



Nonintrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design

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Automated refinement: uniform and dimension-adaptive p- and h-refinement
Gradient enhancement: PCE regression, piecewise Hermite interpolation
Building on UQ foundations: mixed UQ, optimization under uncertainty

Polynomial Chaos Expansions (PCE)

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

i.e.

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

using

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

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

$$\langle \Psi_j^2 \rangle = \prod_{i=1}^n \langle \psi_{m_i}^2 \rangle$$

- **Nonintrusive:** estimate α_j using sampling, regression, tensor-product quadrature, sparse grids, or cubature

Generalized PCE (Wiener-Askey + numerically-generated)

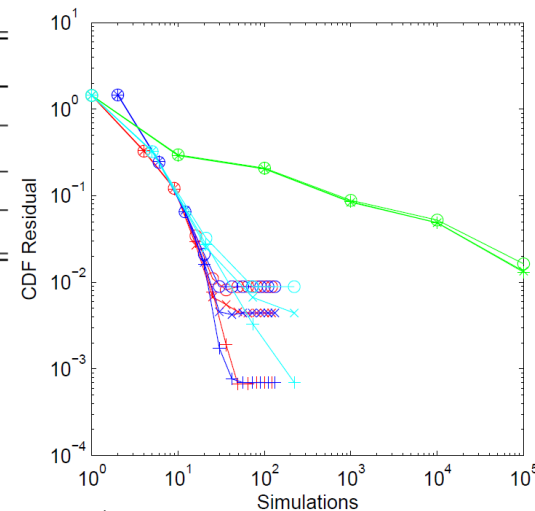
- **Taylor basis:** selection of basis orthogonal to input PDF avoids additional nonlinearity

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 $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

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

- **Taylor expansion form:**

- Dimension p-refinement: anisotropic TPQ/SSG, generalized SSG
- Dimension & region h-refinement: local bases with global & local refinement



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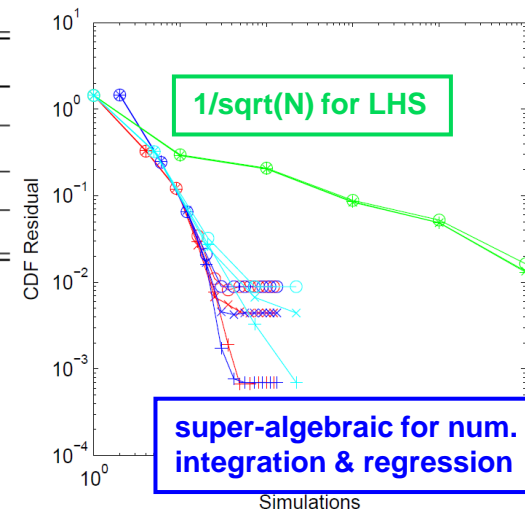
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Stochastic Collocation

(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

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

$$L_i = \prod_{\substack{j=1 \\ j \neq i}}^m \frac{x - x_j}{x_i - x_j}$$

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

Sparse interpolants formed using Σ 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

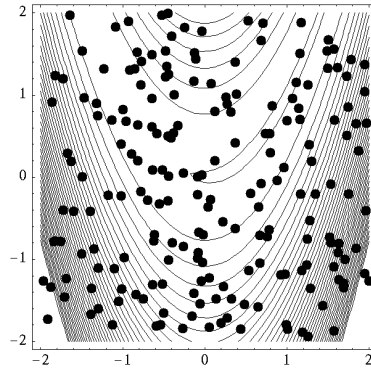
Expectation (sampling):

- Sample w/i distribution of ξ
- Compute expected value of product of R and each Ψ_j

Linear regression

("point collocation"):

- Sample w/i distribution of ξ
- Solves least squares data fit for all coefficients at once:



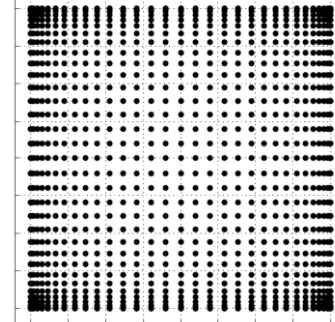
$$\Psi\alpha = R$$

Tensor-product quadrature: PCE/SC

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

$$\mathcal{Q}_i^n f(\xi) = (\mathcal{W}^{i_1} \otimes \dots \otimes \mathcal{W}^{i_n})(f)(\xi) = \sum_{j_1=1}^{m_{i_1}} \dots \sum_{j_n=1}^{m_{i_n}} f(\xi_{j_1}^{i_1}, \dots, \xi_{j_n}^{i_n}) (w_{j_1}^{i_1} \otimes \dots \otimes w_{j_n}^{i_n})$$

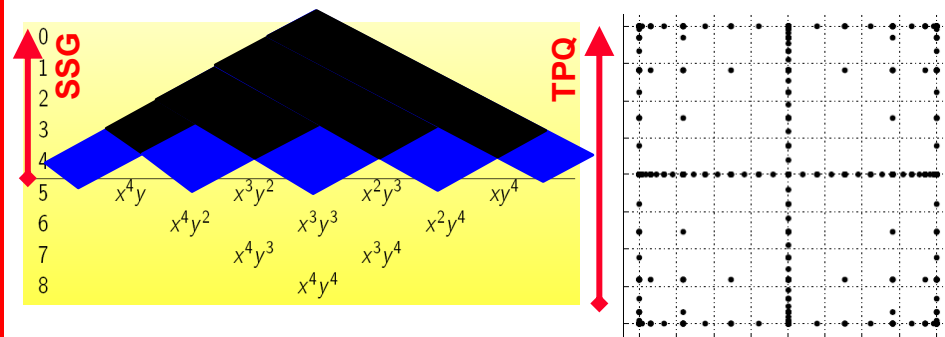
- Every combination of 1-D rules
- Scales as m^n
- 1-D Gaussian rule of order m
→ integrands to order $2m - 1$
- Assuming $R \Psi_j$ of order $2p$,
select $m = p + 1$



Smolyak Sparse Grid: PCE/SC

$$\mathcal{A}(w, n) = \sum_{w+1 \leq |\mathbf{i}| \leq w+n} (-1)^{w+n-|\mathbf{i}|} \binom{n-1}{w+n-|\mathbf{i}|} \cdot (\mathcal{W}^{i_1} \otimes \dots \otimes \mathcal{W}^{i_n})$$

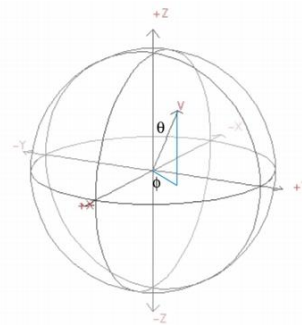
Pascal's triangle (2D):



Cubature: PCE

Stroud and extensions (Xiu, Cools)

- Low order PCE
- global SA, anisotropy detection



Gaussian $i = 2 \rightarrow p = 1$

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

Arbitrary PDF

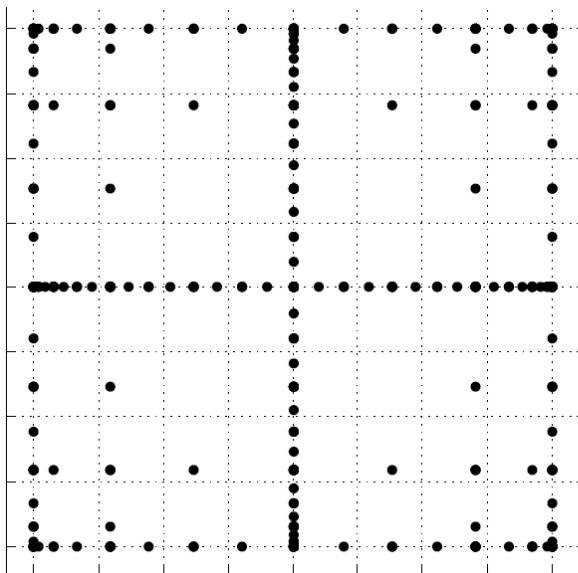
$$t^{(k)} = \frac{1}{\gamma} [\sqrt{\gamma c_1} x^{(k)} - \delta]$$

PCE/SC Expansions: Smolyak Sparse Grids

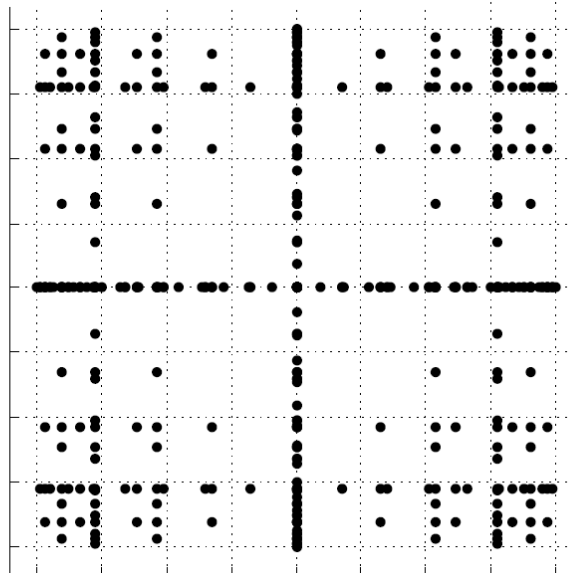
Numerical Integration (Smolyak sparse grids):

$$\mathcal{A}(w, n) = \sum_{|\mathbf{i}| \leq w+n} (\Delta^{i_1} \otimes \dots \otimes \Delta^{i_n}) \quad \text{for} \quad \Delta^i := \mathcal{U}^i - \mathcal{U}^{i-1}$$

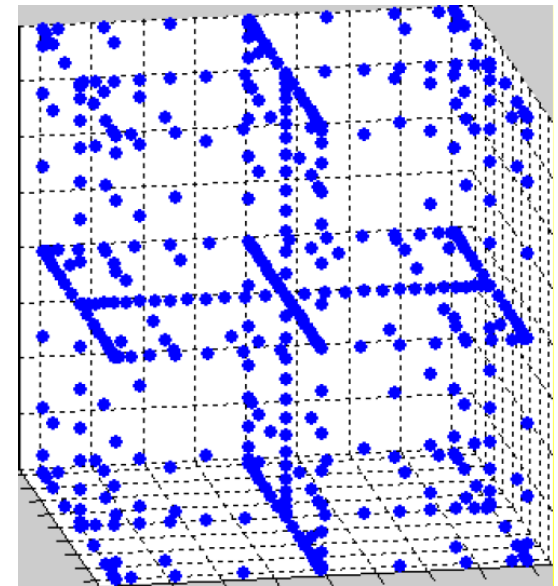
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2D Clenshaw-Curtis sparse grid
(less optimal, more nesting)



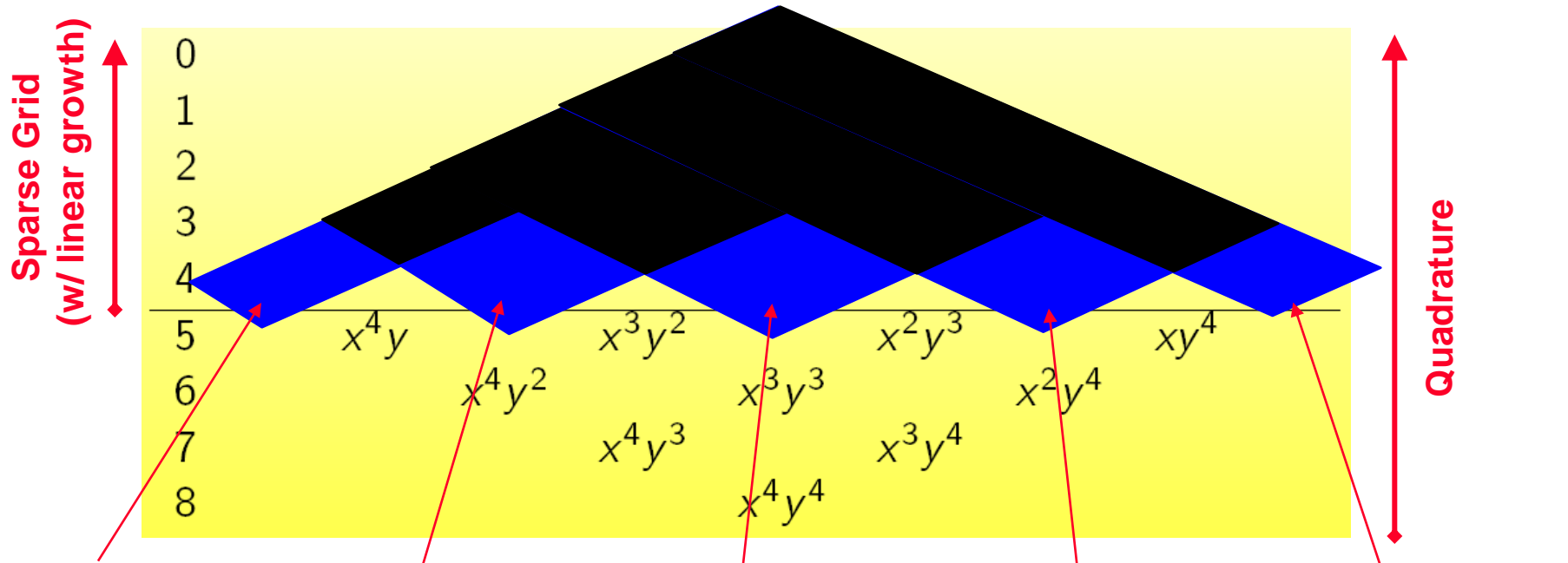
2D Gauss-Legendre sparse grid
(more optimal, less nesting)



3D Clenshaw-Curtis sparse grid

PCE/SC Expansions: Smolyak Sparse Grids (cont.)

Key difference between quadrature & sparse grids: polynomial order coverage



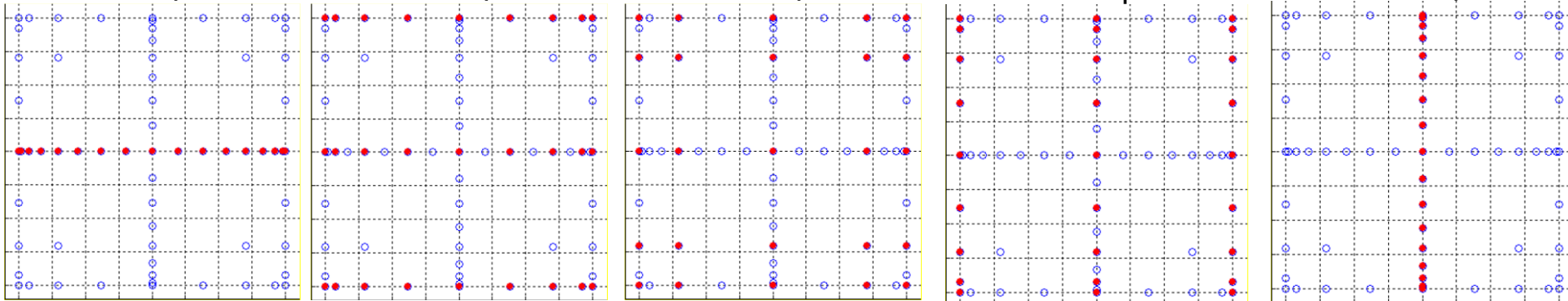
17 x 1 component

9 x 3 component

5 x 5 component

3 x 9 component

1 x 17 component



From J. Burkardt, "A Low Level Introduction to High Dimensional Sparse Grids."

Adaptive Collocation Methods

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

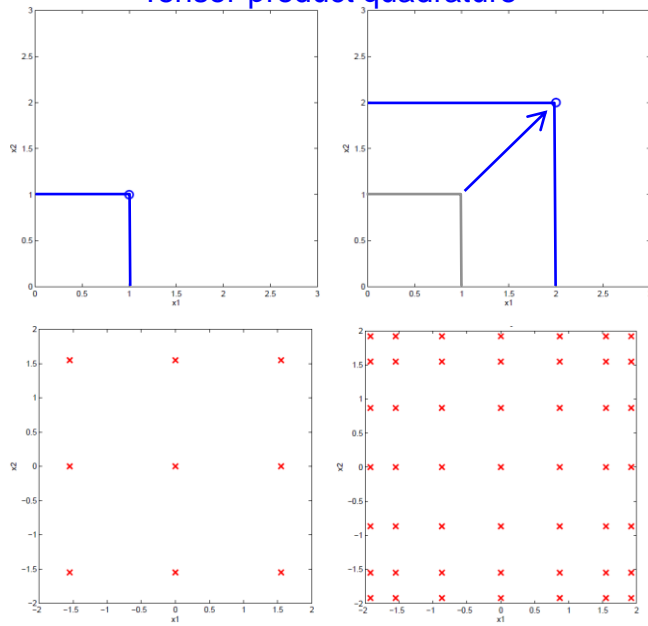
Polynomial order (p -) refinement approaches:

- **Uniform:** isotropic tensor/sparse grids

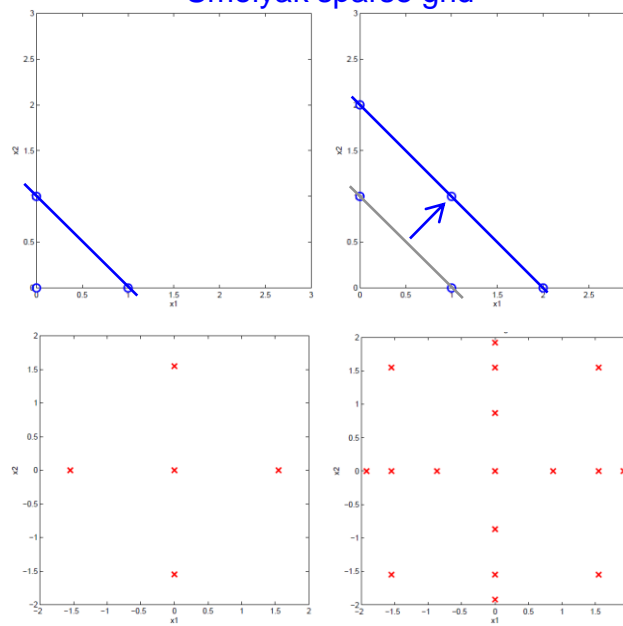
- *Increment grid:* increase order/level, ensure change (restricted growth in nested rules)
- *Assess convergence:* L^2 change in response covariance

$$w+1 \leq |\mathbf{i}| \leq w+n$$

Tensor-product quadrature



Smolyak sparse grid



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- **Uniform:** isotropic tensor/sparse grids
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- **Dimension-adaptive:** anisotropic tensor/sparse grids
 - **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy (dimension preference)

$$\begin{aligned}
 f_{PC}(\mathbf{x}) = & f_0 + \sum_{i=1}^n \sum_{\alpha \in \mathcal{I}_i} f_{\alpha} \Psi_{\alpha}(x_i) \\
 & + \sum_{1 \leq i_1 < i_2 \leq n} \sum_{\alpha \in \mathcal{I}_{i_1, i_2}} f_{\alpha} \Psi_{\alpha}(x_{i_1}, x_{i_2}) + \dots \\
 & + \sum_{1 \leq i_1 < \dots < i_s \leq n} \sum_{\alpha \in \mathcal{I}_{i_1, \dots, i_s}} f_{\alpha} \Psi_{\alpha}(x_{i_1}, \dots, x_{i_s}) \\
 & + \dots + \sum_{\alpha \in \mathcal{I}_{1, 2, \dots, n}} f_{\alpha} \Psi_{\alpha}(x_1, \dots, x_n)
 \end{aligned}$$

$$SU_{i_1 \dots i_s} = \sum_{\alpha \in \mathcal{I}_{i_1, \dots, i_s}} f_{\alpha}^2 E[\Psi_{\alpha}^2] / D_{PC}$$

Main, interaction indices

$$SU_{j_1, \dots, j_t}^T = \sum_{(i_1, \dots, i_s) \in \mathcal{J}_{j_1, \dots, j_t}} SU_{i_1, \dots, i_s}$$

Total indices



$$\underline{w}_{\gamma} < \mathbf{i} \cdot \gamma \leq \underline{w}_{\gamma} + |\gamma|$$

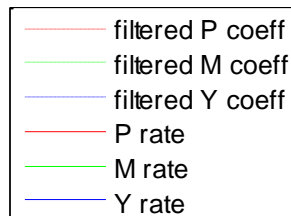
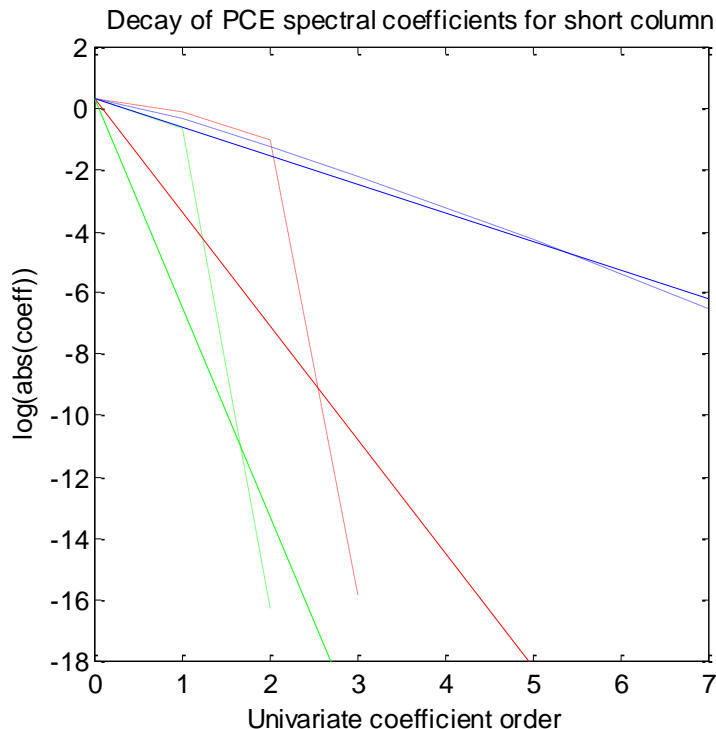
Average Sobol indices over response set

Adaptive Collocation Methods

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 - **PCE:** spectral coefficient decay rates → anisotropy (index set weights)



$$w_{\underline{\gamma}} < \mathbf{i} \cdot \gamma \leq w_{\underline{\gamma}} + |\gamma|$$

Min rates over response set

Adaptive Collocation Methods

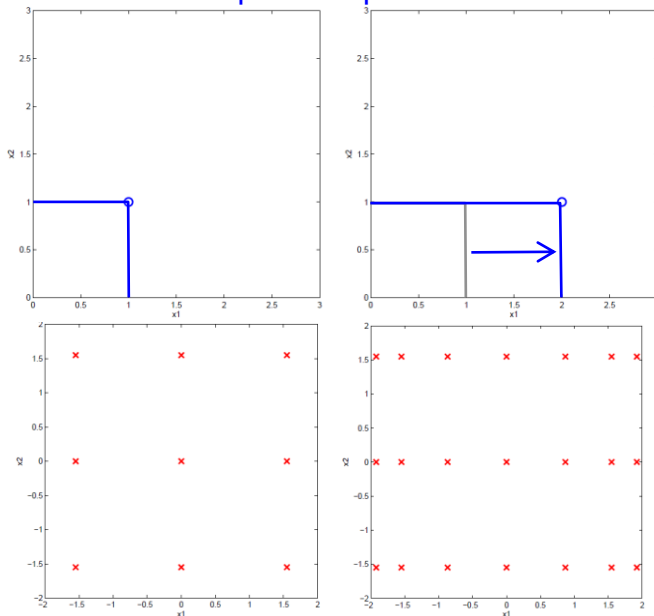
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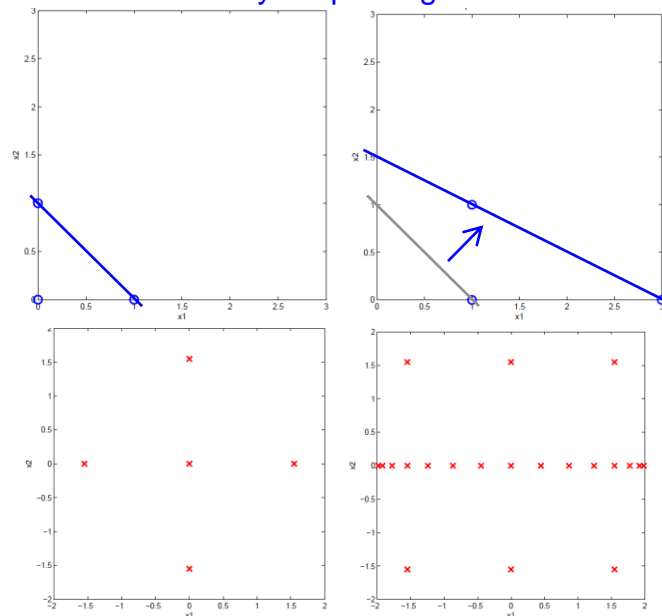
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Tensor-product quadrature



Smolyak sparse grid



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- **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy
- **PCE:** spectral coefficient decay rates → anisotropy

- **Goal-oriented dimension-adaptive:** 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.

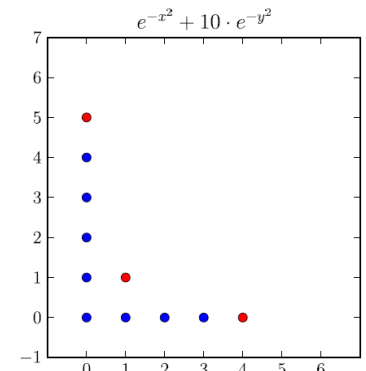
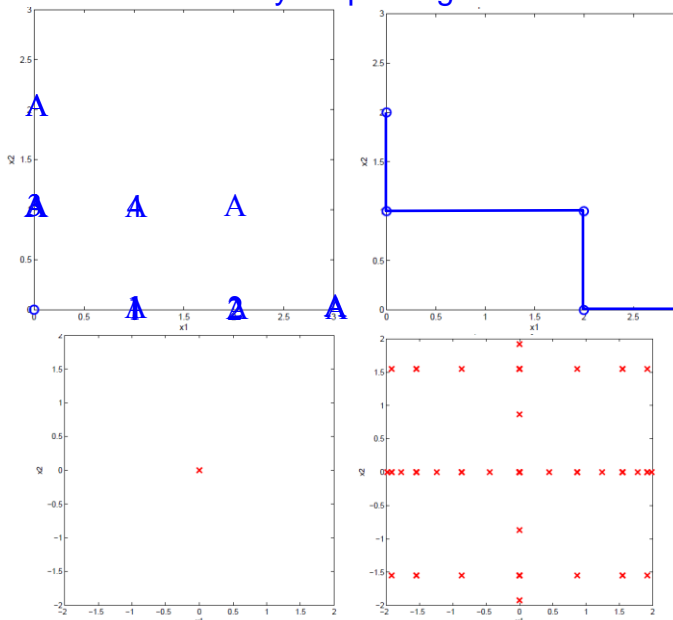
2. Trial set evaluation: For each trial index set, evaluate tensor grid, form tensor expansion, update combinatorial coefficients, and combine with reference expansion. Perform necessary bookkeeping to allow efficient restoration.

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.

Smolyak sparse grid



(Gerstner, 2003)

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

Initial Observations

- **Sobol' anisotropic grids:** target largest contributors to response variance
 - Strengths
 - Most broadly applicable technique: PCE or SC, TPQ or SSG
 - Global variance metrics are robust (i.e., reduces non-monotonicity/drop out issues)
 - Weaknesses
 - Dimensions contributing most to variance may be low order (and vice versa → spectral decay)
 - Refinement logic is not entirely self-consistent, since variance increases with resolution (i.e., reduced refinement pressure for under-resolved dimensions; increased for over-resolved)
- **Spectral decay anisotropic grids:** target dimensions where convergence is slow
 - Strengths
 - Refinement logic is more self-consistent: when under-resolved, rate is low → preference is high and when fully resolved (e.g., a polynomial relationship), rate is higher → preference is reduced
 - Weaknesses
 - PCE only (TPQ or SSG)
 - Vice versa: dimensions with higher order relationships not necessarily dominant QOI contributors
 - Non-monotone drop-outs in univariate coefficients may block refinement
- **Generalized sparse grids:** target index sets that are largest contributors to QOI
 - Strengths
 - Unstructured, fine-grained: resolution of interactions not pre-determined by univariate weights
 - Goal-oriented refinement: index set selection governed by general statistical QOI
 - Start from $w = 0$ (don't need to estimate anisotropy; unimportant interactions not explored → scalability)
 - Weaknesses
 - SSG only (PCE or SC), although a greedy TPQ variant could be constructed
 - Non-monotone drop outs at index set level block refinement
 - Increments are smaller than other methods → precision can be an issue → hierarchical basis

Numerical Experiments

Short Column Test Problem (n=5)

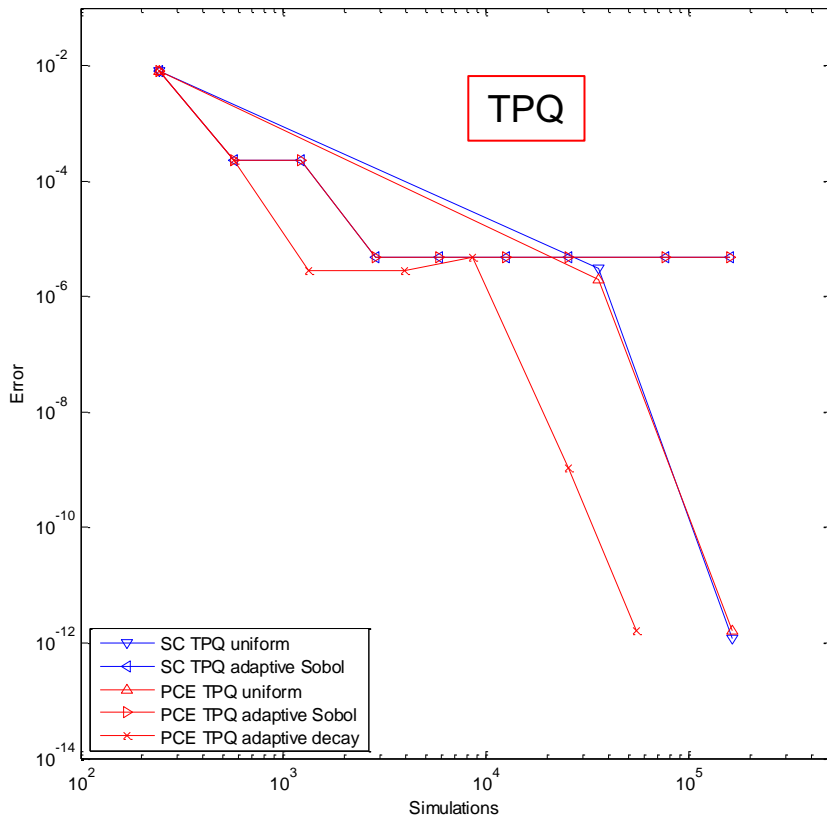
$$g(\mathbf{x}) = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2}$$

Kuschel & Rackwitz, 1997

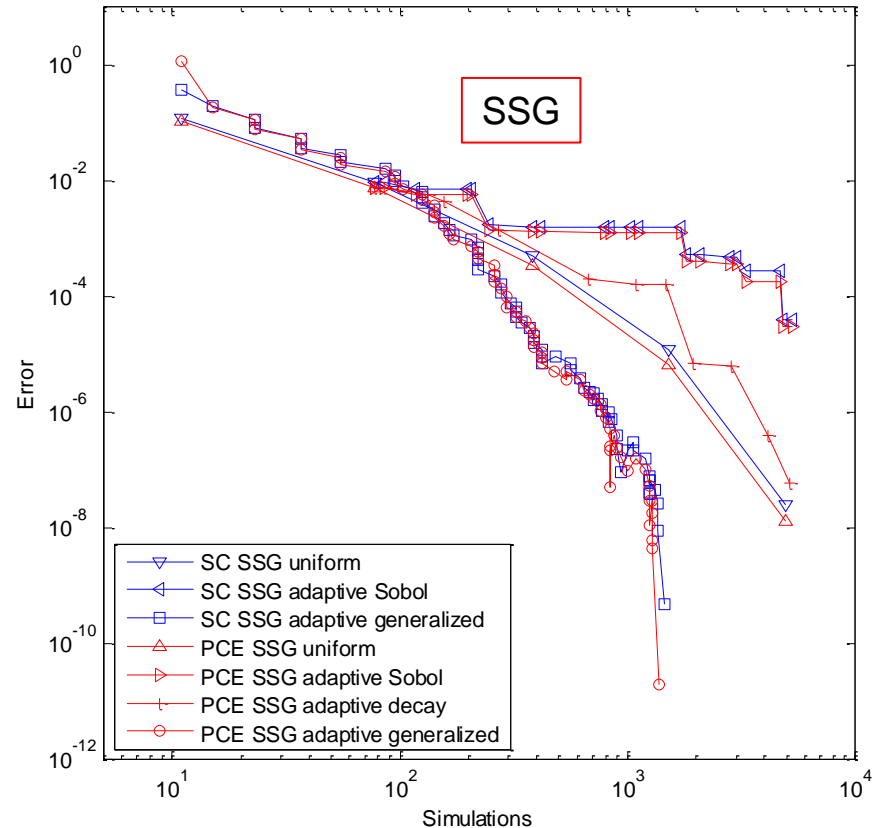
$b = U[5,15]$, $h = U[15,25]$,
 $P = N(500, 100)$,
 $M = N(2000, 400)$, $\rho_{P,M} = 0.5$,
 $Y = \log N(5, 0.5)$

min bh
 s.t. $\beta \geq 2.5$
 $5.0 \leq b \leq 15.0$
 $15.0 \leq h \leq 25.0$

Convergence for Short Column using PCE/SC TPQ uniform/adaptive

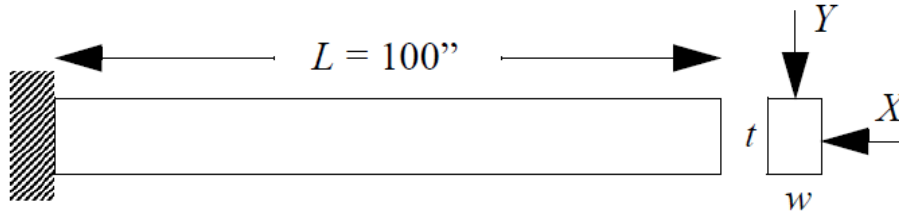


Convergence for Short Column using PCE/SC SSG uniform/adaptive



Numerical Experiments

Cantilever Beam Test Problem (n=6)



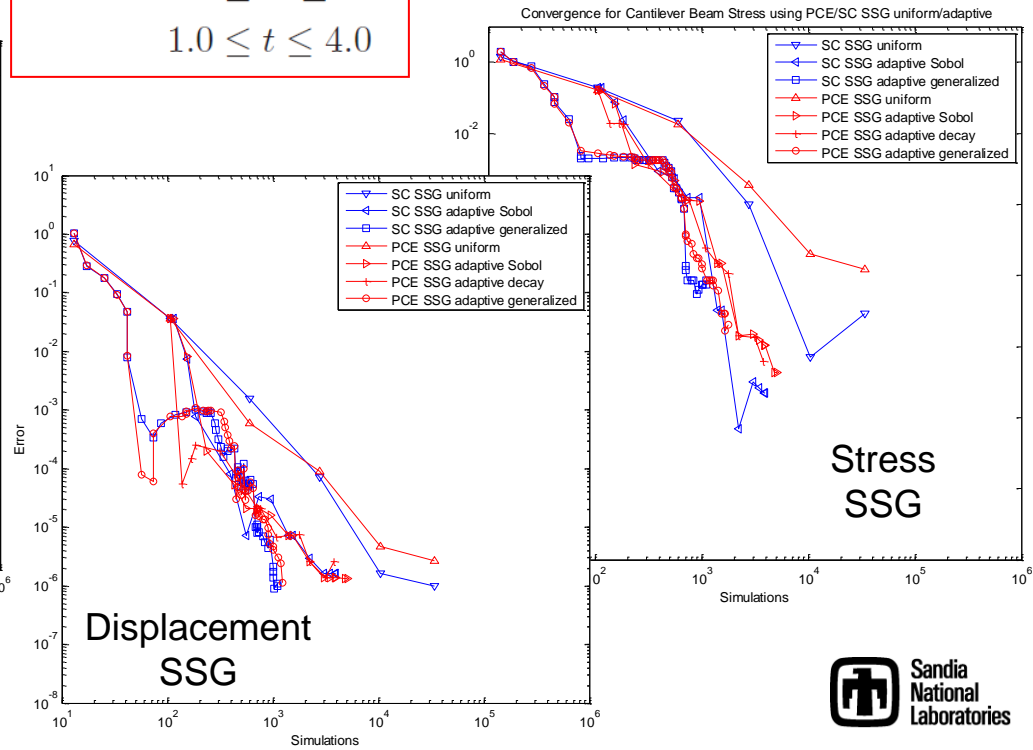
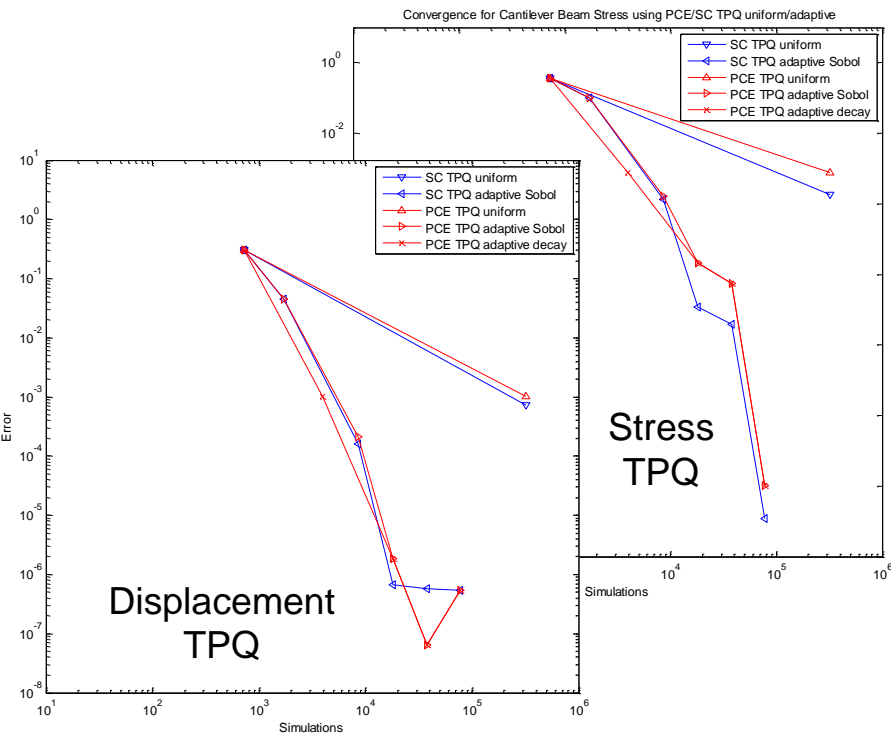
$w, t, R, E, X, Y: U[1,10], U[1,10],$
 $N(4E4, 2E3), N(2.9E7, 1.45E6),$
 $N(500, 100), N(1E3, 100);$
 $D_0 = 2.2535''$

$$S = \frac{600}{wt^2}Y + \frac{600}{w^2t}X \leq R$$

$$D = \frac{4L^3}{Ewt} \sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \leq D_0$$

$$\min wt$$

s.t. $\beta_S \geq 3.0$
 $\beta_D \geq 3.0$
 $1.0 \leq w \leq 4.0$
 $1.0 \leq t \leq 4.0$



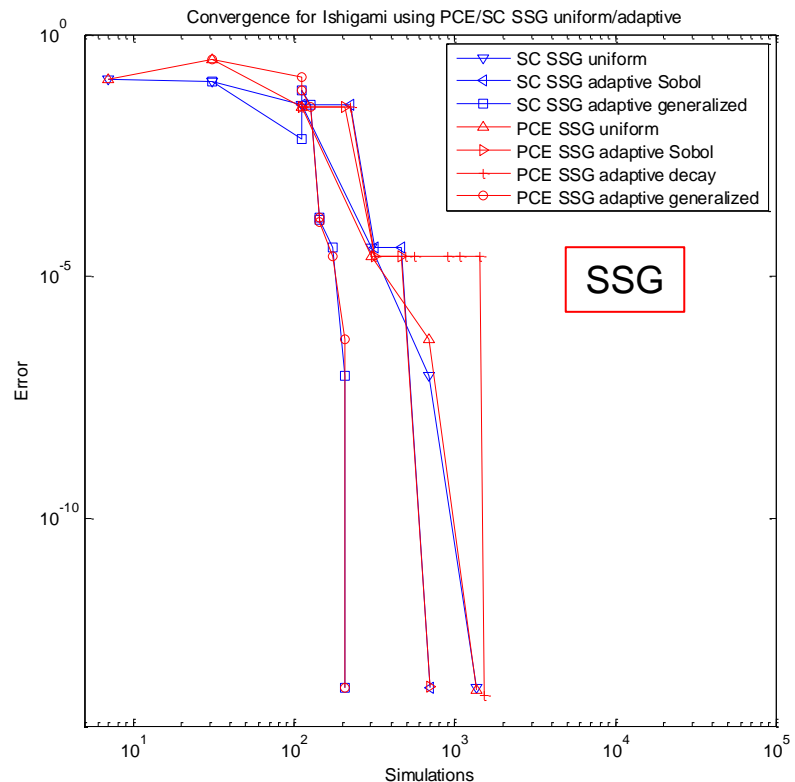
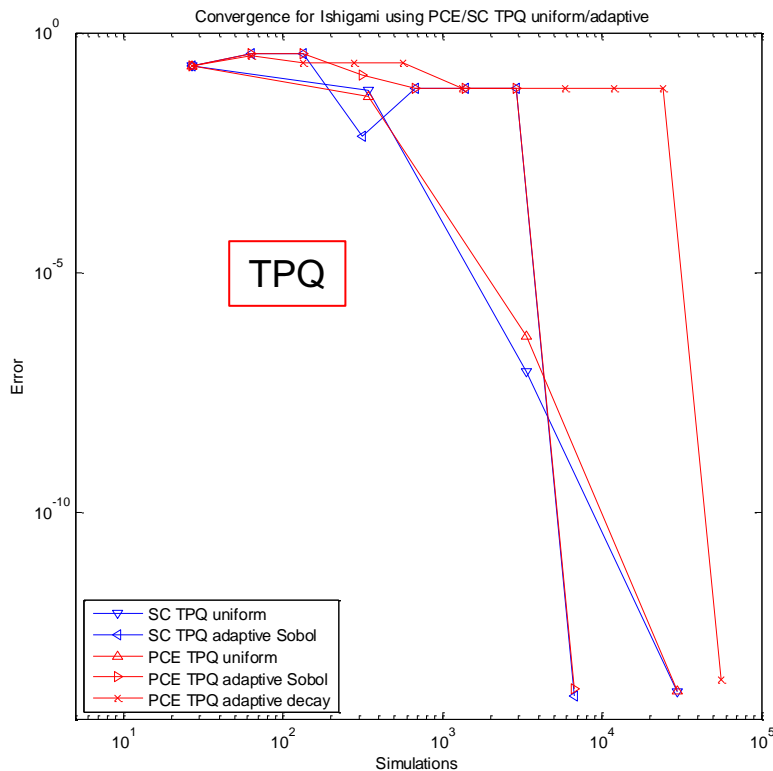
Numerical Experiments

Ishigami Test Problem (n=3)

$$f(\mathbf{x}) = \sin(2\pi x_1 - \pi) + 7 \sin^2(2\pi x_2 - \pi) + 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi)$$

$$x_1, x_2, x_3: iid U[0, 1]$$

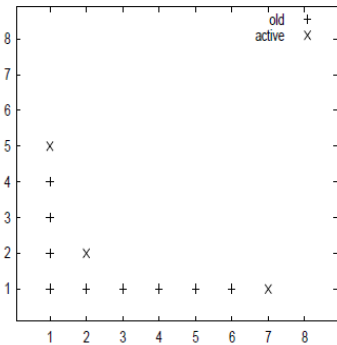
- Specifically designed to be challenging for global SA: term cancellations at mid-point and bounds
- Premature convergence in adaptive methods → start from higher-order grid



Adaptive Collocation Methods

Scalable Gerstner Test Problems (n=10)

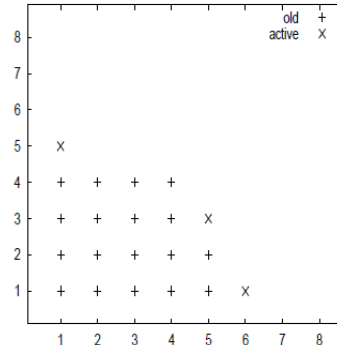
$$e^{-x^2} + 10 \cdot e^{-y^2}$$



$$f = \sum_{i=1}^{n/2} \left[e^{-x_{2i-1}^2} + 10e^{-x_{2i}^2} \right]$$

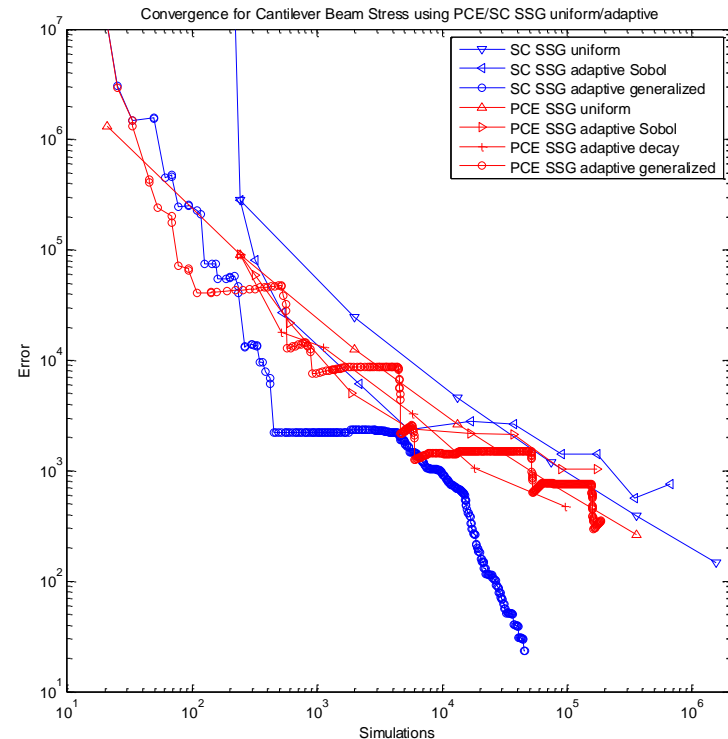
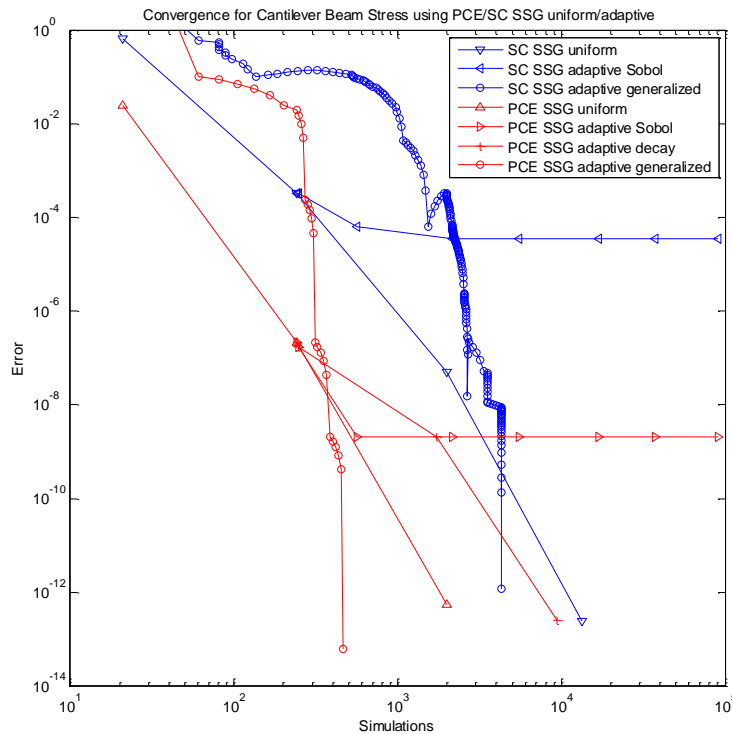
$x_i \text{ iid } U[0, 1]$

$$e^{-10x^2 - 5y^2}$$



$$f = \exp \left(- \sum_{i=1}^{n/2} [10x_{2i-1}^2 + 5x_{2i}^2] \right)$$

$x_i \text{ iid } U[0, 1]$



Remarks on p-refinement

Adaptive p-refinement in nonintrusive stochastic expansions

- PCE and SC with TPQ and SSG
 - Dimension-adaptive p-refinement
 - Uniform p-refinement with isotropic tensor/sparse grids
 - Adaptive p-refinement with anisotropic tensor/sparse grids
 - VBD \rightarrow total Sobol' indices \rightarrow dimension preference
 - PCE spectral coefficient decay rate estimation \rightarrow index weights
 - Goal-oriented adaptive p-refinement with generalized sparse grids
 - Generalized > anisotropic > isotropic

Areas for further study

- Tuning
 - Effect of combining anisotropy/refinement metrics over a response set
 - Scaling of anisotropic preference (VBD/decay rates often too severe)
- Capability extensions
 - Point-wise refinement (finer grain within active index sets)
 - Progression in interpolants: local and global Hermite interpolants (gradient-enhanced)

Extend Scalability through Adjoint Derivative-Enhancement

PCE:

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

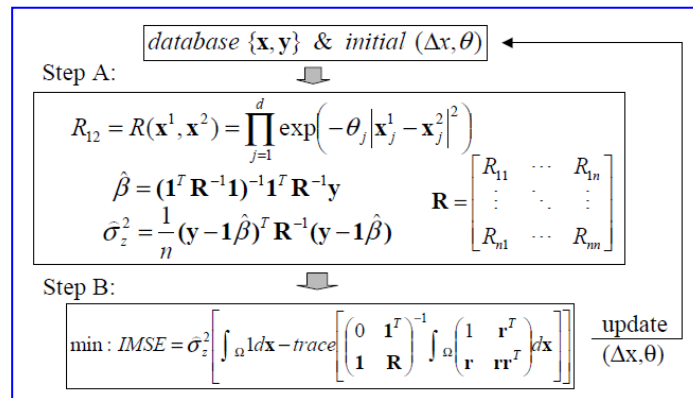
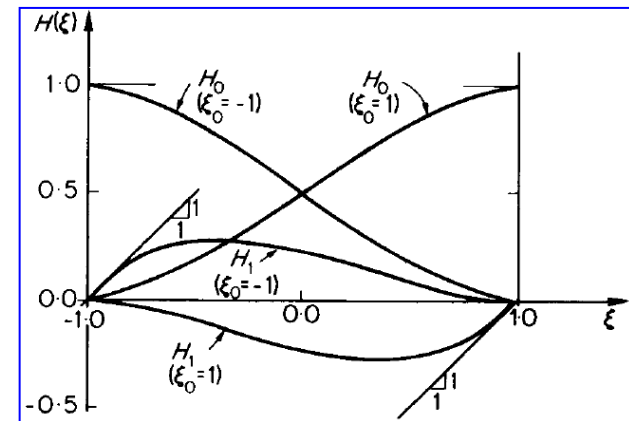
$$\begin{bmatrix}
 \vdots & \vdots & \vdots \\
 \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\
 \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\
 \vdots & \vdots & \ddots & \vdots \\
 \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\
 \vdots & \vdots & \vdots & \vdots
 \end{bmatrix}
 \begin{pmatrix}
 \vdots \\
 \vec{u}^{(m,j)} \\
 \vec{u}^{(m+1,j)} \\
 \vdots \\
 \vec{u}^{(m+n_\xi,j)} \\
 \vdots
 \end{pmatrix}
 =
 \begin{pmatrix}
 \vdots \\
 \vec{u}_i \\
 \frac{\partial \vec{u}_i}{\partial \xi_1} \\
 \vdots \\
 \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\
 \vdots
 \end{pmatrix}$$

SC:

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

EGRA:

- Gradient-enhanced kriging/cokriging
 - Interpolates function values and gradients
 - Scaling: $n^2 \rightarrow n$



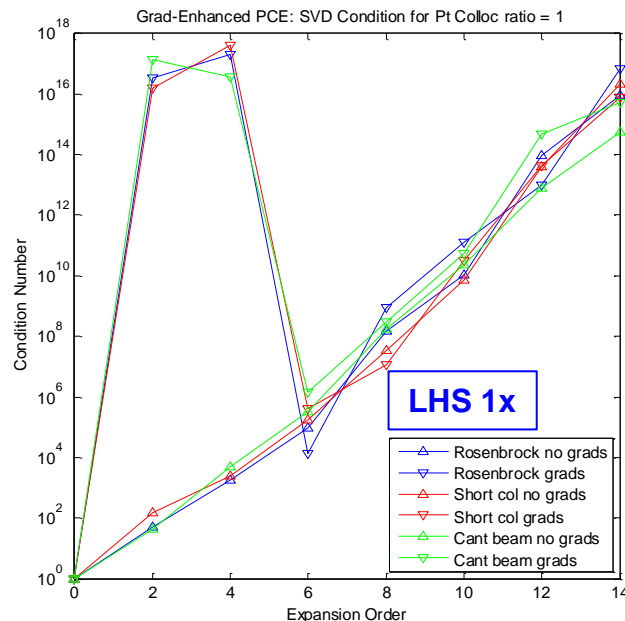
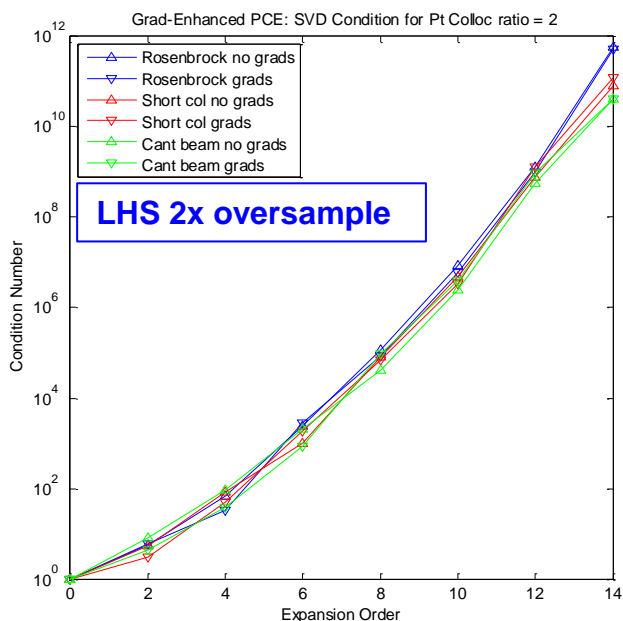
Gradient-Enhanced PCE

Straightforward regression approach implemented in DAKOTA v5.1:

$$\begin{bmatrix} \vdots & \vdots & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{pmatrix} \vdots \\ \vec{u}^{(m,j)} \\ \vec{u}^{(m+1,j)} \\ \vdots \\ \vec{u}^{(m+n_\xi,j)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vec{u}_i \\ \frac{\partial \vec{u}_i}{\partial \xi_1} \\ \vdots \\ \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\ \vdots \end{pmatrix}$$

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

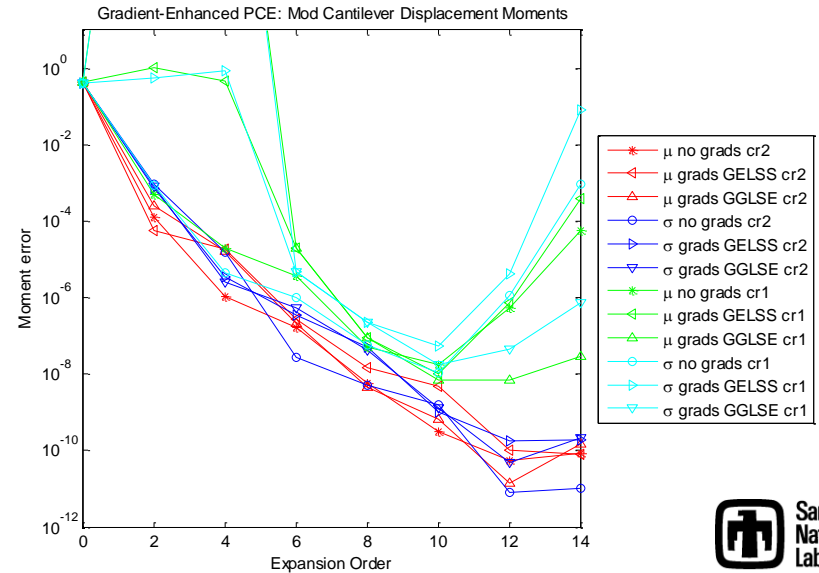
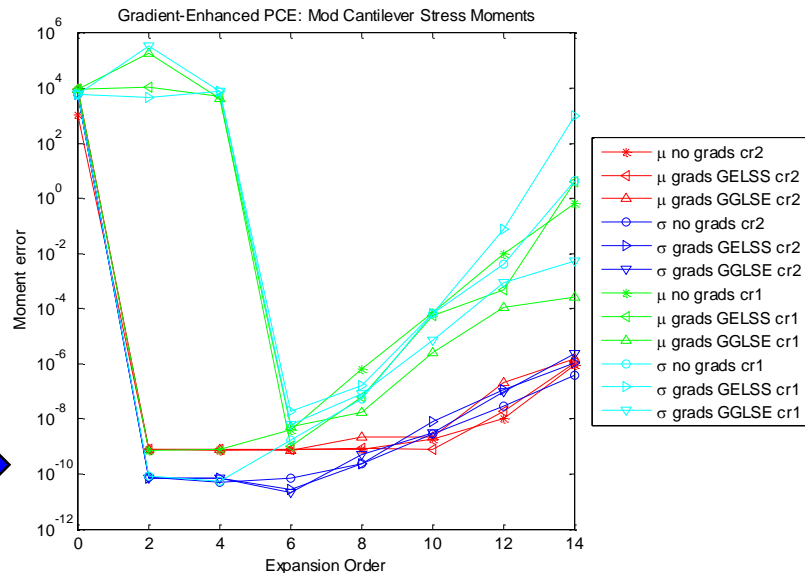
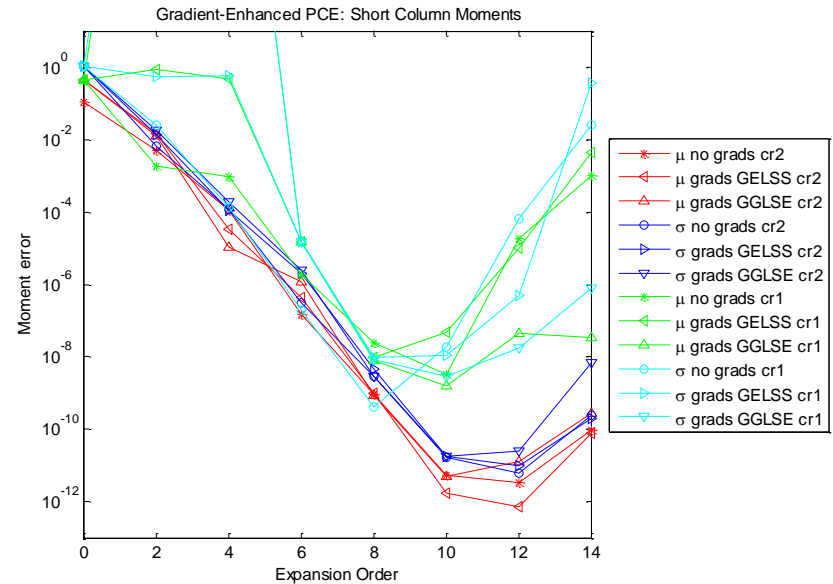
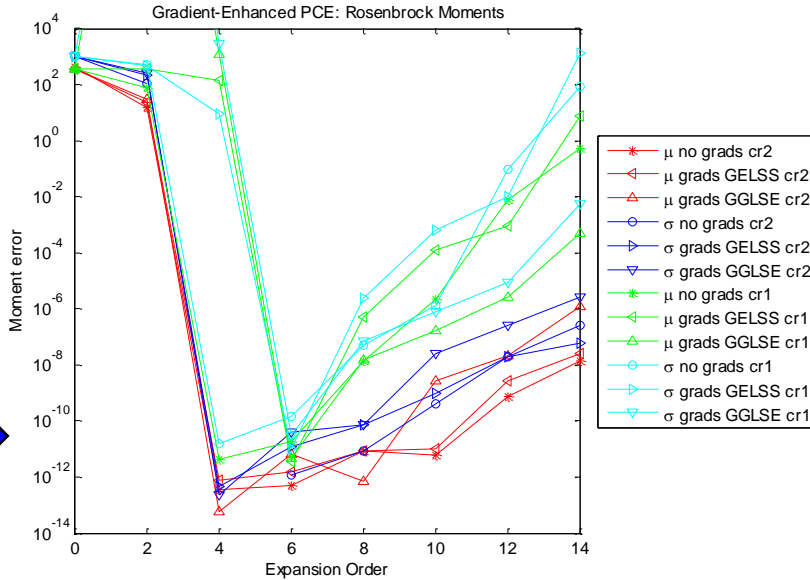
Vandermonde-like systems known to suffer from ill-conditioning



Gradient-Enhanced PCE: "Point Collocation"

LHS with & without gradients, oversample ratio = 1 or 2

Conditioning issues evident as we over-resolve exact solutions



h-refinement with Gradient-Enhanced Interpolants

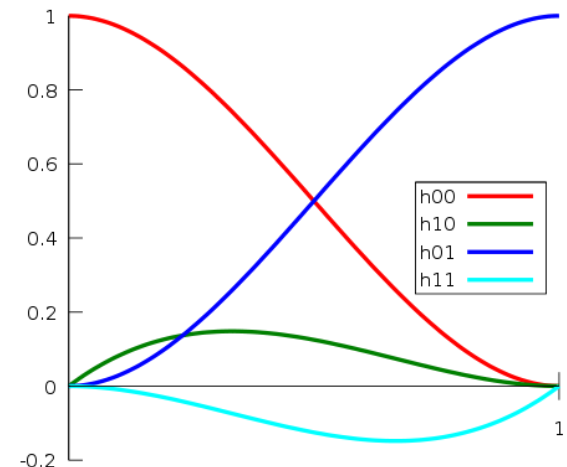
Dimension-adaptive h-refinement: local interpolant bases within global sparse grids:

- Values only: linear spline
- Values only: Quadratic hierarchical spline
- Values+gradients: cubic Hermite spline

$$\Rightarrow p(t) = h_{00}(t)p_0 + h_{10}(t)m_0 + h_{01}(t)p_1 + h_{11}(t)m_1$$

Shape functions – type 1 (value) and type 2 (gradient)

- Rearrange cubic Hermite spline into “hat” functions
- Value (type 1): h01 left half, h00 right half
- Gradient (type 2): h11 left half, h10 right half



Hermite interpolation

- 1D to first-order:

$$W_n(x) = \sum_{v=1}^n f_v h_v^{(1)}(x) + \sum_{v=1}^n f'_v h_v^{(2)}(x)$$

- Multivariate tensor product to arbitrary order (Lalescu):

$$s^{(n)}(x_1, x_2, \dots, x_D) = \sum_{l_1, \dots, l_D=0}^m \sum_{i_1, \dots, i_D=0,1} f^{(l_1, \dots, l_D)}(i_1, \dots, i_D) \prod_{k=1}^D \alpha_{i_k}^{(n, l_k)}(x_k)$$

Global Hermite interpolants also of interest → gradient-enhanced p-refinement

Gradient-Enhanced Interpolation: Explicit formulation eliminates regression error

$$s^{(n)}(x_1, x_2, \dots, x_D) = \sum_{l_1, \dots, l_D=0}^m \sum_{i_1, \dots, i_D=0,1} f^{(l_1, \dots, l_D)}(i_1, \dots, i_D) \prod_{k=1}^D \alpha_{i_k}^{(n, l_k)}(x_k)$$

Example: $n=3$, N pts, 1st-order Hermite

$$f = \sum_{i=1}^N f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^N \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^N \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^N \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3)$$



$$\mu = \sum_{i=1}^N f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^N \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^N \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^N \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)}$$

and similar for higher-order moments

Investigated several variants:

- PW linear vs. PW cubic vs. global
- Newton-Cotes vs. Clenshaw-Curtis
- Restricted growth/delayed sequences vs. unrestricted

Sparse grid gradient-enhanced interpolation of Rosenbrock (w=3, uniform over [-2,2])

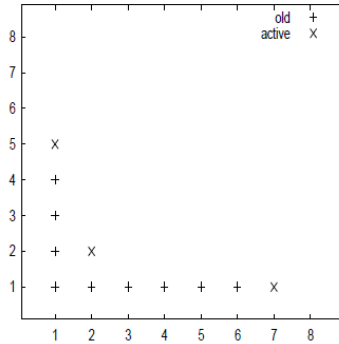
Colloc pt 1:	truth value = 3.6090000000e+03	interpolant = 3.6090000000e+03	error = 0.0000000000e+00
	truth grad_1 = -9.6120000000e+03	interpolant = -9.6120000000e+03	error = 0.0000000000e+00
	truth grad_2 = -2.4000000000e+03	interpolant = -2.4000000000e+03	error = 0.0000000000e+00
Colloc pt 2:	truth value = 2.5090000000e+03	interpolant = 2.5090000000e+03	error = 0.0000000000e+00
	truth grad_1 = -8.0120000000e+03	interpolant = -8.0120000000e+03	error = 0.0000000000e+00
	truth grad_2 = -2.0000000000e+03	interpolant = -2.0000000000e+03	error = 0.0000000000e+00
Colloc pt 3:	truth value = 1.6090000000e+03	interpolant = 1.6090000000e+03	error = 0.0000000000e+00
	truth grad_1 = -6.4120000000e+03	interpolant = -6.4120000000e+03	error = 0.0000000000e+00
	truth grad_2 = -1.6000000000e+03	interpolant = -1.6000000000e+03	error = 0.0000000000e+00
Colloc pt 4:	truth value = 9.0900000000e+02	interpolant = 9.0900000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.8120000000e+03	interpolant = -4.8120000000e+03	error = 0.0000000000e+00
	truth grad_2 = -1.2000000000e+03	interpolant = -1.2000000000e+03	error = 0.0000000000e+00
Colloc pt 5:	truth value = 4.0900000000e+02	interpolant = 4.0900000000e+02	error = 0.0000000000e+00
	truth grad_1 = -3.2120000000e+03	interpolant = -3.2120000000e+03	error = 0.0000000000e+00
	truth grad_2 = -8.0000000000e+02	interpolant = -8.0000000000e+02	error = 0.0000000000e+00
Colloc pt 6:	truth value = 5.1250000000e+02	interpolant = 5.1250000000e+02	error = 0.0000000000e+00
	truth grad_1 = -2.7100000000e+03	interpolant = -2.7100000000e+03	error = 0.0000000000e+00
	truth grad_2 = -9.0000000000e+02	interpolant = -9.0000000000e+02	error = 0.0000000000e+00
Colloc pt 7:	truth value = 9.0400000000e+02	interpolant = 9.0400000000e+02	error = 0.0000000000e+00
	truth grad_1 = -2.4080000000e+03	interpolant = -2.4080000000e+03	error = 0.0000000000e+00
	truth grad_2 = -1.2000000000e+03	interpolant = -1.2000000000e+03	error = 0.0000000000e+00
Colloc pt 8:	truth value = 1.0400000000e+02	interpolant = 1.0400000000e+02	error = 0.0000000000e+00
	truth grad_1 = -8.0800000000e+02	interpolant = -8.0800000000e+02	error = 0.0000000000e+00
	truth grad_2 = -4.0000000000e+02	interpolant = -4.0000000000e+02	error = 0.0000000000e+00
Colloc pt 9:	truth value = 1.0400000000e+02	interpolant = 1.0400000000e+02	error = 0.0000000000e+00
	truth grad_1 = 7.9200000000e+02	interpolant = 7.9200000000e+02	error = 0.0000000000e+00
	truth grad_2 = 4.0000000000e+02	interpolant = 4.0000000000e+02	error = 0.0000000000e+00
Colloc pt 10:	truth value = 8.5000000000e+00	interpolant = 8.5000000000e+00	error = 0.0000000000e+00
	truth grad_1 = -1.0600000000e+02	interpolant = -1.0600000000e+02	error = 0.0000000000e+00
	truth grad_2 = -1.0000000000e+02	interpolant = -1.0000000000e+02	error = 0.0000000000e+00
Colloc pt 11:	truth value = 4.0100000000e+02	interpolant = 4.0100000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = -8.0000000000e+02	interpolant = -8.0000000000e+02	error = 0.0000000000e+00
Colloc pt 12:	truth value = 2.2600000000e+02	interpolant = 2.2600000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = -6.0000000000e+02	interpolant = -6.0000000000e+02	error = 0.0000000000e+00
Colloc pt 13:	truth value = 1.0100000000e+02	interpolant = 1.0100000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = -4.0000000000e+02	interpolant = -4.0000000000e+02	error = 0.0000000000e+00
Colloc pt 14:	truth value = 2.6000000000e+01	interpolant = 2.6000000000e+01	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = -2.0000000000e+02	interpolant = -2.0000000000e+02	error = 0.0000000000e+00
Colloc pt 15:	truth value = 1.0000000000e+00	interpolant = 1.0000000000e+00	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = 0.0000000000e+00	interpolant = 0.0000000000e+00	error = 0.0000000000e+00
Colloc pt 16:	truth value = 2.6000000000e+01	interpolant = 2.6000000000e+01	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = 2.0000000000e+02	interpolant = 2.0000000000e+02	error = 0.0000000000e+00
Colloc pt 17:	truth value = 1.0100000000e+02	interpolant = 1.0100000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = 4.0000000000e+02	interpolant = 4.0000000000e+02	error = 0.0000000000e+00
Colloc pt 18:	truth value = 2.2600000000e+02	interpolant = 2.2600000000e+02	error = 0.0000000000e+00
	truth grad_1 = -4.0000000000e+00	interpolant = -4.0000000000e+00	error = 0.0000000000e+00
	truth grad_2 = 6.0000000000e+02	interpolant = 6.0000000000e+02	error = 0.0000000000e+00

...

Smooth Test Problems

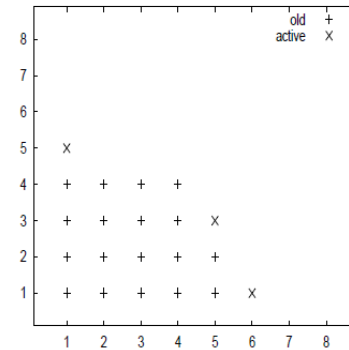
PWL/PWC bases on Gerstner tests (n=2)

$$e^{-x^2} + 10 \cdot e^{-y^2}$$

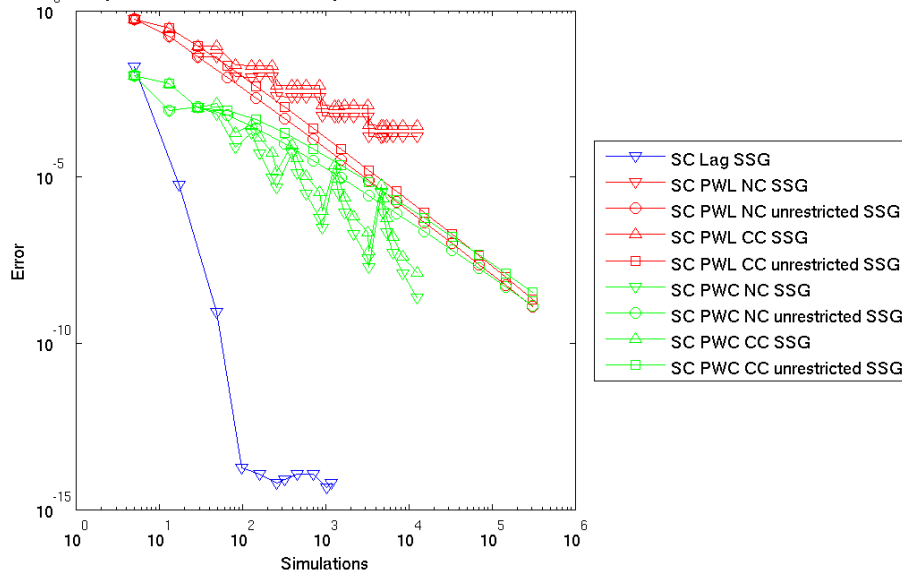


$x_i \text{ iid } U[0, 1]$

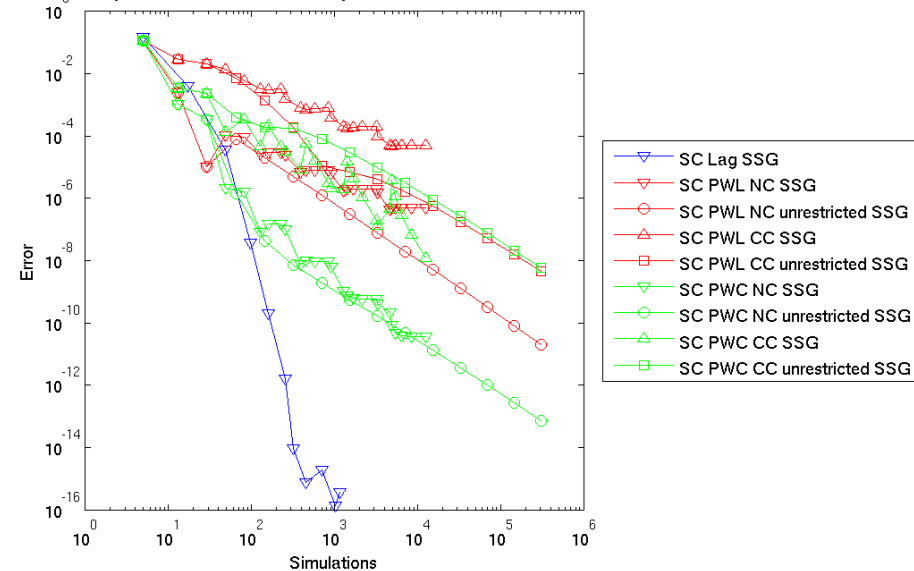
$$e^{-10x^2 - 5y^2}$$



Convergence for Gerstner aniso1 using SC SSG under uniform refinement



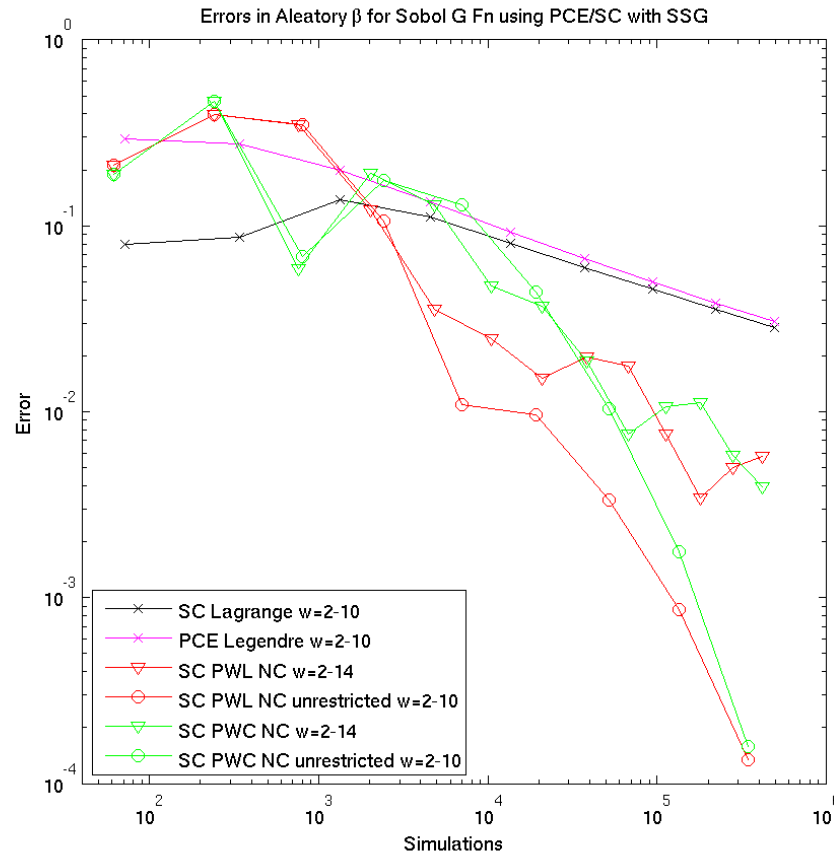
Convergence for Gerstner aniso3 using SC SSG under uniform refinement



Nonsmooth Test Problem

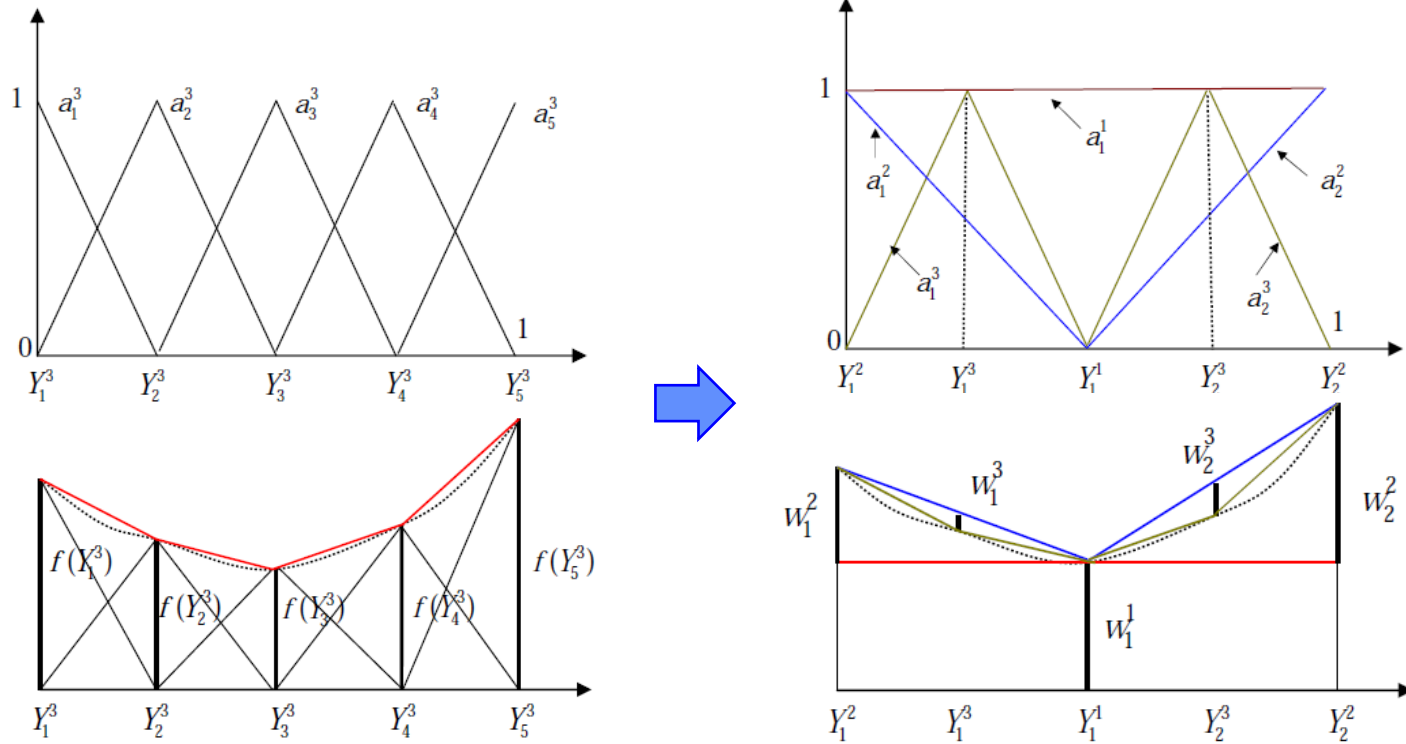
PWL/PWC bases on Sobol's g fn (n=5)

$$f(\mathbf{x}) = 2 \prod_{j=1}^5 \frac{|4x_j - 2| + a_j}{1 + a_j}; \quad a = [0, 1, 2, 4, 8]$$



Gradient-Enhanced Interpolation: Next Steps

- Add hierarchical basis for use alongside nodal basis → local refinement (element splitting, point-wise GSG), improved precision in incremental effects, hybrid metric estimation



Hierarchical linear splines; from Xiang Ma, Ph.D. dissertation, Cornell Univ., 2010

- Extend support for infinite and semi-infinite domains
- Global Hermite interpolation polynomials: stable 1D generators + integration weights

Stochastic Sensitivity Analysis

- **PCE/SC have convenient analytic features**

- Expansions readily differentiated w.r.t. ξ
- Analytic moment expressions

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

$$R = \sum_{j=1}^{N_p} r_j \mathbf{L}_j(\xi)$$

- **Augment w/ nonprobabilistic dimensions s**

- Design, epistemic uncertain

- **Approach 1: PCE/SC over prob. vars for each set of nonprob. vars**

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

$$R(\xi, s) = \sum_{j=1}^{N_p} r_j(s) \mathbf{L}_j(\xi)$$

Moment sensitivity = expectation of response sensitivity

$$\left\{ \begin{array}{l} \frac{d\mu_R}{ds} = \langle \frac{dR}{ds} \rangle \\ \frac{d\sigma_R^2}{ds} = 2 \sum_{j=1}^P \alpha_j \langle \frac{dR}{ds}, \Psi_j \rangle \end{array} \right. \quad \left\{ \begin{array}{l} \mu_R = \sum_{j=1}^{N_p} r_j w_j \\ \sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2 \end{array} \right.$$

→ Additional data requirements (dR/ds), but no additional dimensions

- **Approach 2: PCE/SC over all vars**

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

$$R(\xi, s) = \sum_{j=1}^{N_p} r_j \mathbf{L}_j(\xi, s)$$

Moment sensitivity = expectations over ξ + differentiation of remaining polynomial in s

$$\left\{ \begin{array}{l} \mu_R(s) = \sum_{j=0}^P \alpha_j \langle \Psi_j(\xi, s) \rangle_{\xi} \\ \sigma_R^2(s) = \sum_{j=0}^P \alpha_j^2 \langle \Psi_j^2(\xi, s) \rangle_{\xi} - \mu_R^2(s) \end{array} \right. \quad \left\{ \begin{array}{l} \mu_R(s) = \sum_{j=1}^{N_p} r_j \langle \mathbf{L}_j(\xi, s) \rangle_{\xi} \\ \sigma_R^2(s) = \sum_{j=1}^{N_p} r_j^2 \langle \mathbf{L}_j^2(\xi, s) \rangle_{\xi} - \mu_R^2(s) \end{array} \right.$$

→ Additional dimensions, but no additional data requirements

Optimization Under Uncertainty

Standard NLP

$$\begin{aligned} \min \quad & f(d) \\ \text{s.t.} \quad & g_l \leq g(d) \leq g_u \\ & h(d) = h_t \\ & d_l \leq d \leq d_u \end{aligned}$$

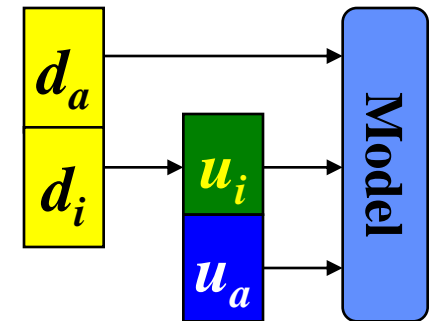
**optimize, accounting
for uncertainty metrics**
(using any UQ method)

Add resp stats $s_u(\mu, \sigma, z/\beta/p)$

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

Input design parameterization

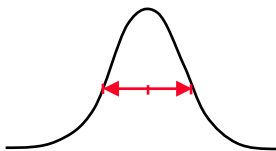
- Design vars may **augment** uncertain vars in simulation
- **Inserted** design vars: an optimization design var may be a parameter of an uncertain dist, e.g., the mean of a normal



Control response statistics to design for...

...robustness:

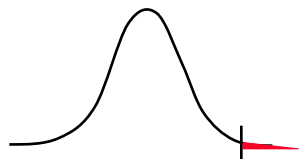
min/constrain moments
 μ, σ^2 , or $z(\beta)$ range



Aleatory

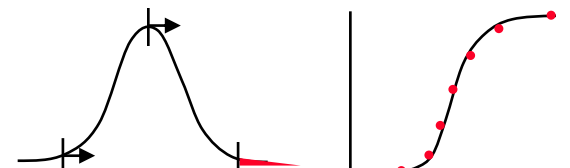
...reliability:

min/max/constrain p/β
(tail stats, failure)



...combined/other:

Pareto, inversion/model
calibration under uncertainty



Optimization Under Uncertainty

Standard NLP

$$\begin{aligned} \min \quad & f(d) \\ \text{s.t.} \quad & g_l \leq g(d) \leq g_u \\ & h(d) = h_t \\ & d_l \leq d \leq d_u \end{aligned}$$

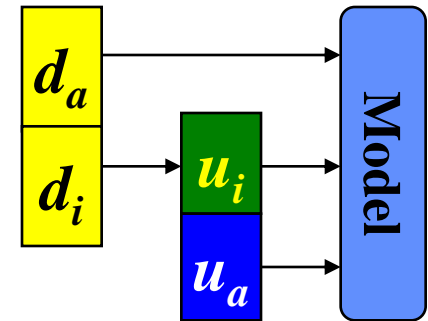
**optimize, accounting
for uncertainty metrics**
(using any UQ method)

Add resp stats $s_u(\mu, \sigma, z/\beta/p)$

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

Input design parameterization

- Design vars may **augment** uncertain vars in simulation
- **Inserted** design vars: an optimization design var may be a parameter of an uncertain dist, e.g., the mean of a normal



Control response statistics to design for...

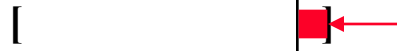
...robustness:

min/constrain moments
 μ, σ^2 , or $z(\beta)$ range



...reliability:

min/max/constrain p/β
(tail stats, failure)



...combined/other:

Pareto, inversion/model
calibration under uncertainty



PCE-based and SC-based OUU

Fully analytic Bi-level:

- Analytic moment/reliability sensitivities (avoid numerical derivs. at design level)
- Uncertain or Combined expansions

Reliability:

$$\left\{ \begin{array}{l} \text{minimize } f \\ \text{subject to } \beta \geq \bar{\beta} \end{array} \right.$$

(β initially based on moment proj)

Robustness:

$$\left\{ \begin{array}{l} \text{minimize } f \\ \text{subject to } \sigma^2 \leq \bar{\sigma}^2 \end{array} \right.$$

Sequential/Surrogate-based:

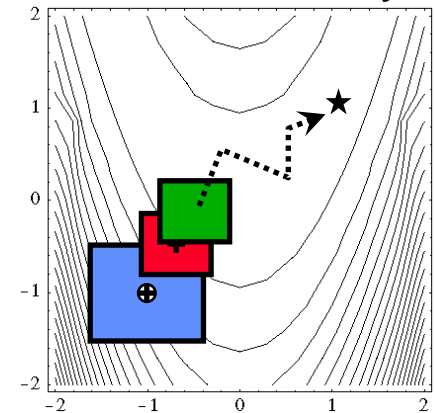
- Break nesting: iterate between opt & UQ w/ (surrogate) linkage
- Uncertain expansions

$$\left\{ \begin{array}{l} \text{minimize } f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T (\mathbf{s} - \mathbf{s}_c) \\ \text{subject to } \beta(\mathbf{s}_c) + \nabla_s \beta(\mathbf{s}_c)^T (\mathbf{s} - \mathbf{s}_c) \geq \bar{\beta} \\ \|\mathbf{s} - \mathbf{s}_c\|_\infty \leq \Delta^k \end{array} \right.$$

$$\left\{ \begin{array}{l} \text{minimize } f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T (\mathbf{s} - \mathbf{s}_c) \\ \text{subject to } \sigma^2(\mathbf{s}_c) + \nabla_s \sigma^2(\mathbf{s}_c)^T (\mathbf{s} - \mathbf{s}_c) \leq \bar{\sigma}^2 \\ \|\mathbf{s} - \mathbf{s}_c\|_\infty \leq \Delta^k \end{array} \right.$$

- 1st-order
- Also QN
- 2nd-order

TR-SBO with local data fit & multifidelity



Multifidelity (focused on UQ fidelity):

- Optimize corrected LF UQ model over TR
 - LF = Combined expansion (over \mathbf{s}), MVFOSM
 - HF = Uncertain expansion (at single design pt)
- Additive corrections enforce LF/HF consistency

$$\begin{array}{l} \bullet \text{ 1}^{\text{st}} \text{ order \&} \\ \bullet \text{ QN 2}^{\text{nd}}\text{-order} \end{array} \quad \begin{array}{l} \hat{\beta}_{hi}(\mathbf{s}) = \beta_{lo}(\mathbf{s}) + \alpha_{\beta}(\mathbf{s}) \\ \hat{\sigma}_{hi}^2(\mathbf{s}) = \sigma_{lo}^2(\mathbf{s}) + \alpha_{\sigma^2}(\mathbf{s}) \end{array}$$

$$\left\{ \begin{array}{l} \text{minimize } f(\mathbf{s}) \\ \text{subject to } \hat{\sigma}_{hi}^2(\mathbf{s}) \leq \bar{\sigma}^2 \\ \|\mathbf{s} - \mathbf{s}_c\|_\infty \leq \Delta^k \end{array} \right.$$

$$\left\{ \begin{array}{l} \text{minimize } f(\mathbf{s}) \\ \text{subject to } \hat{\beta}_{hi}(\mathbf{s}) \geq \bar{\beta} \\ \|\mathbf{s} - \mathbf{s}_c\|_\infty \leq \Delta^k \end{array} \right.$$

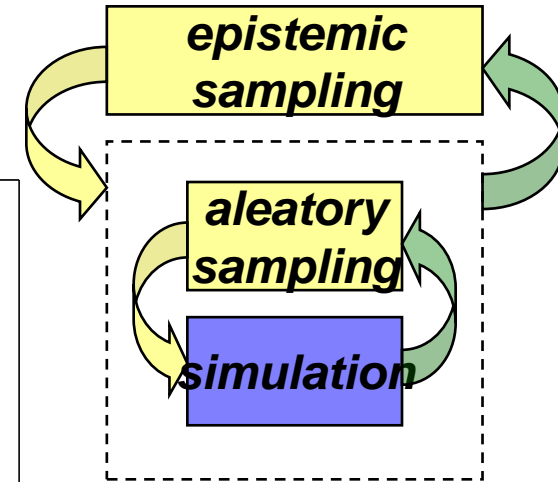
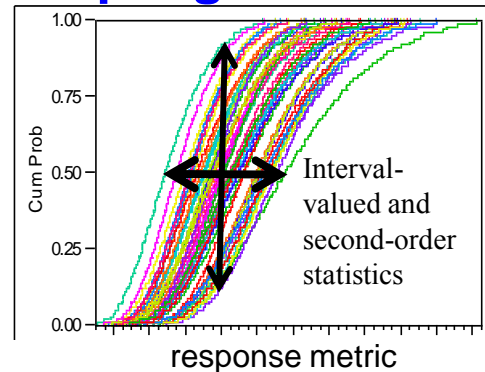
Unilevel approach (sim residuals @ collocation pts)

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 → under-resolved sampling (especially @ outer loop)
- Under-prediction of credible outcomes



Algorithmic approaches

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

Increasing epistemic structure (stronger assumptions)

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)

$$\begin{array}{ll} \text{minimize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \\ \\ \text{maximize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

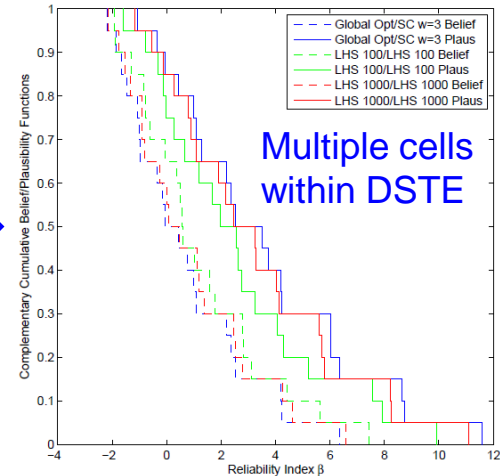
Mixed Aleatory-Epistemic UQ: IVP, SOP, and DSTE based on Stochastic Expansions

Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals					
EGO	SC SSG w = 1	Aleatory	(84/91, 0/0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(372/403, 0/0)	[75.0002, 374.999]	[-2.18735, 11.5900]
EGO	SC SSG w = 3	Aleatory	(1260/1365, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
EGO	SC SSG w = 4	Aleatory	(3564/3861, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 1	Aleatory	(21/77, 21/77)	[75.0000, 375.000]	[-2.26264, 11.8623]
NPSOL	SC SSG w = 2	Aleatory	(93/341, 93/341)	[75.0000, 375.000]	[-2.18735, 11.5901]
NPSOL	SC SSG w = 3	Aleatory	(315/1155, 315/1155)	[75.0000, 375.000]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 4	Aleatory	(891/3267, 891/3267)	[75.0000, 375.000]	[-2.18732, 11.5900]

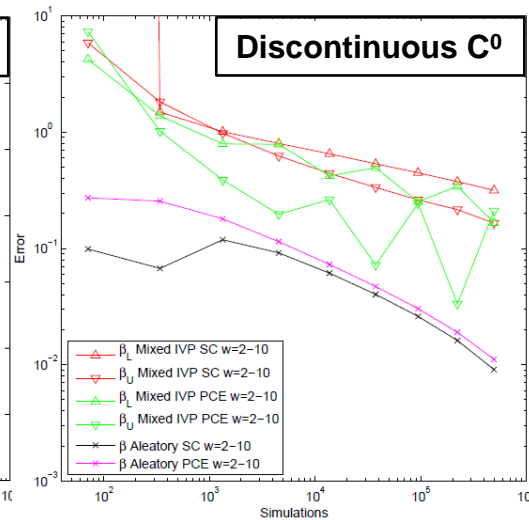
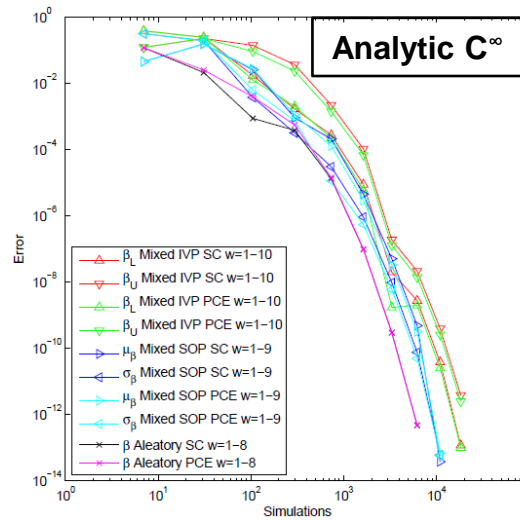
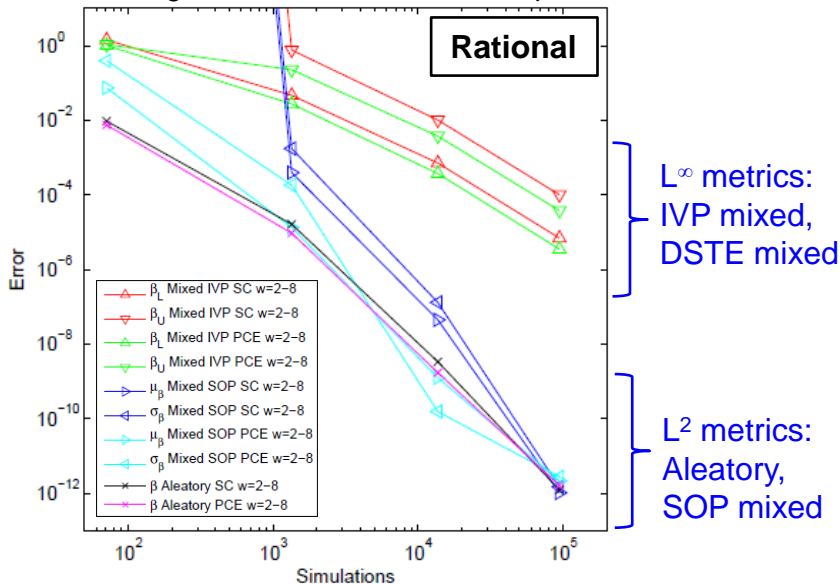
IVP nested LHS sampling: converged to 2-3 digits by 10^8 evals

LHS 100	LHS 100	N/A	($10^4/10^4$, 0/0)	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	($10^6/10^6$, 0/0)	[76.5939, 368.225]	[-2.19883, 11.2353]
LHS 10^4	LHS 10^4	N/A	($10^8/10^8$, 0/0)	[76.4755, 373.935]	[-2.16323, 11.5593]

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



Convergence rates for combined expansions



Concluding Remarks

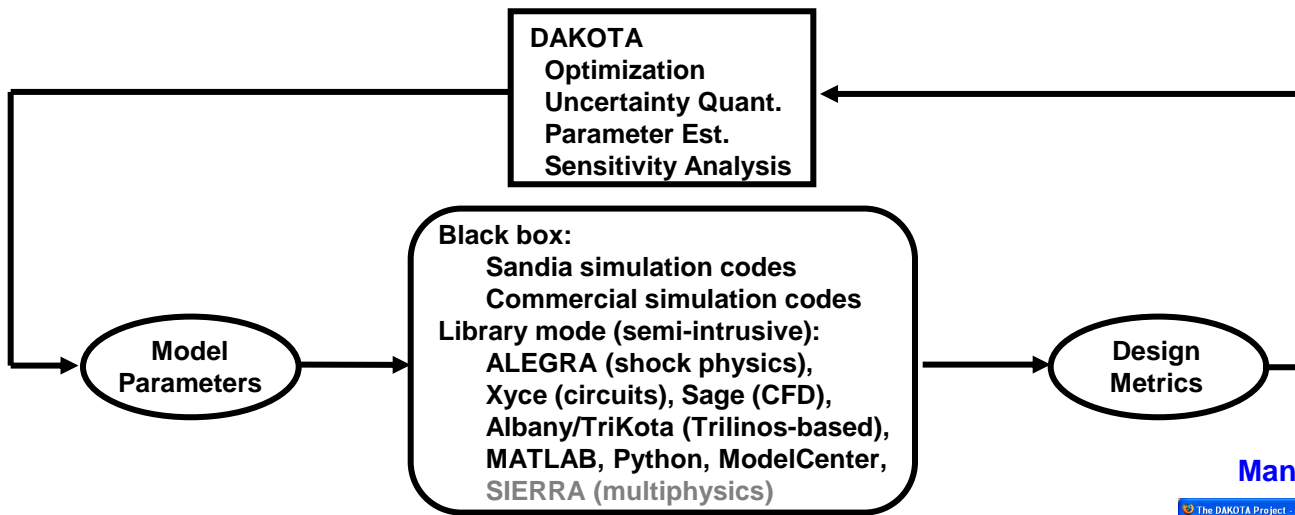
R&D in Adaptive UQ Methods → scalability

- Stochastic expansions: PCE, SC
 - Dimension-adaptive refinement (p- and h-)
 - Uniform p-refinement with *isotropic* grids
 - Adaptive p-refinement with *anisotropic* grids (VBD/Sobol', Spectral decay → anisotropy)
 - Goal-oriented adaptive p-refinement with *generalized* sparse grids (statistical QOI: $\mu, \sigma^2, \beta, \beta^*, p_{fail}$)
 - Adjoint enhancement
 - Hierarchical basis formulations → region-adaptive h-refinement

R&D in UQ Complexity → mixed uncertainties, multiphysics/multiscale

- Stochastic sensitivity analysis → enables OUU/MCUU and mixed UQ
- Design under uncertainty: bilevel, sequential, multifidelity approaches
- Mixed UQ with IVP/SOP/DSTE → greater accuracy/efficiency than nested sampling
 - Inner loop: stochastic expansions (aleatory or combined)
 - Outer loop: opt-based interval est.; global with data reuse (robust) or local with SSA (scalable)
- Multi-* → Multi-physics/Multi-scale/Multifidelity UQ
- Random fields and stochastic processes
- Nondeterministic calibration (MLE, ME, Bayesian inference) → Model Form UQ

DAKOTA Software



Iterative systems analysis
Multilevel parallel computing
Simulation management

<http://dakota.sandia.gov>

Manuals, Publications, Training mats. online

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

