Sparse-Grid Stochastic Collocation Uncertainty Quantification Convergence for Multigroup Diffusion

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INTRODUCTION

Advanced methods in uncertainty quantification for numerical models in computational physics [1] [6] are gaining widespread acceptance in nuclear modeling [5] [8]. However, little attention has been paid to the convergence rates of these methods in stochastic space. We demonstrate the efficiency of sparse-grid stochastic collocation [7] in comparison with analog Monte Carlo for uncertainty quantification through convergence studies.

The physical system we consider is a two-dimensional quarter-core reactor, consisting of 5 materials distributed in 121 regions (see Fig. 1). We solve the two-group neutron diffusion criticality approximation

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

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

We apply vacuum boundaries on the top and right, and reflecting boundaries on the bottom and left. The criticality eigenvalue and quantity of interest $k(\phi)$ is given by

$$k(\phi)=\sum_{g=1}^{2}\iint_D \frac{\nu\Sigma_f^{(g)}\phi_g(\bar{x})}{\left(-\nabla\cdot D_g\nabla+\Sigma_r^{(g)}\right)\phi_g(\bar{x})}\,d\bar{x}. \quad (3)$$

The material properties are shown in Table I, and the domain $\Omega=[0,200\text{ cm}]^2$. The reference value k=1.00007605445.

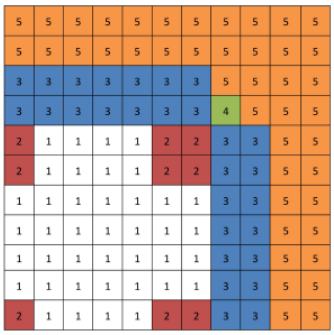

Fig. 1: Core Geometry

The material cross sections, neutron multiplication factors, and diffusion coefficients are potential uncertain input parameters. We introduce uniformly-distributed uncertainty within 10% of the reference values. The uncertain distributions make up the uncertainty space $\Gamma\subset\mathbb{R}^N$, where N is the number of uncertain parameters. We consider the input parameter uncertainties to be independently distributed.

Mat.	g	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	

TABLE I: Reference Material Properties for Benchmark Core

METHODS

We solve our system of equations by imposing a mesh grid on the physical domain using the local and global particle-conserving finite volume method. We solve the system of equations nonlinearly with the criticality eigenvalue, using Jacobian-free Newton-Krylov methods. We use the GMRES algorithm in the `trilinos` solver package from Sandia National Laboratory [4].

Our primary interest in this study is evaluating the practicality of using stochastic collocation on sparse grids [2] [3] [7] to quantify uncertainty in diffusion problems. We use analog Monte Carlo uncertainty quantification as a benchmark, and a high-resolution solution for the moments of k in stochastic space as a reference solution. We compare Monte Carlo and stochastic collocation solutions to the reference as a function of the number of transport solves to contrast convergence rates.

In stochastic solves, we treat the deterministic transport solver non-intrusively as a functional of the uncertain input parameters. To avoid confusion in labels, we will represent $k(Y)$ by a more generic $u(Y)$, where $Y\in\Gamma$ is the vector of uncertain inputs. In Monte Carlo uncertainty quantification, the uncertain vector Y is randomly sampled M times, and moments are derived from the solution realizations. For example,

$$\mathbb{E}[u(Y)]=\int_\Gamma u(Y)\rho(Y)dY\approx\frac{1}{M}\sum_{m=1}^{M}u(Y_m), \quad (4)$$

$$\mathbb{E}[u(Y)^2]=\int_\Gamma u(Y)^2\rho(Y)dY\approx\frac{1}{M}\sum_{m=1}^{M}u(Y_m)^2, \quad (5)$$

where each Y_m is a single realization randomly sampled from the domain of Y.

In stochastic collocation for sparse grids, we approximate $u(Y)$ as the sum of the product of u evaluated at η collocated points and multidimensional Lagrangian polynomials. Using

k as the quadrature index,

$$u(Y) \approx u_{h,\eta,\Lambda(L)}(Y) = \sum_{k=0}^{\eta} u(Y^{(k)}) \mathcal{L}_k(Y), \tag{6}$$

$$\mathcal{L}_k(Y) = \prod_{n=1}^{N} \mathcal{L}_{k_n}(Y_n), \tag{7}$$

$$\mathcal{L}_{k_n}(Y_n) = \prod_{j=1}^{i} \frac{Y_n - Y_n^{(i)}}{Y_n^{(k_n)} - Y_n^{(i)}}, \tag{8}$$

$$\mathbb{E}[u(Y)] \approx \mathbb{E}[u_h(Y)] = \sum_{k=1}^{\eta} w_k \, u_h\Big(Y^{(k)}\Big), \tag{9}$$

where $u_h(Y)$ is the spatially-discretized PDE solution, and $Y^{(k)} = [Y^{(k_1)}, \cdots, Y^{(k_N)}]$ are realizations of Y chosen at quadrature points $Y^{(k)}$ with corresponding weights w_k. We use Gauss-Legendre quadrature to obtain collocation points and weights. The order of the quadrature is obtained based on polynomial expansion orders from an index set $\Lambda(L)$. For a single uncertain parameter ($N = 1$) and a fourth-order polynomial approximation ($L = 4$), Λ includes all polynomial orders from 0 to 4 ($\Lambda = [0, 1, 2, 3, 4]$). Each index point $p \in \Lambda$ corresponds to a polynomial expansion moment of order p.

There are several methods to determine multivariate Λ. The most naive case is a tensor product $\Lambda_{\text{TP}}(L)$ of polynomial expansion orders,

$$\Lambda_{\text{TP}}(L) = \Big\{\bar{p} = [p_1, ..., p_N] : \max_{1 \le n \le N} p_n \le L\Big\}. \tag{10}$$

Other index sets with less cardinality can be employed to reduce the number of collocation points and counteract the Λ_{TP} curse of dimensionality. We consider the *total degree* (Λ_{TD}) set, which is ideal for quantities that are analytic in stochastic space; and the *hyberbolic cross* (Λ_{HC}) index set for quantities that have finite smoothness in stochastic space,

$$\Lambda_{\text{TD}}(L) = \Big\{\bar{p} = [p_1, ..., p_N] : \sum_{n=1}^{N} p_n \le L\Big\}, \tag{11}$$

$$\Lambda_{\text{HC}}(L) = \Big\{\bar{p} = [p_1, ..., p_N] : \prod_{n=1}^{N} p_n + 1 \le L + 1\Big\}. \tag{12}$$

The collocation points used in the Lagrange polynomial expansion are obtained based on the index set chosen. This provides the isotropic sparse grid approximation

$$k(Y) \approx \mathcal{S}_{N,\Lambda(L)}[k](Y) = \sum_{\boldsymbol{i} \in \Lambda(L)} c(\boldsymbol{i}) \bigotimes_{n=1}^{N} \mathcal{U}_{n,p(i_n)}[u](Y), \tag{13}$$

$$c(\boldsymbol{i}) = \sum_{\substack{\boldsymbol{j} = \{0,1\}^N, \\ \boldsymbol{i}+\boldsymbol{j} \in \Lambda(L)}} (-1)^{|\boldsymbol{j}|_1}, \tag{14}$$

$$\bigotimes_{n=1}^{N} \mathcal{U}_{n,p(i_n)}[u](Y) \equiv \sum_{k}^{p(\vec{i})} u_h\Big(Y^{(k)}\Big) \mathcal{L}_k(Y), \tag{15}$$

where we use $p(i) = i$ as the *quadrature rule* used to obtain the number of quadrature points for a polynomial expansion order. The reduction in collocation points due to sparse grids improves with the number of input parameters N and the expansion order L.

Anisotropic Sparse Grids

In many cases, the sensitivity of the stochastic solution to one uncertain dimension is less than another. For example, we heuristically expect the sensitivity of the k-eigenvalue to the reflecting material (material 5) diffusion coefficient to be much less than the sensitivity to the fission cross section in the main fissile material (material 1). We can leverage the varying sensitivity by introducing importance parameters $\vec{\alpha} = [\alpha_1, \cdots, \alpha_N]$ that parametrize the sensitivity of the stochastic solution to each dimension. Using the one-norm $\left|\vec{\alpha}\right|_1 \equiv \frac{1}{N} \sum_{n=1}^{N} \alpha_n$, these weight parameters adjust the index set rules $\Lambda(L)$ for total degree and hyperbolic cross as

$$\tilde{\Lambda}_{\text{TD}}(L) = \Big\{\bar{p} = [p_1, ..., p_N] : \sum_{n=1}^{N} \alpha_n p_n \le \left|\vec{\alpha}\right|_1 L\Big\}, \tag{16}$$

$$\tilde{\Lambda}_{\text{HC}}(L) = \Big\{\bar{p} = [p_1, ..., p_N] : \prod_{n=1}^{N} (p_n + 1)^{\alpha_n} \le (L+1)^{|\vec{\alpha}|_1}\Big\}. \tag{17}$$

In this formulation, greater values of α_n result in less quadrature points for uncertain input Y_n. Smaller values of α_n are assigned to more sensitive dimensions to prioritize collocation points.

RESULTS

Material	Property	Distribution
Material 1	$\nu\Sigma_{2,f}$	$\mathcal{U}(0.0981, 0.1201)$
Material 1	$\Sigma_{2,c}$	$\mathcal{U}(0.0499, 0.0609)$
Material 4	$\nu\Sigma_{2,f}$	$\mathcal{U}(0.0921, 0.1121)$
Material 4	$\Sigma_{2,c}$	$\mathcal{U}(0.03732, 0.04552)$
Material 5	D_2	$\mathcal{U}(0.1432, 0.1752)$

TABLE II: Uncertain Input Parameters

We obtain the error in the moments r of the quantity of interest $k(Y) = u(Y)$, given by

$$\epsilon_h^{(r)} = \frac{|\mathbb{E}[u_h^{(r)}] - \mathbb{E}[u_{\text{ref}}^{(r)}]|}{\mathbb{E}[u_{\text{ref}}^{(r)}]}, \tag{18}$$

$$\mathbb{E}[u_h^{(r)}] = \mathbb{E}[S_{N,\Lambda_{\text{TD}}(L)}[u_h](Y)^{(r)}] = \sum_{k=1}^{\eta} w_k \, u_h^{(r)}\Big(Y^{(k)}\Big). \tag{19}$$

Figs. 2-7 show the comparison of Monte Carlo convergence to stochastic collocation for $N = 1, 3, 5$ where N is the number of uncertain parameters. Both total degree (TD) and hyperbolic cross (HC) index sets have been included for $N > 1$ (they are indistinguishable for $N = 1$). Additionally, we include two low-anisotropy anisotropic grids.

Because of the regularity of $k(Y) = u(Y)$, the total degree index set is as cost-effective as the hyperbolic cross index set. For a less regular stochastic solution, we expect hyperbolic cross would be more efficient. We also expect the convergence rate to diminish with increasing N, and that trend can be seen in the figures for the mean and variance of $k(Y)$. Both the magnitude of the error as well as the convergence rate of stochastic

collocation outperforms Monte Carlo for any number of runs. In addition, heuristic selection of importance weighting improved the accuracy of sparse grid methods by approximately half an order of magnitude.

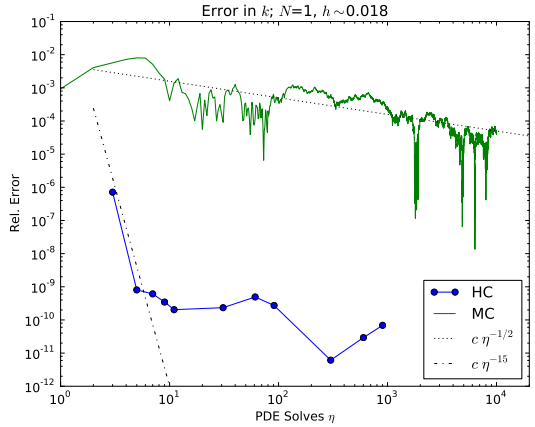

Fig. 2: $N = 1$, Mean

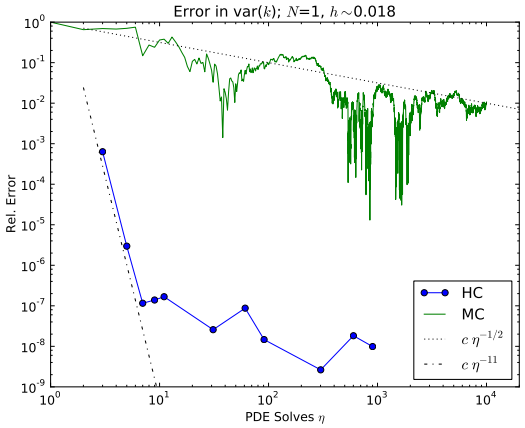

Fig. 3: $N = 1$, Variance

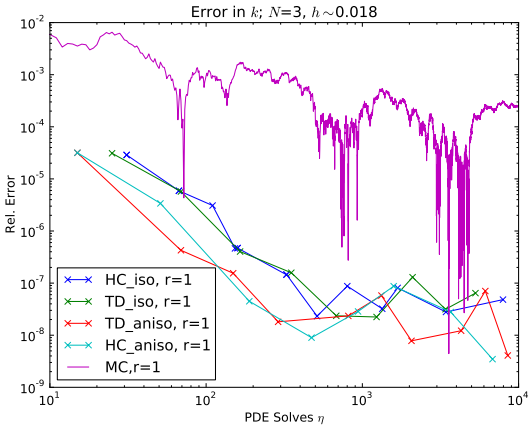

Fig. 4: $N = 3$, Mean

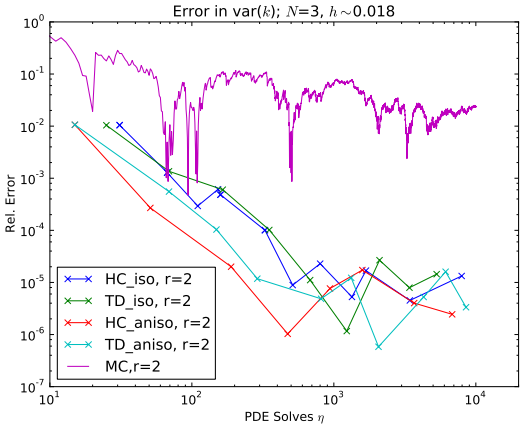

Fig. 5: $N = 3$, Variance

scheme with 8-8-4-4-1 to show worst-case effects of including poor importance weights. The results are compared in Figs. 8 and 9 for the mean and variance.

Anisotropic Sparse Grid

Because of the heuristic nature of anisotropy importance weights, we present here several weight choices and the effect on absolute error and convergence. We consider four cases along with Monte Carlo and isotropic sparse grids. Each case is labeled by its importance weights in order of the input parameters listed in Table II. The choice of weights is informed by considering the convergence rate of each individual parameter alone with increasing quadrature order. We observed material 1 cross sections to converge slowly, while the material 5 diffusion coefficient converges quickly. We choose the sample cases 1-1-2-2-4 and 1-1-4-4-8 to put increasing weight on the material 1 cross sections and remove weight from the material 5 diffusion coefficient. In addition, we choose the case 1-1-2-1-1 as an example of a somewhat arbitrary choice of coefficients. Lastly, we intentionally choose a poor weighting

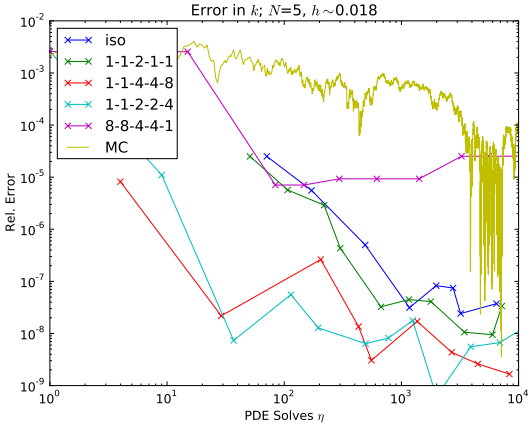

Fig. 8: Anisotropic, Mean

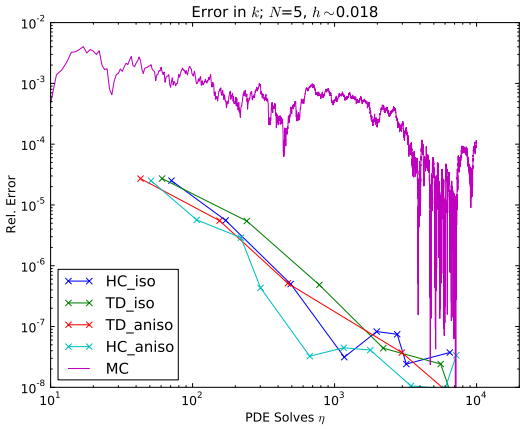

Fig. 6: $N = 5$, Mean

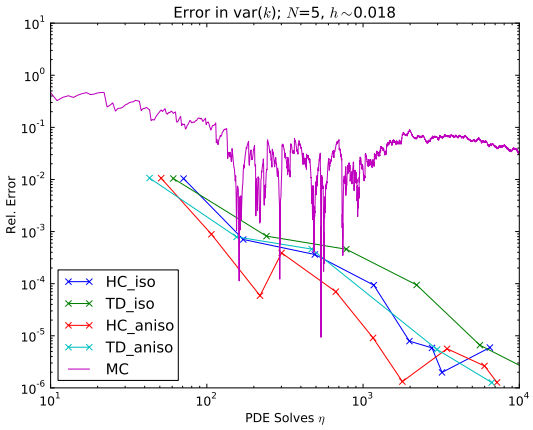

Fig. 7: $N = 5$, Variance

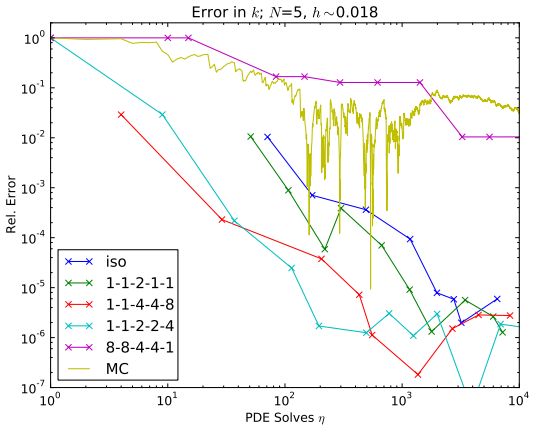

Fig. 9: Anisotropic, Variance

DISCUSSION

We make a few considerations in analyzing our results. First, there is a noticeable plateau in error convergence in many of the stochastic collocation plots. This seems to be an artifact of the algorithm, which uses an iterative tolerance of $\Delta k < 1 \times 10^{-6}$. Because the deterministic solver is only accurate to 6 orders of magnitude, the accuracy of the stochastic solver is limited by this value. We expect reducing the deterministic tolerance to result in further possible convergence in stochastic space.

Additionally, the number of PDE solves for stochastic collocation is determined based on the maximum expansion level L. For higher N, increasing L by only one value increases the number of PDE solves much more than increasing L by one for small N. As a result, there are few data points to power fit for $N = 5$, and the plateau just mentioned around $\epsilon = 10^{-8}$ is more difficult to distinguish from standard convergence. Resolving the issues leading to the plateau should also resolve this difficulty in fitting points.

We can see the possible benefit and harm of applying importance weighting to an anisotropic grid in Figs. 8 and 9. Any application of anisotropic sparse grids in line with our heuristic assessment significantly improves the magnitude of error for a given number of PDE solves. Even the arbitrarily-chosen 1-1-2-1-1 shows improvements over standard isotropic HC. We note, however, that the convergence of 1-1-2-2-4 is quite similar to 1-1-4-4-8. This suggests that with 1-1-2-2-4 we have achieved an optimum efficiency that isn't improved with further anisotropy. However, the anisotropy intentionally chosen poorly shows much worse convergence than the isotropic case, and for the variance is on par with Monte Carlo. Given these limitations, it is clear that for the uncertain spaces presented, stochastic collocation shows much better convergence and magnitude of error for the same cost when compared with Monte Carlo.

REFERENCES

1. Ivo Babuska, Fabio Nobile, and Raul Tempone. A Stochastic Collocation Method for Elliptic Partial Differential Equations with Random Input Data. *SIAM Journal on Numerical Analysis*, 45, 2007.
2. Voker Barthelmann, Erich Novak, and Klaus Ritter. High dimensional polynomial interpolation on sparse grids. *Advances in Computational Mathematics*, 12, 2000.
3. Hans-Joachim Bungartz and Michael Griebel. Sparse Grids. *Acta Numerica*, 13, 2004.
4. Michael Heroux et. al. An Overview of Trilinos. Technical Report SAND2003-2927, Sandia National Laboratories, 2003.
5. E. D. Fichtl and A. K. Prinja. The Stochastic Collocation Method for Radiation Transport in Random Media. *J. Quantitative Spectroscopy & Radiative Transfer*, 12, 2011.
6. O. P. Le Maître and O. M. Knio. *Spectral Methods for Uncertainty Quantification With Applications to Computational Fluid Dynamics*. Springer, 1st edition, 2010.
7. Nobile, Tempone, and Webster. A Sparse Grid Stochastic Collocation Method for Partial Differential Equations with Random Input Data. *SIAM Journal on Numerical Analysis*, 46, 2008.
8. M.E. Rising, A.K. Prinja, and P. Talou. Prompt Fission Neutron Spectrum Uncertainty Propagation Using Polynomial Chaos Expansion. *Nucl. Sci. Eng.*, 175, 2013.