Tests for UQ Framework

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1 Introduction

This work outlines the development of an uncertainty quantification (UQ) framework using generalized polynomial choas expansions and stochastic collocation (PCESC), verified using Monte Carlo (MC) sampling. To verify the several stages of development this framework undergoes in development, we present here several test codes of increasing complexity that the UQ framework will act on. The four test codes solve four problems: a polynomial expression; 1D semi-infinite medium with uniform source and single material; 1D k-eigenvalue neutron diffusion transport with two energy groups and a single material; and a 2D, two energy group k-eigenvalue neutron diffusion transport quarter-core benchmark.

1.1 Algorithm

Each problem-solving code is treated as a black box that reads in an input file and produces a result readable from an output file. We briefly outline the PCESC process here. The problem-solving code can be represented as a function U of certain input parameters p and uncertain parameters $\theta(\omega)$, where θ could be a single parameter or a vector of uncertain parameters and ω is a single realization in the uncertainty space of θ. We expand $U(p,\theta)$ in basis polynomials characteristic of the uncertain parameters:

$$U(p;\theta) \approx \sum_{i=0}^{I} c_i B_I(\theta), \tag{1}$$

where c are expansion coefficients, B are the characteristic orthonormal basis polynomials, and the sum is truncated at some order I. In the limit as I approaches infinity (or if $U(\theta)$ can be expressed exactly as a polynomial of order I), there is no approximation. Often the expansion converges after a reasonably small number of terms.

We make use of the orthonormal nature of the polynomial basis to calculate the coefficients c_i,

$$c_i = \int_\Omega U(\theta) B_i(\theta) d\theta, \tag{2}$$

where Ω is the entire domain of uncertainty space represented by θ. With the right choice of polynomials, we can apply quadrature to solve the integral,

$$c_i = \sum_{\ell=0}^{(i+1)/2} w_\ell U(\theta_\ell) B_i(\theta_\ell). \tag{3}$$

In this case we are applying Gaussian quadrature, where an expansion of order N can exactly integrate a polynomial of order $2N-1$. Once the coefficients are calculated, they in combination with the basis polynomials create a reduced-order model that can be sampled like the original function, but ideally at much less computational expense.

The measure of success for the PCESC algorithm is its ability to preserve the mean and variance of the original function, as well as produce a virtually identical probability density function (pdf) for the solution quantity of interest, $U(p;\theta)$. The mean, variance, and pdf are confirmed using brute-force Monte Carlo sampling of the original code.

2 Polynomial

We include this test case because of the analytic solution, mean, and variance. The test code simple solves the function evaluation

$$U(\theta) = 1 + 2\theta. \tag{4}$$

We consider the cases when θ has a uniform distribution as well as a normal distribution.

type	runs/order	mean	variance
MC	1×10^6	1.26069628111	0.0632432419713
SC	2	1.25774207229	0.0495341371244
SC	4	1.26064320417	0.0604388749588
SC	8	1.26108375978	0.0637370898233
SC	16	1.26112339681	0.0639754882641

Table 1: Statistics for Source Problem with Uniform Uncertainty

3 Semi-Infinite Uniform Source

This case is also simply an evaluation of an analytic function, but can't be exactly represented by a basis polynomial. The solution models the mono-energetic neutron flux at a point inside a 1D semi-infinite homogenous absorbing medium with a uniform source. The governing PDE for this equation is

$$-D\frac{d^2\phi}{d^2x} + \Sigma_a\phi = S, \tag{5}$$

and its solution is

$$\phi(S, D, x, \Sigma_a) = \frac{S}{\Sigma_a}\left(1 - e^{-x/L}\right), \tag{6}$$

$$L^2 \equiv \frac{D}{\Sigma_a}. \tag{7}$$

where S is the uniform source, Σ_a is the material's macroscopic absorption cross sesciton, D is the material's diffusion coefficient, x is a distance into the medium from the boundary, and ϕ is the neutron flux. Restated in the form used by PCESC,

$$U(p;\theta) = \frac{S}{\theta}\left(1 - e^{-\sqrt{\theta}x/\sqrt{D}}\right), \tag{8}$$

where $p = (S, D, x)$. For our calculations, we set a source strength of 1 neutron per square centimeter, a sampling distance of 2 centimeters into the material, and a diffusion coefficent of 0.5 per centimeter.

We consider the cases when the absorption cross section θ has a uniform distribution as well as a normal distribution. For both cases, the other parameters are as follows.

$$S = 1.0 \text{ n/cm}^2\text{/s}, \tag{9}$$

$$D = 0.5 \text{ /cm}, \tag{10}$$

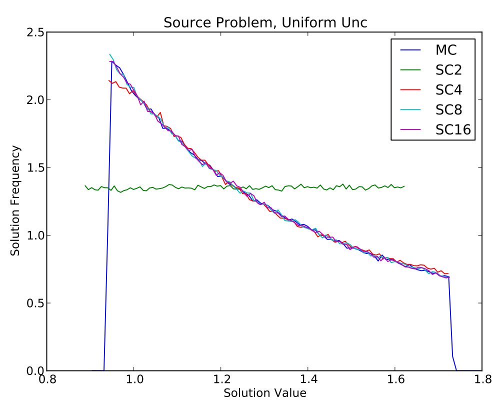
$$x = 2.0 \text{ cm}. \tag{11}$$

We allow Σ_a to vary either uniformly as $\Sigma_a \in [0.5, 1]$ or normally as $\Sigma_a \in \mathcal{N}(0.75, 0.15)$ and quantify the uncertainty using stochastic collocation for generalized polynomial expansion as well as Monte Carlo sampling. For increasing orders of expansion, the mean and variance obtained are shown along with the run time.

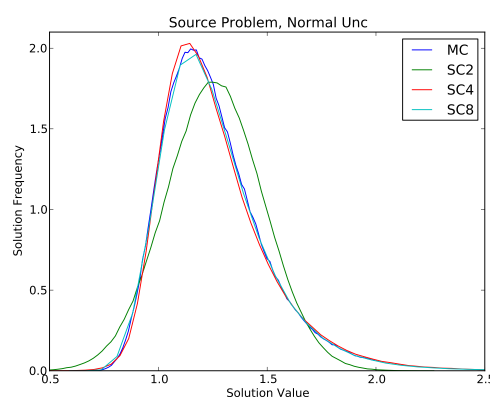
The PDFs were obtained by Monte Carlo sampling of the polynomial expansion for the SC cases, and obtained directly for the Monte Carlo case, shown in Fig. 1. The x-axis is the value of the scalar flux, and the y-axis is the probability of obtaining a particular flux.

type	runs/order	mean	variance	run time (sec)
MC	23400	1.24922240195	0.0488719424418	366.31
SC	2	1.2547221522	0	2.08
SC	4	1.25569029702	0.049198975952	3.11
SC	8	1.25569096924	0.0492316191443	4.74
SC	16	1.25569096924	0.0492316191611	6.88

Table 2: Statistics for Source Problem with Normal Uncertainty



(a) Uniform PDFs



(b) Normal PDFs

Figure 1: Source Problem Solution Distributions

type	runs/order	mean	variance
MC	1×10^6	1.01023757498	0.0092547217648
SC	2	1.00999398244	0.00857615041851
SC	4	1.01022188926	0.00918078062636
SC	8	1.010230418	0.0092238915176
SC	16	1.01023044508	0.00922009179288

Table 3: Convergence of Mean, Variance for Critical Case

4 1D 2G Homogeneous

This problem is a simple version of a k-eigenvalue criticality problem using neutron diffusion. While this problem is 1D, we use a 2D mesh to solve it by imposing reflecting boundary conditions on the top and bottom. The governing PDE for this equation is

$$-\frac{d}{dx}D_g\frac{d\phi_g}{dx} + (\Sigma_{g,a}+\Sigma_{g,s})\phi_g = \sum_{g'}\sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \qquad g\in[1,2], \tag{12}$$

where g denotes the energy group, D is the group diffusion cross section; ϕ is the group flux, x is the location within the problem; $\Sigma_a, \Sigma_s, \Sigma_f$ are the macroscopic absorption, scattering, and fission cross sections respectively; k is the criticality factor eigenvalue and quantity of interest; and χ is the fraction of neutrons born into an energy group. In this case, we consider only downscattering, and fission neutrons are only born into the high energy group ($\Sigma_s^{2\to1} = \chi_2 = 0$).

This problem does not have a convenient general analytic solution. We can express the solver as

$$U(p;\theta) = k(p;\Sigma_{2,a}), \tag{13}$$

where

$$p = (D_g, \Sigma_{1,a}, \Sigma_{g,s}, \nu_g, \Sigma_{g,f}, \chi_g), \qquad g\in[1,2]. \tag{14}$$

While $\phi_g(x)$ might also be considered a parameter, it is an output value solved simultaneously with k.

For this test code we consider $\theta = \Sigma_{2,a}$ in three possible normal distributions. Evaluated at the distribution mean of θ, we consider one each case where $k = (0.9, 1.0, 1.1)$, given by the distributions $\theta \in \mathcal{N}(0.09434, 0.1), \theta \in \mathcal{N}(0.106695, 0.1), \theta \in \mathcal{N}(0.08455, 0.1)$ respectively. A summary of all three cases is shown in Fig. 2. Tabular data for mean and variance convergence is in Tables 3 to 5, and the pdfs for each case are in Figs. 3 to 5. It is important to note that the Monte Carlo sampling was restricted to values within 3 standard deviations of the mean; as such, the means and variances obtained directly through Monte Carlo sampling are not representative of the full uncertainty space. This truncation of the distribution is enforced because without such a restriction, it is possible to sample physically untenable values for $\Sigma_{2,a}$, including negative values.

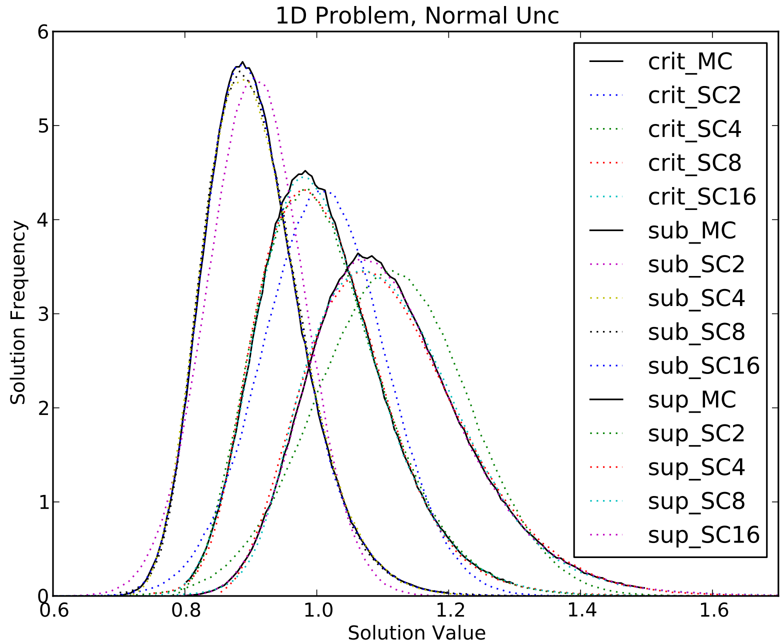


Figure 2: Summary, 1D Criticality

type	runs/order	mean	variance
MC	1×10^6	1.11402940816	0.014621003
SC	2	1.11386614613	0.0133637900516
SC	4	1.11426467694	0.0145502163614
SC	8	1.114283758	0.0146596758645
SC	16	1.11428385746	0.0146501502189

Table 4: Convergence of Mean, Variance for Supercritical Case

type	runs/order	mean	variance
MC	1×10^6	0.90705858894	0.0055124462906
SC	2	0.906911426435	0.00521748368937
SC	4	0.907033407105	0.00550219402953
SC	8	0.907036892243	0.00551754177997
SC	16	0.907036898624	0.00551618720453

Table 5: Convergence of Mean, Variance for Supercritical Case

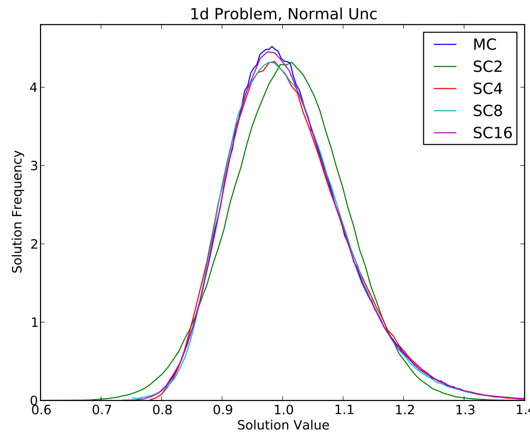


Figure 3: Solution PDF Convergence, 1D Critical Case

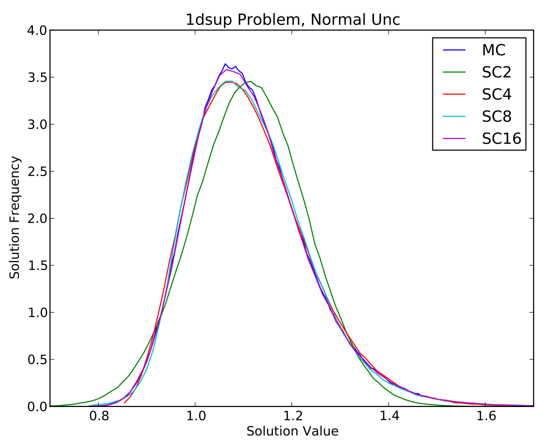


Figure 4: Solution PDF Convergence, 1D Supercritical Case

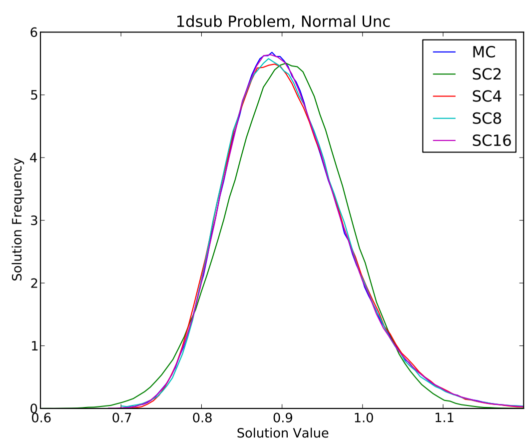


Figure 5: Solution PDF Convergence, 1D Supercritical Case