

Sparse-Grid Stochastic Collocation Uncertainty Quantification Convergence for Multigroup Diffusion

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Supported by Idaho National Laboratory

American Nuclear Society 2014 Winter Meeting

Outline

Discussion Points

- 1 Motivation
- 2 Deterministic Problem
- 3 UQ Methodology
- 4 Results
- 5 Ongoing Work

Motivation

Uncertainty Quantification for Modular Numerical Systems

- Intrusive/Non-Intrusive
- Monte Carlo
 - Dimension Agnostic
 - Slow Convergence
- Stochastic Collocation
 - Improved Convergence*
 - Curse of Dimensionality
- Stochastic Collocation on Sparse Grids

Deterministic Problem

Low-Enrichment Nuclear Reactor

- Homogenized Multiplying Medium
- Steady State Operation

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 3 | 3 | 3 | 3 | 3 | 3 | 3 | 5 | 5 | 5 | 5 | 5 |
| 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 5 | 5 | 5 | 5 |
| 2 | 1 | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 5 | 5 | 5 |
| 2 | 1 | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 5 | 5 | 5 |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3 | 3 | 5 | 5 | 5 |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3 | 3 | 5 | 5 | 5 |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3 | 3 | 5 | 5 | 5 |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3 | 3 | 5 | 5 | 5 |
| 2 | 1 | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 5 | 5 | 5 |

Deterministic Problem

Neutronics

- Diffusion Approximation
- Multigroup, $G = 2$
- Neglect Upscatter
- $\chi(g = 1) = 1$
- Solved using JFNK (GMRES) in `trilinos`

Uncertainties:

- Aleatoric in interaction probability
- Epistemic in measurements of σ

Deterministic Problem

Two-Group, Two-Dimension, Diffusion Approximation

$$-\nabla \cdot (D_1(\bar{x}) \nabla \phi_1(\bar{x})) + \left(\Sigma_a^{(1)}(\bar{x}) + \Sigma_s^{(1 \rightarrow 2)}(\bar{x}) \right) \phi_1(\bar{x}) = \frac{1}{k(\phi)} \sum_{g'=1}^2 \nu_{g'} \Sigma_f^{(g')}(\bar{x}) \phi_{g'}(\bar{x})$$

$$-\nabla \cdot (D_2(\bar{x}) \nabla \phi_2(\bar{x})) + \Sigma_a^{(2)}(\bar{x}) \phi_2(\bar{x}) = \Sigma_s^{(1 \rightarrow 2)}(\bar{x}) \phi_1(\bar{x})$$

Boundary Conditions

$$-D \frac{\partial \phi^{\text{in}}}{\partial x_i} \Big|_{\partial D} = 0, \quad i = 1, 2, \quad x \in \partial_{\text{top}} D \cup \partial_{\text{right}} D$$

$$\frac{\partial \phi}{\partial x_i} \Big|_{\partial D} = 0, \quad i = 1, 2, \quad x \in \partial_{\text{left}} D \cup \partial_{\text{bottom}} D$$

Deterministic Problem

Benchmark

$$k = 1.00007605445$$

| Region | Group | D_g | $\Sigma_{a,g}$ | $\nu\Sigma_{f,g}$ | $\Sigma_s^{1,2}$ |
|--------|-------|----------|----------------|-------------------|------------------|
| 1 | 1 | 1.255 | 8.252e-3 | 4.602e-3 | 2.533e-2 |
| | 2 | 2.11e-1 | 1.003e-1 | 1.091e-1 | |
| 2 | 1 | 1.268 | 7.181e-3 | 4.609e-3 | 2.767e-2 |
| | 2 | 1.902e-1 | 7.047e-2 | 8.675e-2 | |
| 3 | 1 | 1.259 | 8.002e-3 | 4.663e-3 | 2.617e-2 |
| | 2 | 2.091e-1 | 8.344e-2 | 1.021e-1 | |
| 4 | 1 | 1.259 | 8.002e-3 | 4.663e-3 | 2.617e-2 |
| | 2 | 2.091e-1 | 7.3324e-2 | 1.021e-1 | |
| 5 | 1 | 1.257 | 6.034e-4 | 0 | 4.754e-2 |
| | 2 | 1.592e-1 | 1.911e-2 | 0 | |

Introduce 10% Uncertainty

Uncertainty Quantification

UQ Methods

- Analog Monte Carlo
- Stochastic Collocation on Sparse Grids
- Anisotropic Stochastic Collocation

Uncertainty space

$$k(D_g, \Sigma_c^g, \nu \Sigma_f^g, \Sigma_s^{1 \rightarrow 2}, \dots) \rightarrow u(Y) \equiv u(Y_1, Y_2, \dots, Y_N), Y \in \Gamma$$

Compare moments, $P(Y) = \prod_{n=1}^N \rho(Y_n)$

$$\mathbb{E}[u^r] \equiv \int_{\Omega} u(Y)^r P(Y) d\Omega$$

Uncertainty Quantification

Monte Carlo

$$\mathbb{E}[u^r] \approx \frac{1}{M} \sum_{m=1}^M u \left(Y^{(m)} \right)^r$$

Uncertainty Quantification

Stochastic Collocation using Lagrange Polynomials

$$u(Y) \approx u_{h,\eta,\Lambda(L)}(Y) = \sum_{k=0}^{\eta} u(Y^{(k)}) \mathcal{L}_k(Y)$$

$$\mathcal{L}_k(Y) = \prod_{n=1}^N \mathcal{L}_{k_n}(Y_n)$$

$$\mathcal{L}_{k_n}(Y_n) = \prod_{j=1}^i \frac{Y_n - Y_n^{(i)}}{Y_n^{(k_n)} - Y_n^{(i)}}$$

$$\mathbb{E}[u(Y)] \approx \mathbb{E}[u_h(Y)] = \sum_{k=1}^{\eta} w_k u_h(Y^{(k)})$$

Uncertainty Quantification

Stochastic Collocation: Index Set $\Lambda(L)$

■ Tensor Product:

$$\Lambda_{\text{TP}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \max_{1 \leq n \leq N} p_n \leq L \right\}, \eta = (L+1)^N$$

■ Total Degree:

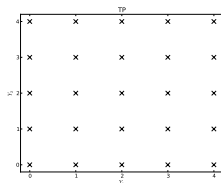
$$\Lambda_{\text{TD}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \sum_{n=1}^N p_n \leq L \right\}, \eta = \binom{L+N}{N}$$

■ Hyperbolic Cross:

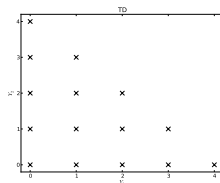
$$\Lambda_{\text{HC}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \prod_{n=1}^N p_n + 1 \leq L + 1 \right\}, \eta \leq (L+1)(1 + \log(L+1))^{N-1}$$

Uncertainty Quantification

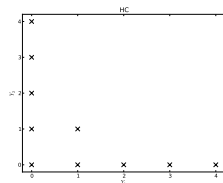
Stochastic Collocation: Index Set $\Lambda(L)$



(a) Tensor Product



(b) Total Degree



(c) Hyperbolic Cross

Figure : Index Set Examples: $N = 2, L = 4$

Uncertainty Quantification

Stochastic Collocation on Sparse Grids

$$u(Y) \approx \mathcal{S}_{N,\Lambda(L)}[u](Y) = \sum_{i \in \Lambda(L)} c(i) \bigotimes_{n=1}^N \mathcal{U}_{n,p(i_n)}[u](Y),$$

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

$$\bigotimes_{n=1}^N \mathcal{U}_{n,p(i_n)}[u](Y) \equiv \sum_{k_1=0}^{p(i_1)} \cdots \sum_{k_N=0}^{p(i_N)} u_h(Y^{(k_1)}, \dots, Y^{(k_N)}) \prod_{n=1}^N \mathcal{L}_{k_n}(Y_n),$$

$$= \sum_k^{\vec{p}(\vec{i})} u_h(Y^{(k)}) \mathcal{L}_k(Y),$$

Uncertainty Quantification

Stochastic Collocation on Sparse Grids

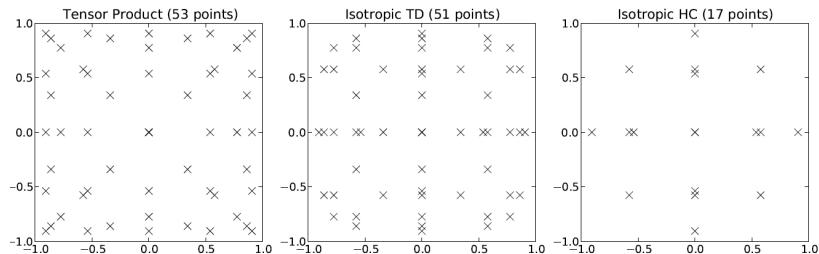


Figure : Sparse Grids, $N = 2$, $L = 4$, $p(i) = i$, Legendre points

Uncertainty Quantification

Stochastic Collocation on Sparse Grids

| N | L | TP | TD | | HC | |
|-----|-----|----------------|----------------|-----------|----------------|--------|
| | | $ \Lambda(L) $ | $ \Lambda(L) $ | η | $ \Lambda(L) $ | η |
| 3 | 4 | 125 | 35 | 165 | 16 | 31 |
| | 8 | 729 | 165 | 2,097 | 44 | 153 |
| | 16 | 4,913 | 969 | 41,857 | 113 | 513 |
| | 32 | 35,737 | 6,545 | 1,089,713 | 309 | 2,181 |
| 5 | 2 | 293 | 21 | 61 | 11 | 11 |
| | 4 | 3,125 | 126 | 781 | 31 | 71 |
| | 8 | 59,049 | 1,287 | 28,553 | 111 | 481 |

Table : Index Set and Collocation Size Comparison

Uncertainty Quantification

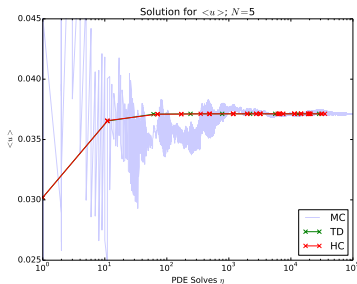
Anisotropic Sparse Grids

$$\tilde{\Lambda}_{\text{TD}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \sum_{n=1}^N \alpha_n p_n \leq |\vec{\alpha}|_1 L \right\}$$

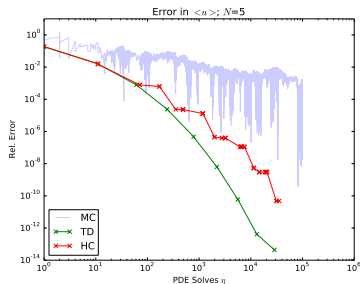
$$\tilde{\Lambda}_{\text{HC}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \prod_{n=1}^N (p_n + 1)^{\alpha_n} \leq (L + 1)^{|\vec{\alpha}|_1} \right\}$$

Sample Results

Attenuation, $u(Y) = \prod_{n=1}^N \exp(-Y_n)$ ($N = 5$)



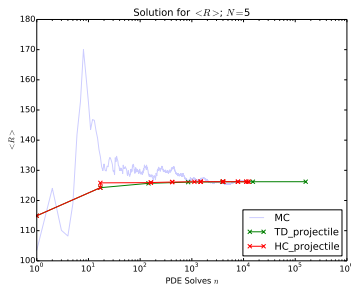
(a) $\langle u \rangle$ Values



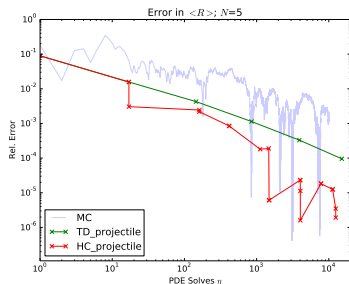
(b) Error in $\langle u \rangle$

Sample Results

Projectile with Drag ($N = 8$)

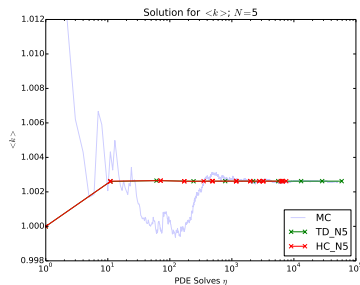
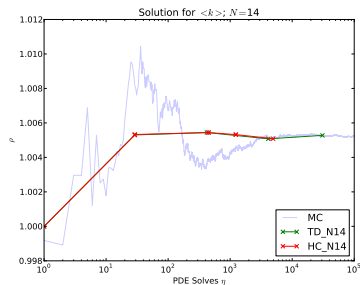


(a) $\langle R \rangle$ Values



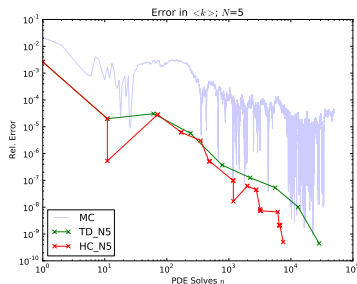
(b) Error in $\langle R \rangle$

Results

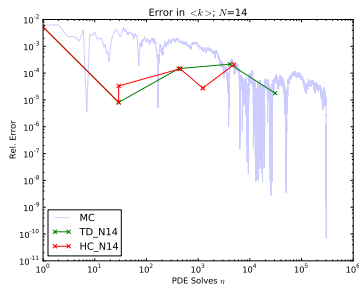
< k > Values(a) < k >, $N=5$ (b) < k >, $N=14$

Results

$\langle k \rangle$ Convergence

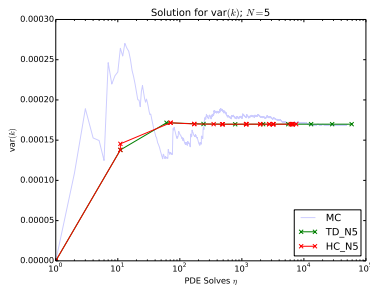
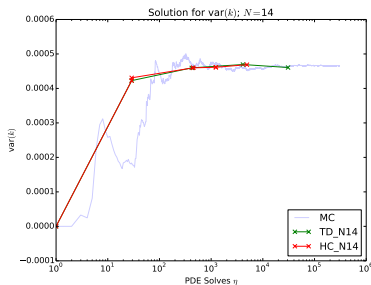


(a) Error in $\langle k \rangle$, $N=5$

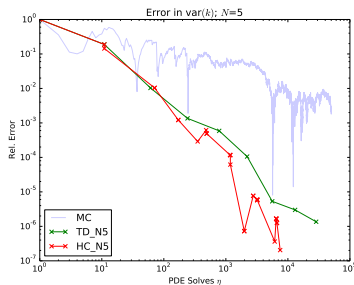
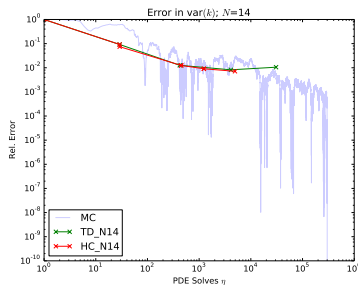


(b) Error in $\langle k \rangle$, $N=14$

Results

 $\text{var}(k)$ Values(a) $\text{var}(k)$, $N=5$ (b) $\text{var}(k)$, $N=14$

Results

var(k) Convergence(a) Error in var(k), $N=5$ (b) Error in var(k), $N=14$

Continuing Efforts

- Increased Material Complexity
- Adaptive Anisotropic Grids
- HDMR
- Multiphysics (Neutronics, Thermal Hydraulics, Materials)

