Tests for UQ Framework

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1   Introduction

This work outlines the development of an uncertainty quantification (UQ) framework using generalized polynomial chaos 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

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

To find the first and second moments of the function $U(\theta)$ analytically,

$$\mathbb{E}[U(\theta)] = \mathbb{E}[1 + 2\theta] = 1 + 2\mathbb{E}[\theta], \tag{5}$$

$$\mathbb{E}[U(\theta)^2]\mathbb{E}[(1 + 2\theta)^2] = 1 + 4\mathbb{E}[\theta] + 4\mathbb{E}[\theta^2]. \tag{6}$$

In general, the moments of θ are given as

$$m_r(\theta) = \mathbb{E}[\theta^r] = \int_\Omega P(\theta)\theta^r d\theta. \tag{7}$$

We consider the cases when θ has a uniform distribution $\theta \in [3, 7]$ as well as a normal distribution $\theta \in \mathcal{N}(5, 4)$. When using PCESC, all coefficients for expansions of polynomial order higher than 1 are zero; thus, only the results for order 2 expansion are shown.

2.1 Uniform Distribution

For a uniformly-distributed variable $\xi \in [a, b]$, the moments are given as

$$m_r(\xi) = \int_{a^r}^{b^r} \frac{1}{b^r - a^r} \xi^r d\xi. \tag{8}$$

Of particular interest are the first moment (expected value) and second moment, which we use to calculate variance.

$$m_1(\xi) \equiv \mathbb{E}[\xi] = \frac{a + b}{2}, \tag{9}$$

$$m_2(\xi) = \mathbb{E}[\xi^2] = \frac{1}{3}(b^2 + ab + a^2). \tag{10}$$

Using the analytic moments given in Eq. 9,

$$\mathbb{E}[\theta] = 5, \tag{11}$$

$$\mathbb{E}[\theta^2] = \frac{79}{3}, \tag{12}$$

$$\mathbb{E}[U(\theta)] = 11, \tag{13}$$

$$\mathbb{E}[U(\theta)^2] = \frac{379}{3}. \tag{14}$$

The variance is given simply as

$$\text{var}[U(\theta)] = \mathbb{E}[U(\theta)^2] - \mathbb{E}[U(\theta)]^2 = \frac{79}{3}. \tag{15}$$

The statistics from MC and PCESC are given in Table 1 and the pdfs are in Fig. 1.

type	runs/order	mean	variance
Analytic	-	11	16/3
MC	1×10^7	10.999555712	5.3374535046
SC	2	11.0	5.33333333333

Table 1: Polynomial Test, Uniform Distribution Statistics

type	runs/order	mean	variance
Analytic	-	11	16
MC	1×10^7	11.0000448162	15.9892244775
SC	2		

Table 2: Polynomial Test, Normal Distribution Statistics

2.2 Normal Distribution

For a normally-distributed variable $\xi \in [\mu, \sigma^2]$, the moments are given as

$$m_r(\xi) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \xi^r d\xi. \tag{16}$$

Of particular interest are the first moment (expected value) and second moment, which we use to calculate variance.

$$m_1(\xi) \equiv \mathbb{E}[\xi] = \mu, \tag{17}$$
$$m_2(\xi) = \mathbb{E}[\xi^2] = \mu^2 + \sigma^2. \tag{18}$$

Using the analytic moments given in Eq. 17,

$$\mathbb{E}[\theta] = 5, \qquad \mathbb{E}[\theta^2] = 29, \tag{19}$$
$$\mathbb{E}[U(\theta)] = 11, \qquad \mathbb{E}[U(\theta)^2] = 137. \tag{20}$$

The variance is given simply as

$$\text{var}[U(\theta)] = \mathbb{E}[U(\theta)^2] - \mathbb{E}[U(\theta)]^2 = 16. \tag{21}$$

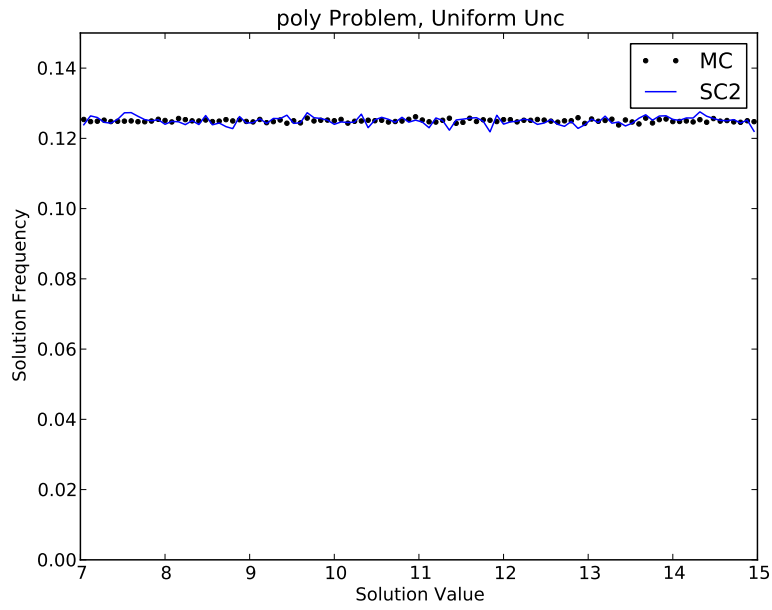The statistics from MC and PCESC are given in Table 2 and the pdfs are in Fig. 2.
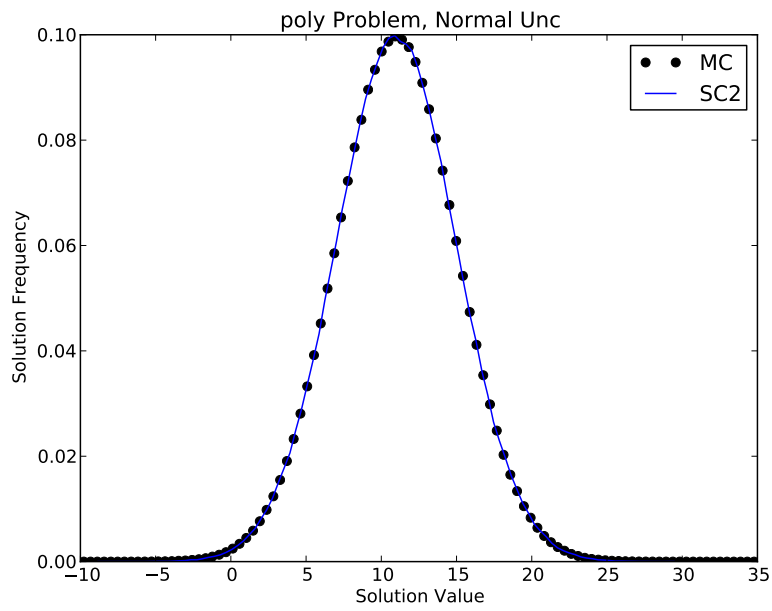
Figure 1: Polynomial Problem, Uniform PDFs

Figure 2: Polynomial Problem, Normal PDFs

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 3: 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

$$-D\frac{d^2\phi}{d^2x} + \Sigma_a\phi = S, \tag{22}$$

and its solution is

$$\phi(S, D, x, \Sigma_a) = \frac{S}{\Sigma_a}\left(1 - e^{-x/L}\right), \tag{23}$$

$$L^2 \equiv \frac{D}{\Sigma_a}. \tag{24}$$

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,

$$U(p; \theta) = \frac{S}{\theta}\left(1 - e^{-\sqrt{\theta}x/\sqrt{D}}\right), \tag{25}$$

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.

$$S = 1.0 \text{ n/cm}^2/\text{s}, \tag{26}$$

$$D = 0.5 \text{ /cm}, \tag{27}$$

$$x = 2.0 \text{ cm}. \tag{28}$$

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. 3. 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

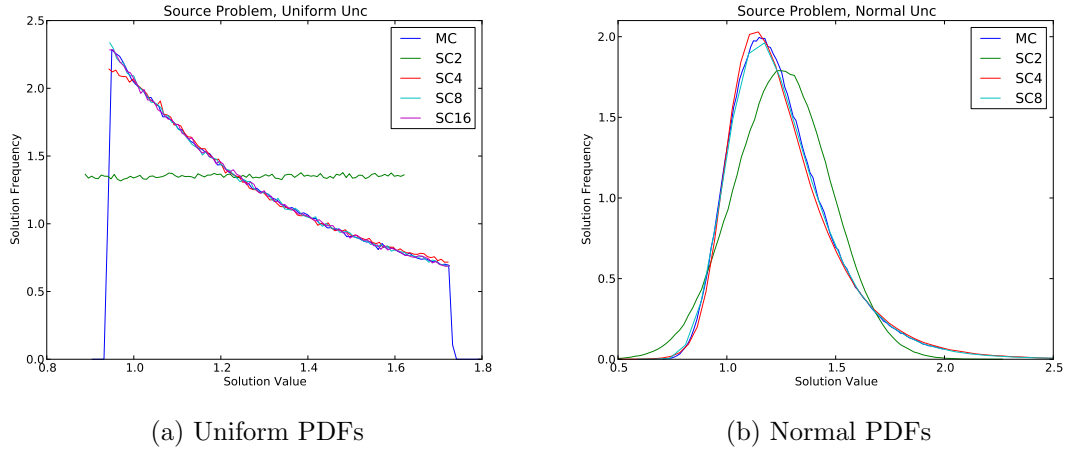Table 4: Statistics for Source Problem with Normal Uncertainty

(a) Uniform PDFs

(b) Normal PDFs

Figure 3: Source Problem Solution Distributions

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type	runs/order	mean	variance	time (s)
MC	1×10^6	1.01144778738	0.0105716289269	15082
SC	2	1.01107577584	0.00974910361412	133
SC	4	1.0113755955	0.0105739848126	231
SC	8	1.01137628238	0.0105785232446	450
SC	16	1.01137628243	0.0105785241745	862

Table 5: 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

$$-\frac{d}{dx}D_g\frac{d\phi_g}{dx} + (\Sigma_{g,a} + \Sigma_{g,s})\phi_g = \sum_{g'}\sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \quad g \in [1,2], \tag{29}$$

$$\Sigma_{g,a} = \Sigma_{g,\gamma} + \Sigma_{g,f}, \tag{30}$$

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; $\Sigma_a, \Sigma_s, \Sigma_f, \Sigma_\gamma$ are the macroscopic absorption, scattering, fission, and capture 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

$$U(p;\theta) = k(p;\Sigma_{2,\gamma}), \tag{31}$$

where

$$p = (D_g, \Sigma_{1,\gamma}, \Sigma_{g,s}, \nu_g, \Sigma_{g,f}, \chi_g), \quad g \in [1,2]. \tag{32}$$

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 $\theta = \Sigma_{2,\gamma}$ 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 $\theta \in \mathcal{N}(0.055969, 0.1), \theta \in \mathcal{N}(0.04438, 0.1), \theta \in \mathcal{N}(0.035181, 0.1)$ respectively.

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.

A summary of all three cases is shown in Fig. 4. Tabular data for mean and variance convergence is in Tables 5 to 7, where the clock time shown makes use of embarrassingly-parallel Monte Carlo sampling with 4 cores. The times for the PCESC runs include the construction of the ROM prior to sampling. The pdfs for each case are in Figs. 5.
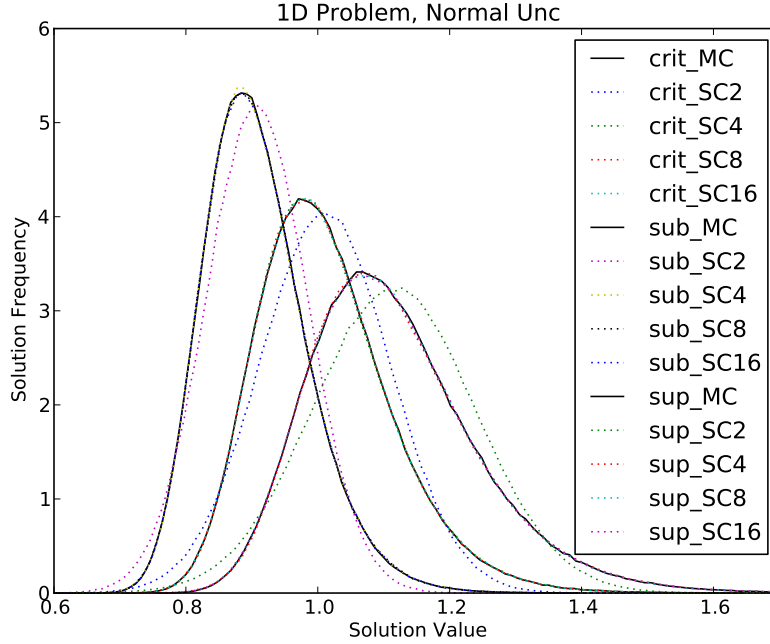
Figure 4: Summary, 1D Criticality

type	runs/order	mean	variance
MC	1×10^6	1.11593980088	0.0168503796482
SC	2	1.11537873568	0.0151539223359
SC	4	1.11590698755	0.016795821961
SC	8	1.11590896034	0.0168106966474
SC	16	1.11590896088	0.0168107061554

Table 6: Convergence of Mean, Variance for Supercritical Case

4.1 Chaos Moment Quadrature Convergence

One concern with using stochastic collocation to build the polynomial chaos moments is the appropriate order of quadrature to use. With Gaussian quadrature, a sum with n terms can exactly integrate a polynomial of order $2n - 1$. The chaos moment expression we integrate is

$$c_i = \int_{\Omega} U(\theta)P(\theta)B_i(\theta)d\theta, \tag{33}$$

$$\approx \sum_{\ell=0}^{L} w_\ell U(\theta_\ell)B_i(\theta_\ell), \tag{34}$$

where P is the probability distribution of θ and B_i is the $i - th$ order basis polynomial. In the simplest case when $U(\theta)$ is a scalar quantity, the order of the expression under the integral is determined solely by the basis polynomial. Thus a quadrature order of $(i + 1)/2$ is the minimum

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type	runs/order	mean	variance
MC	1×10^6	0.907699673282	0.00632790358771
SC	2	0.907653521565	0.00595095987773
SC	4	0.907813174929	0.00633526057266
SC	8	0.907813389468	0.00633649118503
SC	16	0.907813389471	0.00633649126226

Table 7: Convergence of Mean, Variance for Subcritical Case

quadrature order necessary to integrate the chaos moments. In the case $U(\theta)$ is highly nonlinear and ill-approximated by even high-order polynomials, the necessary quadrature order required to accurately determine moments could be much higher.

As an example of chaos moment convergence as a function of quadrature order, we show the PCESC moments of the critical case for 8th-order quadrature in Table 8, as determined by increasing orders of quadrature from the minimum to 12-th order, which assumes $U(\theta)$ is well-approximated by a 7th-order polynomial. As can be seen, the lower moments require smaller quadrature orders, and at least order 8 quadrature is necessary to see reasonable convergence for higher moments. In addition, the moments calculated using quadrature order equal to expansion order are given for expansion orders 2 to 32 in Fig. 9.

Order	1	2	3	4	5	6	7	8
5	1.34648094	-0.13502447	0.02226791	-0.0045477	0.00000000	0.00101863	-0.00092988	0.00313821
6	1.34648100	-0.13502501	0.02227125	-0.00456451	0.0010908	-0.00027317	0.00000000	0.00025291
8	1.34648101	-0.13502506	0.02227158	-0.00456614	0.0010978	-0.00029964	9.01120742e-05	-2.67010906e-05
10	1.34648101	-0.13502506	0.02227158	-0.00456616	0.0010979	-0.00030000	9.13419949e-05	-3.05173759e-05
12	1.34648101	-0.13502506	0.02227158	-0.00456616	0.0010979	-0.00030001	9.13732306e-05	-3.06142832e-05

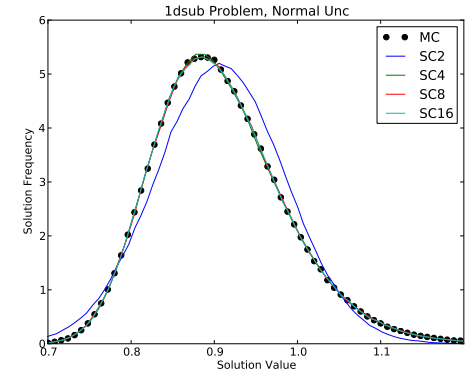Table 8: Chaos Moment Convergence with Increasing Quadrature Order
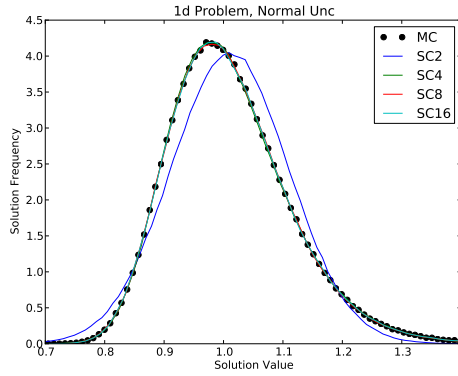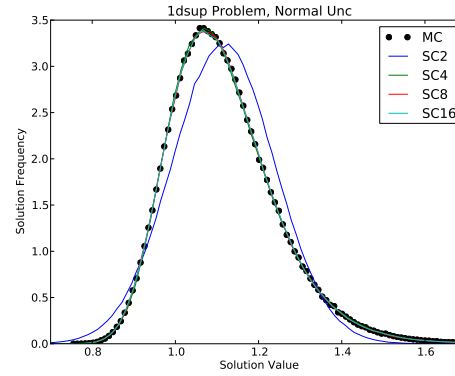
(a) Critical (b) Supercritical (c) Subcritical

Figure 5: 1D Solution PDF Convergences

Moment	SC2	SC4	SC8	SC16	SC32
1	1.34608094	1.3464801	1.34648101	1.34648101	1.34648101
2	-0.13145279	-0.1350169	-0.13502506	-0.13502506	-0.13502506
3	0	0.02222067	0.02227158	0.02227158	0.02227158
4	0	-0.00431037	-0.00456614	-0.00456616	-0.00456616
5	0	0	0.0010978	0.0010979	0.0010979
6	0	0	-0.00029964	-0.00030001	-0.00030001
7	0	0	9.01120742e-05	9.13747084e-05	9.13746830e-05
8	0	0	-2.67010906e-05	-3.06188612e-05	-3.06187650e-05
9	0	0	0	1.11868181e-05	1.11865704e-05
10	0	0	0	-4.42800671e-06	-4.42735312e-06
11	0	0	0	1.89021407e-06	1.88853134e-06
12	0	0	0	-8.66874281e-07	-8.62852707e-07
13	0	0	0	4.24658199e-07	4.15693998e-07
14	0	0	0	-2.18790217e-07	-1.99976426e-07
15	0	0	0	1.12938059e-07	7.56801496e-08
16	0	0	0	-4.90000878e-08	2.05894301e-08
17	0	0	0	0	-1.22580841e-07
18	0	0	0	0	2.51097599e-07
19	0	0	0	0	-4.18278488e-07
20	0	0	0	0	6.25910592e-07
21	0	0	0	0	-8.61060458e-07
22	0	0	0	0	1.09209939e-06
23	0	0	0	0	-1.26866179e-06
24	0	0	0	0	1.32892404e-06
25	0	0	0	0	-1.21597330e-06
26	0	0	0	0	9.01437926e-07
27	0	0	0	0	-4.09433059e-07
28	0	0	0	0	-1.70599526e-07
29	0	0	0	0	6.94034499e-07
30	0	0	0	0	-9.99892578e-07
31	0	0	0	0	9.71463606e-07
32	0	0	0	0	-5.97051529e-07

Table 9: Chaos Moments for 1D Critical Case

5 2D 2G Quarter Core

5.1 Equations

This problem is a more traditional k-eigenvalue criticality problem using neutron diffusion. We simulate a benchmark reactor core by imposing reflecting conditions on the left and bottom boundaries of a quarter-core geometry. The governing PDE for this equation is still

$$-\frac{d}{dx}D_g\frac{d\phi_g}{dx} + (\Sigma_{g,a} + \Sigma_{g,s})\phi_g = \sum_{g'}\sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \quad g \in [1,2], \tag{35}$$

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 ($\Sigma_s^{2\to1} = \chi_2 = 0$). Our coupled equations are

$$-\frac{d}{dx}D_1\frac{d\phi_1}{dx} + (\Sigma_{1,a} + \Sigma_s^{1\to2})\phi_1 = \frac{1}{k}\sum_{g'=1}^{2}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \tag{36}$$

$$-\frac{d}{dx}D_2\frac{d\phi_2}{dx} + \Sigma_{2,a}\phi_2 = \sigma_s^{1'\to2}\phi_1. \tag{37}$$

5.2 Materials and Geometry

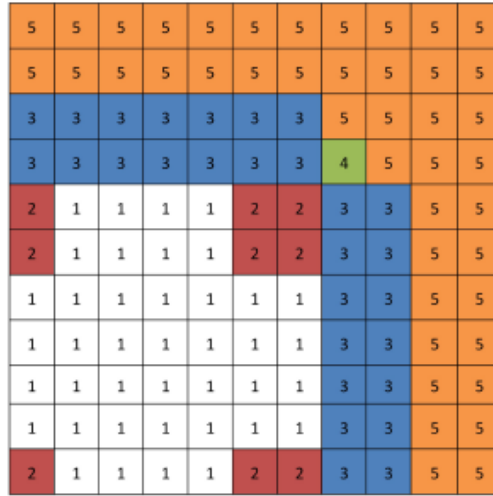The two-dimensional core is shown in Fig. 6 and the material properties are listed in Table 10.

Figure 6: Core Map

Region	Group	D_g	$\Sigma_{a,g}$	$\nu\Sigma_{f,g}$	$\Sigma_{1,2}$
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 10: Basic Material Properties for Core

type	runs/order	mean	variance
MC	1×10^6	1.01488024214	0.00196794483094
SC	2	1.01617227356	0.00103920580302
SC	4	1.01543109812	0.0020042932657
SC	8	1.015592044	0.00192541919329
SC	16	1.01549506606	0.00189209311817
SC	32	1.01061893249	0.00227815756915

Table 11: Convergence of Mean, Variance for 2D2G Case

5.3 Uncertainty Quantification

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

$$U(p;\theta) = k(p;\Sigma_{2,a}), \tag{38}$$

where

$$p = (D_g, \Sigma_{1,a}, \Sigma_{g,s}, \nu_g, \Sigma_{g,f}, \chi_g), \qquad g \in [1,2]. \tag{39}$$

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 $\theta = \Sigma_{2,a}$ normally distributed as $\theta \in \mathcal{N}(0.1003, 0.0001)$. Tabular data for mean and variance convergence is in Table 11, and the pdfs obtained are in Fig. 7. Once again, 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.
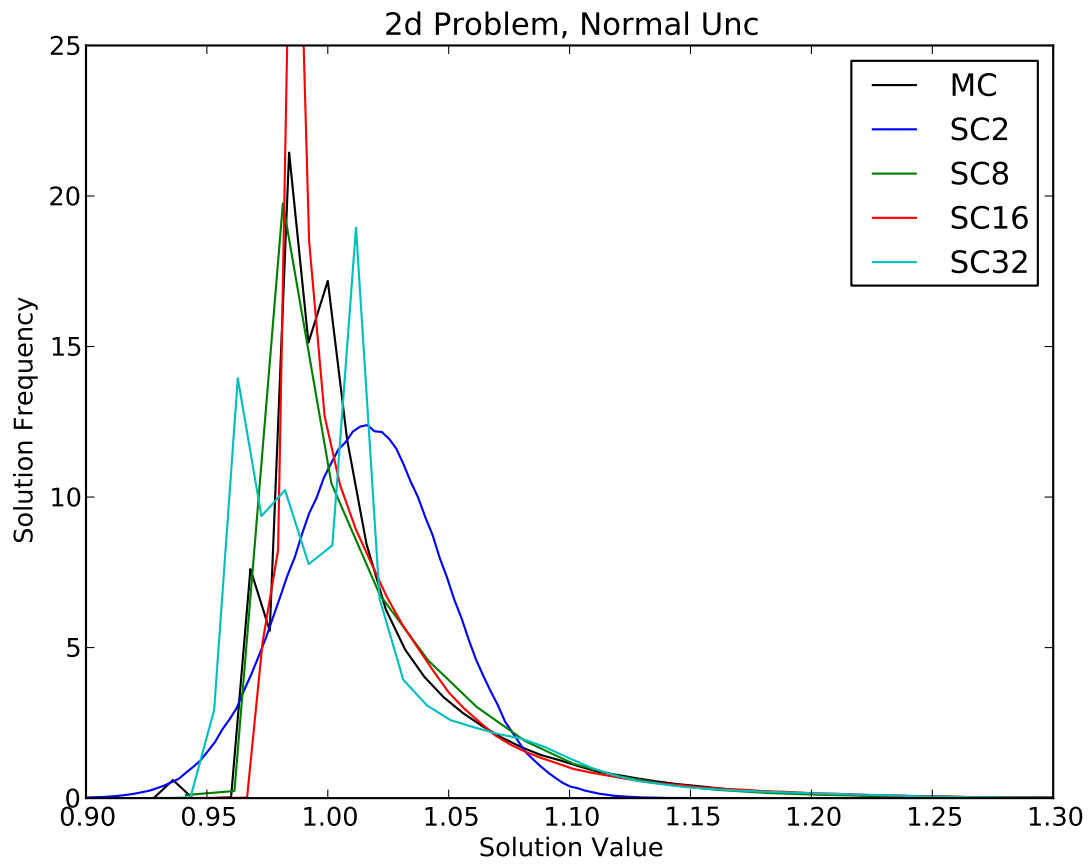
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Figure 7: Solution PDF Convergence, 2D2G Case