Deterministic Uncertainty Quantification with Raven

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1 Introduction

RAVEN (Reactor Analysis and Virtual control ENvironment) is a software framework that acts as the control logic driver for thermal hydraulic code RELAP-7. Central to the purpose of RELAP-7 is determining safety margins in accident-type scenarios for light water nuclear reactors.

Because the inputs to RELAP-7 are likely to have some level of uncertainty in them, RAVEN allows for the capability to use brute-force Monte Carlo to quantify output uncertainty in terms of input uncertainty. This makes it valuable as a PRA (probability risk assessment) code, and allows users to more clearly understand margins calculated with RELAP.

We propose a method of stochastic collocation methods along with generalized polynomial chaos to sample from the uncertainty space of input variables RELAP in an intelligent way and propagate those uncertainties through the code, leveraging RAVEN's interface. This avoids the need to introduce stochastic noise from Monte Carlo calculations and, for a limited number of uncertain inputs, offers significant speedup over brute force Monte Carlo for the same degree of precision. Stochastic collocation may be slower than Monte Carlo as the number of uncertain variables grows, but much of this loss can be gained by employing sparse grid methods to reduce the number of necessary samples. The accuracy cost in stochastic collocation and generalized polynomial chaos originates in truncating infinite sums to a small number of terms; the accuracy of the method generally increases with increasing terms.

We intend eventually to extend the uncertainty quantification tools in RAVEN to propagate uncertainty from inputs of one code through other coupled mutliphysics models in the MOOSE (multiphysics object-oriented simulation environment) system. Of particular interest is BISON, a fuels performance code, which could in turn provide inputs for RAVEN.

2 gPC: Generalized Polynomial Chaos

In general, stochastic processes can be represented efficiently by a basis consisting of an orthogonal set of polynomials, especially if chosen correctly. While homogeneous chaos only makes use of Hermite polynomials, a more generalized polynomial chaos (gPC) intelligently selects basis polynomials based on weighting functions.

Polynomial	Random Distr.	Weighting	Span
Legendre	Uniform	$1/2$	[-1,1]
Hermite	Normal	$\exp(-x^2)/\sqrt{2\pi}$	$(-\infty,\infty)$
Laguerre	Gamma	$x^{k-1}\exp(-x)/\Gamma(k)$	$[0,\infty)$

Consider an uncertain (and therefore treated as stochastic) process $U(p;\zeta)$ that is a function of its "certain" input parameters and phase space p as well as uncertain parameters ζ. In general, ζ may be the combination of many $(\zeta_1,\zeta_2,...,\zeta_n,...,\zeta_N)$ if U depends on many uncertain parameters. We wish to expand U in terms of one of the polynomial bases in order to quantify its uncertainty. The polynomial basis is chosen based on the form and span of the uncertainty, as shown in the table. For any case, U is expanded as

$$U(p;\zeta) \approx \sum_{i=1}^{I} c_i B_i(\zeta), \tag{1}$$

where the approximation is because of term truncation at $P_t < \infty$, c_i are polynomial coefficients, and B_i is the polynomial of order i that best fits the uncertainty in U. Since the polynomials are known, we can solve for the unknown coefficients using the orthogonality of the basis polynomials as

$$c_i = \frac{(U(p;\zeta),B_i(\zeta))}{(B_i(\zeta)^2)}, \tag{2}$$

using $(\cdot)$ as inner product notation

$$\big(f(x),g(x)\big) \equiv \int_S f(x)g(x)dx, \tag{3}$$

where S is the support of x.

3 SCM: Stochastic Collocation Method

The stochastic collocation method (SCM) makes use of quadrature sets to sample from the random space generated by uncertainty. We can make use of quadrature sets consisting of roots of the same polynomials used as basis functions in order to calculate the inner product for the gPC coefficients,

$$(U,B_i) \equiv \int U(\zeta)B_i(\zeta)d\zeta, \tag{4}$$

$$= \left(\int d\zeta_1 \int d\zeta_2 ... \int d\zeta_N\right) U(p;\zeta_1,\zeta_2,...,\zeta_N)B_i(\zeta_1,\zeta_2,...,\zeta_N), \tag{5}$$

$$\approx \left(\sum_{m_1=1}^{M_1} w_{m_1} \sum_{m_2=1}^{M_2} w_{m_2} ... \sum_{m_N=1}^{M_N} w_{m_N}\right) U(p;\zeta_{m_1},\zeta_{m_2},...,\zeta_{m_N})B_i(\zeta_{m_1},\zeta_{m_2},...,\zeta_{m_N}), \tag{6}$$

where w_{m_n} are weights obtained from quadrature sets corresponding to the polynomial basis chosen. The quadrature set may or may not have the same level of truncation as the polynomial expansion; that is, M_n need not be the same as M_1 or I.

We can further modify the inner product calculation by finding the coefficient term at node $\zeta_m \equiv (\zeta_{1,m_1}, ..., \zeta_{n,m_n}, ..., \zeta_{N,m_N})$ so that

$$c_i = \left(\sum_{m_1=1}^{M_1} w_{m_1} \sum_{m_2=1}^{M_2} w_{m_2} ... \sum_{m_N=1}^{M_N} w_{m_N} \right) c_i(\zeta_{1,m_1}, ..., \zeta_{n,m_n}, ..., \zeta_{N,m_N}), \tag{7}$$

$$= \left(\sum_{m_1=1}^{M_1} w_{m_1} \sum_{m_2=1}^{M_2} w_{m_2} ... \sum_{m_N=1}^{M_N} w_{m_N} \right) c_{i,m}, \tag{8}$$

$$c_{i,m} \equiv U(p;\zeta_m) B_i(\zeta_m), \tag{9}$$

where $c_{i,m}$ is the coefficient to the i-th order basis polynomial corresponding to a single sample realization m of $U(p;\zeta)$. Furthermore, we bring weights inward and multiply them to obtain weights that also correspond to a single realization m of U, so that

$$w_m = \prod_{h=1}^{N} w_{m_h}, \tag{10}$$

$$c_i = \left(\sum_{m_1=1}^{M_1} ... \sum_{m_n=1}^{M_n} ... \sum_{m_N=1}^{M_N} \right) w_m c_{i,m}. \tag{11}$$

This form of exansion is the "full tensor product expansion," since it uses all possible combinations of polynomial orders for each uncertain variable. Methods for reducing the number of combinations necessary will be discussed TODO.

3.1 Statistics

One way to compare the validity of stochastic collocation with generalized polynomial chaos expansion with the more standard Monte Carlo uncertainty quantification approach is to compare moments. For TODO REASONS we expect the first and second moment to be preserved in the polynomial expansion of $U(\zeta)$.

The first moment, the mean, is obtained by finding $U(\zeta)$ at the expected value. Since the coefficients of the expansion are constants, this is equivalent to evaluating the expansion at the expected values of the basis polynomials. In turn, these polynomials are evaluated at the expected value from the distribution of the uncertain variable. We use angle brackets $\langle U(\zeta) \rangle$ to indicate the expected value of $U(\zeta)$,

$$\langle U(\zeta) \rangle = \sum_i U_i \langle B_i(\zeta) \rangle, \tag{12}$$

$$= \sum_i U_i B_i(\langle \zeta \rangle), \tag{13}$$

$$= \sum_i U_i B_i(\langle \zeta_1 \rangle, \langle \zeta_2 \rangle, \cdots, \langle \zeta_N \rangle). \tag{14}$$

Assuming the expansion expressed in terms of standardized distributions and only the normal and uniform distributions are considered, the expected value of all ζ_n is zero, so only the first basis function term survives,

$$\langle U(\zeta)\rangle = \sum_i U_i B_i(\langle\zeta_1\rangle, \langle\zeta_2\rangle, \cdots, \langle\zeta_N\rangle), \tag{15}$$

$$= U_0 B_0. \tag{16}$$

The second moment is calculated as the expected value of the square of the function, and is used to compute the variance of the distribution,

$$\langle U^2(\zeta)\rangle = \sum_i U_i B_i(\langle\zeta^2\rangle). \tag{17}$$

For the normal and uniform distribution, general expressions for moments of ζ_n are shown in Table 1. For verification, moments can also be calculated by using Monte Carlo samples of ζ_n from its uncertainty distriubtion, and accumulated as shown in Table 1.

Moment	Uniform $\zeta_n \in (a,b)$	Normal $\zeta_n \in \mathcal{N}(\mu,\sigma^2)$	Monte Carlo
1 $\langle\zeta_n\rangle$	$\frac{1}{2}(b+a)$	μ	$\frac{1}{N}\sum_j \zeta_j$
2 $\langle\zeta_n^2\rangle$	$\frac{1}{2}(b^2+a^2)$	$\mu^2+\sigma^2$	$\frac{1}{N}\sum_j \zeta_j^2$

Table 1: Moments for uniform, normal distributions

The two statistics of interest, the expected value μ and population variance σ^2, are given by

$$\mu = \langle\zeta_n\rangle, \tag{18}$$

$$\sigma^2 = \langle\zeta_n^2\rangle - \langle\zeta_n\rangle^2. \tag{19}$$

3.2 Constructing Multidimensional Bases

We now give examples of expanding a multivariate function in multiple bases. In future sections we explore alternate distributions and polynomials, as well as mapping uncertain spaces onto the [0,1] normalized shifted Legendre polynomial space; for now, we assume all random variables ζ_n are already expressed as uncertain variables with values $\in [0,1]$.

3.2.1 Polynomials and Distributions

We consider a set of eight typical uncertainty distributions and their corresponding polynomials and quadrature. We summarize them in the table below, taken from TODO CITE Xiu and Karniadakis.

	Unc. Distribution	Basis Polynomials	Support
Continuous	Normal	Hermite	$(-\infty,\infty)$
	Gamma	Laguerre	$[0,\infty)$
	Beta	Jacobi	$[a,b]$
	Uniform	Legendre	$[a,b]$
Discrete	Poisson	Charlier	{0,1,2,...}
	Binomial	Krawtchouk	{0,1,...,N}
	Negative Binomial	Meixner	{0,1,2,...}
	Hypergeometric	Hahn	{0,1,...,N}

FIXME get rid of the discontinuous ones? They're not in scipy.
Definitions and examples of these distributions are included in the appendix.

3.2.2 Example: Single-Dimensional expansion, uniform

Starting with the simplest case, we consider a function of single uniform-uncertainty variable $\zeta = \zeta_1$,

$$f(\zeta) = a + b\zeta, \quad \zeta \in [-1, 1], \tag{20}$$

where a and b are arbitrary scalars. We expand $f(\zeta)$ in orthonormalized Legendre polynomials,

$$f(\zeta) = \sum_{i=0}^{\infty} f_i P_i(\zeta), \tag{21}$$

$$= \sum_{i=0}^{1} f_i P_i(\zeta). \tag{22}$$

We can truncate the sum at 1 term because we know a priori $f(\zeta)$ is order 1 in ζ, so it can be exactly represented by Legendre polynomials of up to order 1; in general, this is not known and perfect accuracy can only be guaranteed with infinite terms. Using the orthogonality of the normalized Legendre polynomials, we find the coefficients f_i given by

$$f_i = \int_{-1}^{1} f(\zeta) P_i(\zeta) d\zeta. \tag{23}$$

We can approximate the integral with Gauss-Legendre quadrature,

$$f_i = \sum_{\ell=0}^{\infty} w_\ell f(\zeta_\ell) P_i(\zeta_\ell), \tag{24}$$

$$= \sum_{\ell=0}^{1} w_\ell f(\zeta_\ell) P_i(\zeta_\ell), \tag{25}$$

where once again, because we know the Legendre polynomial order is no greater than 1 and $f(\zeta)$ is order 1, the integral has maximum order 3 and Legendre quadrature can exactly integrate polynomials of order $2n-1$. It is straightforward to insert the values from the Legendre quadrature set and see that the coefficients obtained are

$$f_0 = a\sqrt{2}, \quad f_1 = b\sqrt{\frac{2}{3}}. \tag{26}$$

If we reconstruct $f(\zeta)$ using these coefficients and the first three normalized Legendre polynomials, we obtain our original function $a + b\zeta$.

3.2.3 Example: Single-Dimensional expansion, normal

Starting with the simplest case, we consider a function of single uniform-uncertainty variable $\zeta = \zeta_1$,

$$f(\zeta) = a + b\zeta, \quad \zeta = \mathcal{N}(0, 1), \tag{27}$$

where $\mathcal{N}(0,1)$ indicates a Gaussian normal distribution with mean $\mu = 0$ and standard deviation $\sigma = 1$, and a and b are arbitrary scalars again. We expand using orthonormal (physician's) Hermite polynomials,

$$f(\zeta) = \sum_{i=0}^{1} f_i H_i(\zeta). \tag{28}$$

The Hermite polynomials are orthogonal with respect to the weighting function $W(x) = e^{-x^2}$, so that

$$\int_{-\infty}^{\infty} W(\zeta) H_m(\zeta) H_n(\zeta) d\zeta = \delta_{mn}, \tag{29}$$

The term $W(x)$ did not arise in the Legendre polynomial orthogonality discussion because it is unity, and can be omitted. To find the expansion coefficients f_i, we integrate both sides of Eq. 28 with respect to the weighting function and orthonormal Hermite polynomial,

$$\int_{-\infty}^{\infty} W(\zeta) H_i(\zeta) f(\zeta) d\zeta = \sum_i f_i \int_{-\infty}^{\infty} \rho(\zeta) H_i(\zeta) H_j(\zeta) d\zeta, \tag{30}$$

$$= f_i. \tag{31}$$

Before applying quadrature, it is important to note that Gauss-Hermite quadrature approximates integrals of the form

$$\int_{-\infty}^{\infty} W(x) f(x) dx = \sum_{\ell=0}^{\infty} w_\ell f(x_\ell). \tag{32}$$

Often, if $f(x)$ is known a priori, it's convenient to remove $W(x)$ from $f(x)$ (say, for example, if $f(x) = x^2 e^{-x^2}$). However, with our non-intrusive approach, we have to adjust $f(x)$ with $W^{-1}(x)$ in order to use Gauss-Hermite quadrature accurately. For clarity, we redefine everything under the integral as

$$g(\zeta) \equiv W(\zeta) H_i(\zeta) f(\zeta), \tag{33}$$

$$f_i = \int_{-\infty}^{\infty} g(\zeta) d\zeta. \tag{34}$$

Because we intend to use Gauss-Hermite quadrature, we multiply by $1 = W(\zeta) W^{-1}(\zeta)$,

$$f_i = \int_{-\infty}^{\infty} W(\zeta) \frac{g(\zeta)}{W(\zeta)} d\zeta, \tag{35}$$

$$= \sum_{\ell}^{L} w_\ell \frac{g(\zeta_\ell)}{W(\zeta_\ell)}, \tag{36}$$

$$= \sum_{\ell}^{L} w_\ell \frac{W(\zeta) H_i(\zeta) f(\zeta)}{W(\zeta)}, \tag{37}$$

$$= \sum_{\ell}^{L} w_\ell H_i(\zeta) f(\zeta). \tag{38}$$

In this example, we again truncate at 1st-order expansion and use order 2 quadrature,

$$
\begin{aligned}
f(\zeta) = a + b\zeta &= \sum_{i=0}^{1} f_i H_i(\zeta), && (39)\\
&= f_0 H_0(\zeta) + f_1 H_1(\zeta). && (40)
\end{aligned}
$$

The coefficients are obtained by

$$
\begin{aligned}
f_0 &= w_1 H_0(\zeta_1) f(\zeta_1) + w_2 H_0(\zeta_2) f(\zeta_2), && (41)\\
&= \frac{\sqrt{\pi}}{2}\frac{1}{\sqrt[4]{\pi}}\left(a - \frac{b}{\sqrt{2}}\right) + \frac{\sqrt{\pi}}{2}\frac{1}{\sqrt[4]{\pi}}\left(a + \frac{b}{\sqrt{2}}\right), && (42)\\
&= a\sqrt[4]{\pi}. && (43)
\end{aligned}
$$

$$
\begin{aligned}
f_1 &= w_1 H_1(\zeta_1) f(\zeta_1) + w_2 H_1(\zeta_2) f(\zeta_2), && (44)\\
&= \frac{\sqrt{\pi}}{2}\frac{(-1)}{\sqrt[4]{\pi}}\left(a - \frac{b}{\sqrt{2}}\right) + \frac{\sqrt{\pi}}{2}\frac{1}{\sqrt[4]{\pi}}\left(a + \frac{b}{\sqrt{2}}\right), && (45)\\
&= b\frac{\sqrt[4]{\pi}}{\sqrt{2}}. && (46)
\end{aligned}
$$

Recombining,

$$
\begin{aligned}
f(\zeta) = a + b\zeta &= \sum_{i=0}^{1} f_i H_i(\zeta), && (47)\\
&= f_0 H_0(\zeta) + f_1 H_1(\zeta), && (48)\\
&= a\sqrt[4]{\pi}\frac{1}{\sqrt[4]{\pi}} + b\frac{\sqrt[4]{\pi}}{\sqrt{2}}\frac{2\zeta}{\sqrt{2\sqrt{\pi}}}, && (49)\\
&= a + b\zeta. && (50)
\end{aligned}
$$

3.2.4 Example: Shifted Range

When the uncertain variable is on a non-standard range, it is simple to express the variable in terms of a standardly-distributed variable and make use of the standard weigths and measures. We use the same example as the single-dimensional case above, but using standard Legendre polynomials and uniformly uncertain variables $\zeta \in (a,b), \xi \in (-1,1)$, and define

$$\sigma \equiv \frac{b-a}{2} \text{ (range)}, \qquad \mu \equiv \frac{a+b}{2} \text{ (mean)}. \tag{51}$$

$$\begin{aligned} f(\zeta) &= a + b\zeta, \qquad \zeta \in [a,b], && (52)\\ &= \sum_i f_i P_i(\xi), \quad \xi \in [-1,1], && (53) \end{aligned}$$

$$\zeta = \sigma\xi + \mu, \qquad \xi = \frac{\zeta - \mu}{\sigma}, \tag{54}$$

$$\begin{aligned} f_i &= \int_{-1}^{1} f(\zeta(\xi)) P_i^*(\xi) d\xi, && (55)\\ &= \int_{-1}^{1} f(\sigma\xi + \mu) P_i(\xi) d\xi, && (56)\\ &\approx \sum_\ell w_\ell f(\sigma\xi_\ell + \mu) P_i(\xi_\ell). && (57) \end{aligned}$$

In the specific example case we can truncate at two terms,

$$f_i = \sigma w_1 f(\sigma x_1 + \mu) P_i(x_1) + w_2 f(\sigma x_2 + \mu) P_i(x_2). \tag{58}$$

The two coefficients are

$$\begin{aligned} f_0 &= (1)\left[a + b\left(\frac{-\sigma}{\sqrt{3}} + \mu\right)\right]\left(\frac{1}{\sqrt{2}}\right) + (1)\left[a + b\left(\frac{\sigma}{\sqrt{3}} + \mu\right)\right]\left(\frac{1}{\sqrt{2}}\right), && (59)\\ &= \frac{2}{\sqrt{2}}(a + b\mu), && (60)\\ &= \sqrt{2}(a + b\mu). && (61) \end{aligned}$$

$$\begin{aligned} f_1 &= (1)\left[a + b\left(\frac{-\sigma}{\sqrt{3}} + \mu\right)\right]\left(\sqrt{\frac{3}{2}}\frac{(-1)}{\sqrt{3}}\right) + (1)\left[a + b\left(\frac{\sigma}{\sqrt{3}} + \mu\right)\right]\left(\sqrt{\frac{3}{2}}\frac{1}{\sqrt{3}}\right), && (62)\\ &= b\sqrt{\frac{2}{3}}(\sigma - \mu). && (63) \end{aligned}$$

Reconstructing the original function,

$$\begin{aligned} f(\zeta) = a + b\zeta &= \sum_i f_i P_i(\xi), && (64)\\ &= f_0 P_0(\xi) + f_1 P_1(\xi), && (65)\\ &= (a + b\mu) + (b\sigma\xi), && (66)\\ &= a + b\mu + b\sigma\left(\frac{\zeta - \mu}{\sigma}\right), && (67)\\ &= a + b\zeta. && (68) \end{aligned}$$

3.2.5 Example: Multivariate Expansion

We now consider multidimensional function of ζ_1, ζ_2,

$$f(\zeta) \equiv f(\zeta_1, \zeta_2) = (a - b\zeta_1)(c - d\zeta_2), \tag{69}$$

where (a, b, c, d) are arbitrary scalars. We expand each dimension in normalized shifted Legendre polynomials,

$$f(\zeta) = \sum_{i_1=0}^{\infty} \sum_{i_2=0}^{\infty} f_{i_1,i_2} \tilde{P}_{i_1}(\zeta_1) \tilde{P}_{i_2}(\zeta_2), \tag{70}$$

where f_{i_1,i_2} is the combined coefficient for the multivariate polynomial term. The coefficients can be obtained in the same manner as the single dimension expansion,

$$f_{i_1,i_2} = \int_0^1 \int_0^1 f(\zeta) \tilde{P}_{i_1}(\zeta_1) \tilde{P}_{i_2}(\zeta_2) d\zeta_1 d\zeta_2, \tag{71}$$

and approximated with Legendre quadrature

$$f_{i_1,i_2} = \sum_{\ell_1=0}^{\infty} w_{\ell_1} \sum_{\ell_2=0}^{\infty} w_{\ell_2} f(\zeta_{1,\ell_1}, \zeta_{1,\ell_2}) \tilde{P}_{i_1}(\zeta_{1,\ell_1}) \tilde{P}_{i_2}(\zeta_{2,\ell_2}), \tag{72}$$

$$= \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} w_{\ell_1} w_{\ell_2} f(\zeta_{1,\ell_1}, \zeta_{1,\ell_2}) \tilde{P}_{i_1}(\zeta_{1,\ell_1}) \tilde{P}_{i_2}(\zeta_{2,\ell_2}). \tag{73}$$

Using the first two terms from each sum, we obtain the coefficients

$$f_{0,0} = \frac{(2a+b)(2c+d)}{4}, \tag{74}$$

$$f_{0,1} = \frac{d\sqrt{3}}{12}(2a+b), \tag{75}$$

$$f_{1,0} = \frac{b\sqrt{3}}{12}(2c+d) \tag{76}$$

$$f_{1,1} = \frac{bd}{12}, \tag{77}$$

$$f(x,y) = f_{0,0}\tilde{P}_0(\zeta_1)\tilde{P}_0(\zeta_2) + f_{0,1}\tilde{P}_0(\zeta_1)\tilde{P}_1(\zeta_2) + f_{1,0}\tilde{P}_1(\zeta_1)\tilde{P}_0(\zeta_2) + f_{1,1}\tilde{P}_1(\zeta_1)\tilde{P}_1(\zeta_2), \tag{78}$$

$$= (a + b\zeta_1)(c + d\zeta_2). \tag{79}$$

3.2.6 General Multivariate Expansion

From the two examples above, it is straightforward to extrapolate the general formulation for an expansion in an unknown number of dimensions. We consider a function of $\zeta \equiv (\zeta_1, \zeta_2, \cdots, \zeta_n, \cdots, \zeta_N)$

$$f(\zeta) \equiv f(\zeta_1, \cdots, \zeta_n, \cdots, \zeta_N). \tag{80}$$

We expand it in N dimensions in normalized shifted Legendre polynomials,

$$f(\zeta) = \sum_{i_1}^{\infty} \sum_{i_2}^{\infty} \cdots \sum_{i_N}^{\infty} f_{i_1, i_2, \cdots, i_N} \prod_{n=1}^{N} \tilde{P}_{i_n}(\zeta_n), \tag{81}$$

$$= \sum_{i_1}^{\infty} \cdots \sum_{i_N}^{\infty} f_i \prod_{n=1}^{N} \tilde{P}_{i_n}(\zeta_n), \tag{82}$$

where for simplicity we have defined f_i as the coefficient for the full set of polynomials at a particular set in the sum $i = (i_1, \cdots, i_N)$. As before, the coefficients f_i are determined using orthogonality,

$$f_i = \int_{-1}^{1} \cdots \int_{-1}^{1} \left[f(\zeta) \prod_{n=1}^{N} \tilde{P}_{i_n}(\zeta_n) \right] d\zeta_1 \cdots d\zeta_N, \tag{83}$$

which is approximated with Legendre quadrature as

$$f_i = \sum_{\ell_1=0}^{\infty} \cdots \sum_{\ell_N=0}^{\infty} \left(\prod_{n=1}^{N} w_{\ell_n} \right) f(\zeta_\ell) \prod_{n=1}^{N} \tilde{P}_{i_n}(\zeta_{n,\ell_n}), \tag{84}$$

$$= \sum_{\ell_1=0}^{\infty} \cdots \sum_{\ell_N=0}^{\infty} \left(\prod_{n=1}^{N} w_{\ell_n} \tilde{P}_{i_n}(\zeta_{n,\ell_n}) \right) f(\zeta_\ell), \tag{85}$$

where for convenience we define

$$f(\zeta_\ell) \equiv f(\zeta_{1,\ell_1}, \cdots, \zeta_{n,\ell_n}, \cdots \zeta_{N,\ell_N}). \tag{86}$$

4 Testing: Neutron Criticality

As a simple yet sufficiently complex problem to test stochastic collocation for uncertainty quantification, we make use of a 2-dimensional quarter-core reactor neutron diffusion code, which makes use of two energy groups and 11 distinct regions to nonlinearly solve for the k-eigenvalue of the system using Jacobian-free Newton-Krylov mothods. The sample model uses five materials and, without introducting uncertainty, is nearly exactly critical.

4.1 Problem Description

This test code solves the following equation:

$$-\nabla D_g \nabla \phi_g + \Sigma_{a,g}\phi_g = \sum_{g'} \Sigma_s^{g'g}\phi_{g'} + \frac{\chi_g}{k}\sum_{g'} \nu\Sigma_{f,g'}\phi_{g'}, \qquad g \in (1,2), \tag{87}$$

where k is the k_{eff} eigenvalue, g denotes an energy group (g=1 is high energy, g=2 is low energy), $\Sigma_s^{g'g}$ is the macroscopic scattering cross section from group g' into group g, and χ_g is the group-based neutron fission emission spectrum. For this particlar problem, we consider no upscattering and all fissions in to the high energy group. The two-dimensional core is shown in Fig. 1 and the material properties are listed in Table 2.

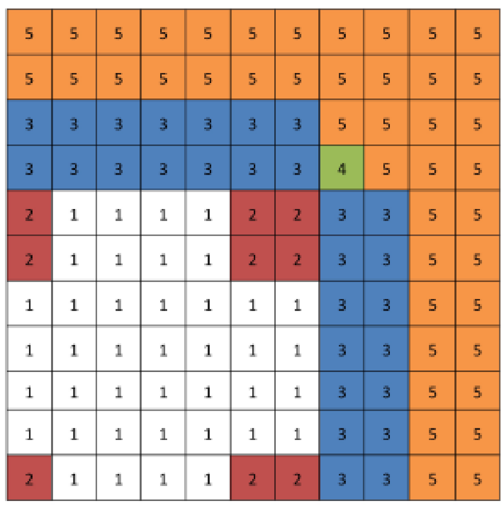


Figure 1: Core Map

4.1.1 Base Results

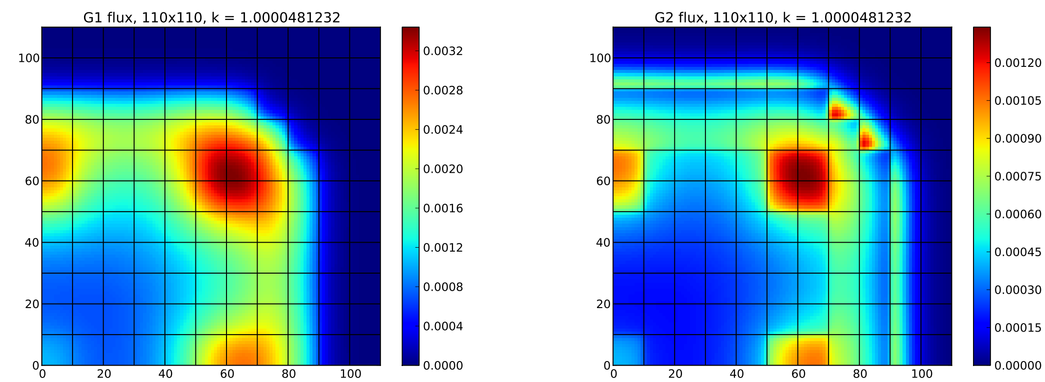
Without introducing uncertainty, the flux profiles by group are shown in Figs. 2a and 2b and $k-$effective is unity to 6 significant digits. Using 100 cells (10 by 10) in each region shown in Fig. 1, k is 1.000048123 converged to 8 orders of magnitude.

4.2 Single Variable Uncertainty

We begin by introducing uncertainty into a single material property; in this case, we chose the Material 1 low-energy absorption cross section. We test both the uniform uncertainty distribution

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 2: Basic Material Properties for Core



(a) High Energy

(b) Low Energy

Figure 2: Base Flux Profiles for Core (no uncertainty)

and normal distribution. In both cases, the mean value is $\Sigma_a^2 = 0.1003$ cm^{-1}.

For the uniform distribution, we allow the value to range uniformly from 30% above to 30% below the mean value, or $\Sigma_a^2 \in (0.07021, 0.13039)$ (this leads to $k \in (0.9707, 1.276)$). The coefficients for the standard orthonormal Legendre expansion are given as follows for several expansion orders, to 4 significant figures:

Similar to the uniform distribution, for the normal distribution we assign a standard deviation of 1% of the mean. The coefficients from the standard orthonormal Hermite expansion are given as follows for expansion orders, to 4 significant figures:

To demonstrate the use of the reduced-order models (ROMs) generated by the code, we sampled each expansion with a million Monte Carlo samples of the uncertain variable. We performed this in both single-processor and embarassingly parallel cases; the run time for an eigth-order expansion was 52 seconds in 4-processor parallel and 195 seconds on a single processor, both for the uniform uncertainty case. The values were then collected in 100 evenly-distributed bins across the range of the values obtained and collected as a numeric PDF. The results for both the uniform uncertainty and normal uncertainty are shown in Figs. 3 and 4.

Coeff	2	4	6	8
f_0	1.479	1.476	1.469	1.476
f_1	-9.698e-2	-1.075e-1	-1.109e-1	-1.081e-1
f_2		5.223e-2	5.946e-2	5.282e-2
f_3		-1.471e-2	-6.970e-3	-1.275e-2
f_4			-5.973e-3	-2.302e-3
f_5			-4.862e-3	2.285e-3
f_6				6.144e-4
f_7				1.245e-3

Table 3: Uniform Uncertainty Expansion Coefficients for Diffusion

Coeff	2	4	6	8
f_0	1.353	1.338	1.321	1.351
f_1	-4.319e-2	-5.928e-2	-6.903e-2	-5.051e-2
f_2		3.083e-2	4.056e-2	2.728e-2
f_3		-2.640e-4	1.144e-2	-8.195e-3
f_4			-6.678e-3	-1.524e-3
f_5			-1.656e-2	2.150e-3
f_6				5.933e-4
f_7				-1.584e-3

Table 4: Uniform Uncertainty Expansion Coefficients for Diffusion

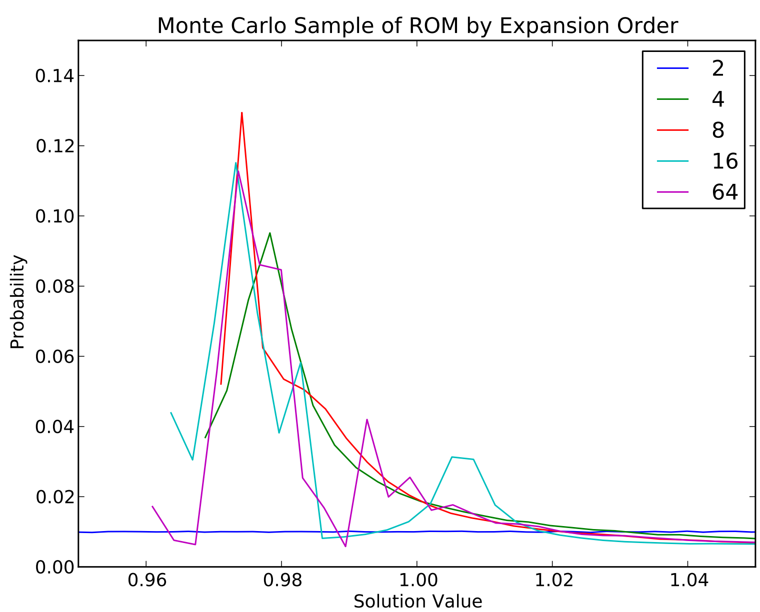


Figure 3: Uniform uncertainty

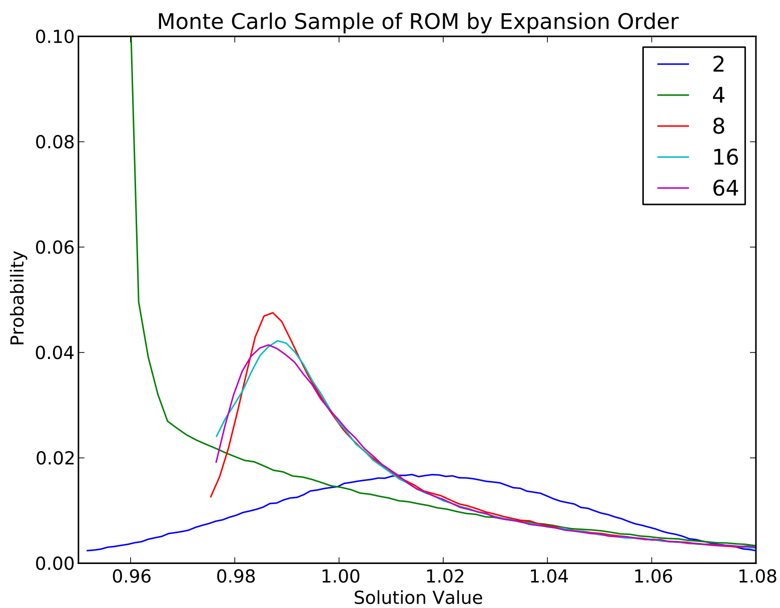


Figure 4: Normal uncertainty

A Polynomials and Distributions

For reference we include the polynomial, distribution, and quadrature definitions for the continuous distributions used in this document. To describe polynomials, we make use of the Pachhammer symbol $(a)_n$

$$(a)_n = a(a+1)(a+2)...(a+n-1), \quad n = 1, 2, 3, ... \tag{88}$$

with $(a)_n = 1$. The generalized hypergeometric series ${}_rF_s$ is given by

$${}_rF_s(a_1, ..., a_r; b_1, ..., b_s; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_r)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!}. \tag{89}$$

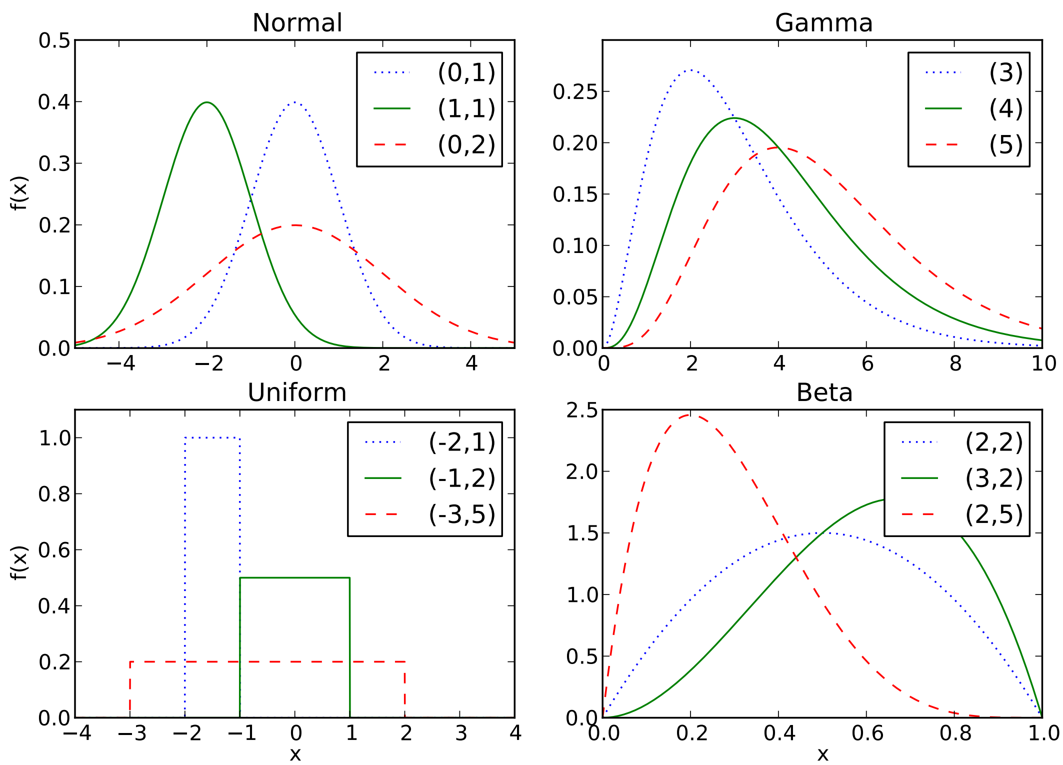


Figure 5: Several Distributions

A.1 Standard Distributions

There are several standard distributions for which quadratures with corresponding polynomials are well-known, making them efficiently represented with small quadratures. We present four here: normal, Gamma, uniform, and Beta.

A.1.1 Normal and Hermite He_n

The normal or Gaussian distribution has support from $-\infty$ to ∞ and is characterized by Hermite polynomials, with the associated Gauss-Hermite quadrature. The pdf of the normal distribution has the form

$$\xi(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \quad x \in (-\infty, \infty), \tag{90}$$

where μ, σ^2 are the mean and variance respectively. Two different kinds of Hermite polynomials exist: one the "probabilist" Hermite polynomial $\mathrm{He}_n(x)$, and the more often seen "physicist" Hermite polynomial $H_n(x)$. The two are essentially the same with the important exception $H_n(x/\sqrt{2}) = \mathrm{He}_n(x)$.

$$\mathrm{He}_n = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2}, \tag{91}$$

$$H_n = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{92}$$

We make use of the probabilist here because of its conformity with the Gaussian distribution. The Hermites are orthogonal,

$$\int_{-\infty}^{\infty} \mathrm{He}_m(x)\mathrm{He}_n(x) e^{-x^2/2} dx = \sqrt{2\pi} n! \delta_{nm}. \tag{93}$$

Hermite quadrature integrates exactly functions of the kind

$$\int_{-\infty}^{\infty} f(x) e^{-x^2/2} dx = \sum_{\ell=0}^{L} w_\ell f(x_\ell). \tag{94}$$

The abscissas of the quadrature are given by roots of the He_n polynomial and weights are given by

$$w_\ell = \frac{L!\sqrt{2\pi}}{n^2[\mathrm{He}_{n-1}(x_\ell)]^2}. \tag{95}$$

A normal distribution is shown with $\mu = 0, \sigma^2 = 1$ in Fig. 5.

A.1.2 Gamma and Laguerre L_n^α

The Gamma distribution has support from 0 to ∞ and is characterized by Laguerre polynomials with the associated Gauss-Laguerre quadrature. The pdf of the Gamma distribution has the form

$$\xi(x;\alpha,\beta) = \frac{x^\alpha e^{-x/\beta}}{\beta^{\alpha+1}\Gamma(\alpha+1)}, \quad \alpha > -1, \beta > 0, x \in (0,\infty), \tag{96}$$

$$\Gamma(\alpha) \equiv \int_0^\infty t^\alpha e^{-t} \frac{dt}{t}, \tag{97}$$

$$\Gamma(\alpha+1) = \alpha\Gamma(\alpha), \tag{98}$$

where α, β are shape and scale constants, respectively. The (generalized) Laguerre polynomials $L_n^{(\alpha)}$ are the solutions to the second order PDE

$$xy'' + (\alpha+1-x)y' + ny = 0, \tag{99}$$

and are given by

$$L_n^{(\alpha)}(x) = \frac{x^{-\alpha}e^x}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^{n+\alpha}\right), \tag{100}$$

$$= \frac{(\alpha+1)_n}{n!}\,{}_1F_1(-n;\alpha+1;x), \tag{101}$$

$$\int_0^\infty e^x x^\alpha L_m^{(\alpha)}(x) L_n^{(\alpha)}(x) dx = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{mn}, \quad \alpha > -1. \tag{102}$$

General Laguerre quadrature exactly integrates functions of the kind

$$\int_0^\infty f(x)e^{-x}x^\alpha dx = \sum_{\ell=0}^{N} w_\ell^{(\alpha)} f(x_\ell^{(\alpha)}). \tag{103}$$

The abscissas of the quadrature are the roots of the polynomial $L_n^{(\alpha)}$, and the weights are given by

$$w_\ell^{(\alpha)} = \frac{1}{x_\ell^{(\alpha)}}\left(\frac{d}{dx}L_N^{(\alpha)}(x_\ell^{(\alpha)})\right)^{-1}. \tag{104}$$

A Gamma distribution with shape $\alpha = 3$ and scale $\beta = 1$ is shown in Fig. 5.

A.1.3 Uniform and Legendre P_n

The uniform distribution has support from a to b, but is typically defined over the domain [-1,1], and is characterized by Legendre polynomials with the associated Gauss-Legendre quadrature. The pdf of the uniform distribution is flat between a and b and zero everywhere else,

$$\xi(x; a, b) = \frac{1}{b-a}, \qquad x \in [a, b], \tag{105}$$

where a, b are the maximum and minimum value, respectively. The Legendre polynomials $P_n(x)$ are solutions to the PDF

$$\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}P_n(x)\right] + n(n+1)P_n(x) = 0, \tag{106}$$

and are given by

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^2\right], \tag{107}$$

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \frac{2}{2n+1}\delta_{mn}. \tag{108}$$

It should be noted that shifting $P_n(x), x \in [-1, 1]$ to $P_n(z), z \in [a, b]$ is performed by the transformation

$$P_n(z) = \frac{b-a}{2}P_n\left(\frac{b-a}{2}x + \frac{a+b}{2}\right), \quad x \in [-1, 1], z \in [a, b]. \tag{109}$$

Legendre quadrature exactly integrates functions of the kind

$$\int_{-1}^{1} f(x)dx = \sum_{\ell=0}^{L} w_\ell f(x_\ell). \tag{110}$$

The abscissas of the quadrature are the roots of the polynomial P_n, and the weights are given by

$$w_\ell = \frac{2}{(1-x_\ell^2)\left[\frac{d}{dx}P_n(x_\ell)\right]^2}. \tag{111}$$

A uniform distribution with minimum -1 and double-range 2 is shown in Fig. 5.

A.1.4 Beta and Jacobi $P_n^{(\alpha,\beta)}$

The Beta distribution has the same support as the uniform distribution, a to b, but is often defined over the domain [0,1], and is characterized by Jacobi polynomials with associated Jacobi quadrature. The Legendre polynomials are a particular type of the Jacobi polynomials with $\alpha = \beta = 0$. The pdf of the beta distribution is given by

$$\xi(x;\alpha,\beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}, \quad x \in [0,1], \tag{112}$$

$$B(\alpha,\beta) = \int_0^1 t^{\alpha-1}(1-t)^{\beta-1}dt, \tag{113}$$

where α, β are shape parameters. The Jacobi polynomials are given by

$$\begin{aligned} P_n^{(\alpha,\beta)}(x) &= \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left[(1-x)^{-}\alpha(1+x)^{\beta}(1-x^2)^n\right], & (114) \\ &= \frac{(\alpha+1)_n}{n!}{}_2F_1\left(-n, 1+\alpha+\beta+n; \alpha+1; \frac{1-x}{2}\right), & (115) \end{aligned}$$

$$\int_{-1}^1 (1-x)^{\alpha}(1+x)^{\beta}P_m^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)dx = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)n!}\delta_{mn}. \tag{116}$$

Jacobi quadrature exactly integrates functions of the kind

$$\int_{-1}^1 f(x)(1-x)^{\alpha}(1+x)^{\beta}dx = \sum_{\ell=0}^{L} w_\ell f(x_\ell). \tag{117}$$

The abscissas of the quadrature are the roots of the polynomial $P_n^{(\alpha,\beta)}$, and the weights are given by

$$w_\ell = -\frac{(2n+\alpha+\beta+2)}{(n+\alpha+\beta+1)}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)(n+1)!}\frac{2^{\alpha+\beta}}{P_{n+1}(x_\ell)\frac{d}{dx}P_n(x_\ell)}. \tag{118}$$

A beta distribution with $\alpha = 2, \beta = 2$ is shown in Fig. 5.

A.2 Non-Standard Distributions

There are many other distributions commonly used in uncertainty, but without a convenient set of polynomials and quadrature to fit them. Because of the widespread use of these distributions, we present some here with approaches to representation by quadrature and polynomials.

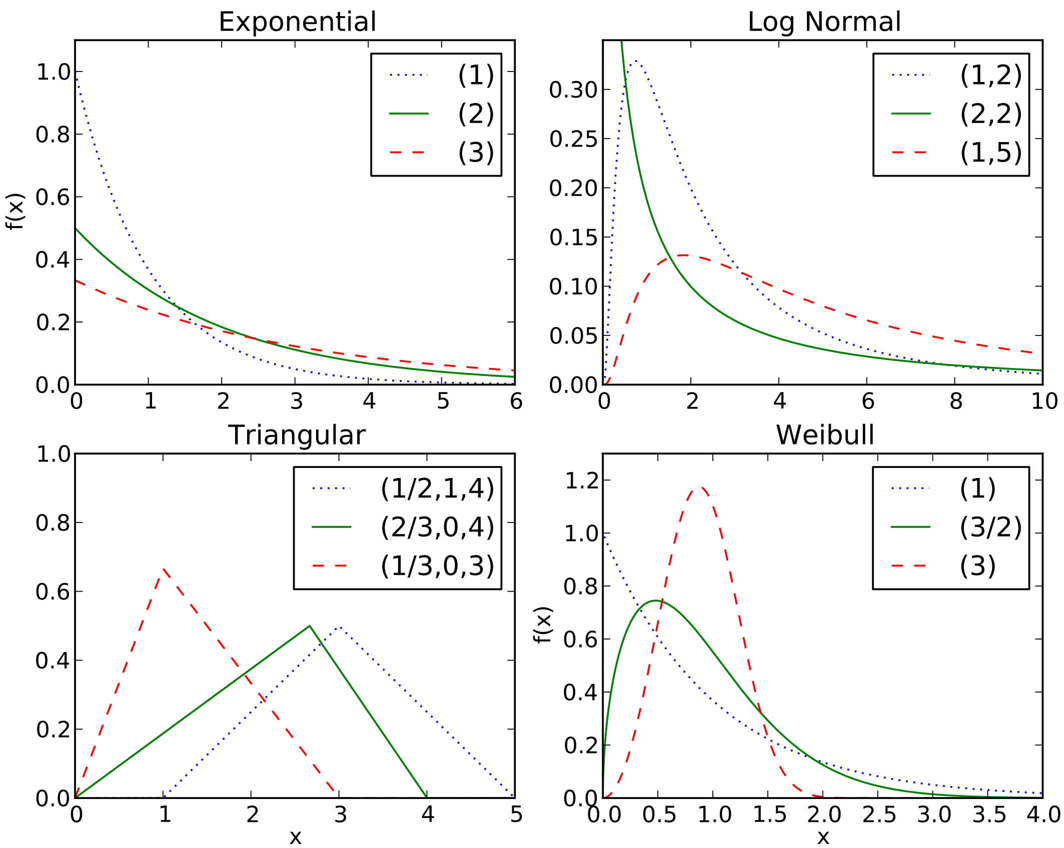


Figure 6: Alternate Distributions

A.3 Exponential

The exponential distribution ranges from 0 to ∞ and has the form

$$\xi(x; \alpha = \alpha e^{-\alpha x}, x \in [0, \infty), \tag{119}$$

where α is a rate scaling factor. TODO finish.

A.3.1 Lognormal

The log normal is descriptively the log of the normal distribution. It ranges from 0 to ∞ and has the form

$$\xi(x;\mu,\sigma^2) = \frac{1}{x\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\ln x - \mu)^2}{2\sigma^2}\right), \quad x \in (0,\infty). \tag{120}$$

where μ, σ^2 are the mean and variance, respectively. TODO finish.

A.3.2 Triangular

The triangular distribution ranges from a to b and rises linearly from a to a point, after which it falls linearly to b. The pdf is given by

$$\xi(x;a,b,c) = \begin{cases} 0, & x < a, \\ \frac{2(x-a)}{(b-a)(c-a)}, & a \leq x \leq c, \\ \frac{2(b-x)}{(b-a)(b-c)}, & c < x \leq b, \\ 0, & b < x, \end{cases} \tag{121}$$

where a, b, c are the minimum, maximum, and location of the highest point, respectively. TODO finish.

A.3.3 Weibull

The Weibull distribution ranges from 0 to ∞ and has the form

$$\xi(x;\lambda,k) = \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k}, \tag{122}$$

where λ, k are the scale and shape parameters, respectively. Often, $\lambda = 1$ and k is the only shaping parameter. TODO finish.

A.3.4 Arbitrary

Many other distributions may arise in characterizing the uncertainty of input parameters. In the event none of the above distributions are close enough, using the distribution's ppf to represent it using shifted Legendre polynomials is recommended, with care for the number of terms used.

B Nonlinear Methodology: JFNK

The diffusion code in Section 4 makes use of the Jabobian-free Newton-Krylov solver method for nonlinear problems. Specifically, the problem is solved using the `GMRES` algortihm found in the Sandia solver package `Trilinos` TODO cite. The three coupled equations to solve, in weak form, are

$$F_k(\phi_1, \phi_2, k) = k - \int_V \sum_g \nu\Sigma_{f,g}\phi_g dV = 0, \tag{123}$$

$$F_{\phi_g}(\phi_1, \phi_2, k) = -\nabla D_g \nabla\phi_g + \Sigma_{a,g}\phi_g - \sum_{g'} \Sigma_s^{g'g}\phi_{g'} - \frac{\chi_g}{k(\phi)} \sum_{g'} \nu\Sigma_{f,g'}\phi_{g'} = 0, \qquad g \in (1,2). \tag{124}$$

Because JFNK has a relatively small radius of convergence, we employ standard power iteration for several iterations before using the `GMRES` package. Since power iteration has a much larger radius of convergence, this assures the flux profiles are near enough to the actual solution that the JFNK method can converge on the base k-eigenvalue. In addition, we employ a very simple preconditioning matrix, which uses only the diagonal of the Jacobian matrix. Allowing $u = (\phi_1, \phi_2, k)$, each Newton step in the solution process is

$$u^{m+1} = u^m + \delta u^m, \tag{125}$$

$$(\mathcal{J}^m M^{-1})(M\delta u^m) = -F(u^m), \tag{126}$$

or, rewritten with $M\delta u^m \equiv \delta x$,

$$\delta x = (\mathcal{J}^m M^{-1})^{-1} F(u^m), \tag{127}$$

and we approximate the Jacobian-preconditioner-vector product as

$$\mathcal{J}^m M^{-1} v = \frac{F(u^m + M^{-1}\epsilon v) - F(u^m)}{\epsilon}, \tag{128}$$

which can be derived by truncating the Taylor expansion of $F(u^m + M^{-1}\epsilon v)$ about u^m. Since the preconditioning matrix M is only the diagonal of the Jacobian,

$$M = \begin{pmatrix} M_{\phi_1\phi_1} & 0 & 0 \\ 0 & M_{\phi_2\phi_2} & 0 \\ 0 & 0 & M_{kk} \end{pmatrix}, \tag{129}$$

$$M_{xy} \equiv \frac{dF_x(x,y)}{dy}. \tag{130}$$

In this particular case,

$$M_{\phi_1\phi_1} = -\nabla \cdot D_1 \nabla + \Sigma_{a_1} - \Sigma_s^{1\to 2} - \nu\Sigma_{f,1}, \tag{131}$$

$$M_{\phi_2\phi_2} = -\nabla \cdot D_2 \nabla + \Sigma_{a,2} - \nu\Sigma_{f,2}, \tag{132}$$

$$M_{kk} = 1. \tag{133}$$