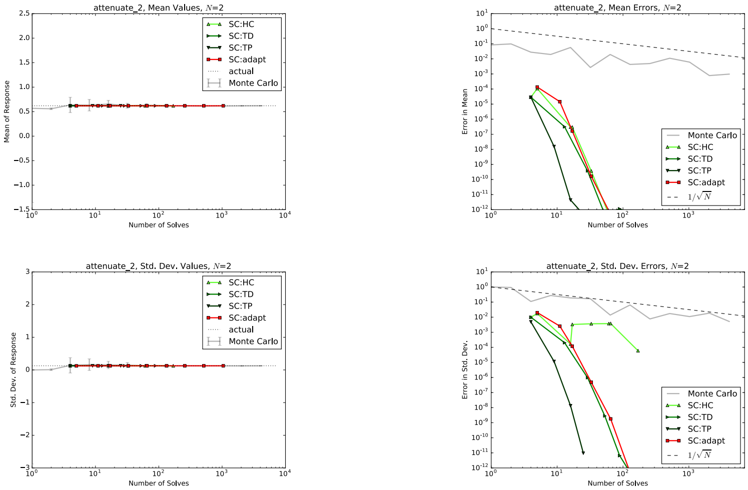
Attenuation, Taylor Expansion

$$e^{-ay} = 1 - ay + \frac{(ay)^2}{2} - \frac{(ay)^3}{6} + \frac{(ay)^4}{24} - \frac{(ay)^5}{120} + \mathcal{O}(y^6)$$

		Polynomial Order (y_1)				
		0	1	2	3	4
Polynomial Order (y_2)	0	1	a	$a^2/2$	$a^3/6$	$a^4/24$
	1	a	a^2	$a^3/2$	$a^4/6$	$a^5/24$
	2	$a^2/2$	$a^3/2$	$a^4/4$	$a^5/12$	$a^6/48$
	3	$a^3/6$	$a^4/6$	$a^5/12$	$a^6/36$	$a^7/144$
	4	$a^4/24$	$a^5/24$	$a^6/48$	$a^7/144$	$a^8/576$

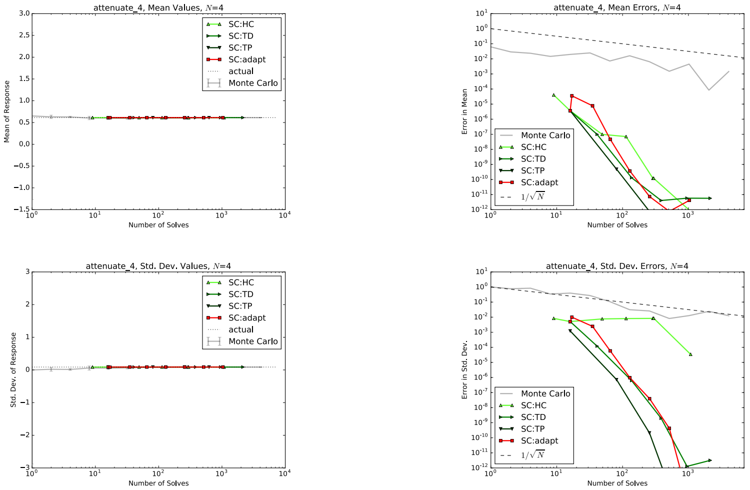
SCgPC Results

Attenuation, $N = 2$



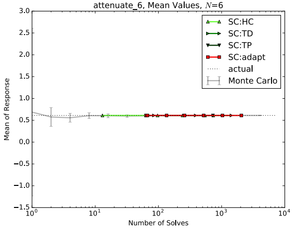
SCgPC Results

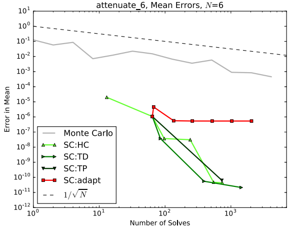
Attenuation, $N = 4$

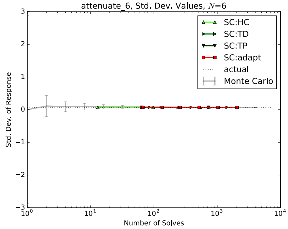


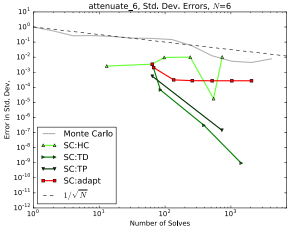
SCgPC Results

Attenuation, $N = 6$







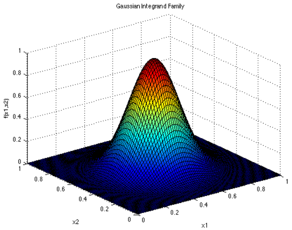


SCgPC Results

Gauss Peak

Gauss Peak

$$u(Y) = \prod_{n=1}^{N} \exp\left(-3^2(y_n - 0.5)^2\right)$$



- Tensor of polynomials
- Slow, inconsistent decay

SCgPC Results

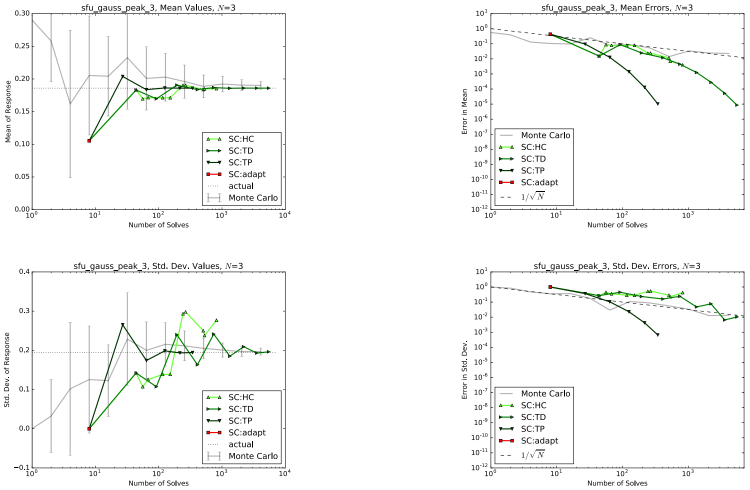
Gauss Peak, Taylor Expansion

$$e^{-a^2y^2} = 1 - a^2y^2 + \frac{a^4}{2}y^4 - \frac{a^6}{6}y^6 + \frac{a^8}{24}y^8 + \mathcal{O}(y^{10})$$

		Polynomial Order (y_1)				
		0	1	2	3	4
Polynomial Order (y_2)	0	1	0	a^2	0	$a^4/2$
	1	0	0	0	0	0
	2	a^2	0	a^4	0	$a^6/2$
	3	0	0	0	0	0
	4	$a^4/2$	0	$a^6/2$	0	$a^8/4$

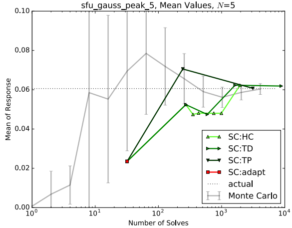
SCgPC Results

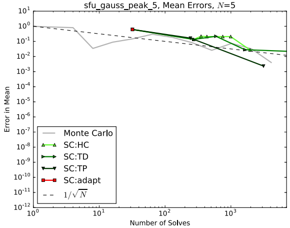
Gauss Peak, $N = 3$

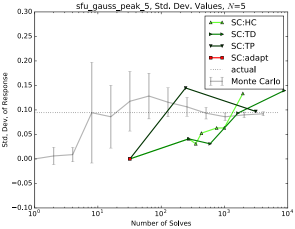


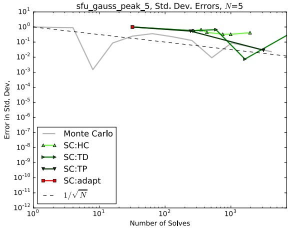
SCgPC Results

Gauss Peak, $N = 5$







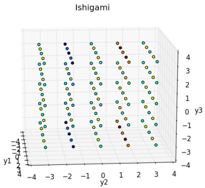


SCgPC Results

Ishigami Function

Ishigami Function

$$u(Y) = \sin y_1 + a \sin^2 y_2 + b\ y_3^4 \sin y_1$$



- Not a tensor combination
- Strange interplay between y_1, y_3

SCgPC Results

Ishigami Function, Taylor Expansion

Ishigami Function

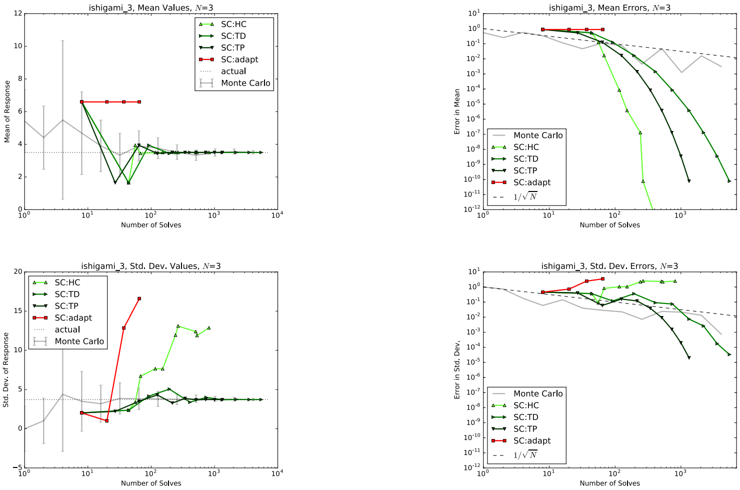
$$u(Y) = \sin y_1 + a\sin^2 y_2 + b\ y_3^4 \sin y_1$$

$$\sin y = x - \frac{x^3}{6} + \frac{x^5}{120} + \mathcal{O}(x^7)$$

$$\sin^2 y = x^2 - \frac{x^4}{3} + \frac{2x^6}{45} + \mathcal{O}(x^8)$$

SCgPC Results

Ishigami Function, $N = 3$

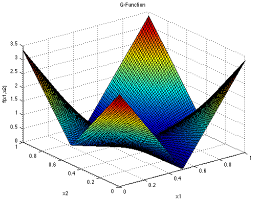


SCgPC Results

Sobol G-Function

Sobol G-Function

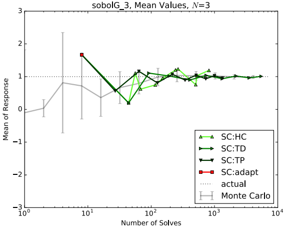
$$u(Y) = \prod_{n=1}^{N} \frac{|4y_n - 2| - a_n}{1 + a_n}, \quad a_n = \frac{n-2}{2}$$

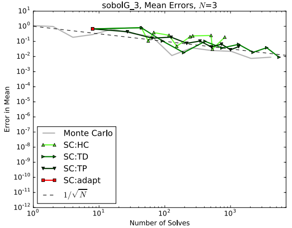


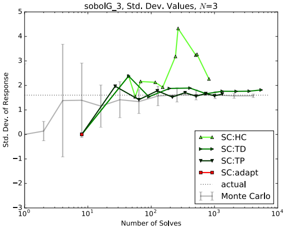
- Tensor combination of terms
- Only zeroth-order continuity

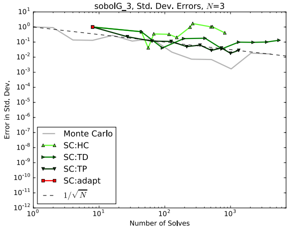
SCgPC Results

Sobol G-Function, $N = 3$



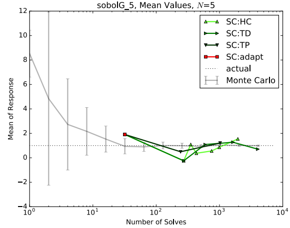


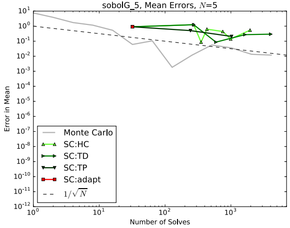


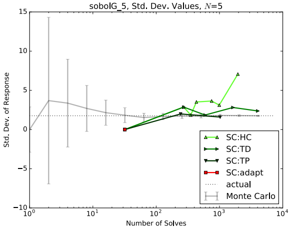


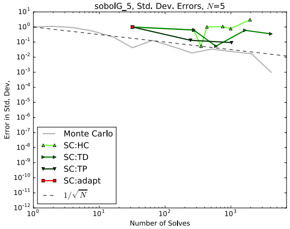
SCgPC Results

Sobol G-Function, $N = 5$









SCgPC Results

Conclusions

Regarding static SCgPC:

- Great in low input space dimensionality
- Better with regular responses
- Total Degree often great choice

Regarding adaptive SCgPC:

- Optimal for small input dimensionality
- Monotonically-decreasing variance moments
- Very poor if oscillating moments

Outline

HDMR

Introduction

HDMR Expansion

$$u(Y) = H[u](Y) = h_0 + \sum_{n=1}^{N} h_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} h_{n_1,n_2} + \cdots$$

$$\hat{Y}_n \equiv (y_1, \cdots, y_{n-1}, y_{n+1}, \cdots, y_N)$$

$$h_0 \equiv \int_{\Omega} u(Y)\, dY, \qquad h_n \equiv \int_{\hat{\Omega}_n} u(Y)\, d\hat{Y}_n - h_0$$

HDMR

HDMR Properties

HDMR Expansion

$$u(Y) = H[u](Y) = h_0 + \sum_{n=1}^{N} h_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} h_{n_1,n_2} + \cdots$$

Properties of HDMR expansion

- Component terms are orthogonal
- Contribution of each input to response
- Truncates to interaction levels
- Sobol sensitivity coefficients
- Requires high-level integration even for h_0

HDMR

cut-HDMR

Cut-HDMR Expansion

$$u(Y) = T[u](Y) = t_r + \sum_{n=1}^{N} t_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} t_{n_1,n_2} + \cdots$$

$$\bar{Y} \equiv (\bar{y}_1, \cdots, \bar{y}_N)$$

$$\hat{\bar{Y}}_n \equiv (\bar{y}_1, \cdots, \bar{y}_{n-1}, \bar{y}_{n+1}, \cdots, \bar{y}_N)$$

$$t_0 \equiv u(\bar{Y}), \qquad t_n \equiv u(y_n, \hat{\bar{Y}}_n) - t_r$$

HDMR

Cut-HDMR Properties

Cut-HDMR Expansion

$$u(Y) = T[u](Y) = t_r + \sum_{n=1}^{N} t_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} t_{n_1,n_2} + \cdots$$

- No integrals required
- Only requires reference value
- Terms are no longer orthogonal
- Variance is not sum of variance of parts
- Converges exactly at no truncation

HDMR

Cut-HDMR and SCgPC

Cut-HDMR Expansion

$$u(Y) = T[u](Y) = t_r + \sum_{n=1}^{N} t_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} t_{n_1,n_2} + \cdots$$

Consider subset terms

- Low-dimension input spaces
- Potentially regular response
- Ideal for SCgPC representation

HDMR

Cut-HDMR and SCgPC

Cut-HDMR Expansion

$$u(Y) = T[u](Y) = t_r + \sum_{n=1}^{N} t_n + \sum_{n_1=1}^{N} \sum_{n_2=1}^{n_1-1} t_{n_1,n_2} + \cdots$$

$$\begin{aligned} t_n &= G[u](y_n, \hat{\hat{Y}}_n) - t_r \\ &= \sum_{k' \in \Lambda'(L')} t_{n;k'} \Phi_{k'}(y_n) - t_r \end{aligned}$$

- $t_{n;k'}$ calculated with Smolyak collocation
- Orthonormality re-introduced
- Can algorithmically recover ANOVA HDMR

HDMR

Cut-HDMR and SCgPC versus SCgPC

Is cut-HDMR with SCgPC better than SCgPC alone?

- Using same polynomial orders and families
- Using same index set type Λ
- Untruncated cut-HDMR is same as SCgPC
- Truncated can approximate with less evaluations
- Most effective when solves very expensive

Outline

HDMR Results

Introduction

Contrast HDMR with SCgPC

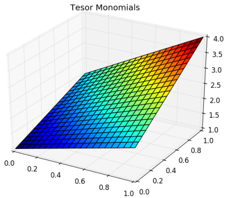
- Same analytic models
- First-, second-, third-order HDMR
- Adaptive HDMR with adaptive SCgPC

HDMR Results

Tensor Monomials

Tensor Monomials

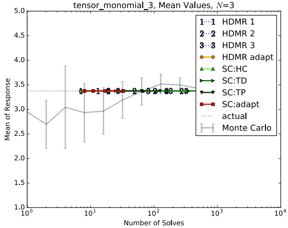
$$u(Y) = \prod_{n=1}^{N} (y_n + 1)$$

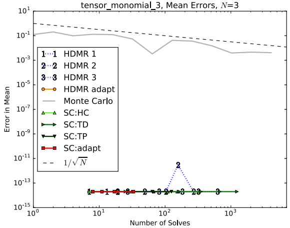


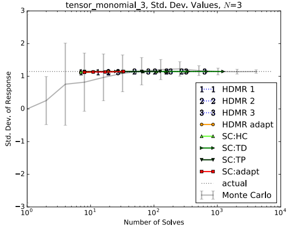
- Linear response
- All polynomial combinations

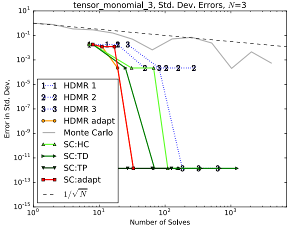
HDMR Results

Tensor Monomials, $N = 3$



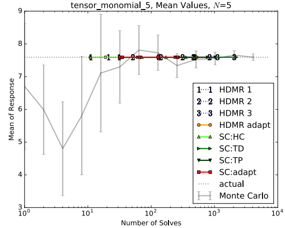


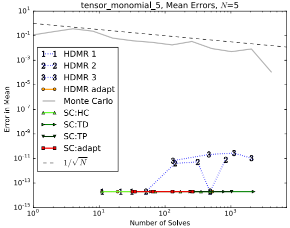


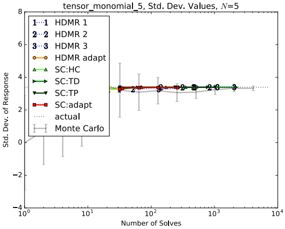


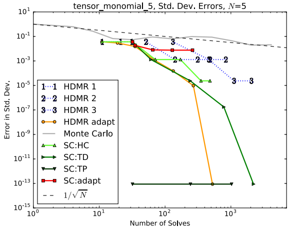
HDMR Results

Tensor Monomials, $N = 5$



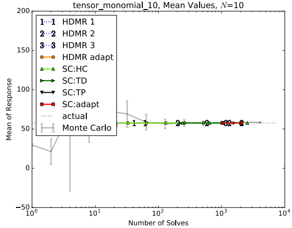


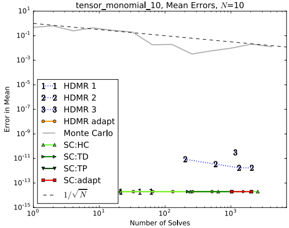


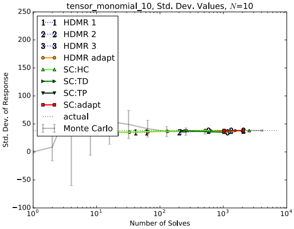


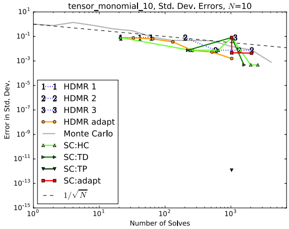
HDMR Results

Tensor Monomials, $N = 10$







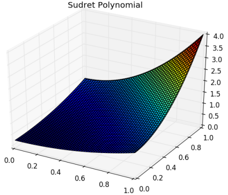


HDMR Results

Sudret Polynomials

Sudret Polynomials

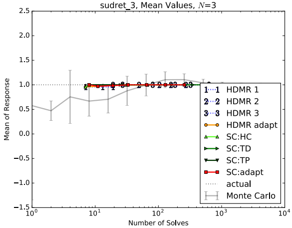
$$u(Y) = \frac{1}{2^N}\prod_{n=1}^{N}(3y_n^2+1)$$

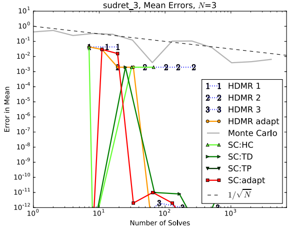


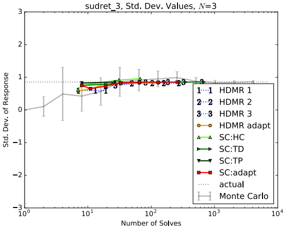
- Exclusively second-order interactions
- All second-order polynomial combinations

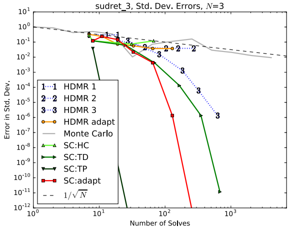
HDMR Results

Sudret Polynomials, $N = 3$



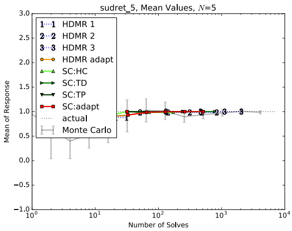


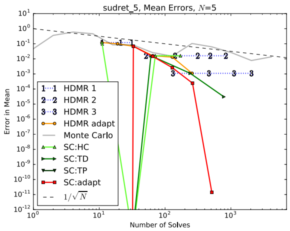


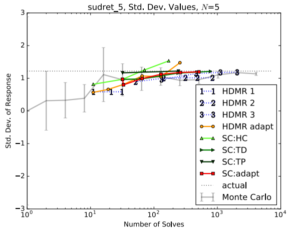


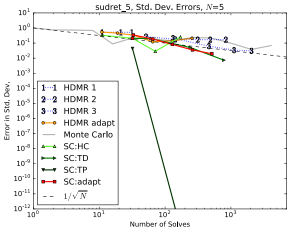
HDMR Results

Sudret Polynomials, $N = 5$







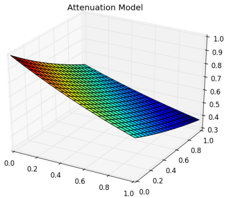


HDMR Results

Attenuation

Attenuation

$$u(Y) = \prod_{n=1}^{N} \exp(-y_n/N)$$



- Tensor of decreasing-importance polynomials
- Combination terms over single-variable

HDMR Results

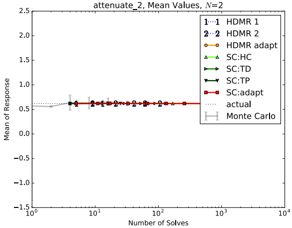
Attenuation, Taylor Expansion

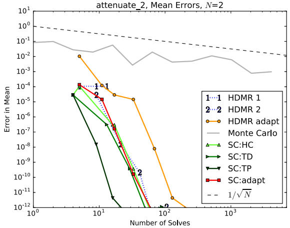
$$e^{-ay} = 1 - ay + \frac{(ay)^2}{2} - \frac{(ay)^3}{6} + \frac{(ay)^4}{24} - \frac{(ay)^5}{120} + \mathcal{O}(y^6)$$

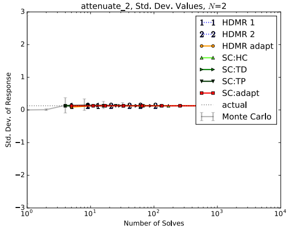
		Polynomial Order (y_1)				
		0	1	2	3	4
Polynomial Order (y_2)	0	1	a	$a^2/2$	$a^3/6$	$a^4/24$
	1	a	a^2	$a^3/2$	$a^4/6$	$a^5/24$
	2	$a^2/2$	$a^3/2$	$a^4/4$	$a^5/12$	$a^6/48$
	3	$a^3/6$	$a^4/6$	$a^5/12$	$a^6/36$	$a^7/144$
	4	$a^4/24$	$a^5/24$	$a^6/48$	$a^7/144$	$a^8/576$

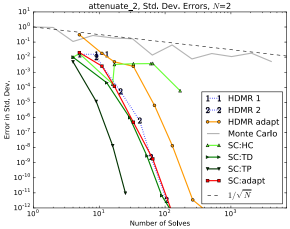
HDMR Results

Attenuation, $N = 2$



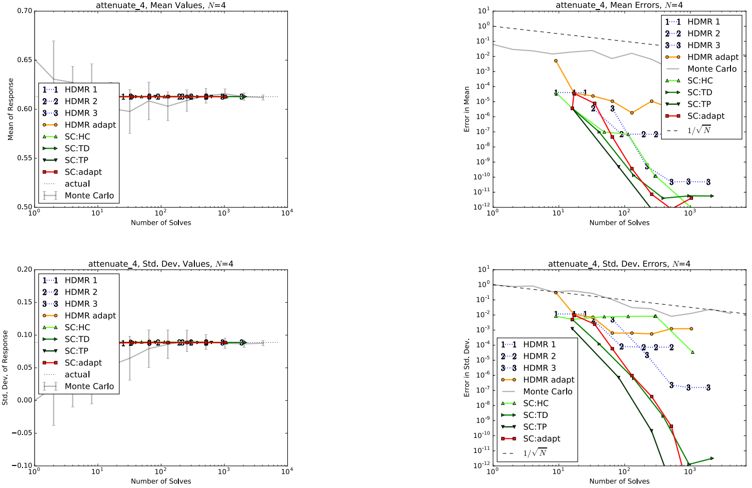






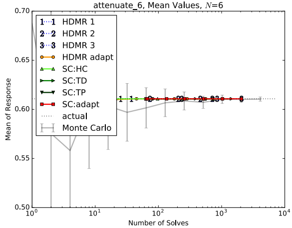
HDMR Results

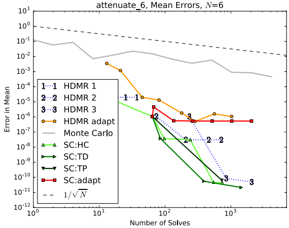
Attenuation, $N = 4$

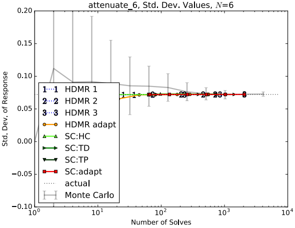


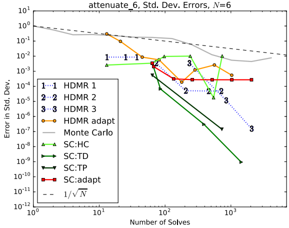
HDMR Results

Attenuation, $N = 6$







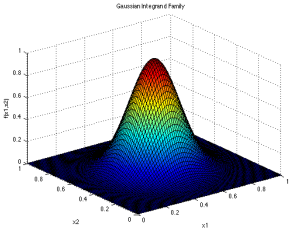


HDMR Results

Gauss Peak

Gauss Peak

$$u(Y) = \prod_{n=1}^{N} \exp\left(-3^2(y_n - 0.5)^2\right)$$



- Tensor of polynomials
- Slow, inconsistent decay

HDMR Results

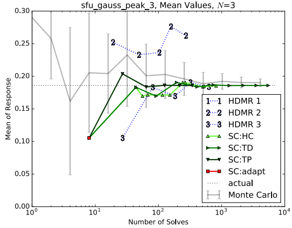
Gauss Peak, Taylor Expansion

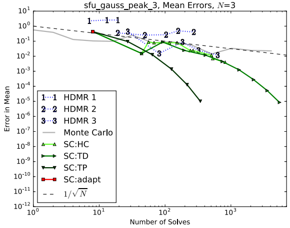
$$e^{-a^2y^2} = 1 - a^2y^2 + \frac{a^4}{2}y^4 - \frac{a^6}{6}y^6 + \frac{a^8}{24}y^8 + \mathcal{O}(y^{10})$$

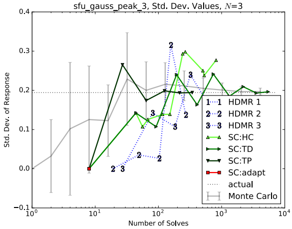
		Polynomial Order (y_1)				
		0	1	2	3	4
Polynomial Order (y_2)	0	1	0	a^2	0	$a^4/2$
	1	0	0	0	0	0
	2	a^2	0	a^4	0	$a^6/2$
	3	0	0	0	0	0
	4	$a^4/2$	0	$a^6/2$	0	$a^8/4$

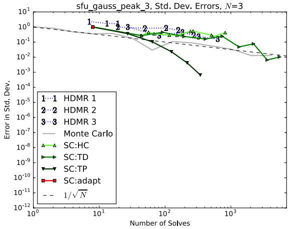
HDMR Results

Gauss Peak, $N = 3$



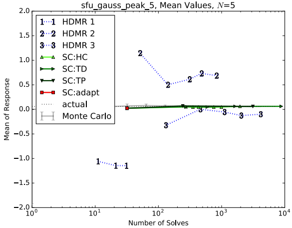


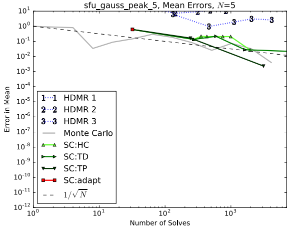


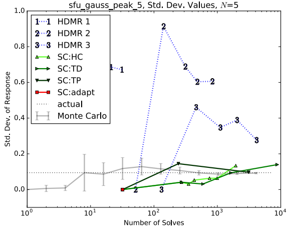


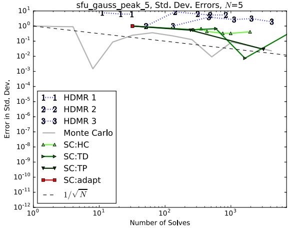
HDMR Results

Gauss Peak, $N = 5$







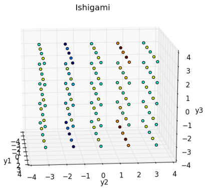


HDMR Results

Ishigami Function

Ishigami Function

$$u(Y) = \sin y_1 + a \sin^2 y_2 + b\ y_3^4 \sin y_1$$



- Not a tensor combination
- Strange interplay between y_1, y_3

HDMR Results

Ishigami Function, Taylor Expansion

Ishigami Function

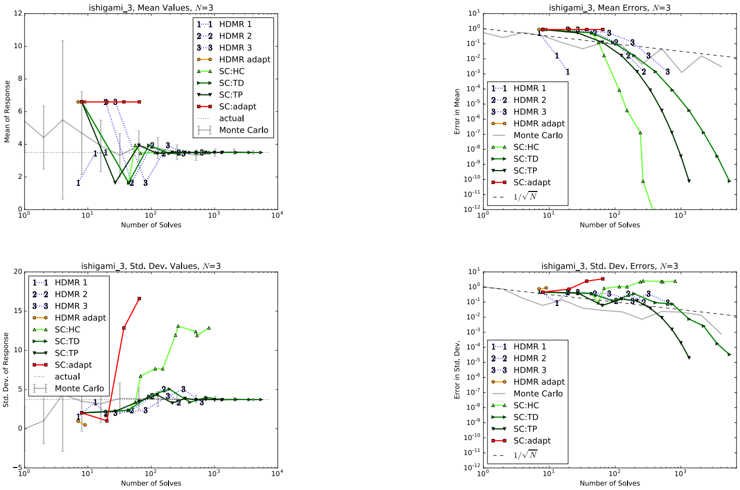
$$u(Y) = \sin y_1 + a \sin^2 y_2 + b\ y_3^4 \sin y_1$$

$$\sin y = x - \frac{x^3}{6} + \frac{x^5}{120} + \mathcal{O}(x^7)$$

$$\sin^2 y = x^2 - \frac{x^4}{3} + \frac{2x^6}{45} + \mathcal{O}(x^8)$$

HDMR Results

Ishigami Function, $N = 3$

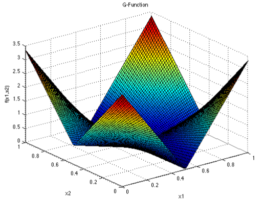


HDMR Results

Sobol G-Function

Sobol G-Function

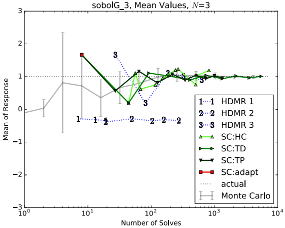
$$u(Y) = \prod_{n=1}^{N} \frac{|4y_n - 2| - a_n}{1 + a_n}, \quad a_n = \frac{n-2}{2}$$

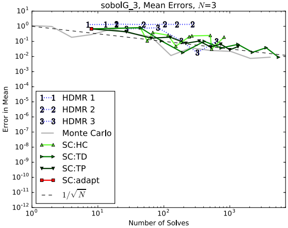


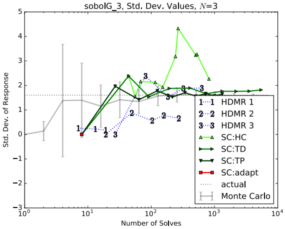
- Tensor combination of terms
- Only zeroth-order continuity

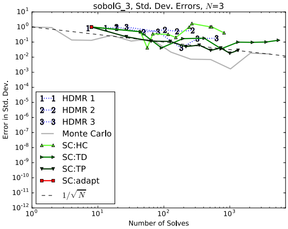
HDMR Results

Sobol G-Function, $N = 3$



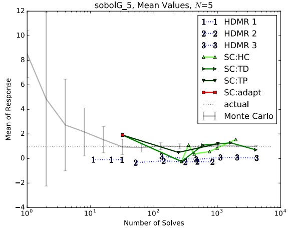


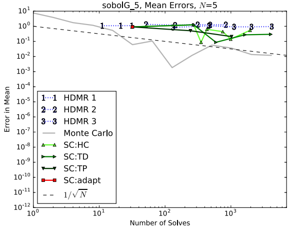


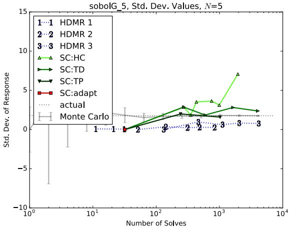


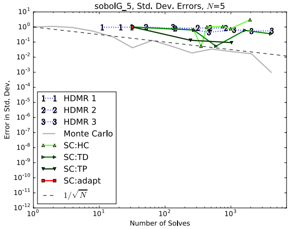
HDMR Results

Sobol G-Function, $N = 5$









HDMR Results

Conclusions

Regarding static HDMR:

- Never outperforms associated SCgPC
- Does produce results with less evaluations

Regarding adaptive HDMR:

- Sometimes outperforms adaptive SCgPC
- Yields results with fewer evaluations

HDMR is most useful when very few evaluations possible

Outline

Neutronics Example

Introduction

More complicated than an analytic case

$$-D_g(\mathbf{r})\nabla^2\phi_g(\mathbf{r}) + \Sigma_{a,g}(\mathbf{r}) = \sum_{g'=1}^{G} \Sigma_{g'\to g}\phi_{g'}(\mathbf{r}) + \frac{\chi_{p,g}}{k}\sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r})$$

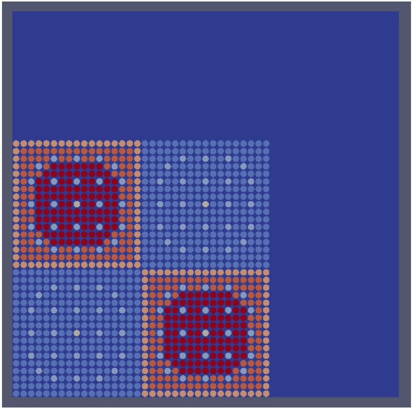
Quantities of interest

- $\phi_g(\mathbf{r})$: Group neutron flux
- k eigenvalue: Neutron multiplication factor

Neutronics Example

Geometry

Quarter-symmetric 4-assembly reactor core



Neutronics Example

Energy Groups

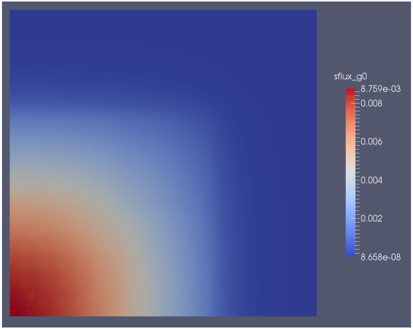
7 energy groups, 7 materials, 32 mesh elements per pin

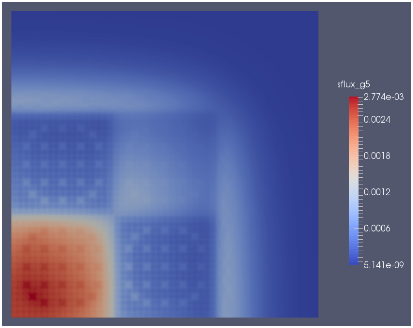
Group	Upper Energy Bound
7	0.02 eV
6	0.1 eV
5	0.625 eV
4	3 eV
3	500 keV
2	1 MeV
1	20 MeV

Solved using `RATTLESNAKE`'s linear CFEM

Neutronics Example

Flux Profiles





Outline

Neutronics Example

Uncertainty

Specific Responses

- k-eigenvalue
- Group 1 flux at reactor center
- Group 5 flux at reactor center

168 correlated uncertain inputs

- Material macroscopic cross sections
- Assigned 10% correlation
  - Same material and reaction, different energies
  - Same material and energy, different reaction
- Relative variance of 5% for all inputs

Neutronics Example

Uncertainty Correlations

Need to de-correlate input space

`RAVEN` has two-step reduction

- Karhunen-Loeve expansion (PCA)
- Sensitivity reduction
- Combined yields *importance rank*

Neutronics Example

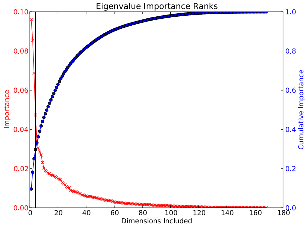
Uncertainty Correlations

	k-eigenvalue		Center Flux, $g = 1$		Center Flux, $g = 5$	
Rank	Dimension	Importance	Dimension	Importance	Dimension	Importance
1	24	0.09606	24	0.07231	24	0.07032
2	9	0.08555	9	0.06472	9	0.06648
3	0	0.06861	0	0.04856	100	0.06474
4	17	0.04737	116	0.03472	13	0.03396
5	23	0.03415	17	0.03470	0	0.03092
6	158	0.03047	10	0.02726	17	0.02716
7	164	0.02852	8	0.02468	10	0.02651
8	50	0.02695	164	0.02174	118	0.02600
9	6	0.02315	20	0.02157	117	0.02420

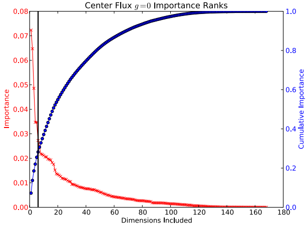
Retained latent dimensions 24, 9, 0, 17, 10, 116, 100, 13

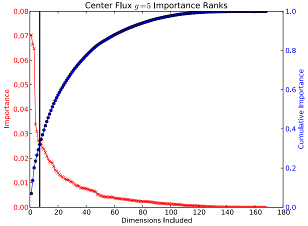
Neutronics Example

Uncertainty Correlations



- Truncated after gradients
- Some importance lost
- Mean preserved well
- Std dev partially preserved

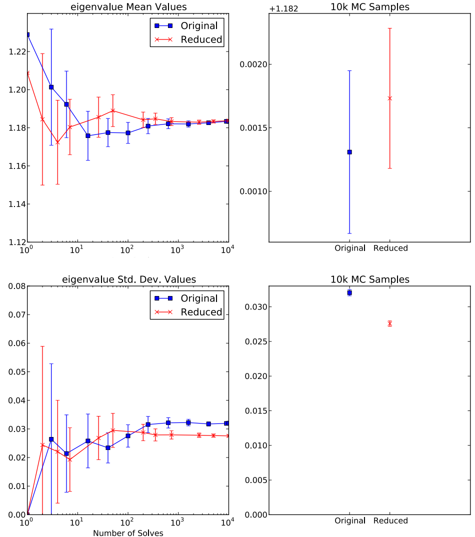




Neutronics Example

Uncertainty Correlations

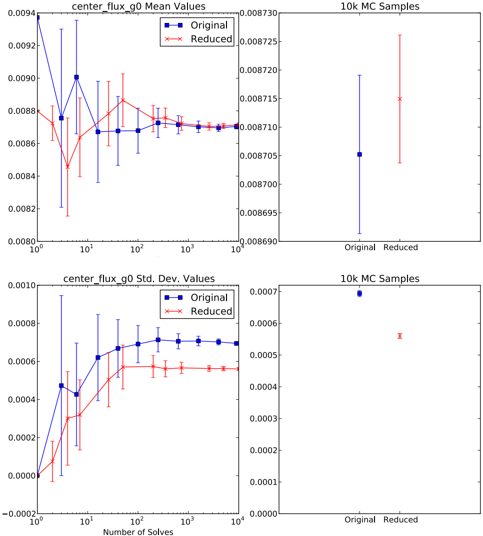
k-Eigenvalue



Neutronics Example

Uncertainty Correlations

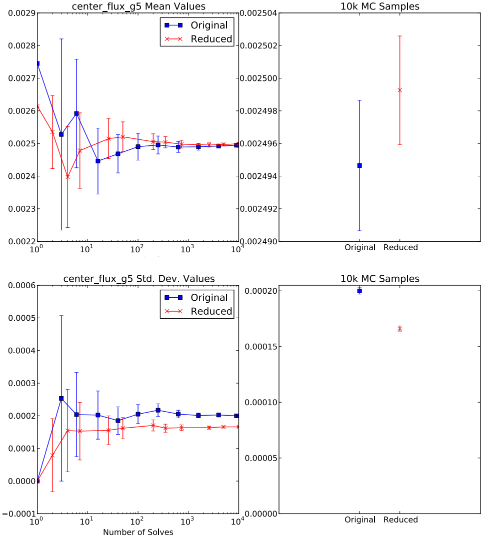
Center Flux, $g = 1$



Neutronics Example

Uncertainty Correlations

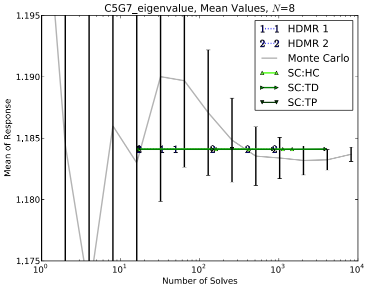
Center Flux, $g = 5$

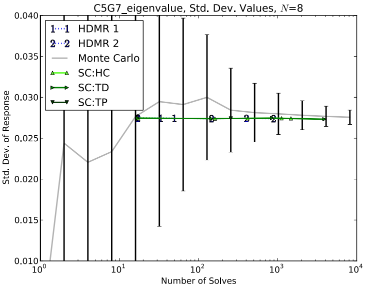


Outline

Neutronics Example

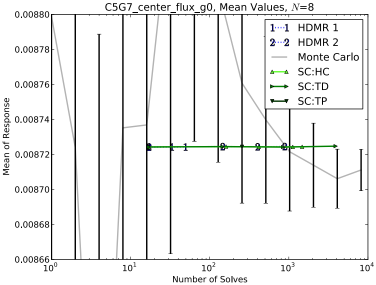
Results: *k*-eigenvalue

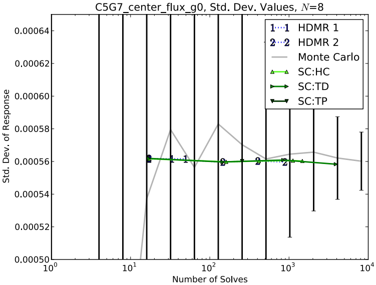




Neutronics Example

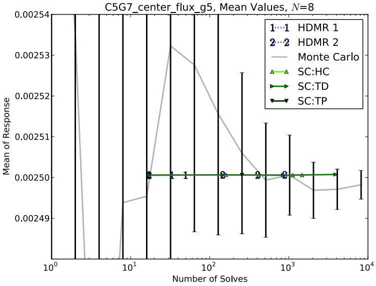
Results: Center Flux, $g = 1$

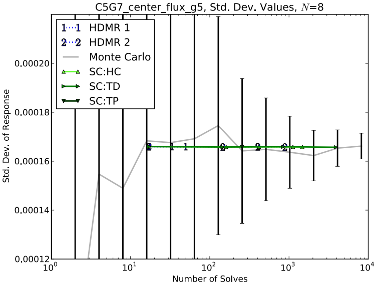




Neutronics Example

Results: Center Flux, $g = 5$





Outline

Multiphysics Example

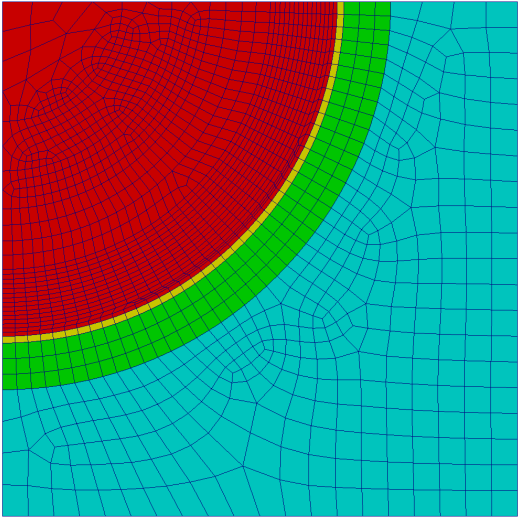
Introduction

Coupled multiphysics problem

- Neutronics
  - neutron transport and interaction
  - Provides flux/power shapes to fuels performance
- Fuels Performance
  - temperature, depletion, fuel oxidation,
  - fission product swelling, densification, fuel fracture,
  - interstitial heat transfer, mechanical contact,
  - cladding creep, thermal expansion, plasticity
  - Provides temperature fields to neutronics

Multiphysics Example

Geometry



Outline

Multiphysics Example

Geometry and Uncertainty

Dimensions

- Domain is 6.3 mm square
- Reflective boundaries
- Fuel pin radius is 4.09575 mm with clad

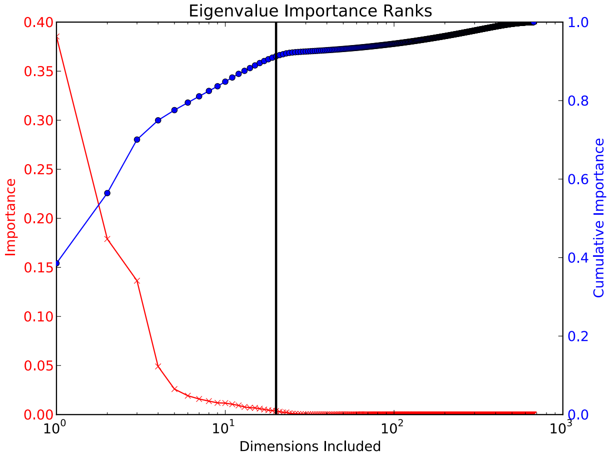
Response is k-eigenvalue

Uncertain inputs

- 671 correlated interaction cross sections
- Fuel thermal expansion coefficient
- Clad thermal conductivity
- Fuel thermal conductivity

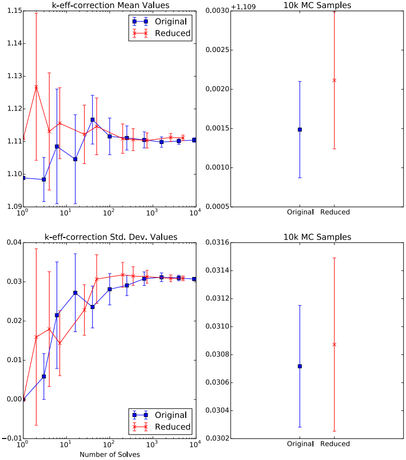
Multiphysics Example

Uncertainty Correlation



Multiphysics Example

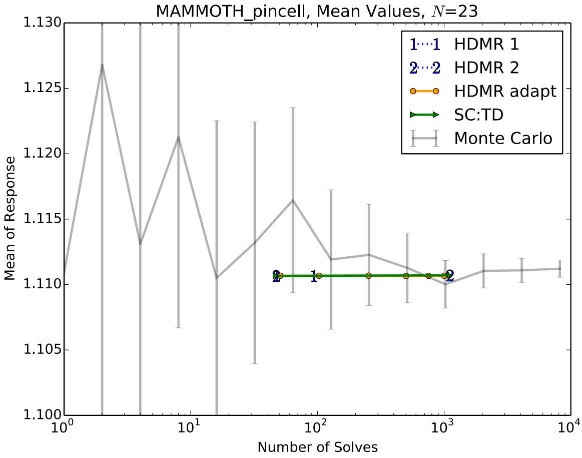
Uncertainty Correlation



Outline

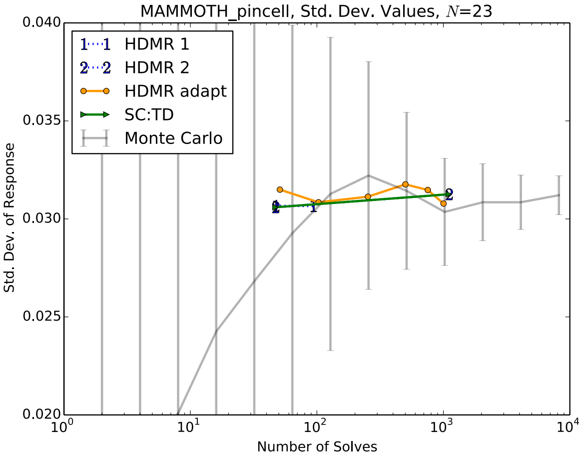
Multiphysics Example

Results



Multiphysics Example

Results



Multiphysics Example

Run Times

Method	Degree	Runs
Total Degree	1	47
Total Degree	2	1105
Total Degree*	3	17389
HDMR (1)	1	47
HDMR (1)	2	47
HDMR (1)	3	93
HDMR (1)	4	93
HDMR (1)	5	139
HDMR (2)	1	47
HDMR (2)	2	1105
HDMR (2)†	3	3221
HDMR (2)†	4	7361
HDMR (2)*	5	13571

Outline

Time-Dependent Analysis

Introduction

Transient Problems

- Response is time-dependent
- Response may evolve in time
- Physics may change in time

"Time" could be any monotonically-increasing parameter

Time-Dependent Analysis

Approach

RAVEN approach

- Divide time into snapshots
- Evaluate ROM on each snapshot
- Interpolate between snapshots

We extended SCgPC and HDMR to do this as well

Limitation: Adaptive methods

Outline

Time-Dependent Example

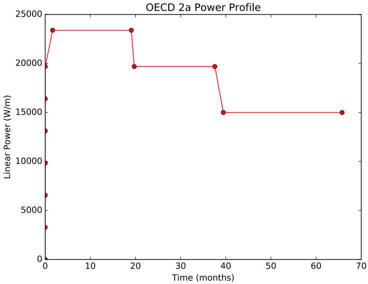
Introduction

Fuels Performance problem

- OECD Benchmark
- PWR Fuel Rod
- "Steady-State"
- Power Changes

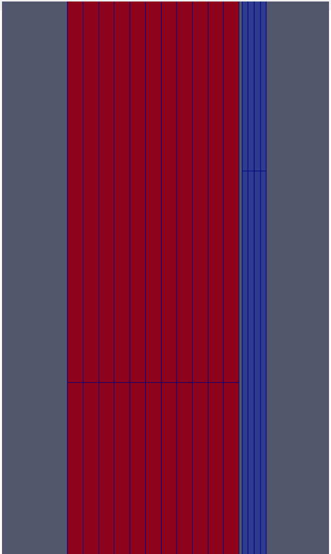
Responses

- max clad temp
- % fission gas released
- clad elongation
- clad creep strain



Time-Dependent Example

Introduction



Geometry

- Fuel and Cladding
- 2D Axisymmetric R-Z
- 4 m by 0.55 cm
- 4290 QUAD8 Elements

Physics

- Displacement/Creep
- Thermal expansion
- Heat conduction
- Heat convection
- Contact stress

UNM

Outline

Time-Dependent Example

Uncertainty

Uncertain Parameter	Mean	Std. Dev.
Clad Thermal Conductivity	16.0	2.5
Cladding Thickness	6.7e-4	8.3e-6
Cladding Roughness	5.0e-7	1.0e-7
Clad Creep Rate	1.0	0.15
Fuel Thermal Conductivity	1.0	0.05
Fuel Density	10299.24	51.4962
Fuel Thermal Expansion	1.0e-5	7.5e-7
Fuel Pellet Radius	4.7e-3	3.335e-6
Fuel Pellet Roughness	2.0e-6	1.6667e-7
Solid Fuel Swelling	5.58e-5	5.77e-6
Gas Conductivity	1.0	0.025
Gap Thickness	9.0e-5	8.33e-6
Mass Flux	3460	57.67
Rod Fill Pressure	1.2e6	40000.0
System Pressure	1.551e7	51648.3
System Power	1.0	0.016667
Uncertain Parameter	**Lower Bound**	**Upper Bound**
Inlet Temperature	558.0	564.0

Time-Dependent Example

Uncertainty

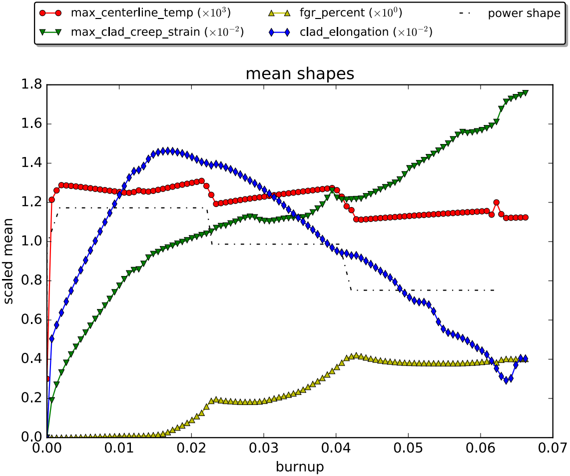
Dependent Parameters

Dependent Parameter	Calculation
Clad inner radius	2*(fuel_rad + gap_width)
Outer Diameter (Hot)	2*(fuel_rad + gap_width + clad_thick)
Outer Diameter (Cool)	2*(fuel_rad + gap_width + clad_thick)
System Pressure (Cool)	sys_press
Thermal Porosity	1 - fuel_dens/10980
Fuel Diameter	2*fuel_rad
Gap Diameter	2*gap_thick
SIFGR Porosity	1 - fuel_dens/10980

Outline

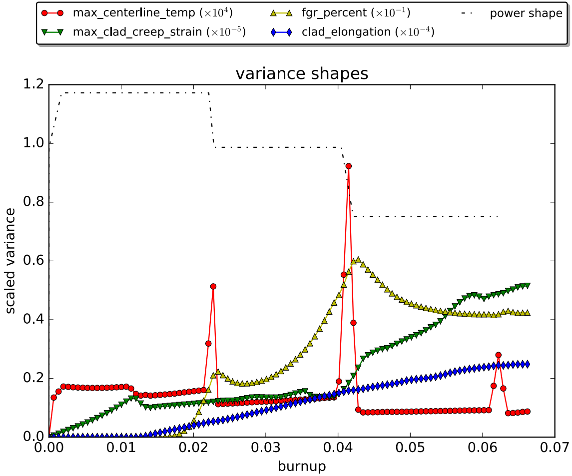
Time-Dependent Example

Results



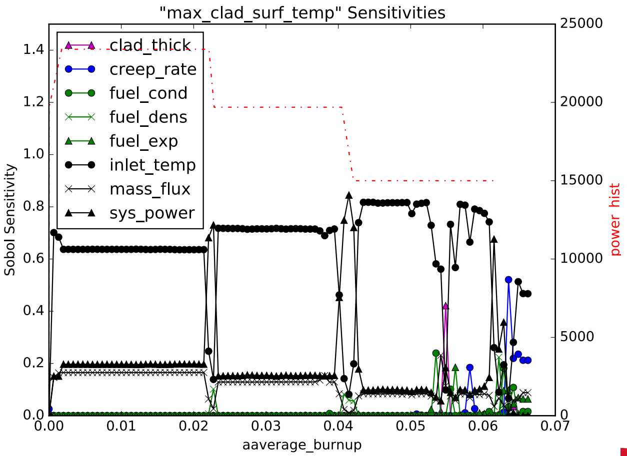
Time-Dependent Example

Results



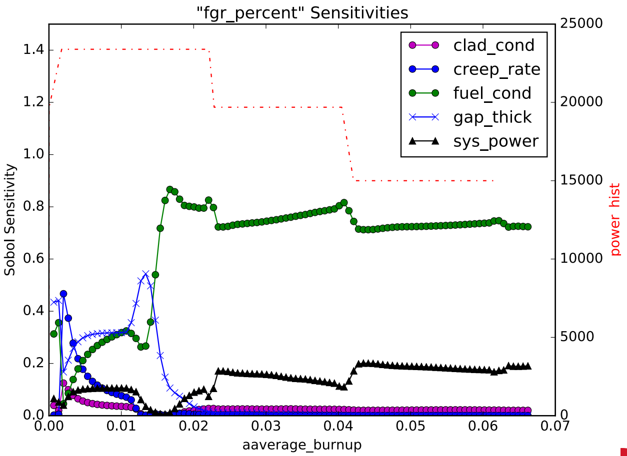
Time-Dependent Example

Results



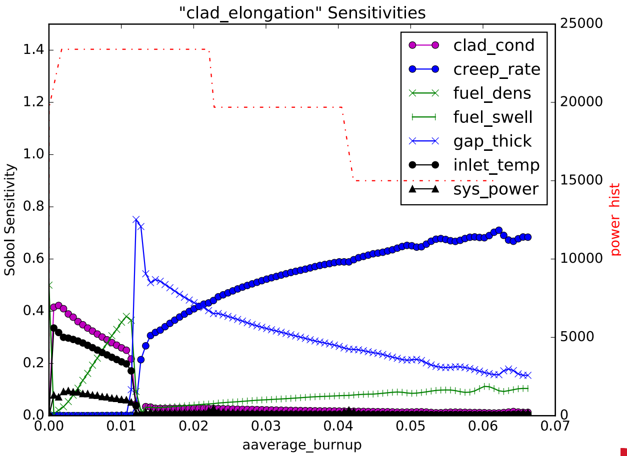
Time-Dependent Example

Results



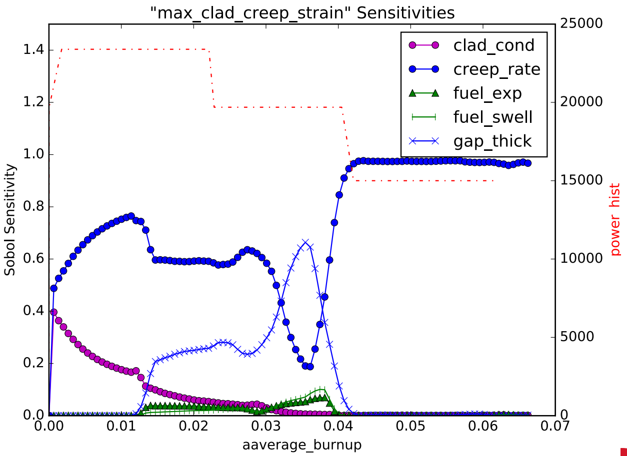
Time-Dependent Example

Results



Time-Dependent Example

Results



Time-Dependent Example

Conclusions

Time-Dependent Analysis with SCgPC and HDMR

- Same benefits as with static analysis
- No additional solves for time-dependent
- Increased understanding of physics
- Informed decision making

Outline

Conclusions

Synopsis

Stochastic Collocation for generalized Polynomial Chaos

- Good for small dimensionality
- Good for regular responses

High-Dimensional Model Reduction

- No more convergent than SCgPC
- Generates solutions more cheaply

Adaptive methods

- Good for anisotropic response
- Good for small dimensionality
- Seldom ideal but often good

Conclusions

Limitations

Collocation-based methods

- Rely on stable simulation models
- Poor for large dimensionality
- Very poor for discontinuous responses

Adaptive collocation methods

- Can be misled
- Stall on inconsistent impacts

Outline

Conclusions

Future Work

Quadrature Order

- “Floor” Quadrature
- Adaptive Quadrature

Adaptive: Impact Inertia

- Currently consider only neighbors
- Consider full history

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- Drs. Prinja, Motamed, Olivera
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- CongJian Wang, Dan Maljovec

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