Adaptive 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, 2] continue to gain acceptance in nuclear modeling [3, 4]. Previously, the efficiency of sparse-grid stochasatic collocation in comparison with Monte Carlo for uncertainty quantification through convergence studies was demonstrated [5]. An adaptive method for anisotropic sparse grid collocation and its convergence compared to previous efforts is considered.

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

$$-\boldsymbol{\nabla}\cdot(D_1(\bar{x})\boldsymbol{\nabla}\phi_1(\bar{x}))+\left(\Sigma_a^{(1)}(\bar{x})+\Sigma_s^{(1\to2)}(\bar{x})\right)\phi_1(\bar{x}) = \frac{1}{k(\phi)}\sum_{g'=1}^{2}\nu_{g'}\Sigma_f^{(g')}(\bar{x})\phi_{g'}(\bar{x}), \quad (1)$$

$$-\boldsymbol{\nabla}\cdot(D_2(\bar{x})\boldsymbol{\nabla}\phi_2(\bar{x}))+\Sigma_a^{(2)}(\bar{x})\phi_2(\bar{x}) = \Sigma_s^{(1\to2)}(\bar{x})\phi_1(\bar{x}). \quad (2)$$

Vacuum boundaries are applied 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 is $[0, 200\text{ cm}]^2$. The reference value k=1.000076.

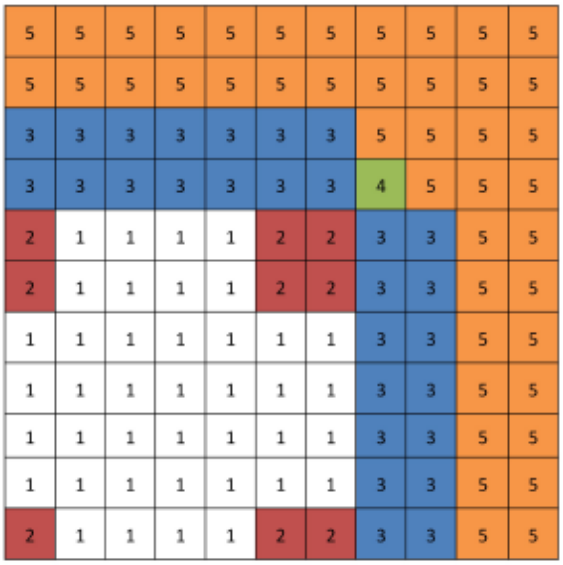

Fig. 1: Core Geometry

TABLE I: Ref. Material Properties for Benchmark Core

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	

The material cross sections, neutron multiplication factors, and diffusion coefficients are potential sources of uncertainty. Uniformly-distributed uncertainty within 5% of the reference values is introduced for material properties. The distribtion of the uncertain parameters make up the uncertainty space $\Gamma\subset\mathbb{R}^N$, where N is the number of uncertain parameters. The input parameter uncertainties are independently distributed.

METHODS

The system of equations is solved by imposing a mesh grid on the physical domain using the local and global particle-conserving finite volume method. They are solved nonlinearly with the criticality eigenvalue, using Jacobian-free Newton-Krylov methods. We use the GMRES algorithm in the `trilinos` solver package in a finite-volume code developed by the author.

Developing an adaptive algorithm for uncertainty quantification builds on the sparse grid formulation used previously [5] and analysis of variance [3]. The k-eigenvalue are represented as a function of input parameters as $u(Y)$. The generalized polynomial chaos expansion is given by

$$u(Y)\approx u_h(Y)=\sum_{k=0}^{\eta}c_k\Phi_k(Y), \quad (4)$$

$$\Phi_k(Y)=\prod_{n=1}^{N}\phi_{k_n}(Y_n), \quad (5)$$

where $u_h(Y)$ is the spatially-discretized PDE solution, and $\phi_{k_n}(y_n)$ are Askey polynomials of order k_n that are orthonormal with respect to the probability distribution function $\rho_n(y_n)$ over the probability space Ω. Using orthonormality, an expression is obtained for the expansion coefficients

c_k as

$$c_k = \langle u(Y)\Phi(Y)\rangle = \int_\Omega u(Y)\Phi(Y)\rho(Y)dY. \tag{6}$$

Because Y are uniformly distributed, Gauss-Legendre quadratures are used to obtain collocation points and weights to evaluate c_k.

Previously static methods were identified to determine the index set Λ [5]. An adaptive method is proposed based on analysis of variance to construct the index set, following a pattern similar to the algorithm in [3]. A property of the gPC expansion is the method of calculating variance, namely

$$\sigma^2 = \mathbb{E}[u_h(Y)^2] - \mathbb{E}[u_h(Y)]^2 = \sum_{k\in\Lambda} c_k^2 - c_0^2. \tag{7}$$

The partial percent variance η due to each polynomial is

$$\eta_k \equiv \frac{c_k^2}{\sigma^2}. \tag{8}$$

The adaptive method is initialized by evaluating the gPC to a first-order polynomial expansion in each dimension. The algorithm then continues by searching the polynomial indices that may be added to the index set, which is dependent on the existing polynomials. The admissibility condition is

$$k - e_j \in \Lambda \text{ for } 1 \le j \le N, k_j > 1, \tag{9}$$

where e_j is a unit vector in the direction j and k_j is the j-th entry in k. The estimated partial variance for a prospective polynomial is the product of immediate subset polynomials,

$$\tilde{\eta}_k = \prod_{j=1,k_j>0}^{N} \eta_{k_j - e_j}. \tag{10}$$

The adaptive algorithm chooses the prospective polynomial with the largest estimated partial variance to add to the index set, and the algorithm continues until estimated remaining variance is less than tolerance.

RESULTS

TABLE II: Uncertain Input Parameters

Material	Property	Distribution
Material 1	$\nu\Sigma_{f,2}$	$\mathcal{U}(0.1036, 0.1146)$
Material 1	$\Sigma_{c,2}$	$\mathcal{U}(0.0526, 0.0582)$
Material 4	$\nu\Sigma_{f,2}$	$\mathcal{U}(0.0970, 0.1072)$
Material 4	$\Sigma_{c,2}$	$\mathcal{U}(0.03935, 0.04349)$
Material 5	D_2	$\mathcal{U}(0.1512, 0.1672)$

The uncertainty quantification algorithm is implemented in `raven` [6], and analysis here is performed using this framework. The uncertain inputs are listed in Table II. Note that while Σ_a was used in the benchmark, Σ_c is used explicitly as an input and Σ_a is derived. The error in the moments r of the quantity of interest $k(Y) = u(Y)$ are given by

$$\epsilon_h^{(r)} = \frac{|\mathbb{E}[u_h^{(r)}] - \mathbb{E}[u_{\text{ref}}^{(r)}]|}{\mathbb{E}[u_{\text{ref}}^{(r)}]}, \tag{11}$$

$$\mathbb{E}[u_h^{(r)}] = \mathbb{E}[S_{N,\Lambda_{\text{TD}}(L)}[u_h](Y)^{(r)}] = \sum_{k=1}^{\eta} w_k\, u_h^{(r)}\left(Y^{(k)}\right). \tag{12}$$

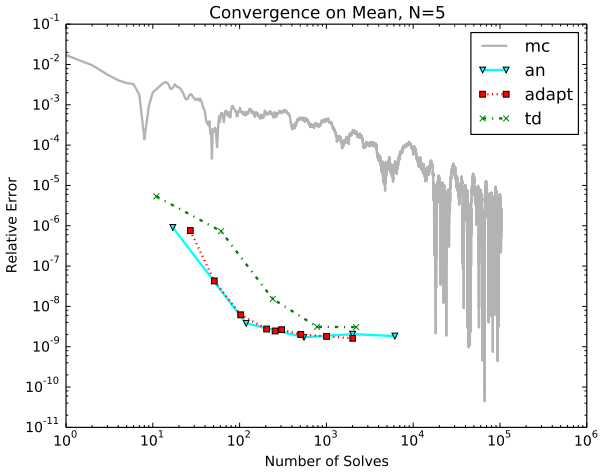

Fig. 2: Mean Convergence

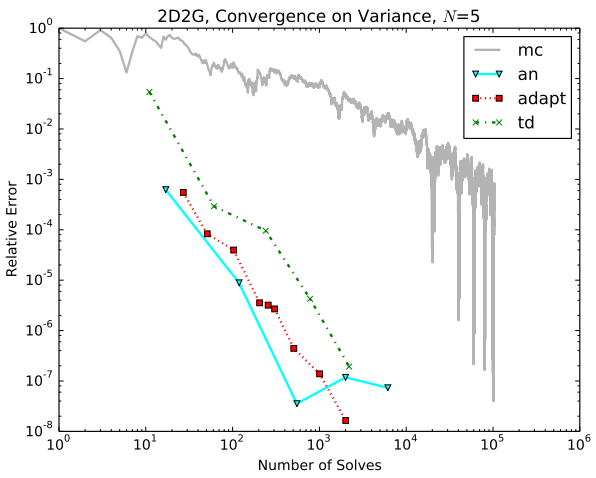

Fig. 3: Variance Convergence

Figs. 2-3 show the comparison of Monte Carlo convergence to stochastic collocation for five uncertain input parameters. The Monte Carlo (mc), total degree (td), and anisotropic total degree (an) methods have been demonstrated previously [5]. The adaptive line is obtained as a result of the work described in this paper. Because of the swift convergence on the mean and the uncertainty of the benchmark value, all presented methods appear to cease converging after 8 orders of magnitude in relative error. However, the same trend can generally be seen in both the mean and variance convergence.

DISCUSSION

As expeected, the convergence of Monte Carlo on the benchmark as a function of computational solves is nearly linear and lethargic compared to the other methods. The static isotropic index set, in which each input dimension is treated with equal importance, converges much more efficiently than Monte Carlo, but lacks the benefit of emphasizing some dimensions over others. The anisotropic case is most efficient, where first-order sensitivity information was used to determine anisotropic weights for polynomials to use in the polynomial chaos expansion.

Interestingly, the adaptive algorithm converges slightly less efficiently than the anisotropic case, while still performing better than the isotropic case. Because the adaptive case has to determine the importance of each input dimension, it occasionally predicts inaccurately and wastes computation solves compared to the more ideal anisotropic case. However, in circumstances when an ideal anisotropy is not understood a priori, the adaptive algorithm may be optimally efficient in representing the original model. Given the potential loss of efficiency when using a poorly-chosen anisotropic weighting, the adaptive algorithm may be an effective choice for initial uncertainty quantification in problems with a low-dimensionality input space.

REFERENCES

1. BABUSKA, NOBILE, and TEMPONE, "A stochastic collocation method for elliptic partial differential equations with random input data," *SIAM Journal on Numerical Analysis*, **45** (2007).
2. L. MAÎTRE and KNIO, *Spectral methods for uncertainty quantification with applications to computational fluid dynamics*, Springer, 1st ed. (2010).
3. AYRES and EATON, "Uncertainty quantification in nuclear criticality modelling using a high dimensional model representation," *Annals of Nuclear Energy*, **80**, 379–402 (May 2015).
4. COOLING, AYRES, PRINJA, and EATON, "Uncertainty and global sensitivity analysis of neutron survival and extinction probabilities using polynomial chaos," *Annals of Nuclear Energy*, **88**, 158–173 (November 2016).
5. TALBOT and PRINJA, "Sparse-grid stochastic collocation uncertainty quantification convergence for multigroup diffusion," *2014 ANS winter conference transactions*, **111**, 747–750 (November 2014).
6. RABITI, ALFONSI, MANDELLI, COGLIATI, and KINOSHITA, "RAVEN, a new software for dynamic risk analysis," in "PSAM 12 Probabilistic Safety Assessment and Management," Honolulu, Hawaii (June 2014).