Overview of Uncertainty Quantification Algorithm R&D in the DAKOTA Project

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NIST UQ Workshop
Boulder, CO; August 1-4, 2011

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

Build on these algorithmic foundations:
Mixed aleatory-epistemic UQ, Opt/model calibration under uncertainty
### Uncertainty Quantification Algorithms @ SNL: New methods bridge robustness/efficiency gap

<table>
<thead>
<tr>
<th></th>
<th>Production</th>
<th>New</th>
<th>Under dev.</th>
<th>Planned</th>
<th>Collabs.</th>
</tr>
</thead>
<tbody>
<tr>
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<td><strong>Reliability</strong></td>
<td>Local: Mean Value, First-order &amp; second-order reliability methods (FORM, SORM)</td>
<td>Global: Efficient global reliability analysis (EGRA)</td>
<td>gradient-enhanced</td>
<td>recursive emulation, TGP</td>
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<td><strong>Stochastic expansion</strong></td>
<td>PCE and SC with uniform &amp; dimension-adaptive p-/h-refinement</td>
<td>local h-refinement, gradient-enhanced</td>
<td>hp-adaptive, discrete, multi-physics</td>
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New methods bridge robustness/efficiency gap

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**Research:** Adaptive Refinement, Basis Enhancement

**Fills Gaps**
Algorithm R&D in Adaptive UQ

**Drivers**

- Efficient/robust/scalable core $\rightarrow$ adaptive methods, adjoint enhancement
- Complex random environments $\rightarrow$ epistemic/mixed UQ, model form/multifidelity, RF/SP, multiphysics/multiscale

**Stochastic expansions:**

- **Polynomial chaos expansions (PCE):** known basis, compute coeffs
- **Stochastic collocation (SC):** known coeffs, form interpolants
- Adaptive approaches: emphasize key dimensions
  - Uniform/dim-adaptive $p$-refinement: iso/aniso/generalized sparse grids
  - Dimension-adaptive $h$-refinement with grad-enhanced interpolants
- Sparse adaptive global methods: scale as $m^{\log r}$ with $r << n$

**EGRA:**

- Adaptive GP refinement for tail probability estimation
- Accuracy similar to exhaustive sampling at cost similar to local reliability assessment
- Global method that scales as $\sim n^2$

**Sampling:**

- Importance sampling (adaptive refinement)
- Incremental MC/LHS (uniform refinement)
Algorithm R&D in UQ Complexity

Drivers

- Efficient/robust/scalable core → adaptive methods, adjoint enhancement
- Complex random env. → mixed UQ, model form/multifidelity, RF/SP, multiphysics/multiscale

Stochastic sensitivity analysis

- Aleatory or combined expansions including nonprobabilistic dimensions s → sensitivities of moments w.r.t. design and/or epistemic parameters

Design and Model Calibration Under Uncertainty

Mixed Aleatory-Epistemic UQ

- SOP, IVP, and DSTE approaches that are more accurate and efficient than traditional nested sampling

Random Fields / Stochastic Processes (Encore, PECOS)

Multiphysics (multiscale) UQ:

- Invert UQ & multiphysics loops → transfer UQ stats among codes

Bayesian Inference:

- Collaborations w/ LANL (GPM), UT (Queso), Purdue/MIT (gPC)

Model form:

- Multifidelity UQ (hierarchy), model averaging/selection (ensemble)
Reliability Methods for UQ
UQ with Reliability Methods

**Mean Value Method**

\[
\mu_g = g(\mu_x)
\]
\[
\sigma_g^2 = \sum_i \sum_j Cov(i, j) \frac{dg}{dx_i}(\mu_x) \frac{dg}{dx_j}(\mu_x)
\]

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

**MPP search methods**

**Reliability Index Approach (RIA)**

minimize \( u^T u \)
subject to \( G(u) = \tilde{z} \)

Find min dist to \( G \) level curve
Used for fwd map \( z \rightarrow p/\beta \)

**Performance Measure Approach (PMA)**

minimize \( \pm G(u) \)
subject to \( u^T u = \beta^2 \)

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

\[
Nataf x \rightarrow u: \quad \Phi(z_i) = F(x_i) \]
\[
z = Lu
\]

Rough statistics
# Reliability Algorithm Variations

## Limit state approximations

<table>
<thead>
<tr>
<th>Variant</th>
<th>Expression</th>
</tr>
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<td>AMV:</td>
<td>$g(x) = g(\mu_x) + \nabla_x g(\mu_x)^T (x - \mu_x)$</td>
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<td>u-space AMV:</td>
<td>$G(u) = G(\mu_u) + \nabla_u G(\mu_u)^T (u - \mu_u)$</td>
</tr>
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<td>$g(x) = g(x^<em>) + \nabla_x g(x^</em>)^T (x - x^*)$</td>
</tr>
<tr>
<td>u-space AMV+:</td>
<td>$G(u) = G(u^<em>) + \nabla_u G(u^</em>)^T (u - u^*)$</td>
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**FORM:** no linearization

- **2nd-order local, e.g. x-space AMV$^2+$:**

$$g(x) \approx g(x^*) + \nabla_x g(x^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla_x^2 g(x^*) (x - x^*)$$

- Hessians may be full/FD/Quasi
- Quasi-Newton Hessians may be BFGS or SR1
Reliability Algorithm Variations

### Limit state approximations

- **AMV:** \( g(x) = g(\mu_x) + \nabla_x g(\mu_x)^T (x - \mu_x) \)
- **u-space AMV:** \( G(u) = G(\mu_u) + \nabla_u G(\mu_u)^T (u - \mu_u) \)
- **AMV+:** \( g(x) = g(x^*) + \nabla_x g(x^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla^2_x g(x^*) (x - x^*) \)
- **u-space AMV+:** \( G(u) = G(u^*) + \nabla_u G(u^*)^T (u - u^*) + \frac{1}{2} (u - u^*)^T \nabla^2_u G(u^*) (u - u^*) \)
- **FORM:** no linearization

- **2nd-order local, e.g. x-space AMV+:**
  \[
g(x) \approx g(x^*) + \nabla_x g(x^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla^2_x g(x^*) (x - x^*)
\]
- **Hessians may be full/FD/Quasi-Newton**
- **Quasi-Newton Hessians may be BFGS or SR1**

### Integrations

- **1st-order:**
  \[
p(g \leq z) = \Phi(-\beta_{cdf})
p(g > z) = \Phi(-\beta_{ccdf})
\]

- **2nd-order:**
  \[
p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta_k} \kappa_i}
\]

### MPP search algorithm

- **[HL-RF], Sequential Quadratic Prog. (SQP), Nonlinear Interior Point (NIP)**

### Warm starting (with projections)

**When:** AMV+ iteration increment, \( z/p/\beta \) level increment, or design variable change

**What:** linearization point & assoc. responses (AMV+), MPP search initial guess

**Multipoint, e.g. TPEA, TANA:**

\[
g(x) \approx g(x_2) + \sum_{i=1}^{n} \frac{\partial g}{\partial x_i} (x_2) \frac{x_{i,2}^{1-p_i}}{p_i} (x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2} \epsilon(x) \sum_{i=1}^{n} (x_i^{p_i} - x_{i,2}^{p_i})^2
\]

\[
p_i = 1 + \ln \left[ \frac{\partial g}{\partial x_i} (x_1) \right] / \ln \left[ \frac{x_{i,1}}{x_{i,2}} \right] - H
\]

\[
\epsilon(x) = \frac{\sum_{i=1}^{n} (x_i^{p_i} - x_{i,1}^{p_i})^2 + \sum_{i=1}^{n} (x_i^{p_i} - x_{i,2}^{p_i})^2}{2 (g(x_1) - g(x_2) - \sum_{i=1}^{n} \frac{\partial g}{\partial x_i} (x_2) \frac{x_{i,2}^{1-p_i}}{p_i} (x_i^{p_i} - x_{i,1}^{p_i}))}
\]

**Additional refinement:**

- **IS, AIS, MMAIS**
- **curvature correction**
Reliability Algorithm Variations:
Algorithm Performance 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>
<td>0.0</td>
</tr>
<tr>
<td>MVSOSM</td>
<td>1</td>
<td>1</td>
<td>0.1127</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space AMV</td>
<td>45</td>
<td>45</td>
<td>0.009275</td>
<td>18.28</td>
</tr>
<tr>
<td>u-space AMV</td>
<td>45</td>
<td>45</td>
<td>0.006408</td>
<td>18.81</td>
</tr>
<tr>
<td>x-space AMV$^2$</td>
<td>45</td>
<td>45</td>
<td>0.006203</td>
<td>2.482</td>
</tr>
<tr>
<td>u-space AMV$^2$</td>
<td>45</td>
<td>45</td>
<td>0.001410</td>
<td>2.031</td>
</tr>
<tr>
<td>x-space AMV+</td>
<td>192</td>
<td>192</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>u-space AMV+</td>
<td>207</td>
<td>207</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space AMV$^2$+</td>
<td>125</td>
<td>131</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>u-space AMV$^2$+</td>
<td>122</td>
<td>130</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space TANA</td>
<td>245</td>
<td>246</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>u-space TANA</td>
<td>296*</td>
<td>278*</td>
<td>6.982e-5</td>
<td>0.05014</td>
</tr>
<tr>
<td>FORM</td>
<td>626</td>
<td>176</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>SORM</td>
<td>669</td>
<td>219</td>
<td>0.0</td>
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<td>0.0</td>
</tr>
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<td>MVSOSM</td>
<td>1</td>
<td>1</td>
<td>6.823</td>
<td>0.0</td>
</tr>
<tr>
<td>x-space AMV</td>
<td>45</td>
<td>45</td>
<td>0.9420</td>
<td>0.0</td>
</tr>
<tr>
<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 AMV$^2$</td>
<td>45</td>
<td>45</td>
<td>2.730</td>
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<tr>
<td>u-space AMV$^2$</td>
<td>45</td>
<td>45</td>
<td>2.828</td>
<td>0.0</td>
</tr>
<tr>
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<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 AMV$^2$+</td>
<td>135</td>
<td>142</td>
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<td>0.0</td>
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<td>132</td>
<td>139</td>
<td>0.0</td>
<td>0.0</td>
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<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>
</tr>
<tr>
<td>FORM</td>
<td>720</td>
<td>192</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>SORM</td>
<td>535</td>
<td>191*</td>
<td>2.410</td>
<td>6.522e-4</td>
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Note: 2nd-order PMA with prescribed $p$ level is harder problem requires $\beta(p)$ update/inversion.
Solution-Verified Reliability Analysis and Design of MEMS

- **Problem:** MEMS subject to substantial variabilities
  - Material properties, manufactured geometry, residual stresses
  - Part yields can be low or have poor durability
  - Data can be obtained → aleatory UQ → probabilistic methods

- **Goal:** account for both uncertainties and errors in design
  - Integrate UQ/OUU (DAKOTA), ZZ/QOI error estimation (Encore), adaptivity (SIERRA), nonlin mech (Aria) → MESA application
  - Perform soln verification in automated, parameter-adaptive way
  - Generate fully converged UQ/OUU results at lower cost

- AMV\(^2\)+ and FORM converge to different MPPs (+ and O respectively)

- Issue: high nonlinearity leading to multiple legitimate MPP solns.

- Challenge: design optimization may tend to seek out regions encircled by the failure domain. 1\(^\text{st}\)-order and even 2\(^\text{nd}\)-order probability integrations can experience difficulty with this degree of nonlinearity. Optimizers can/will exploit this model weakness.

Parameter study over 3\(\sigma\) uncertain variable range for fixed design variables \(d_M^*\). 
**Dashed black line** denotes \(g(x) = F_{\min}(x) = -5.0\).
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)
Efficient Global Reliability Analysis

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<tr>
<th>Reliability Method</th>
<th>Function Evaluations</th>
<th>First-Order $p_f$ (%)</th>
<th>Second-Order $p_f$ (%)</th>
<th>Sampling $p_f$ (%)</th>
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<tr>
<td>No Approximation</td>
<td>70</td>
<td>0.11797 (277.0%)</td>
<td>0.02516 (-19.6%)</td>
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<tr>
<td>x-space AMV$^2$+</td>
<td>26</td>
<td>0.11797 (277.0%)</td>
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<td>LHS solution</td>
<td>10k</td>
<td>—</td>
<td>—</td>
<td>0.03117 (0.385%, 2.847%)</td>
</tr>
<tr>
<td>LHS solution</td>
<td>100k</td>
<td>—</td>
<td>—</td>
<td>0.03126 (0.085%, 1.397%)</td>
</tr>
<tr>
<td>LHS solution</td>
<td>1M</td>
<td>—</td>
<td>—</td>
<td>0.03120 (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>

*10 samples
*28 samples

explore ~ exploit
Stochastic Expansion Methods for UQ
Polynomial Chaos Expansions (PCE)

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

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

i.e.

\[ \alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \Psi_j \varrho(\xi) \, d\xi \]

\[ \langle \Psi_j^2 \rangle = \prod_{i=1}^{n} \langle \psi_i^2 \rangle \]

• Nonintrusive: estimate \( \alpha_j \) using sampling, regression, tensor-product quadrature, sparse grids, or cubature

Generalized PCE (Wiener-Askey + numerically-generated)

• Tailor basis: selection of basis orthogonal to input PDF avoids additional nonlinearity

<table>
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<tr>
<th>Distribution</th>
<th>Density function</th>
<th>Polynomial</th>
<th>Weight function</th>
<th>Support range</th>
</tr>
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<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)^\alpha(1+x)^\beta}{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>

Additional bases generated numerically (discretized Stieltjes + Golub-Welsch)

• Tailor expansion form:
  – Dimension p-refinement: anisotropic TPQ/SSG, generalized SSG
  – Dimension & region h-refinement: local bases with global & local refinement

\[ 1/\sqrt{N} \text{ for LHS} \]

\[ \text{super-algebraic for num. integration & regression} \]
Stochastic Collocation (based on interpolation polynomials)

Instead of estimating coefficients for known basis functions, form interpolants for known coefficients

- **Global:** Lagrange (values) or Hermite (values+derivatives)
- **Local:** linear (values) or cubic (values+gradients) splines

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

Sparse interpolants formed using \( \Sigma \) of tensor interpolants

**Advantages relative to PCE:**
- Somewhat simpler (no expansion order to manage separately)
- Often less expensive (no integration for coefficients)
- Expansion only formed for sampling \( \rightarrow \) probabilities (estimating moments of any order is straightforward)
- Adaptive h-refinement with hierarchical surpluses; explicit gradient-enhancement

**Disadvantages relative to PCE:**
- Less flexible/fault tolerant \( \rightarrow \) structured data sets (tensor/sparse grids)
- Expansion variance not guaranteed positive (important in opt./interval est.)
- No direct inference of spectral decay rates

*With sufficient care on PCE form, PCE/SC performance is essentially identical for many cases of interest (tensor/sparse grids with standard Gauss rules)*
Approaches for forming PCE/SC Expansions

**Random sampling: PCE**

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

*Linear regression (“point collocation”):*
- Sample w/i distribution of $\xi$
- Solves least squares data fit for all coefficients at once:
  $$\Psi\alpha = R$$

**Tensor-product quadrature: PCE/SC**

$$\mathbb{U}^i(f)(\xi) = \sum_{j=1}^{m_i} f(\xi_j^i) w_j^i$$

$$Q^k_i f(\xi) = (\mathbb{U}^{i_1} \otimes \cdots \otimes \mathbb{U}^{i_n}) (f)(\xi) = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} f(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}) (w_{j_1}^{i_1} \otimes \cdots \otimes w_{j_n}^{i_n})$$

- Every combination of 1-D rules
- Scales as $m^n$
- 1-D Gaussian rule of order $m$ → integrands to order $2m - 1$
- Assuming $R\Psi_j$ of order $2p$, select $m = p + 1$

**Smolyak Sparse Grid: PCE/SC**

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

*Pascal’s triangle (2D):*

**Cubature: PCE**

*Stroud and extensions (Xiu, Cools)*
- Low order PCE
- Global SA, anisotropy detection

*Gaussian* $i = 2 \rightarrow p = 1$

$$x_{k,2r-1} = \sqrt{2} \cos \frac{2r k \pi}{n+1}, \quad x_{k,2r} = \sqrt{2} \sin \frac{2r k \pi}{n+1}$$

*Arbitrary PDF*

$$t^{(k)} = \frac{1}{\gamma} \left[ \sqrt{\gamma c_1 x^{(k)}(\delta)} - \delta \right]$$
Adaptive Collocation Methods

**Drivers:** Efficiency, robustness, *scalability* → adaptive methods, adjoint enhancement

**Polynomial order (p-) refinement approaches:**
- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted growth in nested rules)
  - *Assess convergence:* $L^2$ change in response covariance
Adaptive Collocation Methods

Drivers: Efficiency, robustness, \textit{scalability} \rightarrow adaptive methods, adjoint enhancement

Poly\textit{no}\textit{mial order (p-) refinement approaches}:

- **Uniform: \textit{isotropic} tensor/sparse grids**
  - \textit{Increment grid}: increase order/level, ensure change (restricted growth in nested rules)
  - \textit{Assess convergence}: $L^2$ change in response covariance

- **Dimension-adaptive: \textit{anisotropic} tensor/sparse grids**
  - PCE/SC: variance-based decomp. \rightarrow total Sobol’ indices \rightarrow anisotropy (dimension preference)
  - PCE: spectral coefficient decay rates \rightarrow anisotropy (index set weights)

\[
\underline{w_\gamma} < \mathbf{i} \cdot \mathbf{\gamma} \leq \underline{w_\gamma} + |\mathbf{\gamma}|
\]
Adaptive Collocation Methods

Drivers: Efficiency, robustness, \textit{scalability} → adaptive methods, adjoint enhancement

Polynomial order (p-) refinement approaches:

- **Uniform**: \textit{isotropic} tensor/sparse grids
  - \textit{Increment grid}: increase order/level, ensure change (restricted growth in nested rules)
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- **Dimension-adaptive**: \textit{anisotropic} tensor/sparse grids
  - PCE/SC: variance-based decomp. → total Sobol’ indices → anisotropy
  - PCE: spectral coefficient decay rates → anisotropy

- **Goal-oriented dimension-adaptive**: \textit{generalized} sparse grids
  - PCE/SC: change in QOI induced by trial index sets on active front

1. **Initialization**: Starting from reference grid (often $w = 0$ grid), define active index sets using admissible forward neighbors of all old index sets.

2. **Trial set evaluation**: For each trial index set, evaluate tensor grid, form tensor expansion, update combinatorial coefficients, and combine with reference expansion. Perform necessary bookkeeping to allow efficient restoration.

3. **Trial set selection**: Select trial index set that induces largest change in statistical QOI.

4. **Update sets**: If largest change > tolerance, then promote selected trial set from active to old and compute new admissible active sets; return to 2. If tolerance is satisfied, advance to step 5.

5. **Finalization**: Promote all remaining active sets to old set, update combinatorial coefficients, and perform final combination of tensor expansions to arrive at final result for statistical QOI.

\[ w_\gamma < i \cdot \gamma \leq w_\gamma + |\gamma| \]

(Gerstner, 2003)

Fine-grained control: frontier not limited by prescribed shape of index set constraint
Numerical Experiments

Short Column (n=5)

\[ g(x) = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2} \]

\( b = U[5,15], \quad h = U[15,25], \quad P = N(500, 100), \quad M = N(2000, 400), \)
\( \rho_{PM} = 0.5, \quad Y = \log N(5, 0.5) \)

Cantilever Beam (n=6)

\[ S = \frac{600}{w_t^2} Y + \frac{600}{w_r^2} X \leq R \]
\[ D = \frac{4L^3}{Ew_t} \sqrt{(Y/t)^2 + (X/t^2)^2} \leq D_0 \]

\( w, t, R, E, X, Y: U[1,10], U[1,10], N(4E4, 2E3), N(2.9E7, 1.45E6), N(500, 100), N(1E3, 100); D_0 = 2.2535" \)

Ishigami (n=3)

\[ f(x) = \sin(2\pi x_1 - \pi) + 7 \sin^2(2\pi x_2 - \pi) + 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi) \]
\( x_1, x_2, x_3: \text{iid } U[0, 1] \)

- Designed to be challenging for global SA: term cancellations at mid-point & bounds

- Premature convergence in adaptive methods \( \rightarrow \) start from higher-order grid
Extend Scalability through Adjoint Derivative-Enhancement

**PCE:**
- Linear regression with derivatives
  - Gradients/Hessians → addtnl. eqns.

**SC:**
- Gradient-enhanced interpolants
  - Local: cubic Hermite splines
  - Global: Hermite interpolation polynomials

**EGRA:**
- Gradient-enhanced kriging/cokriging
  - Interpolates function values and gradients
  - Scaling: \( n^2 \rightarrow n \)
Gradient-Enhanced PCE

Straightforward regression approach:

\[
\begin{bmatrix}
\frac{\partial \pi_{0,j}}{\partial \xi_1}(\xi_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\xi_i) & \ldots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\xi_i) \\
\frac{\partial \pi_{0,j}}{\partial \xi_n}(\xi_i) & \frac{\partial \pi_{1,j}}{\partial \xi_n}(\xi_i) & \ldots & \frac{\partial \pi_{P,j}}{\partial \xi_n}(\xi_i) \\
\end{bmatrix}
\begin{bmatrix}
\tilde{u}(m,j) \\
\tilde{u}(m+1,j) \\
\vdots \\
\tilde{u}(m+n,\xi,j) \\
\vdots \\
\end{bmatrix}
= 
\begin{bmatrix}
\frac{\partial \pi_{0,j}}{\partial \xi_1} \\
\frac{\partial \pi_{1,j}}{\partial \xi_1} \\
\vdots \\
\frac{\partial \pi_{P,j}}{\partial \xi_1} \\
\vdots \\
\end{bmatrix}
\]

• unweighted LLS by SVD (LAPACK GELSS)
• equality constrained LLS by QR (LAPACK GGLSE) when under-determined by values alone

Vandermonde-like systems known to suffer from ill-conditioning

Error growth as we over-resolve exact solutions
**Dimension-adaptive h-refinement with gradient-enhanced interpolants**

**Dimension-adaptive h-refinement for SC:**
- **Local spline interpolants:** linear Lagrange (value-based), cubic Hermite (gradient-enhanced)
- **Global grids:** iso/aniso tensor, iso/aniso/generalized sparse
- **h-refinement:** uniform, adaptive, goal-oriented adaptive
- **Basis formulations:** nodal, hierarchical

Multivariate tensor product to arbitrary derivative order (Lalescu):

\[
s^{(n)}(x_1, x_2, \ldots, x_D) = \sum_{i_1, \ldots, i_D=0}^{m} \sum_{i_1, \ldots, i_D=0,1}^{m} f^{(i_1, \ldots, i_D)}(i_1, \ldots, i_D) \prod_{k=1}^{D} \alpha_{i_k}^{(n, l_k)}(x_k)
\]

\[
f = \sum_{i=1}^{N} f_{i} H_{i}^{(1)}(x_{i}) H_{i}^{(1)}(x_{2}) H_{i}^{(1)}(x_{3}) + \sum_{i=1}^{N} \frac{df_{i}}{dx_{1}} H_{i}^{(2)}(x_{i}) H_{i}^{(1)}(x_{2}) H_{i}^{(1)}(x_{3}) + \sum_{i=1}^{N} \frac{df_{i}}{dx_{2}} H_{i}^{(1)}(x_{i}) H_{i}^{(2)}(x_{2}) H_{i}^{(1)}(x_{3}) + \sum_{i=1}^{N} \frac{df_{i}}{dx_{3}} H_{i}^{(1)}(x_{i}) H_{i}^{(1)}(x_{2}) H_{i}^{(2)}(x_{3})
\]

\[
\mu = \sum_{i=1}^{N} f_{i} w^{(1)}_{i} w^{(1)}_{i} + \sum_{i=1}^{N} \frac{df_{i}}{dx_{1}} w^{(2)}_{i} w^{(1)}_{i} + \sum_{i=1}^{N} \frac{df_{i}}{dx_{2}} w^{(1)}_{i} w^{(2)}_{i} + \sum_{i=1}^{N} \frac{df_{i}}{dx_{3}} w^{(1)}_{i} w^{(1)}_{i} w^{(2)}_{i}
\]

and similar for higher-order moments
**Build on efficient/scalable UQ core**

**Stochastic sensitivity analysis**

- Aleatory or combined expansions including nonprobabilistic dimensions \( s \) → sensitivities of moments w.r.t. design and/or epistemic parameters

\[
R(\xi, s) = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi, s) \\
\frac{d\mu_R}{ds} = \langle \frac{dR}{ds} \rangle \\
\frac{d\sigma_R^2}{ds} = 2 \sum_{j=1}^{P} \alpha_j \langle \frac{dR}{ds}, \Psi_j \rangle \\
\mu_R(s) = \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\xi, s) \rangle \\
\sigma_R^2(s) = \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \alpha_k \langle \Psi_j(\xi, s) \Psi_k(\xi, s) \rangle \xi - \mu_R^2(s)
\]

**Design and Model Calibration Under Uncertainty**

- Approaches that are more accurate/efficient than nested sampling
  - Interval-valued probability (IVP), aka PBA
  - Dempster-Shafer theory of evidence (DSTE)
  - Second-order probability (SOP), aka PoF

**Mixed Aleatory-Epistemic UQ**

\[
\begin{align*}
\text{min} & \quad f(d) + Ws_u(d) \\
\text{s.t.} & \quad g_l \leq g(d) \leq g_u \\
& \quad h(d) = h_t \\
& \quad d_l \leq d \leq d_u \\
& \quad a_l \leq A_i s_u(d) \leq a_u \\
& \quad A_e s_u(d) = a_t
\end{align*}
\]

**Increasing epistemic structure (stronger assumptions)**
Mixed Aleatory-Epistemic UQ: IVP, DSTE, and SOP

Epistemic uncertainty (aka: subjective, reducible, lack of knowledge uncertainty): insufficient info to specify objective probability distributions

**Traditional approach: nested sampling**

- Expensive sims \( \rightarrow \) under-resolved sampling (especially @ outer loop)
- Under-prediction of credible outcomes

**Algorithmic approaches**

- Interval-valued probability (IVP), *aka* probability bounds analysis (PBA)
- Dempster-Shafer theory of evidence (DSTE)
- Second-order probability (SOP), *aka* probability of frequency

**Address accuracy and efficiency**

- Inner loop: stochastic exp. that are epistemic-aware (aleatory, combined)
- Outer loop:
  - IVP, DSTE: opt-based interval estimation, global (EGO) or local (NLP)
  - SOP: nested stochastic exp. (nested expectation is only post-processing in special cases)
Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

### Interval Estimation

<table>
<thead>
<tr>
<th>Interv Est Approach</th>
<th>UQ Approach</th>
<th>Expansion Variables</th>
<th>Evaluations (Fn, Grad)</th>
<th>Area</th>
<th>β</th>
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<tbody>
<tr>
<td>EGO SC SSG w = 1</td>
<td>Aleatory</td>
<td>84/91, 0/0</td>
<td>75.0002, 374.999</td>
<td>-2.26264, 11.8623</td>
<td></td>
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<tr>
<td>EGO SC SSG w = 2</td>
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<td>372/403, 0/0</td>
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<td></td>
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<tr>
<td>EGO SC SSG w = 3</td>
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<td>1260/1365, 0/0</td>
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<tr>
<td>EGO SC SSG w = 4</td>
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### IVP SC SSG Aleatory:
β interval converged to 5-6 digits by 300-400 evals

### IVP nested LHS sampling:
converged to 2-3 digits by $10^8$ evals

**Fully converged area interval = [75., 375.], β interval = [-2.18732, 11.5900]**

Convergence rates for combined expansions

**L∞ metrics:**
- IVP mixed, DSTE mixed
- Rational

**L² metrics:**
- Aleatory, SOP mixed

**Analytic $C^\infty$**

**Discontinuous $C^0$**
**Mixed Aleatory-Epistemic UQ:**

IVP, SOP, and DSTE based on Stochastic Expansions

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**IVP nested LHS sampling:** converged to 2-3 digits by $10^8$ evals

Fully converged area interval = [75., 375.], β interval = [-2.18732, 11.5900]

**Impact:** render mixed UQ studies practical for large-scale applications

**Current:**
- Global or local opt. for epistemic intervals
  - accuracy or scaling w/ epistemic dimension
- Global or local UQ for aleatory statistics
  - accuracy or scaling w/ aleatory dimension

**Future:**
- *adaptive and adjoint-enhanced* global methods
  - accuracy and scaling
Concluding Remarks

**R&D Drivers:** efficient/robust/scalable core, complex random environments

**Survey of core UQ algorithms:** strengths, weaknesses, research needs

**Sampling (nongradient-based)**
- **Strengths:** Simple and reliable, convergence rate is dimension-independent
- **Weaknesses:** $1/\sqrt{N}$ convergence → expensive for accurate tail statistics

**Local reliability (gradient-based)**
- **Strengths:** computationally efficient, widely used, scalable to large $n$ (w/ efficient derivs.)
- **Weaknesses:** algorithmic failures for limit states with following features
  - Nonsmooth: fail to converge to an MPP
  - Highly nonlinear: low order limit state approxs. insufficient to resolve probability at MPP

**Global reliability (typically nongradient-based)**
- **Strengths:** handles multimodal and/or highly nonlinear limit states
- **Weaknesses:**
  - Conditioning, nonsmoothness → ensemble emulation (recursion, discretization)
  - Scaling to large $n$ → adjoints, additional refinement bias

**Stochastic expansions (typically nongradient-based)**
- **Strengths:** functional representation, exponential convergence rates for smooth problems
- **Weaknesses:**
  - Nonsmoothness → basis enrichment, h-refinement, Pade approx.
  - Scaling to large $n$ → adaptive refinement, adjoints

**Build on algorithmic foundations**

Design under uncertainty, Mixed UQ with IVP/SOP/DSTE
DAKOTA Software

DAKOTA Optimization
Uncertainty Quant.
Parameter Est.
Sensitivity Analysis

Model Parameters

Black box:
- Sandia simulation codes
- Commercial simulation codes

Library mode (semi-intrusive):
- ALEGRA (shock physics), Xyce (circuits), Sage (CFD),
  Albany/TriKota (Trilinos-based), MATLAB, Python, ModelCenter,
  SIERRA (multiphysics)

Design Metrics

Iterative systems analysis
Multilevel parallel computing
Simulation management

http://dakota.sandia.gov
Manuals, Publications, Training

Releases:
Major/Interim, Stable/VOTD; 5.1 released 12/10

Modern SQE:
Linux/Unix, Mac, Windows; Nightly builds/testing;
subversion, TRAC, autotools/Cmake

GNU LGPL:
free downloads worldwide
 (>7000 total ext. registrations, ~3500 distributions last yr.)

Community development:
open checkouts now available

Community support: dakota-users, dakota-help
Iterator

Model

Strategy: control of multiple iterators and models

Coordination:
- Nested
- Layered
- Cascaded
- Concurrent
- Adaptive/Interactive

Parallelism:
- Asynchronous local
- Message passing
- Hybrid
- 4 nested levels with Master-slave/dynamic Peer/static

Model:

Parameters

Design
- continuous
- discrete

Uncertain
- normal/logn
- uniform/logu
- triangular
- exp/beta/gamma
- EV I, II, III
- histogram
- interval

State
- continuous
- discrete

Interface

Application
- system
- fork
- direct
- grid

Approximation
- global
- polynomial 1/2/3, NN, kriging, MARS, RBF
- multipoint – TANAS3
- local – Taylor series
- multifidelity
- ROM

Design

Functions
- objectives
- constraints
- least sq. terms
- generic

Gradients
- numerical
- analytic

Hessians
- numerical
- analytic
- quasi

Strategy

Uncertainty

OptUnderUnc

LeastSq

UncOfOptima

ModelCalUnderUnc

2ndOrderProb

Optimization

Hybrid

SurrBased

Pareto/MStart

Branch&Bound/PICO

DAKOTA Framework
Deployment Initiative: JAGUAR User Interface

- Eclipse-based rendering of full DAKOTA input spec.
- Automatic syntax updates
- Tool tips, Web links, help
- Symbolics, sim. interfacing

- Flat text editor for experienced users
- Keyword completion
- Automatically synchronized with GUI widgets

- Simplified views for high-use applications ("Wizards")
Deployment Initiative: Embedding

Make DAKOTA natively available within application codes

- Streamline problem set-up, reduce complexity, and lower barriers
  - A few additional commands within existing simulation input spec.
  - Eliminate analysis driver creation & streamline analysis (e.g., file I/O)
  - Simplify parallel execution
- Integrated options for algorithm intrusion

SNL Embedding

- Existing: Xyce, Sage, Albany (TriKOTA)
- New: ALEGRA, SIERRA (TriKOTA) → STK

External Embedding

- Existing: ModelCenter, university applications
- New: QUESO (UT Austin), R7 (INL)
- Expanding our external focus:
  - GPL → LGPL; svn restricted → open network
  - Tailored interfaces & algorithms

ModelEvaluator Levels

Non-intrusive

ModelEvaluator: systems analysis
- All residuals eliminated, coupling satisfied
- DAKOTA optimization & UQ

Intrusive to coupling

ModelEvaluator: multiphysics
- Individual physics residuals eliminated; coupling enforced by opt/UQ
- DAKOTA opt/UQ & MOOCHO opt.

Intrusive to physics

ModelEvaluator: single physics
- No residuals eliminated
- MOOCHO opt., Stokhos UQ, NOX, LOCA