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 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 mono-energetic neutron transport in a 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. In all cases, we let (Ω, Σ, P) describe a complete probability space.

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. 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 Σ. 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_i are expansion coefficients, B_i are the characteristic orthonormal basis polynomials, and the sum is truncated at finite 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. Ideally 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,

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

With the right choice of polynomials, we can apply quadrature to solve the integral,

$$c_i = \sum_{\ell=0}^{L} w_\ell U(\theta_\ell) B_i(\theta_\ell). \tag{3}$$

In this case we are applying Gaussian quadrature, where an expansion of order L can exactly integrate a polynomial of order $2L-1$. While the order of the polynomial $B_i(\theta_\ell)$ is i, the equivalent polynomial order of $U(\theta_\ell)$ is unknown and must be determined or approximated. If $U(\theta)$ is scalar, L need only be $(i+1)/2$; this is the low bound for quadrature order. Coefficient convergence as a function of quadrature order is further explored for some of the cases in this report (see, for example, §4.1).

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.

2.1 Univariate

The test code simply 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.

2.1.1 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

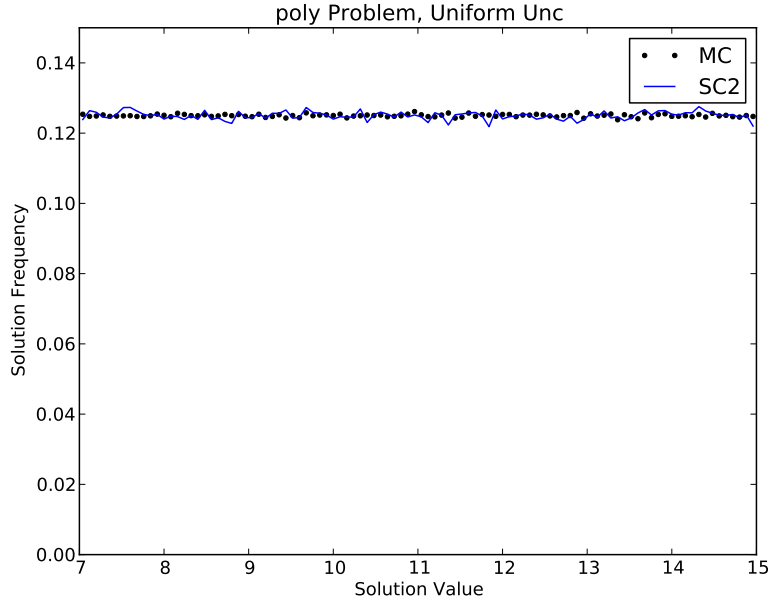Table 1: Polynomial Test, Monovariate Uniform Distribution Statistics

Figure 1: Polynomial Problem, Uniform PDFs

2.1.2 Normal Distribution

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

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

The analytic statistical measures of interest are

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

Using the analytic moments given in Eq. 17,

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

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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.

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

Table 2: Polynomial Test, Monovariate Normal Distribution Statistics
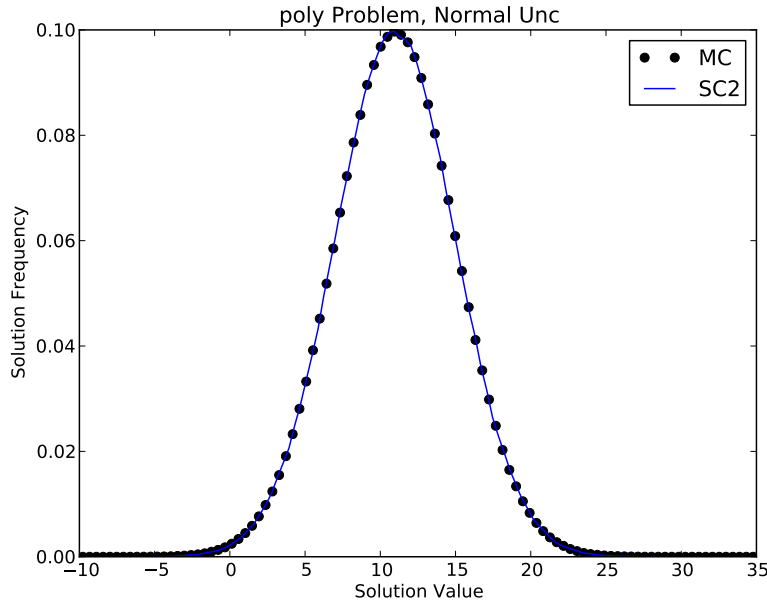

Figure 2: Polynomial Problem, Normal PDFs

2.2 Bivariate

Similar to the univariate case, we add a dimension and define a new function to sample

$$U(\boldsymbol{\theta}) = U(\theta_1, \theta_2) = \theta_1(1 + \theta_2). \tag{22}$$

We impose independence between the uncertain variables in $\boldsymbol{\theta}$. The expected value is given as

$$\langle U \rangle = \langle \theta_1 \rangle + \langle \theta_1 \theta_2 \rangle, \tag{23}$$

$$= \langle \theta_1 \rangle \left(1 + \langle \theta_2 \rangle\right). \tag{24}$$

The second moment is

$$\langle U^2 \rangle = \langle \theta_1^2 \rangle \left(1 + 2 \langle \theta_2 \rangle + \langle \theta_2^2 \rangle\right). \tag{25}$$

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2.2.1 Uniform

We allow $\boldsymbol{\theta}$ to vary uniformly as

$$\theta_1 \in [3, 7], \tag{26}$$
$$\theta_2 \in [1, 6]. \tag{27}$$

Using the derivations for the univariate uniform variable, moments are given explicitly by

$$\langle U \rangle = (5) + (5)\left(\frac{7}{2}\right), \tag{28}$$
$$= \frac{45}{2}. \tag{29}$$
$$\langle U^2 \rangle = \frac{(3)^2 + (3)(7) + (7)^2}{3}\left(1 + (1 + 6) + \frac{(1)^2 + (1)(6) + (6)^2}{3}\right), \tag{30}$$
$$= 588.\bar{1}. \tag{31}$$

The variance is

$$\mathrm{var}[U] = \langle U^2 \rangle - \langle U \rangle^2 = 81.86\bar{1}. \tag{32}$$

The analytic, MC, and PCESC statistics are in Table 3, and the pdfs are show in Fig. 3.

type	runs/order	mean	variance
Analytic	-	$45/2$	$81.86\bar{1}$
MC	1×10^7	22.4962950638	81.8754664265
SC	(1,1)	22.5	81.8611111111

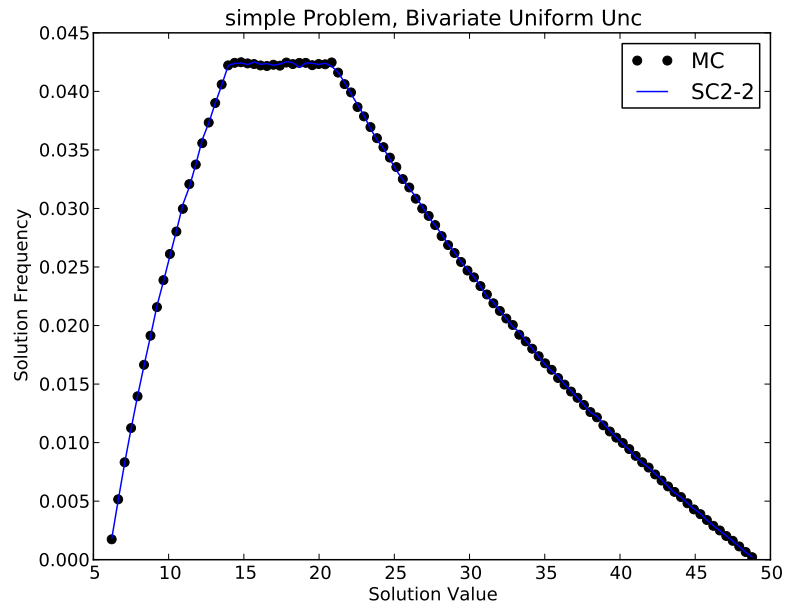Table 3: Polynomial Test, Bivariate Uniform Distribution Statistics

Figure 3: Polynomial Problem, Bivariate Uniform 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 4: Statistics for Source Problem with Uniform Uncertainty

3 Semi-Infinite Uniform Source

This case is also an evaluation of an analytic function, but can't be exactly represented by a finite polynomial expansion. 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

$$-D\frac{d^2\phi}{d^2x} + \Sigma_a\phi = S, \tag{33}$$

and its solution is

$$\phi(S, D, x, \Sigma_a) = \frac{S}{\Sigma_a}\left(1 - e^{-x/L}\right), \tag{34}$$

$$L^2 \equiv \frac{D}{\Sigma_a}. \tag{35}$$

where S is the uniform source, Σ_a is the material's macroscopic absorption cross section, D is the material's diffusion coefficient, x is a distance into the medium from the boundary, and ϕ is the neutron flux.

3.1 Monovariate

Restated in the form used by PCESC,

$$U(p; \theta) = \frac{S}{\theta}\left(1 - e^{-\sqrt{\theta}x/\sqrt{D}}\right), \tag{36}$$

where $p = (S, D, x)$ and $\theta = \Sigma_a$. We consider the cases when the absorption cross section θ has a uniform distribution as well as a normal distribution. For both cases, parameters p are as follows.

$$S = 1.0 \text{ n/cm}^2/\text{s}, \tag{37}$$
$$D = 0.5 \text{ /cm}, \tag{38}$$
$$x = 2.0 \text{ cm}. \tag{39}$$

We allow Σ_a to vary 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 PCESC as well as Monte Carlo sampling. For increasing orders of expansion, the mean and variance obtained are shown along with the run time and are shown in Tables 4 and 5.

The PDFs were obtained by Monte Carlo sampling of the ROM for the PCESC cases, and obtained directly for the Monte Carlo case, shown in Fig. 4. 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	1×10^6	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 5: Statistics for Source Problem with Normal Uncertainty
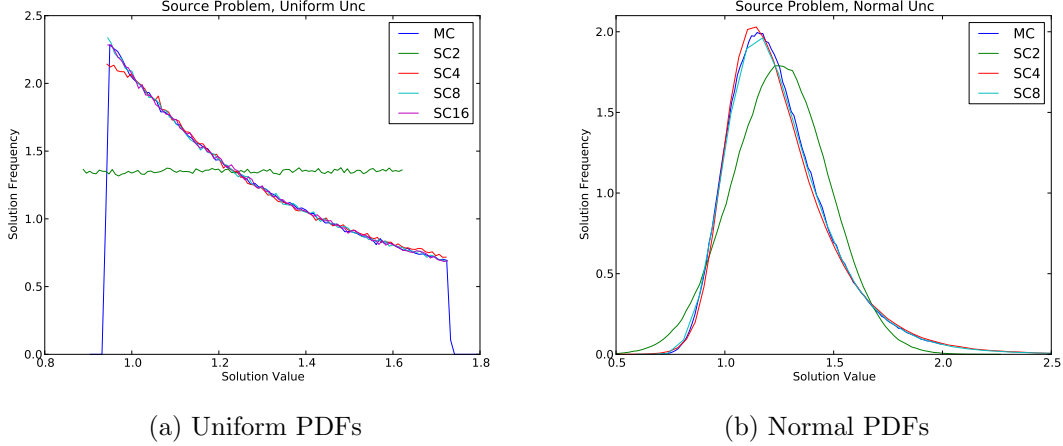

(a) Uniform PDFs (b) Normal PDFs

Figure 4: Source Problem Solution Distributions

3.2 Bivariate

In addition to the absorption cross section, we introduce uncertainty in the location at which the flux is measured. For example, the exact absorption properties of a medium are unknown and a point detector is placed with some uncertainty. Restating the problem,

$$U(p; \boldsymbol{\theta}) = \frac{S}{\theta_1} \left(1 - e^{-\sqrt{\theta_1}\theta_2/\sqrt{D}} \right), \tag{40}$$

where $p = (S, D)$ and $\boldsymbol{\theta} = [\theta_1, \theta_2] = [\Sigma_a, x]$. We consider two cases: when $\theta_1 \sim \mathcal{U}(0.5, 1), \theta_2 \sim \mathcal{U}(1.5, 2.5)$; as well when $\theta_1 \sim \mathcal{N}(0.75, 0.15^2), \theta_2 \sim \mathcal{N}(TODO, TODO)$. For both cases, parameters p are as follows.

$$S = 1.0 \text{ n/cm}^2/\text{s}, \tag{41}$$

$$D = 0.5 \text{ /cm}. \tag{42}$$

We quantify the uncertainty using PCESC as well as Monte Carlo sampling. For increasing orders of expansion, the mean and variance obtained are shown in Tables 6 and 7. The PDFs were obtained by Monte Carlo sampling of the ROM for the PCESC cases, and obtained directly for the Monte Carlo case, shown in Fig. 5. The x-axis is the value of the scalar flux, and the y-axis is the probability of obtaining a particular flux.

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type	order(Σ_a, x)	mean	variance
MC	1×10^6	1.24791828682	0.0508287413676
SC	(2,2)	1.24804231569	0.0506451101763
SC	(2,4)	1.24804212351	0.0506466208388
SC	(4,2)	1.24806746049	0.0507934845282
SC	(4,4)	1.24806726831	0.0507949951904

Table 6: Statistics for Source Problem with Bivariate Uniform Uncertainty

type	runs/order	mean	variance
MC	1×10^6		
SC	(2,2)		
SC	(4,4)		
SC	(8,8)		
SC	(16,16)		

Table 7: Statistics for Source Problem with Bivariate Normal Uncertainty
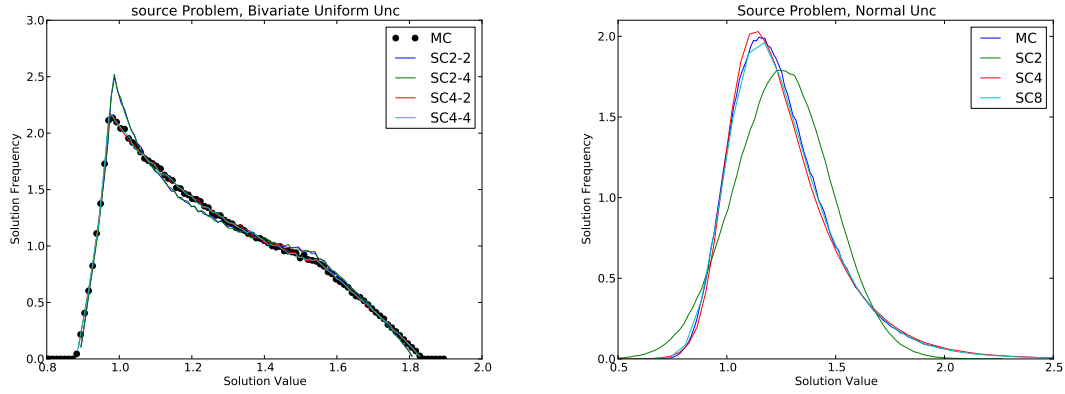
(a) Uniform PDFs   (b) PLACEHOLDERNormal PDFs

Figure 5: Bivariate Source Problem Solution Distributions

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 8: Convergence of Mean, Variance for Critical Case

4 1D 2G Homogeneous

This problem is a simple version of a k-eigenvalue criticality problem using 1D, dual-energy diffusion for neutron transport. 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

$$-\frac{d}{dx}D_g\frac{d\phi_g}{dx} + (\Sigma_{g,a} + \Sigma_{g,s})\phi_g = \sum_{g'}\sigma_s^{g' \to g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \quad g \in [1,2], \tag{43}$$

$$\Sigma_{g,a} = \Sigma_{g,\gamma} + \Sigma_{g,f}, \tag{44}$$

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 ($\Sigma_s^{2 \to 1} = \chi_2 = 0$).

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

$$U(p;\theta) = k(p;\Sigma_{2,\gamma}), \tag{45}$$

where

$$p = (D_g, \Sigma_{1,\gamma}, \Sigma_{g,s}, \nu_g, \Sigma_{g,f}, \chi_g), \quad g \in [1,2]. \tag{46}$$

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 unphysical values for $\Sigma_{2,a}$, including negative values.

A summary of all three cases is shown in Fig. 6. Tabular data for mean and variance convergence is in Tables 8 to 10, 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. 7.
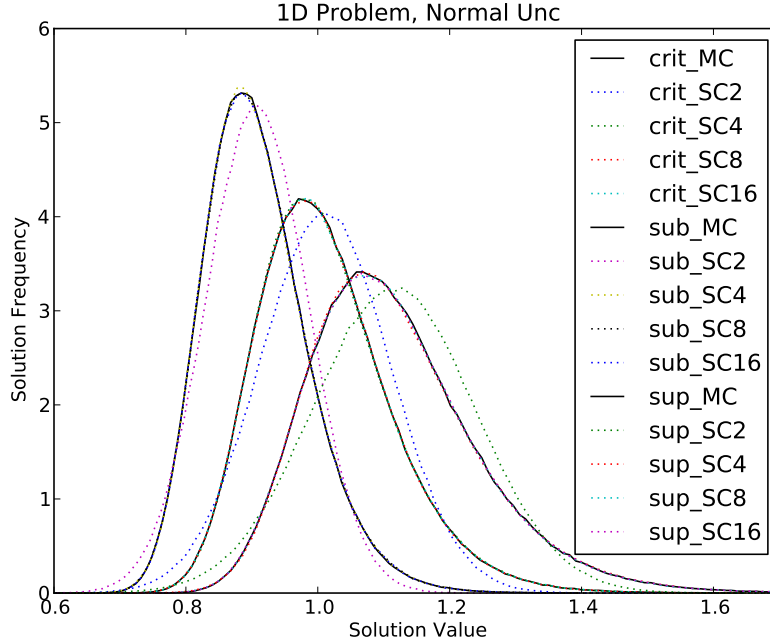
Figure 6: Summary, 1D Criticality

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 9: 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

$$c_i = \int_\Omega U(\theta)P(\theta)B_i(\theta)d\theta, \tag{47}$$

$$\approx \sum_{\ell=0}^{L} w_\ell U(\theta_\ell)B_i(\theta_\ell), \tag{48}$$

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 10: 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 is 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 7th-order quadrature in Table 11, 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. 12.

Quadrature Order	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7
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

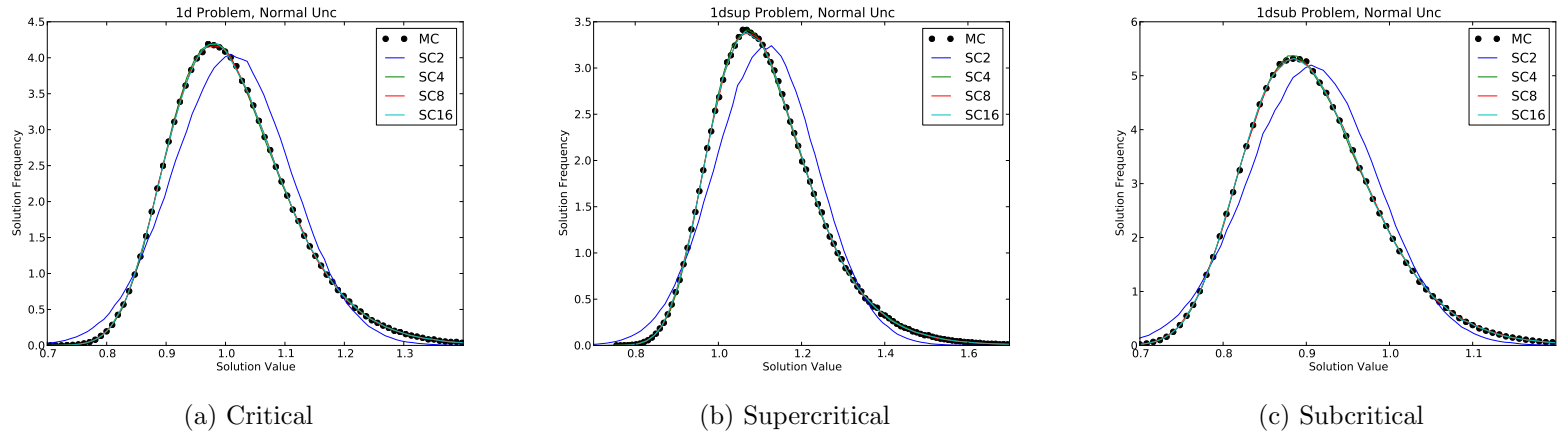Table 11: Chaos Moment Convergence with Increasing Quadrature Order

(a) Critical (b) Supercritical (c) Subcritical

Figure 7: 1D Solution PDF Convergences

Moment	SC1	SC3	SC7	SC15	SC31
0	1.34608094	1.3464801	1.34648101	1.34648101	1.34648101
1	-0.13145279	-0.1350169	-0.13502506	-0.13502506	-0.13502506
2	0	0.02222067	0.02227158	0.02227158	0.02227158
3	0	-0.00431037	-0.00456614	-0.00456616	-0.00456616
4	0	0	0.0010978	0.0010979	0.0010979
5	0	0	-0.00029964	-0.00030001	-0.00030001
6	0	0	9.01120742e-05	9.13747084e-05	9.13746830e-05
7	0	0	-2.67010906e-05	-3.06188612e-05	-3.06187650e-05
8	0	0	0	1.11868181e-05	1.11865704e-05
9	0	0	0	-4.42800671e-06	-4.42735312e-06
10	0	0	0	1.89021407e-06	1.88853134e-06
11	0	0	0	-8.66874281e-07	-8.62852707e-07
12	0	0	0	4.24658199e-07	4.15693998e-07
13	0	0	0	-2.18790217e-07	-1.99976426e-07
14	0	0	0	1.12938059e-07	7.56801496e-08
15	0	0	0	-4.90000878e-08	2.05894301e-08
16	0	0	0	0	-1.22580841e-07
17	0	0	0	0	2.51097599e-07
18	0	0	0	0	-4.18278488e-07
19	0	0	0	0	6.25910592e-07
20	0	0	0	0	-8.61060458e-07
21	0	0	0	0	1.09209939e-06
22	0	0	0	0	-1.26866179e-06
23	0	0	0	0	1.32892404e-06
24	0	0	0	0	-1.21597330e-06
25	0	0	0	0	9.01437926e-07
26	0	0	0	0	-4.09433059e-07
27	0	0	0	0	-1.70599526e-07
28	0	0	0	0	6.94034499e-07
29	0	0	0	0	-9.99892578e-07
30	0	0	0	0	9.71463606e-07
31	0	0	0	0	-5.97051529e-07

Table 12: 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

$$-\frac{d}{dx}D_g\frac{d\phi_g}{dx} + (\Sigma_{g,a} + \Sigma_{g,s})\phi_g = \sum_{g'}\sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \quad g \in [1,2], \qquad (49)$$

$$\Sigma_{g,a} = \Sigma_{g,c} + \Sigma_{g,f}, \qquad (50)$$

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

$$-\frac{d}{dx}D_1\frac{d\phi_1}{dx} + (\Sigma_{1,a} + \Sigma_s^{1\to2})\phi_1 = \frac{1}{k}\sum_{g'=1}^{2}\nu_{g'}\sigma_{f,g'}\phi_{g'}, \qquad (51)$$

$$-\frac{d}{dx}D_2\frac{d\phi_2}{dx} + \Sigma_{2,a}\phi_2 = \sigma_s^{1'\to2}\phi_1, \qquad (52)$$

$$\Sigma_{g,a} = \Sigma_{g,c} + \Sigma_{g,f}. \qquad (53)$$

5.2 Materials and Geometry

The two-dimensional core is shown in Fig. 8 and the material properties are listed in Table 13.

Figure 8: Core Map

Region	Group	D_g	$\Sigma_{c,g}$	$\nu\Sigma_{f,g}$	$\Sigma_s^{1,2}$
1	1	1.255	4.602e-3	4.602e-3	2.533e-2
	2	2.11e-1	5.540e-2	1.091e-1	
2	1	1.268	4.609e-3	4.609e-3	2.767e-2
	2	1.902e-1	8.675e-2	8.675e-2	
3	1	1.259	6.083e-3	4.663e-3	2.617e-2
	2	2.091e-1	4.142e-2	1.021e-1	
4	1	1.259	4.663e-3	4.663e-3	2.617e-2
	2	2.091e-1	3.131e-2	1.021e-1	
5	1	1.257	6.034e-4	0	4.754e-2
	2	1.592e-1	1.911e-2	0	

Table 13: Basic Material Properties for Core

5.3 Uncertainty Quantification

5.3.1 Univariate

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

$$U(p;\theta) = k(p;\Sigma_{2,c}), \tag{54}$$

where

$$p = (D_g, \Sigma_{1,c}, \Sigma_{g,s}, \nu_g, \Sigma_{g,f}, \chi_g), \qquad g \in [1,2]. \tag{55}$$

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

5.3.1.1 Uniform Uncertainty

For this test we consider $\theta = \Sigma_{2,c}$ uniformly distributed as $\theta \in \mathcal{N}(0.0454, 0.0654s)$. Tabular data for mean and variance convergence is in Table 14, and the pdfs obtained are in Fig. 9.

The PCESC runs all made use of order 32 quadrature to integrate chaos moments.

type	runs/order	mean	variance
MC	1×10^6	1.00406413634	0.000446173081079
SC	2	1.00416405471	0.000375112851817
SC	4	1.00416405471	0.000390962150246
SC	8	1.00416405471	0.000406864600682
SC	16	1.00416405471	0.000421349517322
SC	32	1.00416405471	0.000425027572716

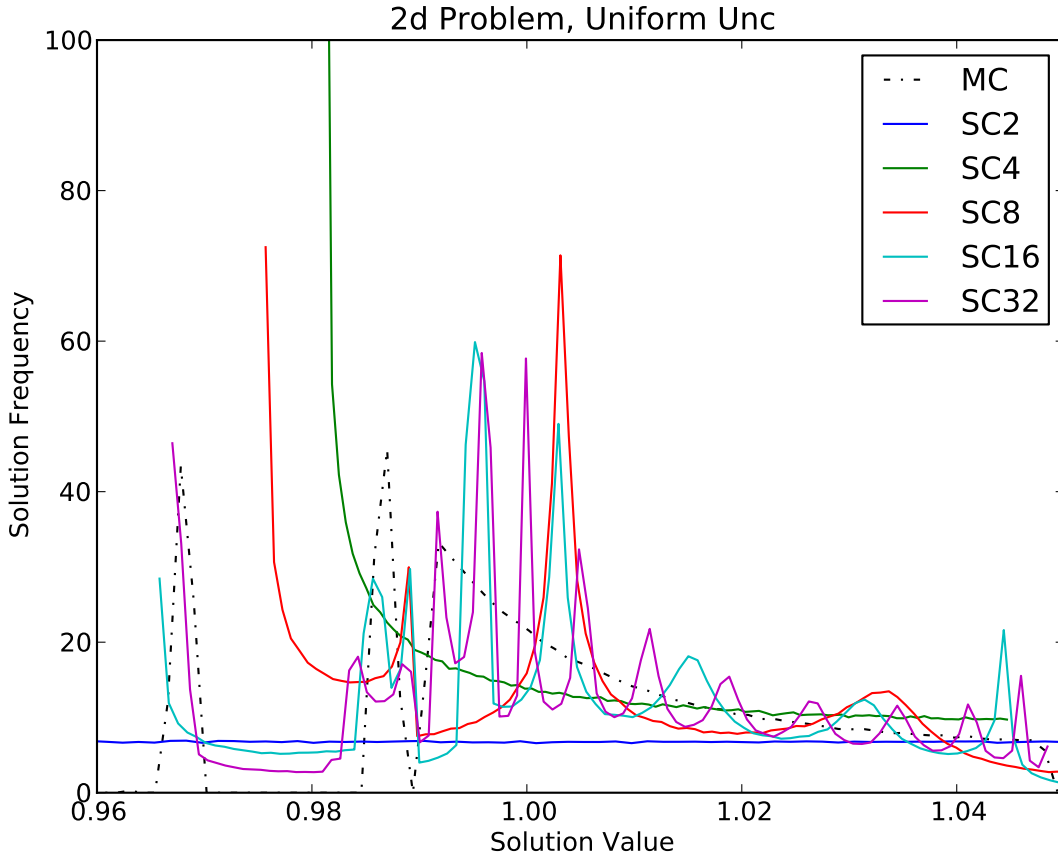Table 14: Convergence of Mean, Variance for 2D2G Case

Figure 9: Solution PDF Convergence, 2D2G Case

5.3.1.2 Normal Uncertainty

For this test we consider $\theta = \Sigma_{2,c}$ normally distributed as $\theta \in \mathcal{N}(0.0554, 0.01^2)$. Tabular data for mean and variance convergence is in Table 15, and the pdfs obtained are in Fig. 10. 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 $\Sigma_{2,c}$, including negative values.

The PCESC runs all made use of order 32 quadrature to integrate chaos moments.

type	runs/order	mean	variance
MC	6×10^5	1.01333702129	0.00160652595587
SC	2	1.01643813464	0.00138703446968
SC	4	1.01643813464	0.00184314998697
SC	8	1.01643813464	0.00184690058216
SC	16	1.01643813464	0.00184724103523
SC	32	1.01643813464	0.00184726152781

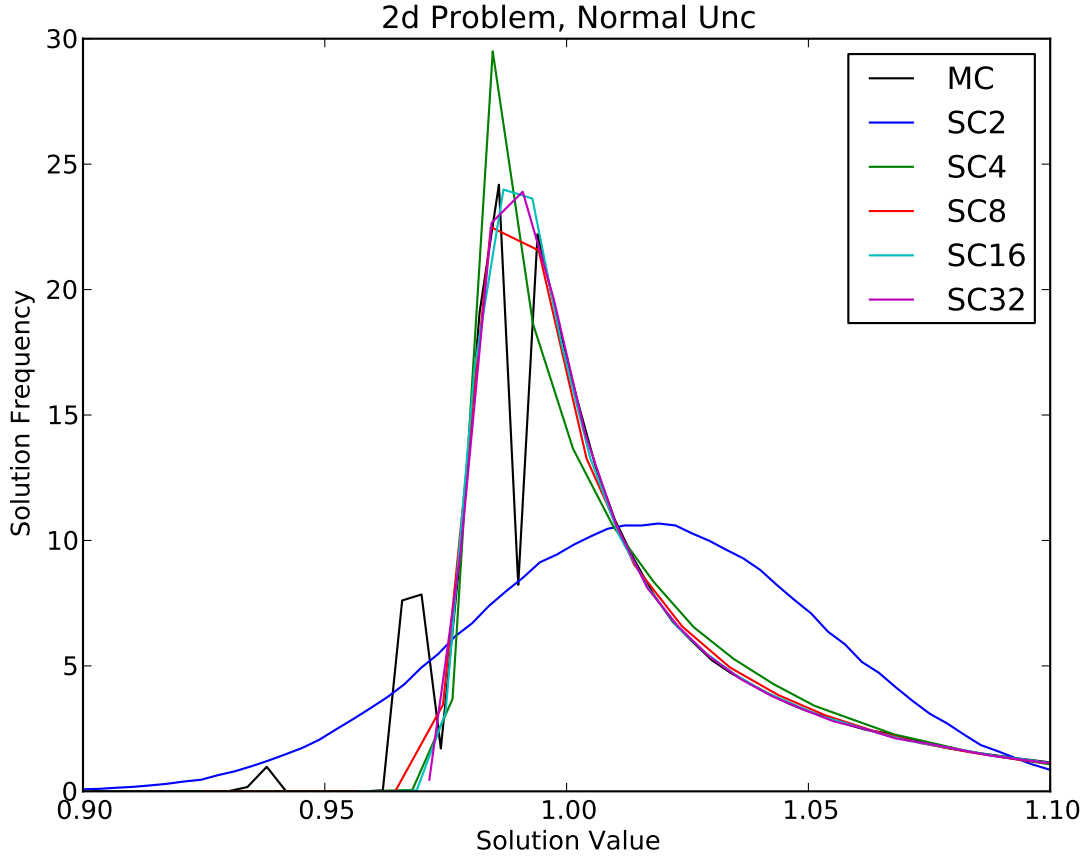Table 15: Convergence of Mean, Variance for 2D2G Case

Figure 10: Solution PDF Convergence, 2D2G Case

5.3.2 Multivariate

In this case we consider five uncertain parameters simultaneously, as in Table 16. Each was given approximately 10% uncertainty from its mean in the benchmark problem.

To explore the input space, we consider a variety of low-order expansions and one of higher order. The results are in Table 17.

Region	Energy Group	Parameter	Uncertainty
1	2	Σ_c	$\mathcal{U}(0.050, 0.061)$
1	2	Σ_f	$\mathcal{U}(0.098, 0.120)$
4	2	Σ_c	$\mathcal{U}(0.037, 0.046)$
4	2	Σ_f	$\mathcal{U}(0.092, 0.112)$
5	2	D	$\mathcal{U}(0.143, 0.175)$

Table 16: Multivariate Uncertainty Space

type	$\mathcal{O}(\Sigma_{2,c}^1, \Sigma_{2,f}^1, \Sigma_{2,c}^4, \Sigma_{2,f}^4, D_2^5)$	mean	variance
MC	1×10^6	0.995950138052	1.34575404516
SC	(2,2,2,2,2)	1.00261445437	0.000173828352441
SC	(4,2,2,2,2)	1.00125722573	0.000245435396045
SC	(2,4,2,2,2)	1.00125489157	0.000244969265818
SC	(2,2,4,2,2)	1.00261445458	0.000173828361529
SC	(2,2,2,4,2)	1.00261445431	0.000173828341974
SC	(2,2,2,2,4)	1.00261445434	0.000173828350938
SC	(4,4,2,2,2)	1.00261444028	0.00017376644541
SC	(6,6,2,2,2)	1.00192854415	0.000216430946449
SC	(8,8,8,8,8)	0.988408029125	1.17178207098

Table 17: Convergence of Mean, Variance for 2D2G Case

5.3.2.1 Convergence Study

There are several factors to consider in the selection of expansion orders for each input parameter. To inform us on appropriate expansion orders, we first consider each input parameter separately. Because they are independent, holding the other parameters at their means while exploring convergence in expansion order of a single parameter gives an appropriate estimate for each expansion order in a multivariate run. To increase run speed, we reduce the mesh refinement to its coarsest level (one grid cell per region). We use 256-order Gauss Legendre quadrature to construct 256 expansion moments for each input parameter separately. The results are shown in Fig. 11. The y-axis is the log of the magnitude of the expansion coefficient, and the x-axis is the expansion moments sorted by order. The coefficient magnitude falls of quickly over the first several terms and plateaus for each case; however, the high value plateau for the Region 1 material cross sections suggests a lack of convergence.
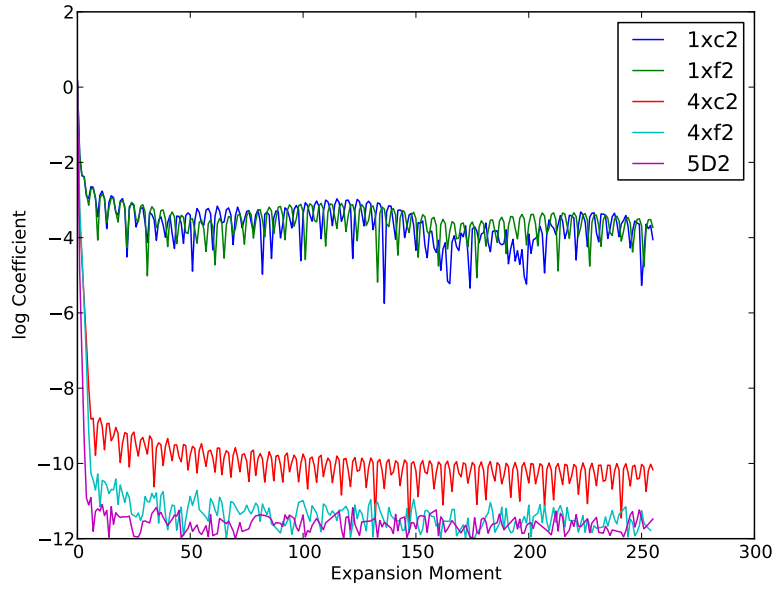
Figure 11: 2G2D: Coarse Mesh Coefficient Decay

We hypothesize that this lack of convergence is because of the discretization error in the solver with such a coarse mesh. To demonstrate the effect of increasing mesh refinement, we consider only the low-energy capture cross section for the first region (1xc2, $\Sigma_c^{(1)}$). The results are shown in Fig. ??.
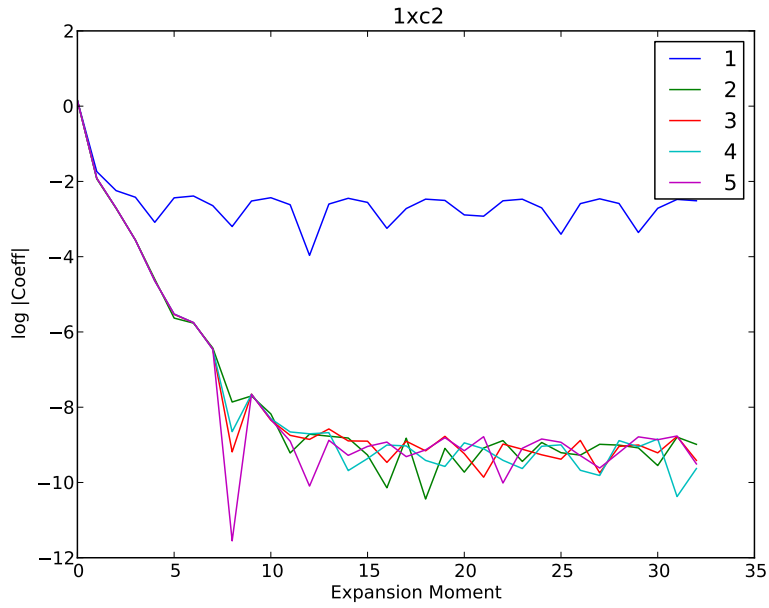

Figure 12: 2G2D: Coefficients over Mesh Refinement

It is worth noting that any integer increase in the mesh refinement per region results in a large increase in mesh refinement overall. The coarsest mesh, using a factor of 1 (1x1 grid cell per region) results in a mesh that is 11x11. A mesh factor of 2 (2x2 grid cells per region) increases the refinement to 22x22. This is equivalent to moving from $h = \Delta_x = \Delta_y = 15$ cm to $h = 7.5$ cm. For this particular set of parameters, increase the mesh factor from 1 to 2 is plenty to assure good convergence for this cross section. It can be the shown that the other Region 1 input parameter in this study behaves similarly and converges much further using a mesh factor of 2.

We perform the same convergence study as before, but using the more refined mesh and only continuing to order 32 expansions. The results are shown in Fig. 13. While the first region material cross sections don't converge as far as the fourth region and reflector (fifth region), they do converge much further. Looking at this plot, we can choose a multivariate expansion order that accurately represents the system. Table 18 shows the results of keeping different expansion orders chosen by imposing a coefficient convergence tolerance. In each case, the quadrature order used is double the expansion order.
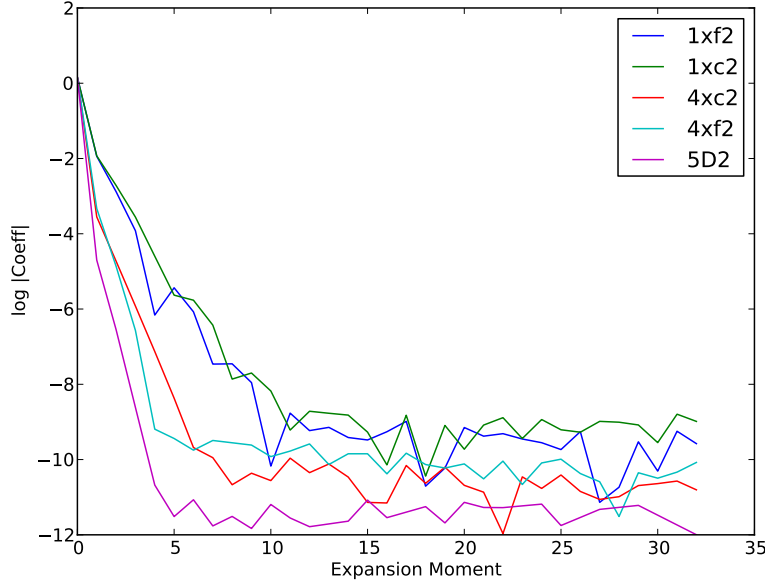

Figure 13: 2G2D: Coarse Mesh Coefficient Decay

type	tol	$\mathcal{P}(\Sigma_{2,c}^1, \Sigma_{2,f}^1, \Sigma_{2,c}^4, \Sigma_{2,f}^4, D_2^5)$	mean	variance
MC	-	-	0.999064586714	0.0262019588485
SC	1e-4	(5, 4, 3, 3, 1)	1.00191085676	0.000202816510815
SC	1e-5	(6, 5, 4, 3, 1)	1.00112487809	0.000554497293737
SC	1e-6	(8, 7, 5, 4, 2)	1.00018130781	0.00245280240592
SC	1e-8	(10, 9, 6, 4, 3)	1.00014901416	0.00207327774315

Table 18: Convergence of Mean, Variance for 2D2G Case, Expansion Tolerances

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