Design Under Uncertainty Employing Stochastic Expansion Methods

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Non-intrusive polynomial chaos expansion (PCE) and stochastic collocation (SC) methods are attractive techniques for uncertainty quantification (UQ) due to their strong mathematical basis and ability to produce functional representations of stochastic variability. PCE estimates coefficients for known orthogonal polynomial basis functions based on a set of response function evaluations, using sampling, linear regression, tensor-product quadrature, or Smolyak sparse grid approaches. SC, on the other hand, forms interpolation functions for known coefficients, and requires the use of structured collocation point sets derived from tensor product or sparse grids. When tailoring the basis functions or interpolation grids to match the forms of the input uncertainties, exponential convergence rates can be achieved with both techniques for general probabilistic analysis problems. Once PCE or SC representations have been obtained for a response metric of interest, analytic expressions can be derived for the moments of the expansion and for the design derivatives of these moments, allowing for efficient design under uncertainty formulations involving moment control (e.g., robust design). This paper presents two approaches for moment design sensitivities, one involving response function expansions over both design and uncertain variables and one involving response derivative expansions over only the uncertain variables. These approaches present a trade-off between increased dimensionality in the expansions (and therefore increased simulation runs required to construct them) with global expansion validity versus increased data requirements per simulation with local expansion validity. Given this capability for analytic moments and their sensitivities, we explore bilevel, sequential, and multifidelity formulations for OUU. Initial experiences with these approaches is presented for a number of benchmark test problems.

I. Introduction

Uncertainty quantification (UQ) is the process of determining the effect of input uncertainties on response metrics of interest. These input uncertainties may be characterized as either aleatory uncertainties, which are irreducible variabilities inherent in nature, or epistemic uncertainties, which are reducible uncertainties resulting from a lack of knowledge. Since sufficient data is generally available for aleatory uncertainties, probabilistic methods are commonly used for computing response distribution statistics based on input probability distribution specifications. Conversely, for epistemic uncertainties, data is generally sparse, making the use of probability theory questionable and leading to nonprobabilistic methods based on interval specifications.

One technique for the analysis of aleatory uncertainties using probabilistic methods is the polynomial chaos expansion (PCE) approach to UQ. In this work, we focus on generalized polynomial chaos using the

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Wiener-Askey scheme,[1] in which Hermite, Legendre, Laguerre, Jacobi, and generalized Laguerre orthogonal polynomials are used for modeling the effect of uncertain variables described by normal, uniform, exponential, beta, and gamma probability distributions, respectively[a]. These orthogonal polynomial selections are optimal for these distribution types since the inner product weighting function and its corresponding support range correspond to the probability density functions for these continuous distributions. In theory, exponential convergence rates can be obtained with the optimal basis. When transformations to independent standard random variables (in some cases, approximated by uncorrelated standard random variables) are used, the variable expansions are uncoupled, allowing the polynomial orthogonality properties to be applied on a per-dimension basis. This allows one to mix and match the polynomial basis used for each variable without interference with the spectral projection scheme for the response.

In non-intrusive PCE, simulations are used as black boxes and the calculation of chaos expansion coefficients for response metrics of interest is based on a set of simulation response evaluations. To calculate these response PCE coefficients, two primary classes of approaches have been proposed: spectral projection and linear regression. The spectral projection approach projects the response against each basis function using inner products and employs the polynomial orthogonality properties to extract each coefficient. Each inner product involves a multidimensional integral over the support range of the weighting function, which can be evaluated numerically using sampling, quadrature, or sparse grid approaches. The linear regression approach (also known as point collocation or stochastic response surfaces) uses a single linear least squares solution to solve for the PCE coefficients which best match a set of response values obtained from a design of computer experiments.

Stochastic collocation (SC) is another stochastic expansion technique for UQ that is closely related to PCE. Whereas PCE estimates coefficients for known orthogonal polynomial basis functions, SC forms Lagrange interpolation functions for known coefficients. Since the i^{th} interpolation function is 1 at collocation point i and 0 for all other collocation points, it is easy to see that the expansion coefficients are just the response values at each of the collocation points. The formation of multidimensional interpolants with this property requires the use of structured collocation point sets derived from tensor product or sparse grids. The key to the approach is performing collocation using the Gauss points and weights from the same optimal orthogonal polynomials used in generalized PCE, which results in the same exponential convergence rates. A key distinction is that, whereas PCE must define an expansion order and a corresponding coefficient estimation approach, SC requires only a collocation grid definition from which the expansion polynomial order is derived based on Lagrange interpolation.

Once PCE or SC representations have been obtained for a response metric of interest, analytic expressions can be derived for the moments of the expansion and for the design derivatives of these moments, allowing for efficient design under uncertainty formulations involving moment control (e.g., robust design). To support reliability-based design involving tail statistics, one simple approach employs projection of these analytic moments to compute approximate reliability indices (used herein), and more sophisticated approaches could involve analytic response PDF fitting based on Pearson/Johnson models using the first four moments (possible future work). This paper presents two approaches for moment design sensitivities, one involving response function expansions over both design and uncertain variables and one involving response derivative expansions over only the uncertain variables. In the former case, the dimensionality of the expansions is increased (requiring increased simulation runs to construct them), but the technique remains zeroth-order and the expansion spans the design space (or potentially some subset of it). In the latter case, the expansion dimensionality is not increased, but accurate design gradients are now required for each simulation and the expansion over random variables must be regenerated for each new design point. The ability to compute analytic statistics and their design derivatives using these two approaches leads to bi-level, sequential, and multifidelity formulations to design under uncertainty.

Section II describes the orthogonal polynomial and interpolation polynomial basis functions, Section III describes the generalized polynomial chaos and stochastic collocation methods in additional detail, Section IV describes non-intrusive approaches for calculating the polynomial chaos coefficients, Section V presents attractive features of PCE methods for performing design under uncertainty, Section VI presents initial computational results, and Section VII provides concluding remarks.

[a]Orthogonal polynomial selections also exist for discrete probability distributions, but are not explored here.

II. Polynomial Basis

A. Orthogonal polynomials in the Askey scheme

Table 1 shows the set of polynomials which provide an optimal basis for different continuous probability distribution types. It is derived from the family of hypergeometric orthogonal polynomials known as the Askey scheme,[2] for which the Hermite polynomials originally employed by Wiener[3] are a subset. The optimality of these basis selections derives from their orthogonality with respect to weighting functions that correspond to the probability density functions (PDFs) of the continuous distributions when placed in a standard form. The density and weighting functions differ by a constant factor due to the requirement that the integral of the PDF over the support range is one.

Table 1. Linkage between standard forms of continuous probability distributions and Askey scheme of continuous hyper-geometric polynomials.

Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}}$	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty, \infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1, 1]$
Beta	$\frac{(1-x)^\alpha (1+x)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^\alpha (1+x)^\beta$	$[-1, 1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0, \infty]$
Gamma	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

Note that Legendre is a special case of Jacobi for $\alpha = \beta = 0$, Laguerre is a special case of generalized Laguerre for $\alpha = 0$, and the Beta function is defined as $B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$. Some care is necessary when specifying the α and β parameters for the Jacobi and generalized Laguerre polynomials since the orthogonal polynomial conventions[4] differ from the common statistical PDF conventions. The former conventions are used in Table 1.

B. Numerically generated orthogonal polynomials

If all random inputs can be described using independent normal, uniform, exponential, beta, and gamma distributions, then PCE can be directly applied. If correlation or other distribution types are present, then additional techniques are required. One solution is to employ nonlinear variable transformations as described in Section III.C such that an Askey basis can be applied in the transformed space. This can be effective as shown in Refs. 5, 6, but convergence rates are typically degraded. In addition, correlation coefficients are warped by the nonlinear transformation,[7] and transformed correlation values are not always readily available. An alternative is to numerically generate the orthogonal polynomials, along with their Gauss points and weights, that are optimal for given random variable sets having arbitrary probability density functions. This not only preserves exponential convergence rates, it also eliminates the need to calculate correlation warping. In this paper, we will explore Golub-Welsch[8] and Gram-Schmidt[9] algorithms for this. Of particular interest is demonstration of the preservation of exponential convergence rates with non-Askey bases.

C. Interpolation polynomials

Lagrange polynomials interpolate a set of points in a single dimension using the functional form

$$L_j = \prod_{\substack{k=1 \\ k \neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k} \tag{1}$$

where it is evident that L_j is 1 at $\xi = \xi_j$, is 0 for each of the points $\xi = \xi_k$, and has order $m - 1$.

For interpolation of a response function R in one dimension over m points, the expression

$$R(\xi) \cong \sum_{j=1}^{m} r(\xi_j)\, L_j(\xi) \tag{2}$$

reproduces the response values $r(\xi_j)$ at the interpolation points and smoothly interpolates between these values at other points. For interpolation in multiple dimensions, a tensor-product approach is used wherein

$$R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right) \tag{3}$$

where $\boldsymbol{i} = (m_1, m_2, \cdots, m_n)$ are the number of nodes used in the n-dimensional interpolation and $\xi_{j_m}^{i_k}$ is the j_mth point in the kth direction. As will be seen later, interpolation on sparse grids involves a summation of these tensor products.

III. Stochastic Expansion Methods

A. Generalized Polynomial Chaos

The set of polynomials from Section II.A are used as an orthogonal basis to approximate the functional form between the stochastic response output and each of its random inputs. The chaos expansion for a response R takes the form

$$R = a_0 B_0 + \sum_{i_1=1}^{\infty} a_{i_1} B_1(\xi_{i_1}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} a_{i_1 i_2} B_2(\xi_{i_1}, \xi_{i_2}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} B_3(\xi_{i_1}, \xi_{i_2}, \xi_{i_3}) + \ldots \tag{4}$$

where each additional set of nested summations indicates an additional order of polynomials in the expansion. This expression can be simplified by reformulating the expansion from an order-based indexing to a term-based indexing

$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi}) \tag{5}$$

where there is a one-to-one correspondence between $a_{i_1 i_2 \ldots i_n}$ and α_j and between $B_n(\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_n})$ and $\Psi_j(\boldsymbol{\xi})$. Each of the $\Psi_j(\boldsymbol{\xi})$ are multivariate polynomials which involve products of the one-dimensional polynomials. For example, a multivariate Hermite polynomial $B(\boldsymbol{\xi})$ of order n is defined from

$$B_n(\xi_{i_1}, \ldots, \xi_{i_n}) = e^{\frac{1}{2}\boldsymbol{\xi}^T \boldsymbol{\xi}} (-1)^n \frac{\partial^n}{\partial \xi_{i_1} \ldots \partial \xi_{i_n}} e^{-\frac{1}{2}\boldsymbol{\xi}^T \boldsymbol{\xi}} \tag{6}$$

which can be shown to be a product of one-dimensional Hermite polynomials involving a multi-index m_i^j:

$$B_n(\xi_{i_1}, \ldots, \xi_{i_n}) = \Psi_j(\boldsymbol{\xi}) = \prod_{i=1}^{n} \psi_{m_i^j}(\xi_i) \tag{7}$$

The first few multidimensional Hermite polynomials for a two-dimensional case (covering zeroth, first, and second order terms) are then

$$\begin{aligned}
\Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\, \psi_0(\xi_2) &&= 1 \\
\Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\, \psi_0(\xi_2) &&= \xi_1 \\
\Psi_2(\boldsymbol{\xi}) &= \psi_0(\xi_1)\, \psi_1(\xi_2) &&= \xi_2 \\
\Psi_3(\boldsymbol{\xi}) &= \psi_2(\xi_1)\, \psi_0(\xi_2) &&= \xi_1^2 - 1 \\
\Psi_4(\boldsymbol{\xi}) &= \psi_1(\xi_1)\, \psi_1(\xi_2) &&= \xi_1 \xi_2 \\
\Psi_5(\boldsymbol{\xi}) &= \psi_0(\xi_1)\, \psi_2(\xi_2) &&= \xi_2^2 - 1
\end{aligned}$$

Thus, a generalized polynomial basis is generated by selecting the univariate basis that is most optimal for each random input and then applying the products as defined by the multi-index to define a mixed set of multivariate polynomials. Similarly, the multivariate weighting functions involve a product of the one-dimensional weighting functions and the multivariate quadrature rules involve a tensor product of the one-dimensional quadrature rules.

The use of independent standard random variables is the critical component that allows decoupling of the multidimensional integrals in a mixed basis expansion. It is assumed in this work that the uncorrelated

standard random variables resulting from the transformation described in Section III.C can be treated as independent. This assumption is valid for uncorrelated standard normal variables (and motivates the approach of using a strictly Hermite basis), but is an approximation for uncorrelated standard uniform, exponential, beta, and gamma variables. For independent variables, the multidimensional integrals involved in the inner products of multivariate polynomials decouple to a product of one-dimensional integrals involving only the particular polynomial basis and corresponding weight function selected for each random dimension. The multidimensional inner products are nonzero only if each of the one-dimensional inner products is nonzero, which preserves the desired multivariate orthogonality properties for the case of a mixed basis.

In practice, one truncates the infinite expansion at a finite number of random variables and a finite expansion order

$$R \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}) \tag{8}$$

where the total number of terms N_t in a complete polynomial chaos expansion of arbitrary order p for a response function involving n uncertain input variables is given by

$$N_t \;=\; 1 + P \;=\; 1 + \sum_{s=1}^{p} \frac{1}{s!} \prod_{r=0}^{s-1} (n+r) \;=\; \frac{(n+p)!}{n!p!} \tag{9}$$

B. Stochastic Collocation

The SC expansion is formed as a sum of a set of multidimensional Lagrange interpolation polynomials, one polynomial per collocation point. Since these polynomials have the feature of being equal to 1 at their particular collocation point and 0 at all other points, the coefficients of the expansion are just the response values at each of the collocation points. This can be written as:

$$R \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi}) \tag{10}$$

where the set of collocation points could involve a tensor product grid as shown in Eq. 3 or a sum of tensor products defined from a sparse grid (refer to Section IV.A.3).

C. Transformations to uncorrelated standard variables

Polynomial chaos and stochastic collocation are expanded using polynomials that are functions of independent standard random variables $\boldsymbol{\xi}$. The dimension of $\boldsymbol{\xi}$ is typically chosen to correspond to the dimension of the original random variables $\boldsymbol{x}$, although this is not required. In fact, the dimension of $\boldsymbol{\xi}$ should be chosen to represent the number of distinct sources of randomness in a particular problem, and if individual x_i mask multiple random inputs, then the dimension of $\boldsymbol{\xi}$ can be expanded to accommodate.[10] For simplicity, all subsequent discussion will assume a one-to-one correspondence between $\boldsymbol{\xi}$ and $\boldsymbol{x}$.

This notion of independent standard space is extended over the notion of "u-space" used in reliability methods[11,12] in that in includes not just independent standard normals, but also independent standardized uniforms, exponentials, betas and gammas. For problems directly involving independent normal, uniform, exponential, beta, and gamma distributions for input random variables, conversion to standard form involves a simple linear scaling transformation (to the form of the density functions in Table 1) and then the corresponding chaos/collocation points can be employed. For correlated normal, uniform, exponential, beta, and gamma distributions, the same linear scaling transformation is applied followed by application of the inverse Cholesky factor of the correlation matrix (similar to Eq. 12 below, but the correlation matrix requires no modification for linear transformations). As described previously, the subsequent independence assumption is valid for uncorrelated standard normals but introduces error for uncorrelated standard uniform, exponential, beta, and gamma variables. For other distributions with a close relationship to variables supported in the Askey scheme (i.e., lognormal, loguniform, and triangular distributions), a nonlinear transformation is employed to transform to the corresponding Askey distributions (i.e., normal, uniform, and uniform distributions, respectively) and the corresponding chaos polynomials/collocation points are employed. For other less directly-related distributions (e.g., extreme value distributions), the nonlinear Nataf transformation is

employed to transform to uncorrelated standard normals as described below and Hermite polynomials are employed.

The transformation from correlated non-normal distributions to uncorrelated standard normal distributions is denoted as $\boldsymbol{\xi} = T(\mathbf{x})$ with the reverse transformation denoted as $\mathbf{x} = T^{-1}(\boldsymbol{\xi})$. These transformations are nonlinear in general, and possible approaches include the Rosenblatt,[13] Nataf,[7] and Box-Cox[14] transformations. The nonlinear transformations may also be linearized, and common approaches for this include the Rackwitz-Fiessler[15] two-parameter equivalent normal and the Chen-Lind[16] and Wu-Wirsching[17] three-parameter equivalent normals. The results in this paper employ the Nataf nonlinear transformation, which is suitable for the common case when marginal distributions and a correlation matrix are provided, but full joint distributions are not known[b]. The Nataf transformation occurs in the following two steps. To transform between the original correlated x-space variables and correlated standard normals ("z-space"), a CDF matching condition is applied for each of the marginal distributions:

$$\Phi(z_i) = F(x_i) \tag{11}$$

where $\Phi()$ is the standard normal cumulative distribution function and $F()$ is the cumulative distribution function of the original probability distribution. Then, to transform between correlated z-space variables and uncorrelated ξ-space variables, the Cholesky factor $\mathbf{L}$ of a modified correlation matrix is used:

$$\mathbf{z} = \mathbf{L}\boldsymbol{\xi} \tag{12}$$

where the original correlation matrix for non-normals in x-space has been modified to represent the corresponding "warped" correlation in z-space.[7]

IV. Non-intrusive methods for expansion formation

The major practical difference between PCE and SC is that, in PCE, one must estimate the coefficients for known basis functions, whereas in SC, one must form the interpolants for known coefficients. PCE estimates its coefficients using any of the approaches to follow: random sampling, tensor-product quadrature, Smolyak sparse grids, or linear regression. In SC, the multidimensional interpolants need to be formed over structured data sets, such as point sets from quadrature or sparse grids; approaches based on random sampling may not be used.

A. Spectral projection

The spectral projection approach projects the response against each basis function using inner products and employs the polynomial orthogonality properties to extract each coefficient. Similar to a Galerkin projection, the residual error from the approximation is rendered orthogonal to the selected basis. From Eq. 8, it is evident that

$$\alpha_j \;=\; \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} \;=\; \frac{1}{\langle \Psi_j^2 \rangle} \int_\Omega R\, \Psi_j\, \varrho(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{13}$$

where each inner product involves a multidimensional integral over the support range of the weighting function. In particular, $\Omega = \Omega_1 \otimes \cdots \otimes \Omega_n$, with possibly unbounded intervals $\Omega_j \subset \mathbb{R}$ and the tensor product form $\varrho(\boldsymbol{\xi}) = \prod_{i=1}^n \varrho_i(\xi_i)$ of the joint probability density (weight) function. The denominator in Eq. 13 is the norm squared of the multivariate orthogonal polynomial, which can be computed analytically using the product of univariate norms squared

$$\langle \Psi_j^2 \rangle \;=\; \prod_{i=1}^{n} \langle \psi^2_{m_i^j} \rangle \tag{14}$$

where the univariate inner products have simple closed form expressions for each polynomial in the Askey scheme.[4] Thus, the primary computational effort resides in evaluating the numerator, which is evaluated numerically using sampling, quadrature or sparse grid approaches (and this numerical approximation leads to use of the term "pseudo-spectral").

[b] If joint distributions are known, then the Rosenblatt transformation is preferred.

1. Sampling

In the sampling approach, the integral evaluation is equivalent to computing the expectation (mean) of the response-basis function product (the numerator in Eq. 13) for each term in the expansion when sampling within the density of the weighting function.

In computational practice, coefficient estimations based on sampling benefit from first estimating the response mean (the first PCE coefficient) and then removing the mean from the expectation evaluations for all subsequent coefficients.[10] While this has no effect for quadrature/sparse grid methods (see following two sections) and little effect for fully-resolved sampling, it does have a small but noticeable beneficial effect for under-resolved sampling.

2. Tensor product quadrature

In quadrature-based approaches, the simplest general technique for approximating multidimensional integrals, as in Eq. 13, is to employ a tensor product of one-dimensional quadrature rules. In the case where Ω is a hypercube, i.e. $\Omega = [-1,1]^n$, there are several choices of nested abscissas, included Clenshaw-Curtis, Gauss-Patterson, etc.[18–20] In the more general case, we propose to use Gaussian abscissas, i.e. the zeros of the orthogonal polynomials with respect to some positive weight, e.g. Gauss-Hermite, Gauss-Legendre, Gauss-Laguerre, generalized Gauss-Laguerre, or Gauss-Jacobi.

We first introduce an index $i \in \mathbb{N}_+$, $i \geq 1$. Then, for each value of i, let $\{\xi_1^i, \ldots, \xi_{m_i}^i\} \subset \Omega_i$ be a sequence of abscissas for quadrature on Ω_i. For $f \in C^0(\Omega_i)$ and $n = 1$ we introduce a sequence of one-dimensional quadrature operators

$$\mathscr{U}^i(f)(\xi) = \sum_{j=1}^{m_i} f(\xi_j^i)\, w_j^i, \tag{15}$$

with $m_i \in \mathbb{N}$ given. When utilizing Gaussian quadrature, Eq. 15 integrates exactly all polynomials of degree less than $2m_i - 1$, for each $i = 1, \ldots, n$. Given an expansion order p, the highest order coefficient evaluations (Eq. 13) can be assumed to involve integrands of at least polynomial order $2p$ (Ψ of order p and R modeled to order p) in each dimension such that a minimal Gaussian quadrature order of $p+1$ will be required to obtain good accuracy in these coefficients.

Now, in the multivariate case $n > 1$, for each $f \in C^0(\Omega)$ and the multi-index $\mathbf{i} = (i_1, \ldots, i_n) \in \mathbb{N}_+^n$ we define the full tensor product quadrature formulas

$$\mathcal{Q}_{\mathbf{i}}^n f(\xi) = \left(\mathscr{U}^{i_1} \otimes \cdots \otimes \mathscr{U}^{i_n}\right)(f)(\boldsymbol{\xi}) = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} f\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(w_{j_1}^{i_1} \otimes \cdots \otimes w_{j_n}^{i_n}\right). \tag{16}$$

Clearly, the above product needs $\prod_{j=1}^n m_{i_j}$ function evaluations. Therefore, when the number of input random variables is small, full tensor product quadrature is a very effective numerical tool. On the other hand, approximations based on tensor product grids suffer from the *curse of dimensionality* since the number of collocation points in a tensor grid grows exponentially fast in the number of input random variables. For example, if Eq. 16 employs the same order for all random dimensions, $m_{i_j} = m$, then Eq. 16 requires m^n function evaluations.

3. Smolyak sparse grids

If the number of random variables is moderately large, one should rather consider sparse tensor product spaces as first proposed by Smolyak[21] and further investigated by Refs. 18–20, 22–24 that reduce dramatically the number of collocation points, while preserving a high level of accuracy.

Here we follow the notation and extend the description in Ref. 18 to describe the Smolyak *isotropic* formulas $\mathscr{A}(\mathrm{w}, n)$, where w is a level that is independent of dimension[c]. The Smolyak formulas are just linear combinations of the product formulas in Eq. 16 with the following key property: only products with a relatively small number of points are used. With $\mathscr{U}^0 = 0$ and for $i \geq 1$ define

$$\Delta^i = \mathscr{U}^i - \mathscr{U}^{i-1}. \tag{17}$$

[c]Other common formulations use a dimension-dependent level q where $q \geq n$. We use $w = q - n$, where $w \geq 0$ for all n.

and we set $|\mathbf{i}| = i_1 + \cdots + i_n$. Then the isotropic Smolyak quadrature formula is given by

$$\mathscr{A}(\mathrm{w}, n) = \sum_{|\mathbf{i}| \leq \mathrm{w}+n} \left(\Delta^{i_1} \otimes \cdots \otimes \Delta^{i_n} \right). \tag{18}$$

Equivalently, formula Eq. 18 can be written as[25]

$$\mathscr{A}(\mathrm{w}, n) = \sum_{\mathrm{w}+1 \leq |\mathbf{i}| \leq \mathrm{w}+n} (-1)^{\mathrm{w}+n-|\mathbf{i}|} \binom{n-1}{\mathrm{w}+n-|\mathbf{i}|} \cdot \left(\mathscr{U}^{i_1} \otimes \cdots \otimes \mathscr{U}^{i_n} \right). \tag{19}$$

Given an index set of levels, growth rules must be defined for the one-dimensional quadrature orders. In order to take advantage of nesting and provide similar growth behavior for fully nested and weakly nested integration rules, the following growth rules are currently employed:

$$\text{Clenshaw} - \text{Curtis}: \quad m = \begin{cases} 1 & w = 0 \\ 2^w + 1 & w \geq 1 \end{cases} \tag{20}$$

$$\text{Gaussian}: \quad m = 2^{w+1} - 1 \tag{21}$$

Examples of isotropic sparse grids, constructed from the fully nested Clenshaw-Curtis abscissas and the weakly-nested Gaussian abscissas are shown in Figure 1, where $\Omega = [-1, 1]^2$. There, we consider a two-dimensional parameter space and a maximum level $\mathrm{w} = 5$ (sparse grid $\mathscr{A}(5, 2)$). To see the reduction in function evaluations with respect to full tensor product grids, we also include a plot of the corresponding Clenshaw-Curtis isotropic full tensor grid having the same maximum number of points in each direction, namely $2^{\mathrm{w}} + 1 = 33$. Whereas an isotropic tensor-product quadrature scales as m^n, an isotropic sparse grid scales as $m^{\log\, n}$, significantly mitigating the curse of dimensionality.

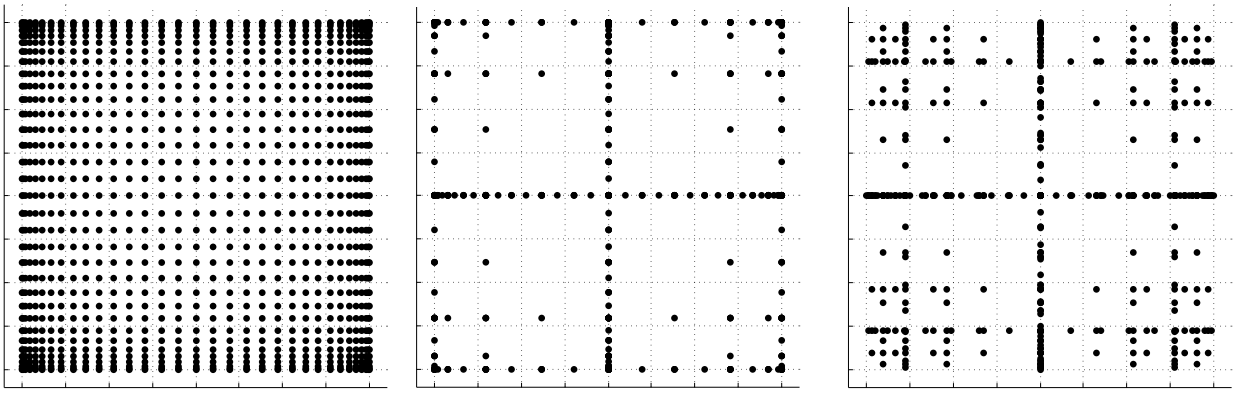


Figure 1. For a two-dimensional parameter space ($n = 2$) and maximum level $\mathrm{w} = 5$, we plot the full tensor product grid using the Clenshaw-Curtis abscissas (left) and isotropic Smolyak sparse grids $\mathscr{A}(5, 2)$, utilizing the Clenshaw-Curtis abscissas (middle) and the Gaussian abscissas (right).

B. Linear regression

The linear regression approach (also known as point collocation or stochastic response surfaces[26,27]) uses a single linear least squares solution of the form:

$$\boldsymbol{\Psi}\boldsymbol{\alpha} = \boldsymbol{R} \tag{22}$$

to solve for the complete set of PCE coefficients $\boldsymbol{\alpha}$ that best match a set of response values $\boldsymbol{R}$. The set of response values is typically obtained by performing a design of computer experiments within the density function of $\boldsymbol{\xi}$, where each row of the matrix $\boldsymbol{\Psi}$ contains the N_t multivariate polynomial terms Ψ_j evaluated at a particular $\boldsymbol{\xi}$ sample. An over-sampling is generally advisable (Ref. 27 recommends $2N_t$ samples), resulting in a least squares solution for the over-determined system. In the case of $2N_t$ oversampling, the simulation

requirements for this approach scale as $\frac{2(n+p)!}{n!p!}$, which can be significantly more affordable than isotropic tensor-product quadrature (e.g., $(p+1)^n$) for larger problems.

A closely related technique is known as the "probabilistic collocation" approach. Rather than employing random over-sampling, this technique uses a selected subset of N_t Gaussian quadrature points (those with highest tensor-product weighting), which provides more optimal collocation locations and preserves interpolation properties.

V. Design Under Uncertainty Using Stochastic Expansions

A. Stochastic Sensitivity Analysis

Stochastic expansion methods have a number of convenient analytic features that make them attractive for use within design under uncertainty algorithms. First, moments of the response expansion are available analytically, which enable convenient moment control in design under uncertainty. Second, the response expansions themselves are readily differentiated with respect to the underlying expansion variables.

1. Analytic moments

Mean and variance of the polynomial chaos expansion are available in simple closed form:

$$\mu_R = \langle R \rangle \cong \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}) \rangle = \alpha_0 \tag{23}$$

$$\sigma_R^2 = \langle (R-\mu_R)^2 \rangle \cong \langle (\sum_{j=1}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}))^2 \rangle = \sum_{j=1}^{P}\sum_{k=1}^{P} \alpha_j \alpha_k \langle \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle = \sum_{j=1}^{P} \alpha_j^2 \langle \Psi_j^2 \rangle \tag{24}$$

where the norm squared of each multivariate polynomial is computed from Eq. 14. The moments μ_R and σ_R are exact moments of the expansion, which converge to moments of the true response function. Higher moments are also available analytically and could be employed in moment fitting approaches (i.e., Pearson and Johnson models) in order to approximate a response PDF, although this is outside the scope of the current paper.

Similar expressions can be derived for stochastic collocation:

$$\mu_R = \langle R \rangle \cong \sum_{j=1}^{N_p} r_j \langle \boldsymbol{L}_j(\boldsymbol{\xi}) \rangle = \sum_{j=1}^{N_p} r_j w_j \tag{25}$$

$$\sigma_R^2 = \langle R^2 \rangle - \mu_R^2 \cong \sum_{j=1}^{N_p}\sum_{k=1}^{N_p} r_j r_k \langle \boldsymbol{L}_j(\boldsymbol{\xi}) \boldsymbol{L}_k(\boldsymbol{\xi}) \rangle - \mu_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2 \tag{26}$$

where the expectation of a particular Lagrange polynomial constructed at Gauss points and then integrated at these same Gauss points leaves only the weight corresponding to the point for which the interpolation value is one.

2. Design variable sensitivity analysis: random variable expansions

With the introduction of design variables $\boldsymbol{s}$, a polynomial chaos expansion only over the random variables $\boldsymbol{\xi}$ has the functional relationship:

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=0}^{P} \alpha_j(\boldsymbol{s}) \Psi_j(\boldsymbol{\xi}) \tag{27}$$

In this case, design sensitivities for the mean and variance in Eqs. 23 and 24 are as follows:

$$\frac{d\mu_R}{ds} = \frac{d\alpha_0}{ds} = \frac{d}{ds}\langle R \rangle = \langle \frac{dR}{ds} \rangle \tag{28}$$

$$\frac{d\sigma_R^2}{ds} = \sum_{j=1}^{P} \langle \Psi_j^2 \rangle \frac{d\alpha_j^2}{ds} = 2\sum_{j=1}^{P} \alpha_j \langle \frac{dR}{ds}, \Psi_j \rangle \tag{29}$$

since

$$\frac{d\alpha_j}{ds} = \frac{\langle \frac{dR}{ds}, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} \tag{30}$$

The coefficients calculated in Eq. 30 may be interpreted as either the design sensitivities of the chaos coefficients for the response expansion or the chaos coefficients of an expansion for the response design sensitivities. The evaluation of integrals involving $\frac{dR}{ds}$ extends the data requirements for the PCE approach to include response sensitivities at each of the sampling points for the quadrature, sparse grid, sampling, or point collocation coefficient estimation approaches. The resulting expansions are valid only for a particular set of design variables and must be recalculated each time the design variables are modified.

Similarly for stochastic collocation,

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=1}^{N_p} r_j(\boldsymbol{s}) \boldsymbol{L}_j(\boldsymbol{\xi}) \tag{31}$$

leads to

$$\frac{d\mu_R}{ds} = \frac{d}{ds}\langle R \rangle = \sum_{j=1}^{N_p} \frac{dr_j}{ds} \langle \boldsymbol{L}_j \rangle = \sum_{j=1}^{N_p} w_j \frac{dr_j}{ds} \tag{32}$$

$$\frac{d\sigma_R^2}{ds} = \sum_{j=1}^{N_p} 2 w_j r_j \frac{dr_j}{ds} - 2\mu_R \frac{d\mu_R}{ds} = \sum_{j=1}^{N_p} 2 w_j (r_j - \mu_R) \frac{dr_j}{ds} \tag{33}$$

based on differentiation of Eqs. 25-26.

3. Design variable sensitivity analysis: combined variable expansions

Alternatively, a stochastic expansion can be formed over both $\boldsymbol{\xi}$ and $\boldsymbol{s}$. Assuming a bounded design domain $\boldsymbol{s}_L \leq \boldsymbol{s} \leq \boldsymbol{s}_U$ (with no implied probability content), a Legendre chaos basis would be appropriate for each of the dimensions in $\boldsymbol{s}$ within a polynomial chaos expansion.

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \tag{34}$$

In this case, design sensitivities for the mean and variance do not require response sensitivity data, but this comes at the cost of forming the PCE over additional dimensions. For this combined variable expansion, the mean and variance are evaluated by evaluating the expectations over only the random variables, which eliminates the polynomial dependence on $\boldsymbol{\xi}$, leaving behind the desired polynomial dependence on $\boldsymbol{s}$:

$$\mu_R(\boldsymbol{s}) = \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \tag{35}$$

$$\sigma_R^2(\boldsymbol{s}) = \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \alpha_k \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \Psi_k(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} - \mu_R^2(\boldsymbol{s}) \tag{36}$$

The remaining polynomials may then be differentiated with respect to $\boldsymbol{s}$. In this approach, the combined PCE is valid for the full design variable range ($\boldsymbol{s}_L \leq \boldsymbol{s} \leq \boldsymbol{s}_U$) and does not need to be updated for each change in design variables, although adaptive localization techniques (i.e., trust region model management approaches) can be employed when improved local accuracy of the sensitivities is required.

Similarly for stochastic collocation,

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \tag{37}$$

leads to

$$\mu_R(\boldsymbol{s}) = \sum_{j=1}^{N_p} r_j \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \tag{38}$$

$$\sigma_R^2(\boldsymbol{s}) = \sum_{j=1}^{N_p} \sum_{k=1}^{N_p} r_j r_k \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \boldsymbol{L}_k(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \; - \; \mu_R^2(\boldsymbol{s}) \tag{39}$$

where the remaining polynomials not eliminated by the expectation over $\boldsymbol{\xi}$ are again differentiated with respect to $\boldsymbol{s}$.

4. Inputs and outputs

There are two types of design variables for which design sensitivities must be calculated: "augmented," where the design variables are separate from and augment the random variables, and "inserted," where the design variables define distribution parameters for the random variables. While one could artificially augment the dimensionality of a combined variable expansion approach with inserted design variables, this is not currently explored in this paper. Thus, any inserted design variable sensitivities must be handled using Eqs. 28-29 and Eqs. 32-33 where $\frac{dR}{ds}$ is calculated as $\frac{dR}{dx}\frac{dx}{ds}$ and $\frac{dx}{ds}$ is the design Jacobian if the variable transformation $\mathbf{x} = T^{-1}(\boldsymbol{\xi})$.

While moment sensitivities directly enable robust design optimization formulations which seek to control response variance, design for reliability requires design sensitivities of tail statistics. In this abstract, we initially focus on design sensitivity of simple moment projections for this purpose. In reliability analysis using the Mean Value method, forward ($\bar{z} \rightarrow \beta$) and inverse ($\bar{\beta} \rightarrow z$) mappings employing the reliability index are approximated as:[11,12]

$$\beta_{cdf} = \frac{\mu_R - \bar{z}}{\sigma_R} \tag{40}$$

$$\beta_{ccdf} = \frac{\bar{z} - \mu_R}{\sigma_R} \tag{41}$$

$$z = \mu_R - \sigma_R \bar{\beta}_{cdf} \tag{42}$$

$$z = \mu_R + \sigma_R \bar{\beta}_{ccdf} \tag{43}$$

such that it is straightforward to form approximate design sensitivities of β and z from the PCE moment sensitivities. From here, approximate design sensitivities of probability levels may also be formed given a probability expression (such as $\Phi(-\beta)$) for the reliability index. The current alternative of numerical design sensitivities of sampled probability levels would employ fewer simplifying approximations, but would also be much more expensive to compute accurately and is avoided for now. Future capabilities for analytic probability sensitivities could be based on Pearson/Johnson model for analytic response PDFs or sampling sensitivity approaches.

B. Optimization Formulations

Given the capability to compute analytic statistics of the response along with design sensitivities of these statistics, we pursue bi-level, sequential, and multifidelity approaches for optimization under uncertainty (OUU). The latter two approaches apply surrogate modeling approaches (data fits and multifidelity modeling) to the uncertainty analysis and then apply trust region model management to the optimization process.

1. Fully analytic bi-level

The simplest and most direct approach is to employ these analytic statistics and their design derivatives directly within an optimization loop. This approach is known as bi-level OUU, since there is an inner level uncertainty analysis nested within an outer level optimization.

Consider the common reliability-based design example of a deterministic objective function with a reliability constraint:

$$\begin{aligned} &\text{minimize} && f \\ &\text{subject to} && \beta \geq \bar{\beta} \end{aligned} \tag{44}$$

where β is computed relative to a prescribed threshold response value $\bar{z}$ and is constrained by a prescribed reliability level $\bar{\beta}$. Another common example is robust design in which the constraint enforcing a reliability lower-bound has been replaced with a constraint enforcing a variance upper-bound:

$$\begin{aligned} \text{minimize} \quad & f \\ \text{subject to} \quad & \sigma^2 \leq \bar{\sigma}^2 \end{aligned} \tag{45}$$

Solving these problems using a bi-level approach involves computing $\beta(\boldsymbol{s})$ and $\frac{d\beta}{d\boldsymbol{s}}$ for Eq. 44 or σ^2 and $\frac{d\sigma^2}{d\boldsymbol{s}}$ for Eq. 45 for each set of design variables $\boldsymbol{s}$ passed from the optimizer. This approach is explored for both Uncertain and Combined expansions using PCE and SC.

2. Sequential

An alternative OUU approach is the sequential approach, in which additional efficiency is sought through breaking the nested relationship of the UQ and optimization loops. The general concept is to iterate between optimization and uncertainty quantification, updating the optimization goals based on the most recent uncertainty assessment results. This approach is common with the reliability methods community, for which the updating strategy may be based on safety factors[28] or other approximations.[29]

A particularly effective approach for updating the optimization goals is to use data fit surrogate models, and in particular, local Taylor series models allow direct insertion of stochastic sensitivity analysis capabilities. In Ref. 11, first-order Taylor series approximations were explored, and in Ref. 12, second-order Taylor series approximations are investigated. In both cases, a trust-region model management framework[30] is used to adaptively manage the extent of the approximations and ensure convergence of the OUU process. Surrogate models are used for both the objective and the constraint functions, although the use of surrogates is only required for the functions containing statistical results; deterministic functions may remain explicit is desired.

In particular, trust-region surrogate-based optimization for reliability-based design employs surrogate models of f and β within a trust region Δ^k centered at $\mathbf{s}_c$:

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} \quad & \beta(\mathbf{s}_c) + \nabla_s \beta(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \geq \bar{\beta} \\ & \| \mathbf{s} - \mathbf{s}_c \|_\infty \leq \Delta^k \end{aligned} \tag{46}$$

and trust-region surrogate-based optimization for robust design employs surrogate models of f and σ^2 within a trust region Δ^k centered at $\mathbf{s}_c$:

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} \quad & \sigma^2(\mathbf{s}_c) + \nabla_s \sigma^2(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \leq \bar{\sigma}^2 \\ & \| \mathbf{s} - \mathbf{s}_c \|_\infty \leq \Delta^k \end{aligned} \tag{47}$$

Second-order local surrogates may also be employed, where the Hessians are typically approximated with quasi-Newton updates. The sequential approach will be explored for Uncertain expansions using PCE and SC.

3. Multifidelity

The multifidelity OUU approach is another trust-region surrogate-based approach. Instead of the surrogate UQ model being a simple data fit (in particular, first-/second-order Taylor series model) of the truth UQ model results, we now employ distinct UQ models of differing fidelity. This differing UQ fidelity could stem from the fidelity of the underlying simulation model, the fidelity of the UQ algorithm, or both. In this paper, we focus on the fidelity of the UQ algorithm. For reliability methods, this could entail varying fidelity in approximating assumptions (e.g., Mean Value for low fidelity, SORM for high fidelity), and for stochastic expansion methods, it could involve differences in selected levels of p and k refinement.

In this paper, we define UQ fidelity as point-wise accuracy in the design space and take the low fidelity model, whose validity over the design space will be adaptively controlled, to be the Combined expansion PCE/SC model, and the high fidelity truth model to be the Uncertain expansion PCE/SC model, with

validity only at a single design point. This will allow us to take advantage of the design space spanning and lower cost of the Combined expansion approach to the extent possible, with fallback to the greater accuracy and higher expense of the Uncertain expansion approach when needed. The Combined expansion approach will span only the current trust region of the design space and will need to be reconstructed for each new trust region. The design derivatives of each model provide the necessary data to correct the low fidelity model to first-order consistency with the high fidelity model at the center of each trust region.

Multifidelity optimization for reliability-based design can be formulated as:

$$\begin{array}{rc} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\beta_{hi}}(\mathbf{s}) \geq \bar{\beta} \\ & \| \mathbf{s} - \mathbf{s}_c \|_\infty \leq \Delta^k \end{array} \tag{48}$$

and multifidelity optimization for robust design can be formulated as:

$$\begin{array}{rc} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\sigma_{hi}}^2(\mathbf{s}) \leq \bar{\sigma}^2 \\ & \| \mathbf{s} - \mathbf{s}_c \|_\infty \leq \Delta^k \end{array} \tag{49}$$

where the deterministic objective function is not approximated and $\hat{\beta_{hi}}$ and $\hat{\sigma_{hi}}^2$ are the approximated high-fidelity UQ results resulting from correction of the low-fidelity UQ results. In the case of an additive correction function:

$$\hat{\beta_{hi}}(\mathbf{s}) = \beta_{lo}(\mathbf{s}) + \alpha_\beta(\mathbf{s}) \tag{50}$$

$$\hat{\sigma_{hi}}^2(\mathbf{s}) = \sigma^2_{lo}(\mathbf{s}) + \alpha_{\sigma^2}(\mathbf{s}) \tag{51}$$

where correction functions $\alpha(\mathbf{s})$ enforcing first-order consistency[31] will be explored.

VI. Computational Results

Generalized polynomial chaos and stochastic collocation have been implemented in DAKOTA,[32] an open-source software framework for design and performance analysis of computational models on high performance computers. This section presents computational results on the performance of stochastic expansion-based OUU methods for several analytic test problems, building on the UQ results presented in Ref. 5.

A. Rosenbrock

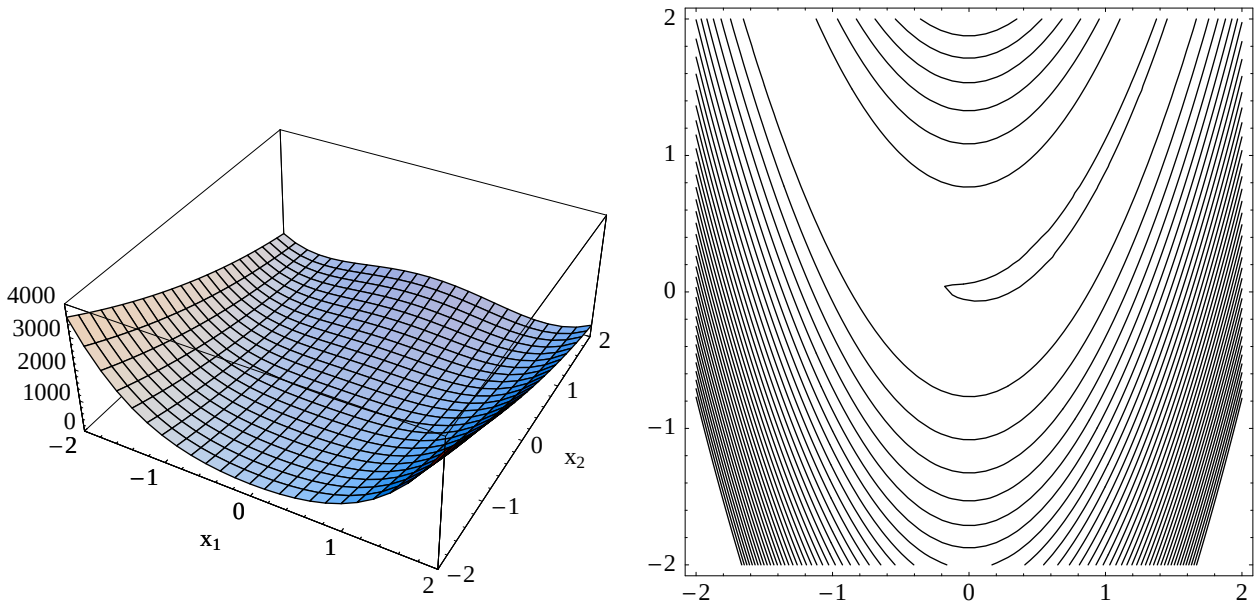
The two-dimensional Rosenbrock function is a popular test problem for gradient-based optimization algorithms due to its difficulty for first-order methods. It turns out that this is also a challenging problem for certain UQ methods (especially local reliability methods), since a particular response level contour involves a highly nonlinear curve that encircles the mean point. The function is a fourth order polynomial of the form:

$$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \tag{52}$$

A three-dimensional plot of this function is shown in Figure 2(a), where both x_1 and x_2 range in value from -2 to 2. Figure 2(b) shows a contour plot for Rosenbrock's function where the encircling of the mean at (0,0) is evident.

1. Design under uncertainty

Since exact results can be obtained for Rosenbrock using stochastic expansions, a simple OUU formulation is demonstrated that provides exact results for both analytic design sensitivity formulations. Taking x_1 to be a design variable with initial value -0.75 and bounds $-2 \leq x_1 \leq 2$ and taking x_2 to be a standard normal random variable ($\mu = 0, \sigma = 1$), Table 2 shows the computational results for maximizing β_{cdf} for $\bar{z} = 10$. with either SC or fourth-order Hermite PCE and either Gauss-Hermite quadrature order = 5 or Gauss-Hermite sparse grid level = 2. Sparse grids are not yet supported for anisotropic distribution types so Combined PCE and Combined SC are not available for the mixture of normal uncertain and uniform design variables.



(a) 3-D plot.

(b) Contours.

Figure 2. Rosenbrock's function.

Sequential results are shown for first-order and quasi-second-order Taylor series linkages and multifidelity results are shown for first-order additive corrections. For the bi-level approaches, the analytic sensitivity results are verified against results using finite difference sensitivities for the objective function. NPSOL's sequential quadratic programming (SQP) method is used as the optimizer.

For this problem, the functional input/output relationship is captured exactly and all techniques are equally successful in locating the optimum at the lower bound of x_1. No difference is discernible between the PCE and SC results, and sparse grids are slightly more expensive than tensor-product quadrature for this low dimensional problem. As expected, the Analytic-Uncertain approach, relative to the Analytic-Combined approach, trades a reduction in simulation evaluations for a requirement of higher order information per simulation. Both the Analytic-Combined and the Numerical-Combined approaches form only a single expansion for which both analytic and finite difference sensitivity evaluations for all design variable values involve only post-processing of the expansion. The sequential and multifidelity approaches require only a single trust region iteration to achieve hard convergence (Karush-Kuhn-Tucker optimality conditions satisfied), such that quasi-second-order linkages (which require at least two iterations to accumulate curvature information) provide no benefit. Overall, the sequential approaches are the most efficient of the techniques by a small margin.

B. Short Column

This test problem involves the plastic analysis of a short column with rectangular cross section (width $b = 5$ and depth $h = 15$) having uncertain material properties (yield stress Y) and subject to uncertain loads (bending moment M and axial force P).[33] The limit state function is defined as:

$$g(\mathbf{x}) = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2} \tag{53}$$

The distributions for P, M, and Y are Normal(500, 100), Normal(2000, 400), and Lognormal(5, 0.5), respectively, with a correlation coefficient of 0.5 between P and M (uncorrelated otherwise).

Table 2. PCE-based and SC-based design results, Rosenbrock test problem.

OUU Approach	Sensitivity Approach	Expansion Variables	Integration Approach	Evaluations (Fn, Grad)	β
PCE Bi-level	Analytic	Uncertain	Quadrature	(15, 15)	2.091
PCE Bi-level	Analytic	Combined	Quadrature	(25, 0)	2.091
PCE Bi-level	Numerical	Uncertain	Quadrature	(45, 0)	2.091
PCE Bi-level	Numerical	Combined	Quadrature	(25, 0)	2.091
PCE Sequential 1	Analytic	Uncertain	Quadrature	(15, 10)	2.091
PCE Sequential Q2	Analytic	Uncertain	Quadrature	(15, 10)	2.091
PCE Multifidelity	Analytic	LF Comb, HF Unc	Quadrature	(40, 10)	2.091
PCE Bi-level	Analytic	Uncertain	Sparse Grid	(21, 21)	2.091
PCE Bi-level	Numerical	Uncertain	Sparse Grid	(63, 0)	2.091
PCE Sequential 1	Analytic	Uncertain	Sparse Grid	(21, 14)	2.091
PCE Sequential Q2	Analytic	Uncertain	Sparse Grid	(21, 14)	2.091
SC Bi-level	Analytic	Uncertain	Quadrature	(15, 15)	2.091
SC Bi-level	Analytic	Combined	Quadrature	(25, 0)	2.091
SC Bi-level	Numerical	Uncertain	Quadrature	(45, 0)	2.091
SC Bi-level	Numerical	Combined	Quadrature	(25, 0)	2.091
SC Sequential 1	Analytic	Uncertain	Quadrature	(15, 10)	2.091
SC Sequential Q2	Analytic	Uncertain	Quadrature	(15, 10)	2.091
SC Multifidelity	Analytic	LF Comb, HF Unc	Quadrature	(40, 10)	2.091
SC Bi-level	Analytic	Uncertain	Sparse Grid	(21, 21)	2.091
SC Bi-level	Numerical	Uncertain	Sparse Grid	(63, 0)	2.091
SC Sequential 1	Analytic	Uncertain	Sparse Grid	(21, 14)	2.091
SC Sequential Q2	Analytic	Uncertain	Sparse Grid	(21, 14)	2.091

1. Design under uncertainty

An objective function of cross-sectional area and a target reliability index of 2.5 are used in the design problem:

$$\begin{aligned} \min \quad & bh \\ \text{s.t.} \quad & \beta \geq 2.5 \\ & 5.0 \leq b \leq 15.0 \\ & 15.0 \leq h \leq 25.0 \end{aligned} \tag{54}$$

The initial design of $(b, h) = (5, 15)$ is infeasible and the optimization must add material to obtain the target reliability at the optimal design $(b, h) = (8.114, 25.00)$.

For PCE, a fourth-order Hermite expansion is again used, although in order to scale better for a slightly higher dimensional problem, tensor-product quadrature is replaced with point collocation using a factor of two oversampling (70 simulations per uncertain expansion over three variables and 252 simulations per combined expansion over five variables). For SC, point collocation is not available and tensor-product quadrature with order = 5 is retained, at considerable expense. Both PCE and SC are also explored with Smolyak sparse grids at level = 2. Again, combined variable expansions cannot currently be performed over sparse grids, which restricts the bi-level and multifidelity options. NPSOL SQP method is again used as the optimizer, SR1 updates are used for quasi-second-order linkages in sequential approaches, and analytic sensitivity results are verified against results using numerical derivatives for the bi-level methods. Table 3 shows the computational results. For this problem, the functional input/output relationship is

Table 3. PCE-based and SC-based design results, short column test problem.

OUU Approach	Sensitivity Approach	Expansion Variables	Integration Approach	Evaluations (Fn, Grad)	Area	β
PCE Bi-level	Analytic	Uncertain	Pt Colloc	(490, 210)	202.86	2.5001
PCE Bi-level	Analytic	Combined	Pt Colloc	(252, 0)	204.37	2.5002
PCE Bi-level	Numerical	Uncertain	Pt Colloc	(1120, 0)	202.86	2.5001
PCE Bi-level	Numerical	Combined	Pt Colloc	(252, 0)	204.37	2.5002
PCE Sequential 1	Analytic	Uncertain	Pt Colloc	(840, 420)	202.86	2.5000
PCE Sequential Q2	Analytic	Uncertain	Pt Colloc	(770, 420)	202.86	2.5000
PCE Multifidelity	Analytic	LF Comb, HF Unc	Pt Colloc	(952, 360)	202.86	2.5000
PCE Bi-level	Analytic	Uncertain	Sparse Grid	(259, 111)	203.19	2.5001
PCE Bi-level	Numerical	Uncertain	Sparse Grid	(592, 0)	203.19	2.5001
PCE Sequential 1	Analytic	Uncertain	Sparse Grid	(444, 222)	203.18	2.5000
PCE Sequential Q2	Analytic	Uncertain	Sparse Grid	(407, 222)	203.18	2.5000
SC Bi-level	Analytic	Uncertain	Quadrature	(875, 375)	202.87	2.5001
SC Bi-level	Analytic	Combined	Quadrature	(3125, 0)	202.28	2.5001
SC Bi-level	Numerical	Uncertain	Quadrature	(2000, 0)	202.87	2.5001
SC Bi-level	Numerical	Combined	Quadrature	(3125, 0)	202.28	2.5001
SC Sequential 1	Analytic	Uncertain	Quadrature	(1500, 750)	202.87	2.5000
SC Sequential Q2	Analytic	Uncertain	Quadrature	(1375, 750)	202.87	2.5000
SC Multifidelity	Analytic	LF Comb, HF Unc	Quadrature	(4375, 625)	202.86	2.5000
SC Bi-level	Analytic	Uncertain	Sparse Grid	(259, 111)	202.87	2.5001
SC Bi-level	Numerical	Uncertain	Sparse Grid	(592, 0)	202.87	2.5001
SC Sequential 1	Analytic	Uncertain	Sparse Grid	(444, 222)	202.86	2.5000
SC Sequential Q2	Analytic	Uncertain	Sparse Grid	(407, 222)	202.86	2.5000

not captured exactly by the PCE and SC expansions and performance differences are evident. For PCE-based approaches, the Combined expansion results are less expensive to obtain, since they employ only a

single expansion for all design variable sets, but these optima are approximate and the Uncertain expansion approaches can be seen to converge more accurately. Since the sequential approach takes more than a single iteration to converge, benefit from quasi-second-order linkage is evident: accumulated curvature information converges the sequential iteration more quickly. In addition, the multifidelity machinery converges to the high fidelity result based on Uncertain expansions despite the optimizer being interfaced only with the low fidelity Combined expansions. For SC, the Combined expansion results still employ only a single expansion for all design variable sets, but the increased dimensionality is prohibitive for tensor-product quadrature and is only competitive for Smolyak sparse grids. SC appears to slightly outperform PCE in terms of accuracy for this problem, as evidenced by the bi-level Combined expansion results and each of the sparse grid Uncertain expansion results. Overall, SC-based bi-level Uncertain expansions on sparse grids is the most accurate and efficient technique for this problem.

C. Cantilever Beam

The next test problem involves the simple uniform cantilever beam[28, 34] shown in Figure 3.

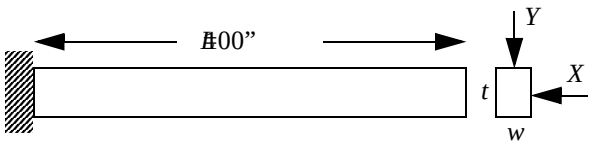


Figure 3. Cantilever beam test problem.

Random variables in the problem include the yield stress R and Youngs modulus E of the beam material and the horizontal and vertical loads, X and Y, which are modeled with normal distributions using N(40000, 2000), N(2.9E7, 1.45E6), N(500, 100), and N(1000, 100), respectively. Problem constants include $L = 100$ in. and $D_0 = 2.2535$ in. The beam response metrics have the following analytic form:

$$\text{stress} = \frac{600}{wt^2}Y + \frac{600}{w^2t}X \leq R \tag{55}$$

$$\text{displacement} = \frac{4L^3}{Ewt}\sqrt{(\frac{Y}{t^2})^2 + (\frac{X}{w^2})^2} \leq D_0 \tag{56}$$

1. *Design under uncertainty*

The design problem is to minimize the weight (or, equivalently, the cross-sectional area) of the beam subject to the displacement and stress constraints. If the random variables are fixed at their means, the resulting deterministic design problem has the solution $(w,\ t) = (2.352,\ 3.326)$ with an objective function of 7.824. When seeking a 3-sigma reliability level (where reliability index β is based on moment projection) on these constraints, the design problem can be summarized as follows:

$$\begin{aligned} \min \quad & wt \\ \text{s.t.} \quad & \beta_S \geq 3.0 \\ & \beta_D \geq 3.0 \\ & 1.0 \leq w \leq 4.0 \\ & 1.0 \leq t \leq 4.0 \end{aligned} \tag{57}$$

For PCE, a second-order Hermite expansion is employed using either point collocation with a factor of two oversampling (30 simulations per uncertain expansion over four variables and 56 simulations per combined expansion over six variables) or Smolyak sparse grids with level = 2. For SC, tensor-product quadrature with order = 3 or Smolyak sparse grids with level = 2 are employed. Again, combined variable expansions over sparse grids are not yet supported (restricts the bi-level and multifidelity options), NPSOL SQP is the optimizer, SR1 updates provide quasi-second-order linkages in sequential approaches, and analytic sensitivity results are verified against numerical derivative results for the bi-level methods. Table 4 shows

Table 4. PCE-based and SC-based design results, cantilever beam test problem.

OUU Approach	Sensitivity Approach	Expansion Variables	Integration Approach	Evaluations (Fn, Grad)	Area	β_S	β_D
PCE Bi-level	Analytic	Uncertain	Pt Colloc	(330, 330)	9.410	3.000	3.033
PCE Bi-level	Analytic	Combined	Pt Colloc	(56, 0)	45.29	1.952	1.177
PCE Bi-level	Numerical	Uncertain	Pt Colloc	(1650, 0)	9.410	3.000	3.033
PCE Bi-level	Numerical	Combined	Pt Colloc	(56, 0)	45.29	1.952	1.177
PCE Sequential 1	Analytic	Uncertain	Pt Colloc	(1050, 510)	4.198	-7.169	-8.332
PCE Sequential Q2	Analytic	Uncertain	Pt Colloc	(810, 420)	9.410	3.000	3.033
PCE Multifidelity	Analytic	LF Comb, HF Unc	Pt Colloc	(536, 240)	9.408	2.997	2.998
PCE Bi-level	Analytic	Uncertain	Sparse Grid	(627, 627)	9.412	3.000	3.048
PCE Bi-level	Numerical	Uncertain	Sparse Grid	(3135, 0)	9.412	3.000	3.048
PCE Sequential 1	Analytic	Uncertain	Sparse Grid	(1881, 912)	4.192	-7.162	-8.318
PCE Sequential Q2	Analytic	Uncertain	Sparse Grid	(969, 513)	9.412	3.000	3.048
SC Bi-level	Analytic	Uncertain	Quadrature	(891, 891)	9.411	3.000	3.048
SC Bi-level	Analytic	Combined	Quadrature	(729, 0)	6.543	7.982	3.000
SC Bi-level	Numerical	Uncertain	Quadrature	(4455, 0)	9.411	3.000	3.048
SC Bi-level	Numerical	Combined	Quadrature	(729, 0)	6.543	7.982	3.000
SC Sequential 1	Analytic	Uncertain	Quadrature	(2673, 1296)	4.192	-7.162	-8.318
SC Sequential Q2	Analytic	Uncertain	Quadrature	(2187, 1134)	9.411	3.000	3.048
SC Multifidelity	Analytic	LF Comb, HF Unc	Quadrature	(4779, 2025)	4.387	-7.026	-8.289
SC Bi-level	Analytic	Uncertain	Sparse Grid	(627, 627)	9.412	3.000	3.048
SC Bi-level	Numerical	Uncertain	Sparse Grid	(3135, 0)	9.412	3.000	3.048
SC Sequential 1	Analytic	Uncertain	Sparse Grid	(1881, 912)	4.192	-7.161	-8.318
SC Sequential Q2	Analytic	Uncertain	Sparse Grid	(969, 513)	9.412	3.000	3.048

the computational results. For this problem, the functional input/output relationship is captured accurately enough by second-order Uncertain expansions to converge to the correct solution. The Combined expansion results, while again inexpensive, do not have sufficient accuracy to locate the correct solution for either PCE or SC. The first-order sequential approaches also fail to converge for PCE and SC, whereas accumulation of curvature information mitigates this problem in both cases. The multifidelity approach is successful in forcing the low fidelity results toward the high fidelity optimum for PCE, but fails in this regard for SC. Overall, PCE-based bi-level Uncertain expansions using point collocation is the most efficient technique for this problem, followed by the PCE multifidelity approach and the PCE and SC bi-level Uncertain expansion approaches on sparse grids.

D. Steel Column

The final analytic test problem involves the trade-off between cost and reliability for a steel column.[33] The cost is defined as

$$Cost = bd + 5h \tag{58}$$

where b, d, and h are the means of the flange breadth, flange thickness, and profile height, respectively. This problem demonstrates the efficiency of different coefficient estimation approaches when scaled to larger dimensional UQ problems. Nine uncorrelated random variables are used in the problem to define the yield stress F_s (lognormal with $\mu/\sigma = 400/35$ MPa), dead weight load P_1 (normal with $\mu/\sigma = 500000/50000$ N), variable load P_2 (gumbel with $\mu/\sigma = 600000/90000$ N), variable load P_3 (gumbel with $\mu/\sigma = 600000/90000$ N), flange breadth B (lognormal with $\mu/\sigma = b/3$ mm), flange thickness D (lognormal with $\mu/\sigma = d/2$ mm), profile height H (lognormal with $\mu/\sigma = h/5$ mm), initial deflection F_0 (normal with $\mu/\sigma = 30/10$ mm), and Youngs modulus E (weibull with $\mu/\sigma = 21000/4200$ MPa). The limit state has the following analytic form:

$$g = F_s - P\left(\frac{1}{2BD} + \frac{F_0}{BDH}\frac{E_b}{E_b - P}\right) \tag{59}$$

where

$$P = P_1 + P_2 + P_3 \tag{60}$$

$$E_b = \frac{\pi^2 EBDH^2}{2L^2} \tag{61}$$

and the column length L is 7500 mm.

1. *Design under uncertainty*

This design problem demonstrates design variable insertion into random variable distribution parameters through the design of the mean flange breadth, flange thickness, and profile height. Since there are no augmented design variables in this problem, the two design sensitivity approaches collapse into one. The following design formulation maximizes the reliability subject to a cost constraint:

$$\begin{aligned} \max \quad & \beta \\ \text{s.t.} \quad & Cost \leq 4000. \\ & 200.0 \leq b \leq 400.0 \\ & 10.0 \leq d \leq 30.0 \\ & 100.0 \leq h \leq 500.0 \end{aligned} \tag{62}$$

For PCE, the limit state is modeled using a fourth-order expansion and the coefficients are estimated using either point collocation with 1000 samples (minimum required is 715 samples) or sparse grid level = 2. For SC, only sparse grid level = 2 is employed. Table 5 shows the results for analytic cost and reliability design sensitivities and for a mixture of analytic cost and numerical reliability sensitivities. For this problem, the input/output relationship is captured accurately enough by fourth-order Uncertain expansions to converge to the correct solution at $(b, d, h) = (200., 175., 100.)$. Whereas a sparse grid level of 2 is sufficient to converge the SC statistics, a sparse grid level of 3 (at an increased cost of (35701, 11274) for analytic and (92071, 0) for numerical) is required to generate the correct reliability index within the PCE statistics. Thus, SCBDO outperforms PCBDO in this problem. Overall, the SC-based bi-level approach on sparse grids is the most accurate and efficient of the methods.

Table 5. PCE-based and SC-based design results, steel column test problem.

OUU Approach	Sensitivity Approach	Expansion Variables	Integration Approach	Evaluations (Fn, Grad)	β	Cost
PCE Bi-level	Analytic	Uncertain	Pt Colloc	(18000, 6000)	3.236	4000.
PCE Bi-level	Mixed	Uncertain	Pt Colloc	(48000, 0)	3.236	4000.
PCE Sequential 1	Analytic	Uncertain	Pt Colloc	(10000, 5000)	3.236	4000.
PCE Sequential Q2	Analytic	Uncertain	Pt Colloc	(14000, 7000)	3.236	4000.
PCE Bi-level	Analytic	Uncertain	Sparse Grid	(3255, 1085)	3.143	4000.
PCE Bi-level	Numerical	Uncertain	Sparse Grid	(8680, 0)	3.143	4000.
PCE Sequential 1	Analytic	Uncertain	Sparse Grid	(11274, 5637)	3.236	4000.
PCE Sequential Q2	Analytic	Uncertain	Sparse Grid	(11274, 5637)	3.236	4000.
SC Bi-level	Analytic	Uncertain	Sparse Grid	(3255, 1085)	3.236	4000.
SC Bi-level	Numerical	Uncertain	Sparse Grid	(8680, 0)	3.236	4000.
SC Sequential 1	Analytic	Uncertain	Sparse Grid	(11274, 5637)	3.236	4000.
SC Sequential Q2	Analytic	Uncertain	Sparse Grid	(11274, 5637)	3.236	4000.

VII. Conclusions

This paper has investigated the relative performance of non-intrusive generalized polynomial chaos and stochastic collocation methods applied to several algebraic benchmark problems with known solutions. The primary distinction between these methods is that PCE must estimate coefficients for a known basis of orthogonal polynomials (using sampling, linear regression, quadrature, or sparse grids) whereas SC must form an interpolant for known coefficients (using quadrature or sparse grids).

Performance between these methods is shown to be very similar and both demonstrate impressive convergence behavior. However, when a difference is observed, SC has been the consistent winner, generally manifesting in the reduction of the required integration by one order or level. This difference can be attributed to practical issues. The elimination of the need to prescribe an expansion order in SC not only leads to a simpler method, it also eliminates issues with nonoptimal synchronization between this prescribed expansion order and the selected integration approach. In Gaussian quadrature for example, integration of polynomials of even order $2p$ in PCE based on quadratures which can resolve integrals of odd order $2m-1$ result in slight over or under-integration by one polynomial order. In addition, tensor-product quadratures can resolve polynomials of a particular order in each dimension independently, which over-integrates expansions of fixed total polynomial order. In a sense, SC automatically adapts the expansion polynomials to the integration point set based on the Lagrange construction, eliminating inefficiencies caused by nonoptimal integration of polynomial chaos expansions. This observation appears to hold for both Gaussian rules and Clenshaw-Curtis rules.

These preferred UQ approaches are carried forward in design under uncertainty studies employing two stochastic sensitivity approaches, one based on expansions of response design sensitivities over uncertain variables and another based on combined expansions of response functions over design and uncertain variables. While it is shown that both approaches are capable of exact results, computational experiments indicate that the former approach is more reliable (so long as the underlying response derivatives are reliable) for use in gradient-based design optimization. The two stochastic sensitivity approaches provide the foundation for exploration of bi-level, sequential, and multifidelity formulations to design under uncertainty. Quasi-second order linkages are shown to be preferred to first-order linkages within sequential formulations and multifidelity approaches are shown to be capable of coercing the low fidelity optimization to converge to the high fidelity optimum; however, neither approach consistently outperforms the simpler bi-level approach when it employs an efficient gradient-based optimizer such as sequential quadratic programming.

The current direction of the stochastic expansion work is focused on the development of adaptive schemes that can tailor either a polynomial chaos basis and expansion/integration order or a stochastic collocation interpolation grid to the problem at hand. This entails supporting arbitrary input PDFs by numerically generating orthogonal polynomials and their Gauss points/weights and developing a capability to adapt the

expansions per dimension based on stochastic error estimation.

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