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

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Outline

Discussion Points

Motivation

Uncertainty Quantification for Modular Numerical Systems

- Uncertain inputs $\rightarrow$ Distribution of QoI
- 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
- Quantity of Interest: k-eigenvalue

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
3	3	3	3	3	3	3	4	5	5	5
2	1	1	1	1	2	2	3	3	5	5
2	1	1	1	1	2	2	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
2	1	1	1	1	2	2	3	3	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

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Deterministic Problem

Two-Group, Two-Dimension, Diffusion Approximation

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

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

Boundary Conditions

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

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

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

Uncertainty space

$$k(D_g^{(m)}, \Sigma_{g,c}^{(m)}, \nu\Sigma_{g,f}^{(m)}, \Sigma_{g'\to g,s}^{(m)}, \ldots) \to u(Y) \equiv u(Y_1, Y_2, \ldots, Y_N),$$

$$Y \in \Omega, \qquad \text{span}(Y) = \Omega.$$

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

- Randomly sample $Y^{(m)} \in \Omega$
- Compute statistics

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

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Uncertainty Quantification

Stochastic Collocation using Lagrange Polynomials

Interpolate u using Lagrange polynomials at points $Y^{(k)}$

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

$$\mathcal{L}_k(Y) = \prod_{n=1}^{N} \mathcal{L}_{k_n}(Y_n), \qquad \mathcal{L}_{k_n}(Y_n) = \prod_{j=1}^{i} \frac{Y_n - Y_n^{(i)}}{Y_n^{(k_n)} - Y_n^{(i)}}$$

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

Uncertainty Quantification

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

- Tensor Product:

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

- Total Degree:

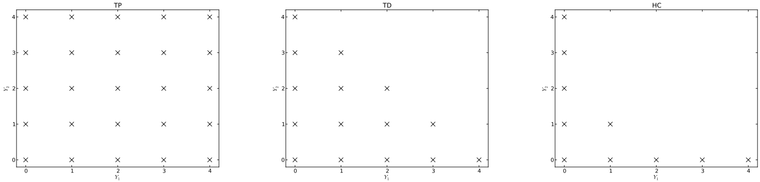
$$\Lambda_{\mathrm{TD}}(L) = \left\{\bar{p} = [p_1, ..., p_N] : \sum_{n=1}^{N} p_n \leq L\right\}, \eta = \binom{L+N}{N}$$

- Hyperbolic Cross:

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

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

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

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

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

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

Uncertainty Quantification

Stochastic Collocation on Sparse Grids

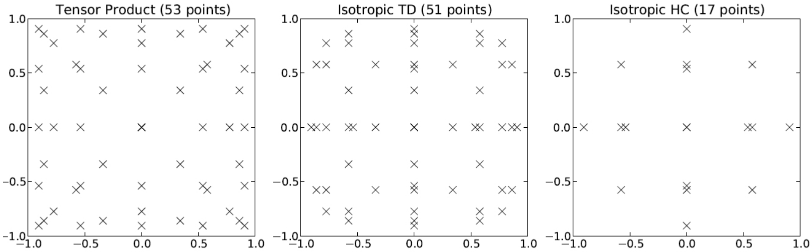


Figure : Sparse Grids, $N = 2$, $L = 4$, $p(i) = i$, Legendre points

Uncertainty Quantification

Stochastic Collocation on Sparse Grids

		TP	TD		HC	
N	L	$\lvert\Lambda(L)\rvert$	$\lvert\Lambda(L)\rvert$	η	$\lvert\Lambda(L)\rvert$	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

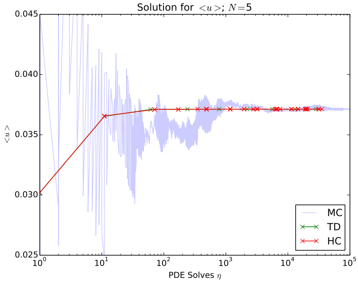
Anisotropic Sparse Grids

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

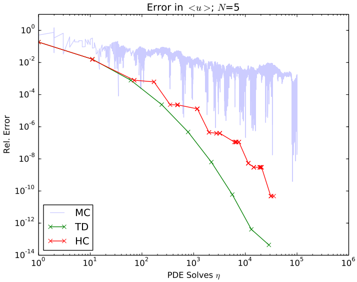
$$\tilde{\Lambda}_{HC}(L) = \left\{ \bar{p} = [p_1, ..., p_N] : \prod_{n=1}^{N} (p_n + 1)^{\alpha_n} \leq (L+1)^{|\vec{\alpha}|_1} \right\}$$

Sample Results

Attenuation, $u(Y) = \prod_n^N \exp(-Y_n)$ $(N = 5)$



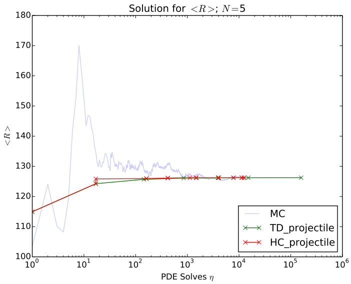
(a) $< u >$ Values



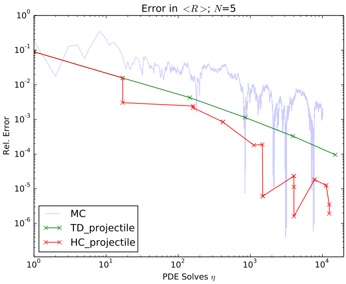
(b) Error in $< u >$

Sample Results

Projectile with Drag ($N = 8$)



(a) $< R >$ Values



(b) Error in $< R >$

Results

Cases

$N = 5$

- $Y = \left\{\Sigma_{2,f}^{(1)}, \Sigma_{2,c}^{(1)}, \Sigma_{2,f}^{(4)}, \Sigma_{2,c}^{(4)}, D_2^{(5)}\right\}$

$N = 14$

- $Y = \left\{\Sigma_{2,f}^{(1)}, \Sigma_{2,c}^{(1)}, D_2^{(1)}, \Sigma_{2,f}^{(2)}, \Sigma_{2,c}^{(2)}, D_2^{(2)}, \Sigma_{2,f}^{(3)}, \Sigma_{2,c}^{(3)}, D_2^{(3)}, \Sigma_{2,f}^{(4)}, \Sigma_{2,c}^{(4)}, D_2^{(4)}, \Sigma_{2,c}^{(5)}, D_2^{(5)}\right\}$

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
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1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
2	1	1	1	1	2	2	3	3	5	5

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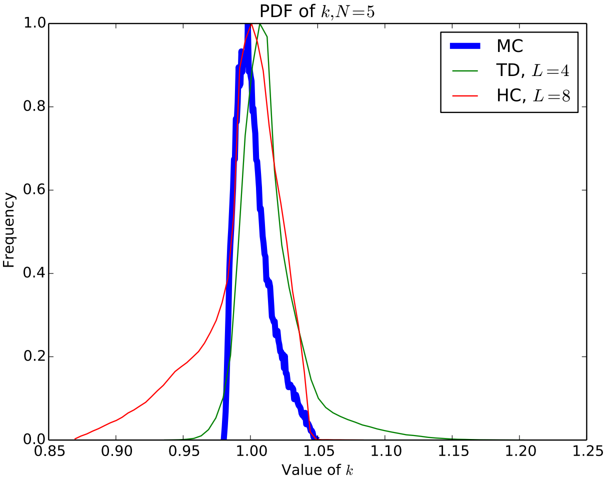
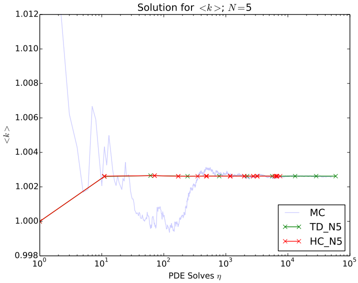
Results
PDF

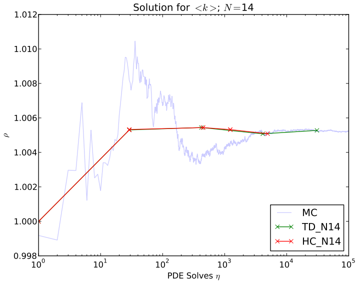

PDF of $k, N=5$
Frequency
Value of k
MC
TD, $L=4$
HC, $L=8$
0.0
0.2
0.4
0.6
0.8
1.0
0.85
0.90
0.95
1.00
1.05
1.10
1.15
1.20
1.25

Results

$< k >$ Values



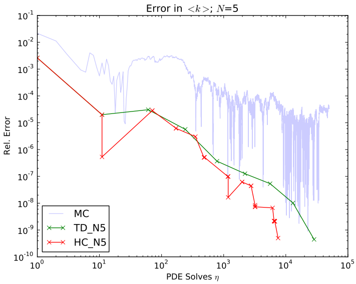
(a) $< k >$, N=5



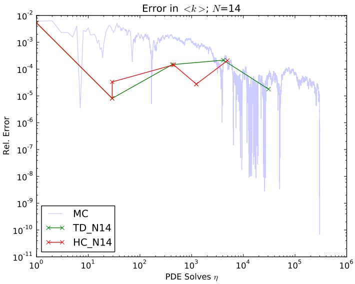
(b) $< k >$, N=14

Results

$< k >$ Convergence



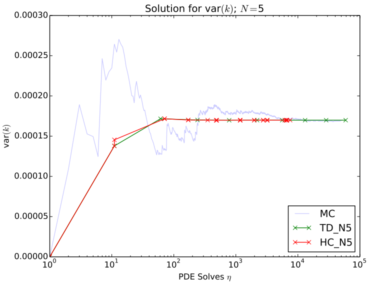
(a) Error in $< k >$, N=5



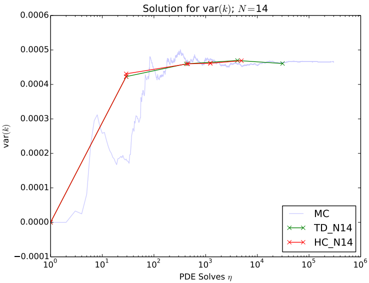
(b) Error in $< k >$, N=14

Results

var(k) Values



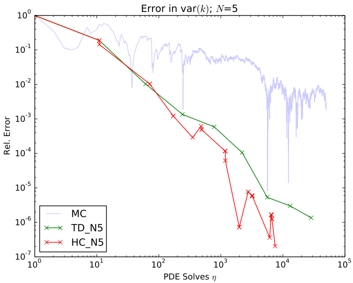
(a) var(k), N=5



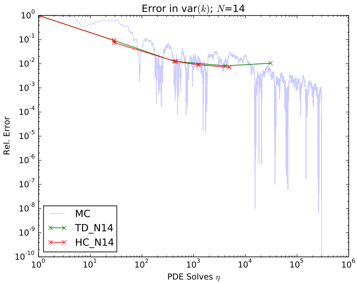
(b) var(k), N=14

Results

var(k) Convergence



(a) Error in var(k), N=5



(b) Error in var(k), N=14

Continuing Efforts

- Increased Material Complexity
- Polynomial Chaos Expansion
- Adaptive Anisotropic Grids
- High-Density Model Reduction (HDMR)
- Multiphysics (Neutronics, Thermal Hydraulics, Materials)