

Advanced Stochastic Collocation Methods for Polynomial Chaos in RAVEN

Paul W. Talbot

University of New Mexico

Dissertation Defense, November 3, 2016

Funded by a Laboratory Directed Research effort at
Idaho National Laboratory

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)

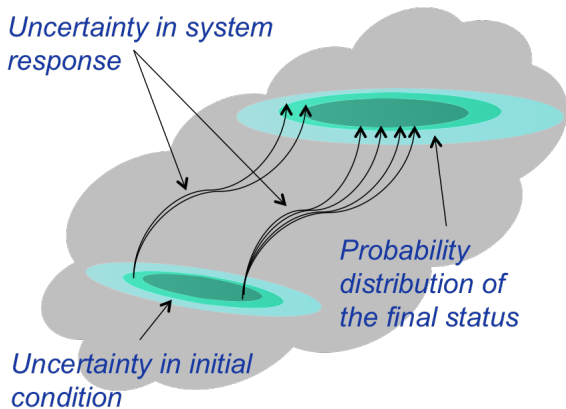
- ▶ Analyze models as accurately as possible
- ▶ Propagate uncertainty to determine safety margins
- ▶ Example: RISMC



Introduction

Uncertainty Quantification

Uncertainty Quantification as explained by RAVEN



Nomenclature

- ▶ 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
- ▶ $Y = (y_1, y_2, \dots, y_N)$ 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, $Y = (y_1, \dots, y_N)$
- ▶ 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 $u(Y(\omega))$

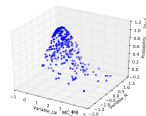


Introduction

Traditional Uncertainty Quantification Methods

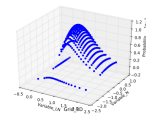
Monte Carlo

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



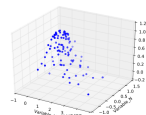
Grid

- ▶ 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

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions

Outline

- 1 Introduction
- 2 SCgPC
 - Theory
 - Results
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions

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

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

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

$$\Lambda_{TP}(L) = \left\{ k = (k_1, \dots, k_N) : \max_{1 \leq n \leq N} k_n \leq L \right\}$$

Example: $N = 2, L = 3$

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



SCgPC

gPC: Polynomial Set Λ

Total Degree Index Set

$$\Lambda_{\text{TD}}(L) = \left\{ k = (k_1, \dots, k_N) : \sum_{n=1}^N k_n \leq L \right\}$$

Example: $N = 2, L = 3$

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



SCgPC

gPC: Polynomial Set Λ

Hyperbolic Cross Index Set

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

Example: $N = 2, L = 3$

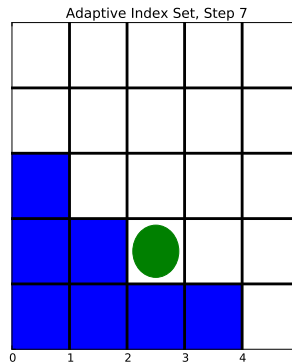
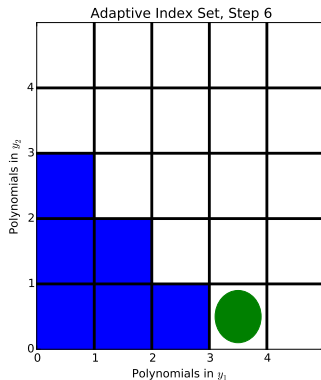
$$\Lambda_{\text{HC}}(3) = \begin{array}{cccc} (3,0) & & & \\ (2,0) & & & \\ (1,0) & (1,1) & & \\ (0,0) & (0,1) & (0,2) & (0,3) \end{array}$$



SCgPC

Adaptive SCgPC

Add polynomials adaptively



SCgPC

Adaptive SCgPC

Choose polynomials to add adaptively

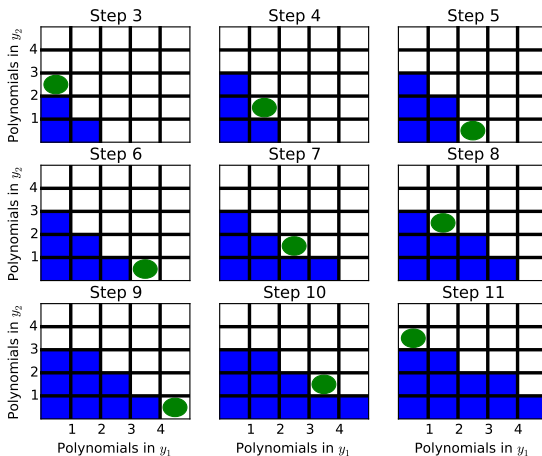
Estimated Polynomial Impact

$$\tilde{\eta}_k = \frac{1}{N} \sum_{n=1}^N \eta_{k-e_n}$$

Average of predecessor polynomials

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

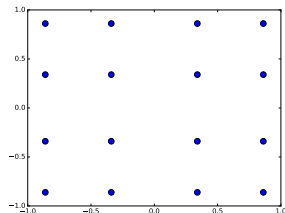
Stochastic Collocation

Multidimensional Numerical Integrals

Basic choice: tensor combination

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

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



SCgPC

Smolyak Sparse Grid

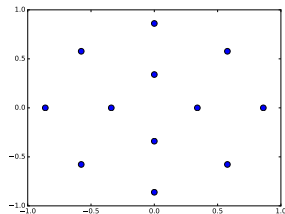
Tensor quadrature can be wasteful

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

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

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

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



SCgPC

Smolyak sparse grid

Expansion Moments

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

Calculate using Smolyak sparse grid

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

gPC Expansion

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

Outline

- 1 Introduction
- 2 SCgPC
 - Theory
 - Results
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions

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

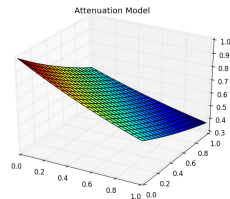
- ▶ Tensor Monomials
- ▶ Sudret Polynomial
- ▶ **Attenuation**
- ▶ **Gauss Peak**
- ▶ Ishigami
- ▶ Sobol G-Function

SCgPC Results

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

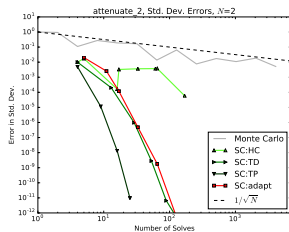
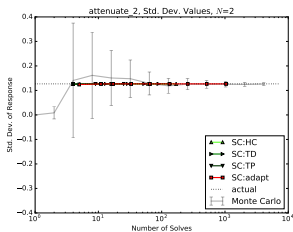
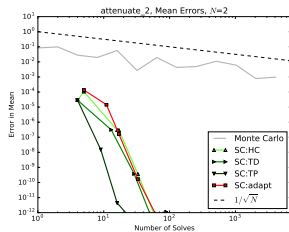
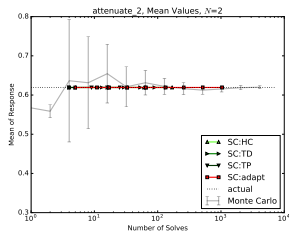
$$e^{-ay} = 1 - ay + \frac{(ay)^2}{2} - \frac{(ay)^3}{6} + \frac{(ay)^4}{24} - \frac{(ay)^5}{120} + \mathcal{O}(y^6)$$

		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	$a^4/24$	$a^5/24$	$a^6/48$	$a^7/144$	$a^8/576$



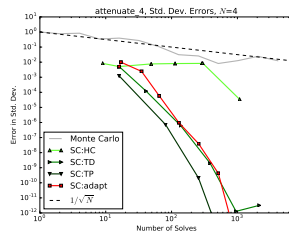
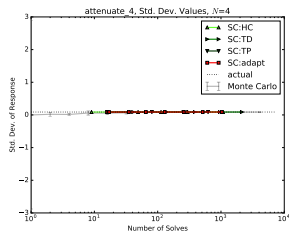
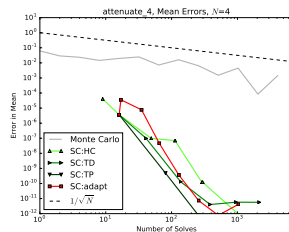
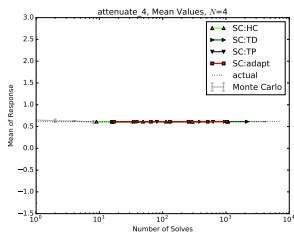
SCgPC Results

Attenuation, $N = 2$

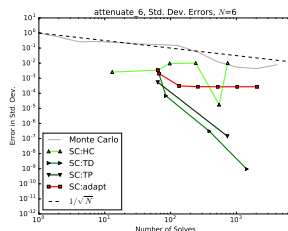
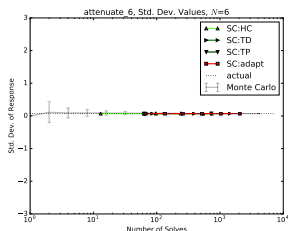
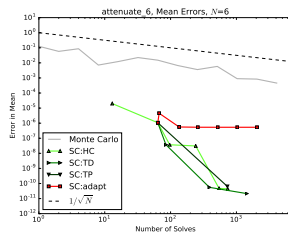
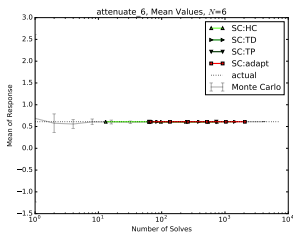


SCgPC Results

Attenuation, $N = 4$



SCgPC Results

Attenuation, $N = 6$ 

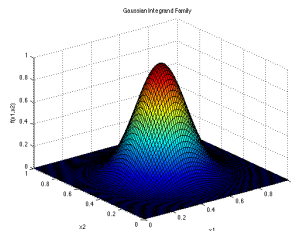
SCgPC Results

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

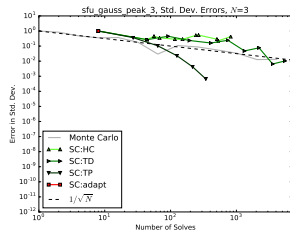
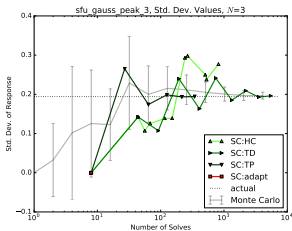
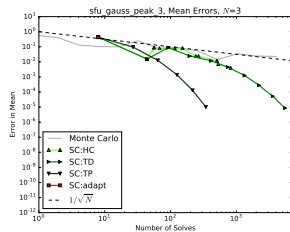
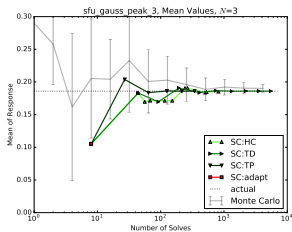
$$e^{-a^2 y^2} = 1 - a^2 y^2 + \frac{a^4}{2} y^4 - \frac{a^6}{6} y^6 + \frac{a^8}{24} y^8 + \mathcal{O}(y^{10})$$

		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	$a^8/4$



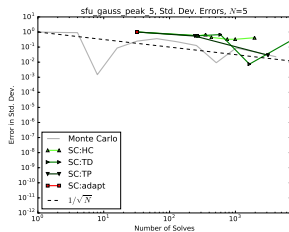
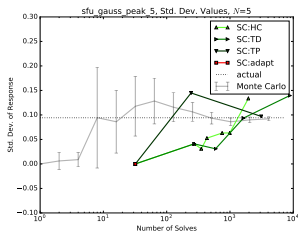
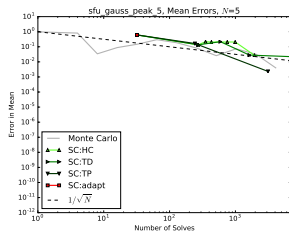
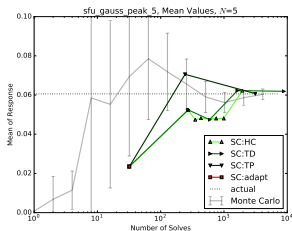
SCgPC Results

Gauss Peak, $N = 3$



SCgPC Results

Gauss Peak, $N = 5$



Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR**
 - Theory
 - Results
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions

HDMR

Introduction

HDMR Expansion

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

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

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



HDMR

HDMR Properties

HDMR Expansion

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

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

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

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

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

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

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

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

Consider subset terms

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

HDMR

Cut-HDMR and SCgPC

Cut-HDMR Expansion

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

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

- ▶ $t_{n; k'}$ 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

HDMR

Adaptive HDMR

Construct cut-HDMR with SCgPC adaptively:

- ▶ Choose:
 - ▶ Add a new subset
 - ▶ Add polynomial to existing subset
- ▶ Subset impact: Sobol sensitivity
- ▶ Polynomial impact: local \times subset

HDMR

Cut-HDMR and SCgPC versus SCgPC

Estimated Subset Impact

$$S_{\beta} = \frac{\text{var}[h_{\beta}]}{\text{var}[T(Y)]}$$

Estimated Polynomial Impact

$$\tilde{\xi}_k = \tilde{\eta}_k \cdot S_{\beta}$$

$$\tilde{\eta}_k = \frac{1}{N} \sum_{n=1}^N \eta_{k-e_n}$$

$$\eta_k = c_k^2$$

Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR**
 - Theory
 - Results**
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions



HDMR Results

Introduction

Contrast HDMR with SCgPC

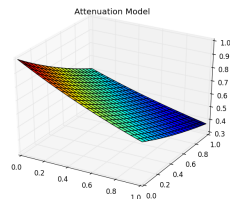
- ▶ Same analytic models
- ▶ First-, second-, third-order HDMR
- ▶ Adaptive HDMR with adaptive SCgPC

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

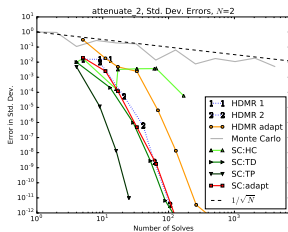
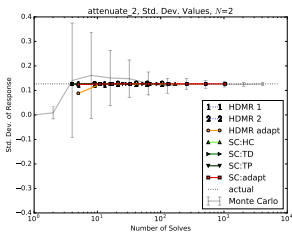
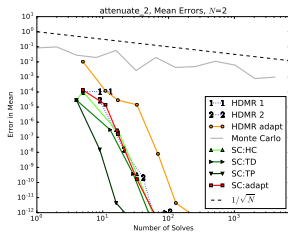
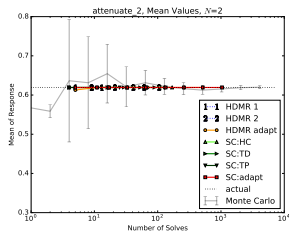
$$e^{-ay} = 1 - ay + \frac{(ay)^2}{2} - \frac{(ay)^3}{6} + \frac{(ay)^4}{24} - \frac{(ay)^5}{120} + \mathcal{O}(y^6)$$

		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	$a^4/24$	$a^5/24$	$a^6/48$	$a^7/144$	$a^8/576$



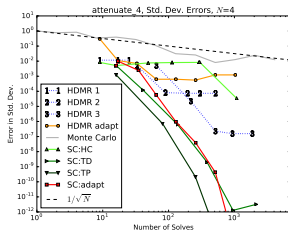
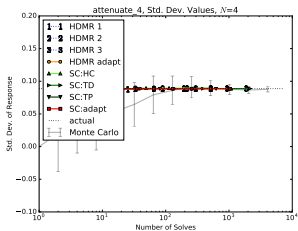
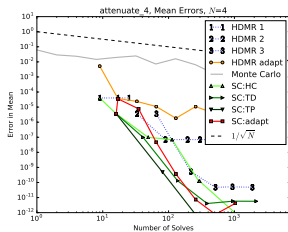
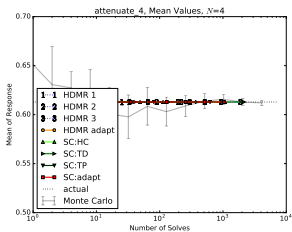
HDMR Results

Attenuation, $N = 2$

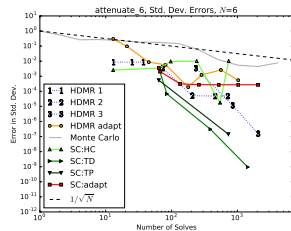
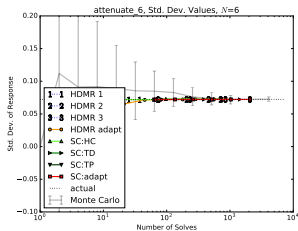
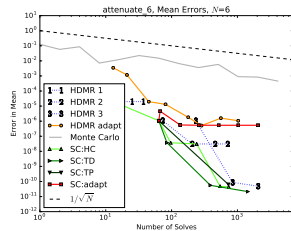
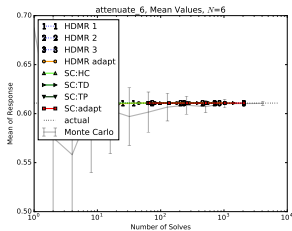


HDMR Results

Attenuation, $N = 4$



HDMR Results

Attenuation, $N = 6$ 

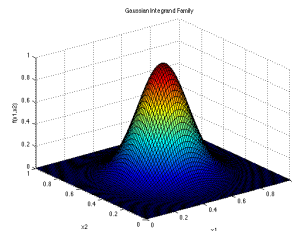
HDMR Results

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

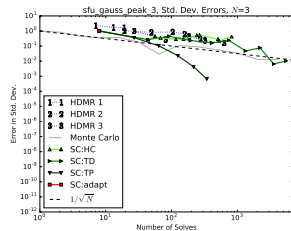
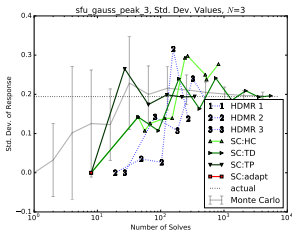
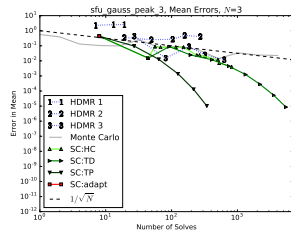
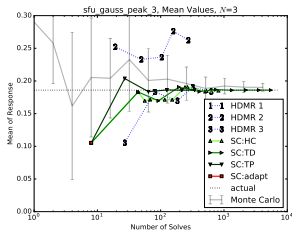
Gauss Peak, Taylor Expansion

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

		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	$a^8/4$

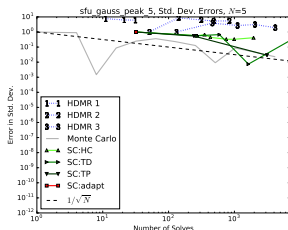
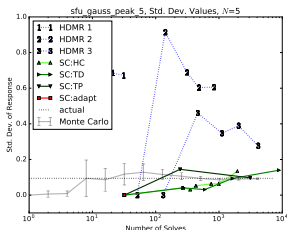
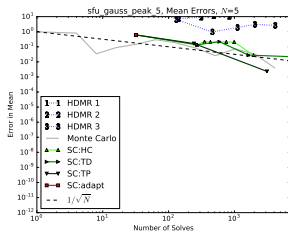
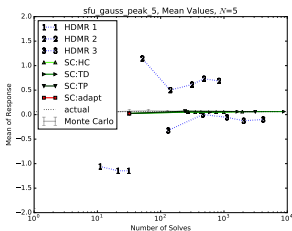
HDMR Results

Gauss Peak, $N = 3$



HDMR Results

Gauss Peak, $N = 5$



Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example**
 - Problem
 - Uncertainty
 - Results
- 5 Multiphysics Example
- 6 Conclusions

Neutronics Example

Introduction

More complicated than an analytic case

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

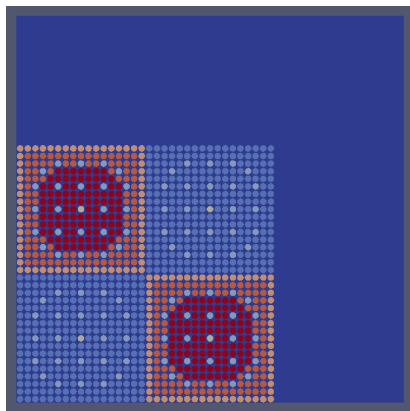
Quantities of interest

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

Neutronics Example

Geometry

Quarter-symmetric 4-assembly reactor core



Neutronics Example

Energy Groups

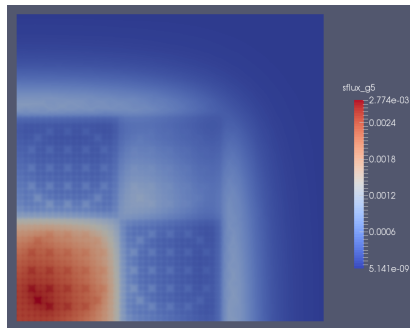
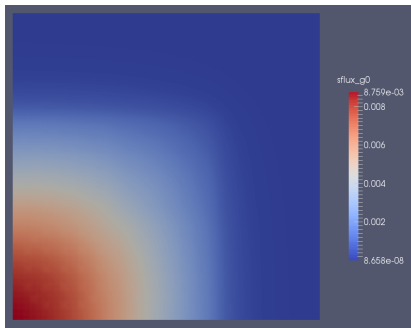
7 energy groups, 7 materials, 32 mesh elements per pin

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

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example**
 - Problem
 - Uncertainty**
 - Results
- 5 Multiphysics Example
- 6 Conclusions

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

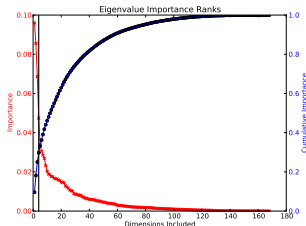
Rank	<i>k</i> -eigenvalue		Center Flux, $g = 1$		Center Flux, $g = 5$	
	Dimension	Importance	Dimension	Importance	Dimension	Importance
1	24	0.09606	24	0.07231	24	0.07032
2	9	0.08555	9	0.06472	9	0.06648
3	0	0.06861	0	0.04856	100	0.06474
4	17	0.04737	116	0.03472	13	0.03396
5	23	0.03415	17	0.03470	0	0.03092
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

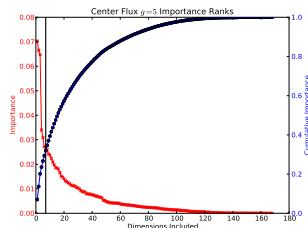
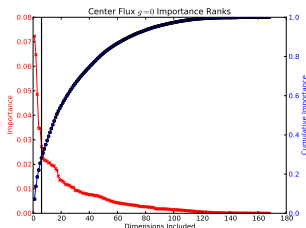


Neutronics Example

Uncertainty Correlations



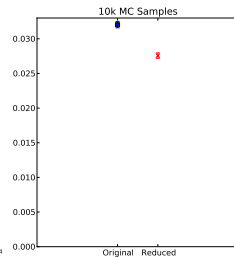
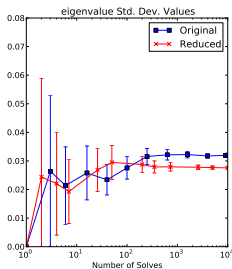
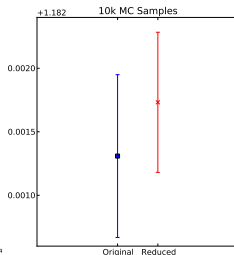
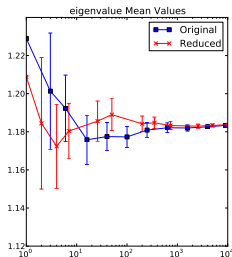
- ▶ Truncated after gradients
- ▶ Some importance lost
- ▶ Mean preserved well
- ▶ Std dev partially preserved



Neutronics Example

Uncertainty Correlations

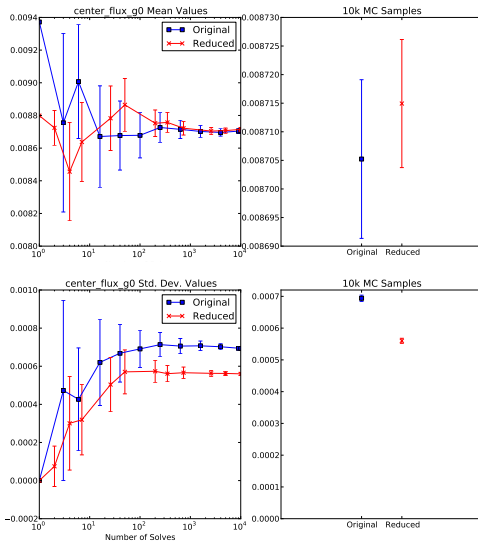
k -Eigenvalue



Neutronics Example

Uncertainty Correlations

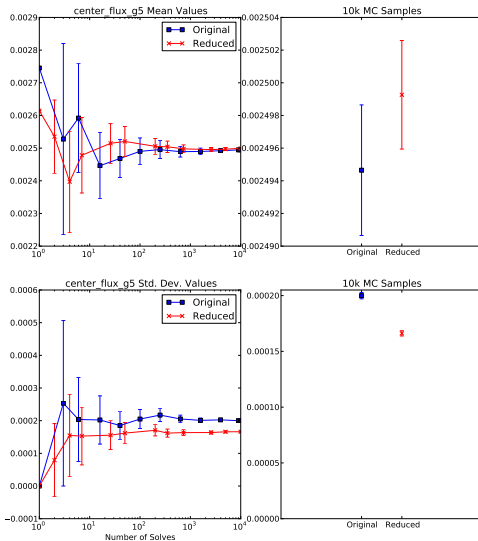
Center Flux, $g = 1$



Neutronics Example

Uncertainty Correlations

Center Flux, $g = 5$

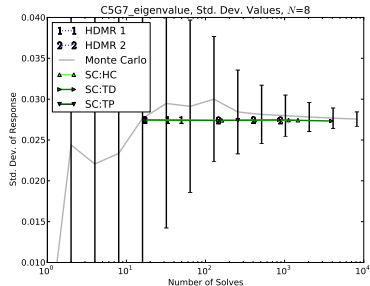
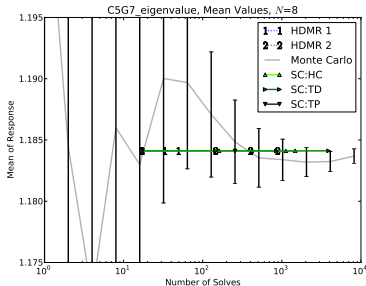


Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example**
 - Problem
 - Uncertainty
 - **Results**
- 5 Multiphysics Example
- 6 Conclusions

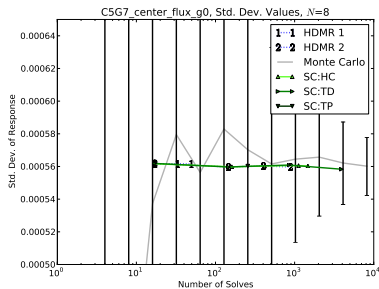
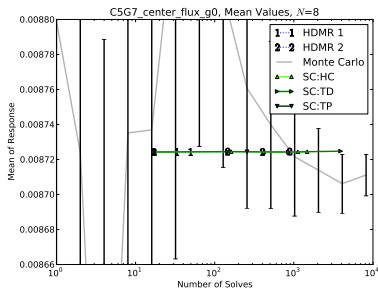
Neutronics Example

Results: k -eigenvalue



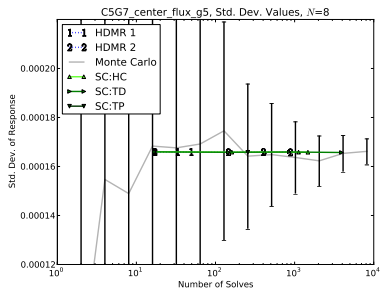
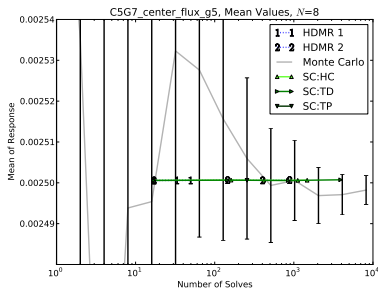
Neutronics Example

Results: Center Flux, $g = 1$



Neutronics Example

Results: Center Flux, $g = 5$



Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example**
 - Problem
 - Uncertainty
 - Results
- 6 Conclusions

Multiphysics Example

Introduction

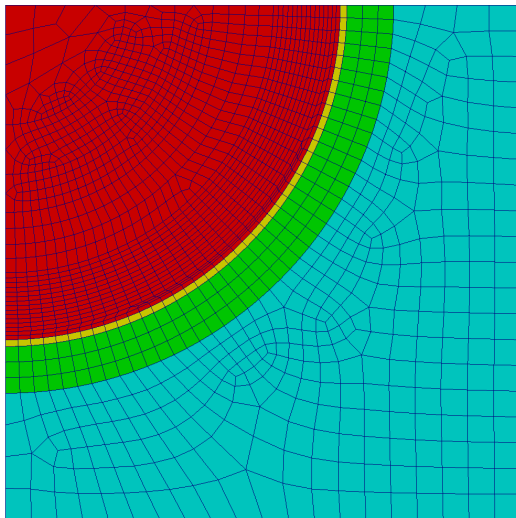
Coupled multiphysics problem

- ▶ 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

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example**
 - Problem
 - **Uncertainty**
 - Results
- 6 Conclusions

Multiphysics Example

Geometry and Uncertainty

Dimensions

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

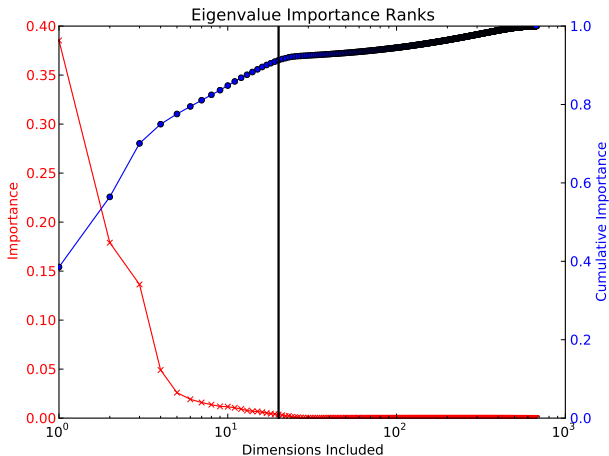
Response is k -eigenvalue

Uncertain inputs

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

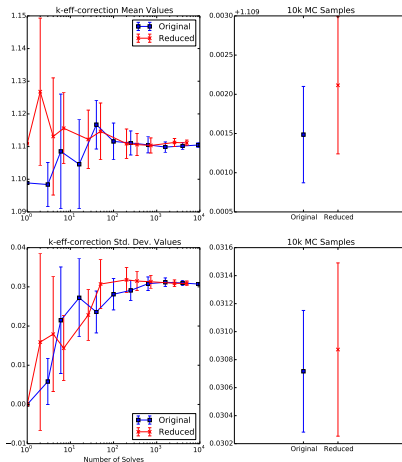
Multiphysics Example

Uncertainty Correlation



Multiphysics Example

Uncertainty Correlation

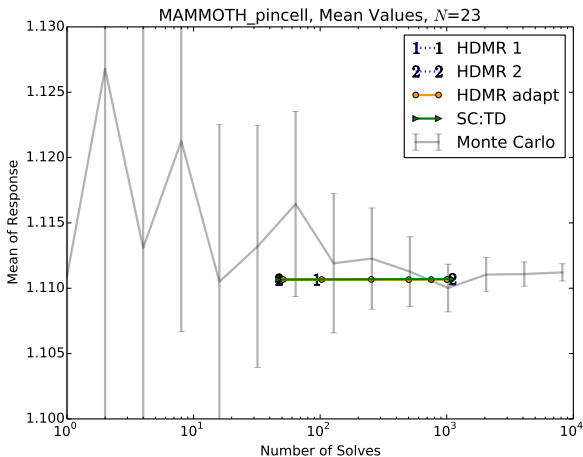


Outline

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example**
 - Problem
 - Uncertainty
 - **Results**
- 6 Conclusions

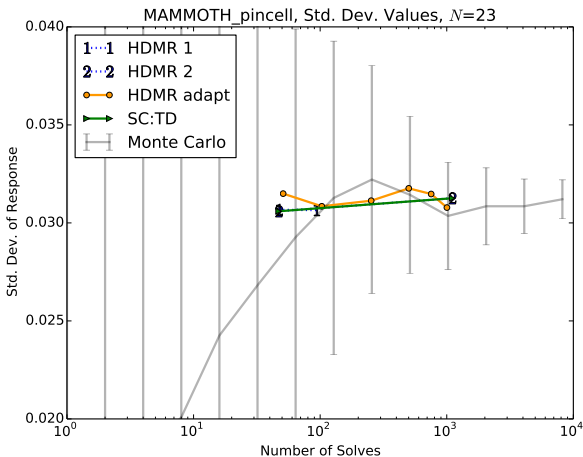
Multiphysics Example

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

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions**
 - Synopsis
 - Future Work

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

- 1 Introduction
- 2 SCgPC
- 3 HDMR
- 4 Neutronics Example
- 5 Multiphysics Example
- 6 Conclusions**
 - Synopsis
 - Future Work

Conclusions

Future Work

Quadrature Order

- ▶ “Floor” Quadrature
- ▶ Adaptive Quadrature

Adaptive: Impact Inertia

- ▶ Currently consider only neighbors
- ▶ Consider full history

Acknowledgments

Thanks!

UNM Faculty and Peers

- ▶ Drs. Prinja, Motamed, Olivera
- ▶ Mike Rising, Aaron Olson, Matt Gonzalez, Japan Patel

INL Staff, Post-Docs, and Interns

- ▶ Drs. Rabiti, Alfonsi, Cogliatti, Mandelli, Kinoshita
- ▶ CongJian Wang, Dan Maljovec

Funded through a Laboratory-Directed Research and Development opportunity at Idaho National Laboratory