Nonintrusive Methods for Uncertainty Quantification

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Introduction: Risk-informed Decision Making, QMU, and UQ

In order to support risk-informed decision making using modeling and simulation, the following key elements are required:

– **Predictive simulations**: verified and validated for application of interest
– **Quantified uncertainties**: the effect of random variability is fully understood

Formal DOE process for Quantification of Margins and Uncertainties (QMU): process of providing *best estimate + uncertainty* in the decision context

**Uncertainty Quantification**

Critical component of QMU: credible M&S capability for stockpile stewardship

Uncertainty can be categorized to be one of two different types:

– **Aleatory/irreducible**: inherent variability with sufficient data → probabilistic models
– **Epistemic/reducible**: uncertainty from lack of knowledge → nonprobabilistic models
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Uncertainty applications: penetration, joint mechanics, abnormal environments, shock physics, …
# Uncertainty Quantification Algorithms @ SNL:
New methods bridge robustness/efficiency gap

<table>
<thead>
<tr>
<th>Category</th>
<th>Production</th>
<th>New</th>
<th>Under dev.</th>
<th>Planned</th>
<th>Collabs.</th>
</tr>
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<tr>
<td>Sampling</td>
<td>LHS/MC, QMC/CVT</td>
<td>IS/AIS/MMAIS,</td>
<td></td>
<td>Bootstrap, Jackknife</td>
<td>Gunzburger</td>
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<td></td>
<td></td>
<td>Incremental LHS</td>
<td></td>
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<tr>
<td>Reliability</td>
<td>1&lt;sup&gt;st&lt;/sup&gt;/2&lt;sup&gt;nd&lt;/sup&gt;-order local: MV/MV&lt;sup&gt;2&lt;/sup&gt;, x/u AMV/AMV&lt;sup&gt;2&lt;/sup&gt;/AMV+/ AMV&lt;sup&gt;2&lt;/sup&gt;+, x/u TANA, FORM/SORM</td>
<td>Global: EGRA</td>
<td></td>
<td></td>
<td>Local: Renaud, Global: Mahadevan</td>
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<tr>
<td>expansion</td>
<td></td>
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<tr>
<td>Other</td>
<td>Random fields/stochastic proc.</td>
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<tr>
<td>probabilistic</td>
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<tr>
<td>Epistemic</td>
<td>Second-order probability</td>
<td>Dempster-Shafer evidence theory</td>
<td>Opt-based interval est.</td>
<td>Bayesian, Imprecise probability</td>
<td>Higdon, Williams, Ferson</td>
</tr>
<tr>
<td>Metrics</td>
<td>Importance factors, Partial correlations</td>
<td>Main effects, Variance-based decomposition</td>
<td>Stepwise regression</td>
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</table>
Sampling

- Assume distributions on the uncertain input values, repeatedly sample from those distributions and run the model with the sampled values; yields corresponding distributions of the outputs.
- Considerable work has led to more efficient Monte Carlo (MC) sampling methods, including pseudo-MC sampling (Latin hypercube sampling) or quasi-MC sampling which more uniformly distribute samples over the space.
- Sampling is not the most efficient UQ method, but it is easy to implement, robust, and transparent.

**Input Distributions**
- N samples of X

**Output Distributions**
- N realizations of X
  - Measure 1
  - Measure 2

**Simulation Model**

**Final Temperature Values**

Goals: assess nominal, variability, tail statistics, probability of failure.
Motivations:

- DACE $\rightarrow$ global sensitivity analysis
- UQ $\rightarrow$ output moments, probabilities

Types:

- Monte Carlo: basic random sampling
- Pseudo Monte Carlo: Latin Hypercube Sampling (LHS) is a stratified, structured sampling method that picks random samples from equal probability bins for all 1-D projections.
- Quasi Monte Carlo: deterministic sequences constructed to uniformly cover a unit hypercube with low discrepancy. E.g., Halton, Hammersley, Sobol
- Centroidal Voronoi Tesselation (CVT): generates nearly uniform spacing over arbitrarily shaped parameter spaces; originally developed for “meshless” mechanics methods.
- (Multimodal, Adaptive) Importance Sampling: generates samples with recentered density to emphasize areas of importance (i.e., tails)

Associated Tools:

- Correlation analysis
- Variance-based decomposition
Latin Hypercube Sampling

- LHS is stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples.
  - Early work by McKay and Conover
  - Further refinement by Iman → enforce prescribed input

A two-dimensional representation of one possible LHS of size 5 utilizing X1 (normal) and X2 (uniform)

Intervals Used with a LHS of Size N = 5 in Terms of the PDF and CDF for a Normal Random Variable
UQ with Reliability Methods

Mean Value Method

\[
\begin{align*}
\mu_g &= g(\mu_x) \\
\sigma_g &= \sum_i \sum_j \text{Cov}(i, j) \frac{dg}{dx_i}(\mu_x) \frac{dg}{dx_j}(\mu_x)
\end{align*}
\]

\[
\begin{align*}
\beta_{cdf} &= \frac{\mu_g - \bar{z}}{\sigma_g} \\
\beta_{ccdf} &= \frac{\bar{z} - \mu_g}{\sigma_g}
\end{align*}
\]

Rough statistics

MPP search methods

Reliability Index Approach (RIA)

minimize \( u^T u \)

subject to \( G(u) = \bar{z} \)

Find min dist to \( G \) level curve

Used for fwd map \( z \to p/\beta \)

Performance Measure Approach (PMA)

minimize \( \pm G(u) \)

subject to \( u^T u = \bar{\beta}^2 \)

Find min \( G \) at \( \beta \) radius

Used for inv map \( p/\beta \to z \)

Nataf \( x \to u: \)

\[
\Phi(z_i) = F(x_i)
\]

\( z = Lu \)
UQ with Reliability Methods

Mean Value Method

\[ \mu_g = g(\mu_x) \]
\[ \sigma_g = \sum_i \sum_j \text{Cov}(i, j) \frac{dg}{dx_i}(\mu_x) \frac{dg}{dx_j}(\mu_x) \]

\[ \tilde{z} \rightarrow p, \beta \]
\[ \beta_{cdf} = \frac{\mu_g - \tilde{z}}{\sigma_g} \]
\[ \beta_{ccdf} = \frac{\tilde{z} - \mu_g}{\sigma_g} \]

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\[ \text{minimize } \mathbf{u}^T \mathbf{u} \]
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Performance Measure Approach (PMA)

\[ \text{minimize } \pm G(\mathbf{u}) \]
subject to \( \mathbf{u}^T \mathbf{u} = \bar{\beta}^2 \)

Find min \( G \) at \( \beta \) radius
Used for inv map \( p/\beta \rightarrow z \)

Many algorithm variations in limit state approximations, probability integrations, MPP search algorithm, warm starting, etc.
## Reliability Algorithm Variations

<table>
<thead>
<tr>
<th>MPP search</th>
<th>Order of approximation and integration</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>First order</td>
</tr>
<tr>
<td>none</td>
<td>MVFOSM</td>
</tr>
<tr>
<td>x_taylor_mean</td>
<td>AMV</td>
</tr>
<tr>
<td>u_taylor_mean</td>
<td>u-space AMV</td>
</tr>
<tr>
<td>x_taylor_mpp</td>
<td>AMV+</td>
</tr>
<tr>
<td>u_taylor_mpp</td>
<td>u-space AMV+</td>
</tr>
<tr>
<td>x_two_point</td>
<td>TANA</td>
</tr>
<tr>
<td>u_two_point</td>
<td>u-space TANA</td>
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<tr>
<td>no_approx</td>
<td>FORM</td>
</tr>
</tbody>
</table>
Reliability Algorithm Variations: Sample Results

Analytic benchmark test problems: lognormal ratio, short column, cantilever

<table>
<thead>
<tr>
<th>RIA Approach</th>
<th>SQP Function Evaluations</th>
<th>NIP Function Evaluations</th>
<th>CDF p Error Norm</th>
<th>Target z Offset Norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVFOSM</td>
<td>1</td>
<td>1</td>
<td>0.1548</td>
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<tr>
<td>MVSOSM</td>
<td>1</td>
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<td>45</td>
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<td>45</td>
<td>0.006408</td>
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<td>45</td>
<td>0.002063</td>
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<td>45</td>
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<td>x-space AMV+</td>
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<td>192</td>
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<td>0.0</td>
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<tr>
<td>u-space AMV+</td>
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<td>207</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>x-space AMV²+</td>
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<td>131</td>
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<td>u-space AMV²+</td>
<td>122</td>
<td>130</td>
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<td>x-space TANA</td>
<td>245</td>
<td>246</td>
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<tr>
<td>u-space TANA</td>
<td>296*</td>
<td>278*</td>
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<td>FORM</td>
<td>626</td>
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<td>0.0</td>
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<tr>
<td>SORM</td>
<td>669</td>
<td>219</td>
<td>0.0</td>
<td>0.0</td>
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</table>

<table>
<thead>
<tr>
<th>PMA Approach</th>
<th>SQP Function Evaluations</th>
<th>NIP Function Evaluations</th>
<th>CDF z Error Norm</th>
<th>Target p Offset Norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVFOSM</td>
<td>1</td>
<td>1</td>
<td>7.454</td>
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<tr>
<td>MVSOSM</td>
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<td>1</td>
<td>6.823</td>
<td>0.0</td>
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<td>u-space AMV</td>
<td>45</td>
<td>45</td>
<td>0.5828</td>
<td>0.0</td>
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<tr>
<td>x-space AMV²</td>
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<td>45</td>
<td>2.730</td>
<td>0.0</td>
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<tr>
<td>u-space AMV²</td>
<td>45</td>
<td>45</td>
<td>2.828</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space AMV+</td>
<td>171</td>
<td>179</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>u-space AMV+</td>
<td>205</td>
<td>205</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>x-space AMV²+</td>
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<td>142</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>u-space AMV²+</td>
<td>132</td>
<td>139</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space TANA</td>
<td>293*</td>
<td>272</td>
<td>0.04259</td>
<td>1.598e-4</td>
</tr>
<tr>
<td>u-space TANA</td>
<td>325*</td>
<td>311*</td>
<td>2.208</td>
<td>5.600e-4</td>
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<tr>
<td>FORM</td>
<td>720</td>
<td>192</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>SORM</td>
<td>535</td>
<td>191*</td>
<td>2.410</td>
<td>6.522e-4</td>
</tr>
</tbody>
</table>

Note: 2nd-order PMA with prescribed p level is harder problem → requires β(p) update/inversion
New UQ Method: Efficient Global Reliability Analysis (EGRA)

• Address known failure modes of local reliability methods:
  – Nonsmooth: fail to converge to an MPP
  – Multimodal: only locate one of several MPPs
  – Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP

• Based on EGO (surrogate-based global opt.), which exploits special features of GPs
  – Mean and variance predictions: formulate expected improvement (EGO) or expected feasibility (EGRA)
  – Balance explore and exploit in computing an optimum (EGO) or locating the limit state (EGRA)
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Accurate and efficient global estimation of failure surfaces
EGRA (cont.):
Benchmark performance

Rosenbrock Test

Multimodal Test

CDF Comparison

<table>
<thead>
<tr>
<th>Reliability Method</th>
<th>Function Evaluations</th>
<th>First-Order $p_f$ (Error%)</th>
<th>Second-Order $p_f$ (Error%)</th>
<th>Sampling $p_f$ (Error, Avg. Error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Approximation</td>
<td>70</td>
<td>0.11797 (277.0%)</td>
<td>0.02516 (-19.6%)</td>
<td>—</td>
</tr>
<tr>
<td>x-space AMV²⁺</td>
<td>26</td>
<td>0.11797 (277.0%)</td>
<td>0.02516 (-19.6%)</td>
<td>—</td>
</tr>
<tr>
<td>u-space AMV²⁺</td>
<td>26</td>
<td>0.11777 (277.0%)</td>
<td>0.02516 (-19.6%)</td>
<td>—</td>
</tr>
<tr>
<td>u-space TANA</td>
<td>131</td>
<td>0.11797 (277.0%)</td>
<td>0.02516 (-19.6%)</td>
<td>—</td>
</tr>
<tr>
<td>LHS solution</td>
<td>10k</td>
<td>—</td>
<td>—</td>
<td>0.03117 (0.385%, 2.847%)</td>
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<tr>
<td>LHS solution</td>
<td>100k</td>
<td>—</td>
<td>—</td>
<td>0.03126 (0.085%, 1.397%)</td>
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<tr>
<td>LHS solution</td>
<td>1M</td>
<td>—</td>
<td>—</td>
<td>0.03129 (truth, 0.339%)</td>
</tr>
<tr>
<td>x-space EGRA</td>
<td>35.1</td>
<td>—</td>
<td>—</td>
<td>0.03134 (0.155%, 0.433%)</td>
</tr>
<tr>
<td>u-space EGRA</td>
<td>35.2</td>
<td>—</td>
<td>—</td>
<td>0.03133 (0.136%, 0.296%)</td>
</tr>
</tbody>
</table>

Accuracy similar to exhaustive sampling at cost similar to local reliability assessment
Generalized Polynomial Chaos Expansions

Approximate response w/ spectral proj. using orthogonal polynomial basis fns

\[ R = \sum_{j=0}^{P} \alpha_j \psi_j(\xi) \]

using

\[ \psi_0(\xi) = \psi_0(\xi_1) \psi_0(\xi_2) = 1 \]
\[ \psi_1(\xi) = \psi_1(\xi_1) \psi_0(\xi_2) = \xi_1 \]
\[ \psi_2(\xi) = \psi_0(\xi_1) \psi_1(\xi_2) = \xi_2 \]
\[ \psi_3(\xi) = \psi_2(\xi_1) \psi_0(\xi_2) = \xi_1^2 - 1 \]
\[ \psi_4(\xi) = \psi_1(\xi_1) \psi_1(\xi_2) = \xi_1 \xi_2 \]
\[ \psi_5(\xi) = \psi_0(\xi_1) \psi_2(\xi_2) = \xi_2^2 - 1 \]

- **Nonintrusive:** estimate \( \alpha_j \) using sampling (expectation), pt collocation (regression), tensor-product quadrature or Smolyak sparse grids (numerical integration)

**Wiener-Askey Generalized PCE**

- **Tailor basis:** optimal basis selection leads to exponential conv rates

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Density function</th>
<th>Polynomial</th>
<th>Weight function</th>
<th>Support range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>( \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} )</td>
<td>Hermite ( H_n(x) )</td>
<td>( e^{-\frac{x^2}{2}} )</td>
<td>([-\infty, \infty])</td>
</tr>
<tr>
<td>Uniform</td>
<td>( \frac{1}{2} )</td>
<td>Legendre ( P_n(x) )</td>
<td>1</td>
<td>([-1, 1])</td>
</tr>
<tr>
<td>Beta</td>
<td>( \frac{(1-x)^a (1+x)^b}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)} )</td>
<td>Jacobi ( P_n^{(\alpha, \beta)}(x) )</td>
<td>( (1 - x)^\alpha (1 + x)^\beta )</td>
<td>([-1, 1])</td>
</tr>
<tr>
<td>Exponential</td>
<td>( e^{-x} )</td>
<td>Laguerre ( L_n(x) )</td>
<td>( e^{-x} )</td>
<td>([0, \infty])</td>
</tr>
<tr>
<td>Gamma</td>
<td>( \frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)} )</td>
<td>Generalized Laguerre ( L_n^{(\alpha)}(x) )</td>
<td>( x^\alpha e^{-x} )</td>
<td>([0, \infty])</td>
</tr>
</tbody>
</table>

- **Tailor expansion type/order/range:** TP or TO PCE, p/k-adapt based on PCE error est.
  - Dimension p-refinement: anisotropic quadrature/sparse grid
  - Dimension k-refinement: discretization of random domain
Stochastic Collocation
(based on Lagrange interpolation)

Instead of estimating coeffs for known basis fns, form interpolants for known coefficients

\[ R = \sum_{j=1}^{N_p} r_j L_j(\xi) \]

\[ R = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r \left( \xi_{j_1}, \ldots, \xi_{j_n} \right) \left( L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n} \right) \]

Form sparse interpolant using \( \Sigma \) of tensor products (same as forming sparse grid)

Key is use of same Gauss points/weights from the orthogonal polynomials for specified input PDFs → same exponential convergence rates

Advantages relative to PCE:
• Simpler (no expansion order)
• Adapts to integration approach / collocation pt set: doesn’t over-/under-integrate a (nonsynchronized) expansion
• Estimating moments of any order is easy: \( E[R^k] = \sum r_{j}^k w_{j} \) (formation of interpolant only reqd for CDF sampling)
• No intrusive variant: intrusive approach decouples into collocation

Disadvantages relative to PCE:
• Requires structured data sets: quadrature/sparse grid (cubature?), no random sampling sets as in PCE
PCE Coefficient Estimation: Spectral Projection, Sampling

Orthogonality of multivariate polynomials allows coefficient extraction using spectral projection

\[ R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi) \]  \[ \alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_\Omega R \Psi_j Q(\xi) \, d\xi \]

Denominator available analytically:

\[ \langle \Psi_j^2 \rangle = \prod_{i=1}^{n} \langle \psi_{m,i}^2 \rangle \]

Key requirement is evaluation of numerator for each polynomial

**Expectation (sampling):**
- Sample within distribution of \( \xi \)
- Compute expected value of product of \( R \) and each \( \Psi_j \)

**Linear regression ("point collocation"):**
- Sample within distribution of \( \xi \)
- Solves a least squares data fit for all coefficients at once:

\[ \Psi \alpha = R \]
PCE/SC Expansions:
Tensor Product Quadrature

**Numerical integration: tensor-product quadrature**

\[ \mathcal{W}^i(f)(\xi) = \sum_{j=1}^{m_i} f(\xi^i_j) w^i_j \]

\[ Q^n_i f(\xi) = (\mathcal{W}^{i_1} \otimes \cdots \otimes \mathcal{W}^{i_n})(f)(\xi) = \sum_{j_1=1}^{m_1} \cdots \sum_{j_n=1}^{m_n} f(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}) (w_{j_1}^{i_1} \otimes \cdots \otimes w_{j_n}^{i_n}) \]

- Evaluate response at every combination of 1-D integration rules
- Weights for each point are product of 1-D weights
- Scales as \( m^n \)
- 1-D Gaussian rule of order \( m \) exactly integrates any polynomial up to order \( 2m - 1 \)
- Assuming \( R \mathcal{Y}_j \) of order \( 2p \), select \( m = p + 1 \)

Clenshaw-Curtis tensor-product
PCE/SC Expansions: Smolyak Sparse Grids

**Numerical Integration (Smolyak sparse grids):**

\[ \mathcal{I}(w, n) = \sum_{|i| \leq w+n} (\Delta_{i_1} \otimes \cdots \otimes \Delta_{i_n}) \]

for

\[ \Delta^i := \mathcal{U}^i - \mathcal{U}^{i-1} \]

\[ \mathcal{I}(w, n) = \sum_{w+1 \leq |i| \leq w+n} (-1)^{w+n-|i|} \binom{n-1}{w+n-|i|} \cdot (\mathcal{U}_{i_1} \otimes \cdots \otimes \mathcal{U}_{i_n}) \]

Nonlinear growth rules promote nesting of collocation pts

Linear growth rules provide finer granularity & integrand uniformity

**Clements – Curtis:**

\[ m = \begin{cases} 
1 & i = 1 \\
2^{i-1} + 1 & i > 1 
\end{cases} \]

**Gaussian nonlinear:**

\[ m = 2^i - 1 \]

**Gaussian linear:**

\[ m = 2^i - 1 \]
PCE/SC Expansions: Smolyak Sparse Grids

Numerical Integration (Smolyak sparse grids):

\[
\mathcal{A}(w, n) = \sum_{|i| \leq w+n} (\Delta^{i_1} \otimes \cdots \otimes \Delta^{i_n})
\]

for

\[
\Delta^i := U^i - U^{i-1}
\]

\[
\mathcal{A}(w, n) = \sum_{w+1 \leq |i| \leq w+n} (-1)^{w+n-|i|} \binom{n-1}{w+n-|i|} \cdot (U^{i_1} \otimes \cdots \otimes U^{i_n})
\]

2D Clenshaw-Curtis sparse grid (less optimal, more nesting)

2D Gauss-Legendre sparse grid (more optimal, less nesting)

3D Clenshaw-Curtis sparse grid
### PCE/SC Expansions: Smolyak Sparse Grids (cont.)

**Key difference between quadrature & sparse grids:** polynomial order coverage

<table>
<thead>
<tr>
<th>Sparse Grid (w/ linear growth)</th>
<th>Quadrature</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>x^2</td>
</tr>
<tr>
<td>3</td>
<td>x^3</td>
</tr>
<tr>
<td>4</td>
<td>x^4</td>
</tr>
<tr>
<td>5</td>
<td>x^4\cdot y</td>
</tr>
<tr>
<td>6</td>
<td>x^4\cdot y^2</td>
</tr>
<tr>
<td>7</td>
<td>x^4\cdot y^3</td>
</tr>
<tr>
<td>8</td>
<td>x^4\cdot y^4</td>
</tr>
</tbody>
</table>

From J. Burkardt, “A Low Level Introduction to High Dimensional Sparse Grids.”
**PCE/SC Expansions: Smolyak Sparse Grids (cont.)**

*Key difference between quadrature & sparse grids:* polynomial order coverage

From J. Burkardt, “A Low Level Introduction to High Dimensional Sparse Grids.”
Performance of traditional (total-order) PCE

Traditional PCE: super-algebraic convergence for numerical integration and regression approaches. $\sqrt{N}$ for $\alpha$ sampling

But, SC outperforms traditional PCE for all quadrature/sparse grid cases
Poor synchronization of traditional total-order PCE w/ numerical integration $\rightarrow$ \textit{PCE tailoring}
Tailoring of Polynomial Chaos Expansions

\[ R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi) \]

\[ \Psi_j(\xi) = \prod_{i=1}^{n} \psi_{m_i}(\xi_i) \]

Multi-index length & content

Tensor-product

\[ N_t = 1 + P = \prod_{i=1}^{n} (p_i + 1) \]

Total-order

\[ N_t = 1 + P = 1 + \sum_{s=1}^{p} \frac{1}{s!} \prod_{r=0}^{s-1} (n + r) = \frac{(n + p)!}{n!p!} \]

Monomial coverage

Tensor-prod quadrature (m=5)

Sparse grid (nonlinear growth, w=4)

Sparse grid (linear growth, w=4)
Tailoring of Polynomial Chaos Expansions

\[ R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi) \]

\[ \Psi_j(\xi) = \Pi_{i=1}^{n} \psi_{m_i^j}(\xi_i) \]

Tensor-product

\[ N_t = 1 + P = \Pi_{i=1}^{n}(p_i + 1) \]

Total-order

\[ N_t = 1 + P = 1 + \sum_{s=1}^{p} \frac{1}{s!} \Pi_{r=0}^{s-1}(n + r) = \frac{(n + p)!}{n!p!} \]

Monomial coverage

**Tensor-prod quadrature (m=5)**

**Sparse grid (nonlinear growth, w=4)**

**Sparse grid (linear growth, w=4)**

Traditional PCE: total-order \( p = m-1 \)

**Tailored PCE: tensor-product** \( p = m-1 \)

Traditional PCE: heuristic total-order

**Tailored PCE: synchronized total-order**

\[ \Psi_0(\xi) = \psi_0(\xi_1) \psi_0(\xi_2) = 1 \]

\[ \Psi_1(\xi) = \psi_1(\xi_1) \psi_0(\xi_2) = \xi_1 \]

\[ \Psi_2(\xi) = \psi_2(\xi_1) \psi_0(\xi_2) = \xi_1^2 - 1 \]

\[ \Psi_3(\xi) = \psi_3(\xi_1) \psi_1(\xi_2) = \xi_2 \]

\[ \Psi_4(\xi) = \psi_4(\xi_1) \psi_1(\xi_2) = \xi_1 \xi_2 \]

\[ \Psi_5(\xi) = \psi_5(\xi_1) \psi_1(\xi_2) = (\xi_1^2 - 1) \xi_2 \]

\[ \Psi_6(\xi) = \psi_6(\xi_1) \psi_2(\xi_2) = \xi_2^3 - 1 \]

\[ \Psi_7(\xi) = \psi_7(\xi_1) \psi_2(\xi_2) = \xi_1 \xi_2^2 - 1 \]

\[ \Psi_8(\xi) = \psi_8(\xi_1) \psi_2(\xi_2) = (\xi_1^2 - 1)(\xi_2^2 - 1) \]
Computational Results: Lognormal Ratio (n=2)

Compare CDF convergence for traditional PCE, tailored PCE, and SC using TPQ and SSG (linear and nonlinear growth)

Tailored PCE shows improvement over traditional PCE
Computational Results: Lognormal Ratio (n=2)

Compare CDF convergence for traditional PCE, tailored PCE, and SC using TPQ and SSG (linear and nonlinear growth).

- Tailored PCE shows improvement over traditional PCE
  - TPQ: tailored PCE eliminates perf. gap
  - Nonlinear SSG: modest improvement for tailored
  - Linear SSG: both PCE and SC are improved; PCE closes perf. gap

While this work closes the performance gap, in no direct comparison has nonintrusive PCE outperformed SC → PCE motivated by flexibility in collocation sets (i.e., Genz cubature, unstructured/random sets supporting fault tolerance).
Algebraic Benchmarks:
Steel Column

\[ g = F_s - P \left( \frac{1}{2BD} + \frac{F_0}{BDH} \frac{E_b}{E_b - P} \right) \]
\[ P = P_1 + P_2 + P_3 \]
\[ E_b = \frac{\pi^2 E BDH^2}{2L^2} \]

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 \( \mu/\sigma = 300/3 \) mm)
flange thickness \( D \) (lognormal with \( \mu/\sigma = 20/2 \) mm)
profile height \( H \) (lognormal with \( \mu/\sigma = 300/5 \) mm)
initial deflection \( F_0 \) (normal with \( \mu/\sigma = 30/10 \) mm)
Youngs modulus \( E \) (weibull with \( \mu/\sigma = 21000/4200 \) MPa)
Algebraic Benchmarks: Steel Column

\begin{align*}
g &= F_s - P \left( \frac{1}{2BD} + \frac{F_0}{BDH \, E_b - P} \right) \\
P &= P_1 + P_2 + P_3 \\
E_b &= \frac{\pi^2 E \cdot BDH^2}{2L^2}
\end{align*}

- 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)
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Singularity:
- Local methods (reliability) are fine
- LHS to \( 10^6 \) is also divergent
Algebraic Benchmarks: Steel Column

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

\[ P = P_1 + P_2 + P_3 \]

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Youngs modulus \( E \) (weibull with \( \mu/\sigma = 21000/4200 \) MPa)

Singularity:
- Local methods (reliability) are fine
- LHS to 10^6 is also divergent

(a) CDF convergence.  
(b) Mean convergence.  
(c) Standard deviation convergence.
Algorithmic Strengths, Weaknesses, R&D Needs

**Sampling**
- **Strengths**: Simple and reliable, convergence rate is dimension-independent
- **Weaknesses**: $\sqrt{N}$ convergence → expensive for accurate tail statistics

**Local reliability**
- **Strengths**: Computationally efficient, widely used, scales to large $n$
- **Weaknesses**: algorithmic failures for limit states with following features
  - **Nonsmooth**: fail to converge to an MPP
  - **Multimodal**: only locate one of several MPPs
  - **Highly nonlinear**: low order limit state approxs. insufficient to resolve probability at MPP

**Global reliability**
- **Strengths**: handles nonsmooth, multimodal, highly nonlinear limit states
- **Weaknesses**: global surrogate → scaling to large $n$

**Stochastic expansions**
- **Strengths**: functional representation, exponential convergence rates
- **Issues**: Discontinuity → Gibbs phenomena
- **Issues**: Singularity → divergence in moments
- **Issues**: Scaling to large $n$ → exponential growth in simulation reqmts

**Research**:
- Pade approximation
- Basis enrichment / discretization (→ local basis functions)
- Dimension adaptive methods
Build on Foundation Provided by these Probabilistic UQ Methods

Stochastic sensitivity analysis
- Local reliability ($p/\beta$)
- Stochastic expansions ($\mu/\sigma$)

\[
\begin{align*}
\nabla_d z &= \nabla_d g \\
\nabla_d \beta_{cdf} &= \frac{1}{\| \nabla_u G \|} \nabla_d g \\
\nabla_d \mu_{cdf} &= -\phi(-\beta_{cdf}) \nabla_d \beta_{cdf}
\end{align*}
\]

(1st order)

If $d = \text{distr param}$, then expand $\nabla_d g = \nabla_d x \nabla_x g$

\[
\begin{align*}
\mu_R &= \alpha_0 \\
\sigma^2_R &= \sum_{j=1}^{P} \alpha_j^2 \langle \Psi_j \rangle^2 \\
\frac{d\mu_R}{ds} &= \langle \frac{dR}{ds} \rangle \\
\frac{d\sigma^2_R}{ds} &= 2 \sum_{j=1}^{P} \alpha_j \langle \frac{dR}{ds} \Psi_j \rangle
\end{align*}
\]

Augment NLP w/ $s_u (\mu, \sigma, z/\beta/p)$

\[
\begin{align*}
\min & \quad f(d) + W s_u(d) \\
s.t. & \quad g_t \leq g(d) \leq g_u \\
& \quad h(d) = h_t \\
& \quad d_l \leq d \leq d_u \\
& \quad \omega_l \leq A_i s_u(d) \leq \omega_u \\
& \quad A_e s_u(d) = a_t
\end{align*}
\]

OUU/MCUU
- Reliability-based design ($p/\beta$)
- Robust design ($\mu/\sigma$)

Mixed aleatory/epistemic UQ
- SOP
- DSTE
Epistemic UQ

Epistemic UQ: one does not know enough to specify probability distributions
Sometimes referred to as subjective, reducible, or lack of knowledge uncertainty

Second-order probability
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).

Dempster-Shafer theory of evidence
- Basic probability assignment (interval-based)
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals

<table>
<thead>
<tr>
<th>Source</th>
<th>Bel(&gt;Y)</th>
<th>P(&gt;Y)</th>
<th>P(I(&gt;Y))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>10%</td>
<td>90%</td>
<td>10%</td>
</tr>
<tr>
<td>Source 2</td>
<td>10%</td>
<td>70%</td>
<td>20%</td>
</tr>
<tr>
<td>Source 3</td>
<td>33%</td>
<td>33%</td>
<td>33%</td>
</tr>
</tbody>
</table>
SOP using Stochastic Expansions

Second-order probability
- Traditional approach employs nested sampling
- Expensive sims lead to under-resolved sampling, especially at outer loop
- As for OUU, epistemic interval vars may be augmented or inserted
- In limiting case, inner loop collapses to a single deterministic analysis

Address accuracy and efficiency
- Inner loop: stochastic expansions which are epistemic-aware ($0^{th}$-order combined. $1^{st}$-order prob.)
- Outer loop: opt-based interval estimation, exploiting data reuse within global min/max
  - EGO, DIRECT, et al.

minimize $M(s)$
subject to $s_L \leq s \leq s_U$

maximize $M(s)$
subject to $s_L \leq s \leq s_U$
Dempster-Shafer

- Dempster-Shafer belief structures: for each uncertain input variable, one specifies “basic probability assignment” for each potential interval where variable may exist
- Intervals may be contiguous, overlapping, or have “gaps”

![Variable 1](BPA=0.5, BPA=0.2, BPA=0.3)

![Variable 2](BPA=0.5, BPA=0.3, BPA=0.2)

- Look at various combinations of intervals. In each joint interval “box”, one needs to find the maximum and minimum value in that box (by sampling or optimization)
- Belief: lower bound on the probability that is consistent with the evidence
- Plausibility: upper bound on the probability that is consistent with the evidence
- Order these beliefs and plausibilities to get CDFs

![Graph](Original LHS samples used
To generate a surrogate

Million sample points generated from the surrogate, used to determine the max and min in each “cell” to calculate plausibility and belief)
D-S Epistemic Uncertainty Results: Cantilever Beam Test Problem

**Example 1**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Intervals</th>
<th>BPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>[0.97, 1.03] m</td>
<td>1.0</td>
</tr>
<tr>
<td>P</td>
<td>[85,115] N</td>
<td>1.0</td>
</tr>
<tr>
<td>E</td>
<td>[27.6,110.4]GPa</td>
<td>1.0</td>
</tr>
</tbody>
</table>

**Example 2**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Intervals</th>
<th>BPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>[0.97, 0.98] [0.98, 1.02] [1.02,1.03] m</td>
<td>0.25, 0.5, 0.25</td>
</tr>
<tr>
<td>P</td>
<td>[85,90] [90,110] [110,115] N</td>
<td>0.25, 0.5, 0.25</td>
</tr>
<tr>
<td>E</td>
<td>[27.6,41.4] [41.4, 96.6] [96.6,110.4]GPa</td>
<td>0.25, 0.5, 0.25</td>
</tr>
</tbody>
</table>

Displacement (cm)
Solution-Verified Reliability Analysis and Design of MEMS

**Application:** Probabilistic analysis and design of compliant bi-stable MEMS accounting for manufacturing uncertainties and solution errors

**Approach:** Integration of multiple Sandia modeling & simulation capabilities:
- uncertainty analysis and probabilistic design (DAKOTA)
- global norm and quantity of interest error estimates (Coda)
- nonlinear mechanics analysis (Aria) + data structures and h-refinement (SIERRA)

**Strategy:** On-line soln verification → project UQ/OUU results towards ∞—discretization

- Reduce/eliminate errors (adaptive mesh refinement)
- Include error estimates as deterministic quantity
- Include error estimates as random variables
- Include error bounds as epistemic intervals
Solution-Verified Reliability Analysis and Design of MEMS

**Application:** Probabilistic analysis and design of compliant bi-stable MEMS accounting for manufacturing uncertainties and solution errors

**Bi-stable MEMS Switch**

**Approach:** Integration of multiple Sandia modeling & simulation capabilities:
- uncertainty analysis and probabilistic design (DAKOTA)
- global norm and quantity of interest error estimates (Coda)
- nonlinear mechanics analysis (Aria) + data structures and h-refinement (SIERRA)

**Strategy:** On-line soln verification $\rightarrow$ project UQ/OUU results towards $\infty$—discretization

- **Reduce/eliminate errors** (adaptive refinement)
- **Include error estimates** as deterministic quantities
- **Include error estimates** as random variables
- **Include error bounds** as epistemic intervals

**Error-informed:** ZZ/QOI EE as indicators for uniform/adaptive refinement (tight tols: eliminate correction)

**Error-corrected:** QOI EE as analysis correction factors

**Combined:** control QOI error levels (loose tols: assure correction accuracy) and use correction factors
For particular geometric design parameters and realizations of uncertain variables:

1. generate 2-D geometric model and (re-)mesh (also ongoing smooth mesh movement work at SNL)

2. simulate displacement steps with Sierra/Aria (via new nonlinear quasistatic mechanics capability) to determine reaction forces

3. postprocess force—displacement curve and interpolate to find maximum and minimum

2 uncertain vars \( x \): edge bias \( \Delta w \) and residual stress \( S_r \)

<table>
<thead>
<tr>
<th>variable</th>
<th>mean</th>
<th>std. dev.</th>
<th>distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta w )</td>
<td>-0.2 ( \mu m )</td>
<td>0.08</td>
<td>normal</td>
</tr>
<tr>
<td>( S_r )</td>
<td>-11 Mpa</td>
<td>4.13</td>
<td>normal</td>
</tr>
</tbody>
</table>
Bistable Switch: Problem Formulation

**Typical design specifications:**
- actuation force $F_{\min}$ reliably $< \text{target (-5 } \mu\text{N)}$
- bistable ($F_{\max} > 0, F_{\min} < 0$)
- maximum force: $50 < F_{\max} < 150$
- equilibrium $E_2 < 8 \mu m$
- maximum stress < 1200 MPa

**simultaneously reliable and robust designs**

\[
\begin{align*}
\text{max} & \quad E \left[ F_{\min}(d, x) \right] \\
\text{s.t.} & \quad 2 \leq \beta_{ccdf}(d) \\
& \quad 50 \leq E \left[ F_{\max}(d, x) \right] \leq 150 \\
& \quad E \left[ E_2(d, x) \right] \leq 8 \\
& \quad E \left[ S_{\max}(d, x) \right] \leq 3000
\end{align*}
\]

**combined RIA/PMA to control both tails**
(reliable/robust):

\[
\begin{align*}
\text{max} & \quad z_{\beta=-2}(d) \\
\text{s.t.} & \quad 2 \leq \beta_{ccdf}(d) \\
& \quad \text{nln. constr.}
\end{align*}
\]

**RIA/PMA combination:**
\(\text{twice the cost}\)
ASC 2006 L2 Milestone Results

- Reliability analysis: compute error-corrected CDFs and assess accuracy/efficiency

- RBDO: carry best fwd to design switch for max robustness s.t. reliability constraint

Conclusions: UQ/OUU with error corrected/informed approaches can be:
- more accurate: controlling/correcting errors leads to higher confidence in UQ/RBDO results
- less expensive: Linear800+EE analysis above < 10% cost of fully converged reference
- more reliable: on-line approach accounts for any parameter dependence (esp. shape vars)
- more convenient: can eliminate need for manual *a priori* convergence studies

Reliability constraint: $\beta > 2$
Max $F_{\min}$ (10x robustness)
Concluding Remarks

Survey of nonintrusive UQ methods:
- Sampling
- Local and global reliability
- Stochastic expansions: polynomial chaos, stochastic collocation

• Strengths, weaknesses, research needs
• Highlighted new methods that bridge critical gap → reliability of LHS at much lower cost

Build on algorithmic foundations
• SSA for local reliability and PCE/SC → OUU/MCUU and mixed aleatory-epistemic UQ
• SOP/DSTE that are more accurate/efficient than nested sampling
  – Inner loop: Stochastic expansions that are epistemic-aware (with SSA of moments)
  – Outer loop: opt-based interval estimation; global min/max with data reuse

Demonstration of integration of UQ/Opt/EE → Soln-verified MEMS UQ/OUU

Current directions:
• Additional tailoring and fine-grained algorithmic control (stochastic expansions)
  – Sparse grids: anisotropy in level
  – Numerically generated orthog polys for arbitrary input PDFs (Golub-Welsch, Gramm-Schmidt)
  – Stochastic error estimation & p/k adaptivity (towards unification w/ h/p FE adaptivity)
DAKOTA Software

Access

- GNU GPL – freely available worldwide (~5000 registered users)
- Releases: Major, Interim, Stable, VOTD 4.2 released Nov. 2008
- Manuals: Users, Reference, Developers
- Support: dakota-users, dakota-developers

Platforms

- Linux, Solaris, AIX, Windows (Cygwin/MINGW), Mac
- MPICH, MVAPICH, OpenMPI on IP, GM, IB

DAKOTA

Optimization
Uncertainty Quant.
Parameter Est.
Sensitivity Analysis

Black Box:
- Sandia simulation codes
- Commercial simulation codes

Semi-intrusive:
- SIERRA (multiphysics), SALINAS (structural dynamics), Xyce (circuits), Sage (CFD), MATLAB, Mathematica, ModelCenter, FIPER

Model Parameters

Design Metrics