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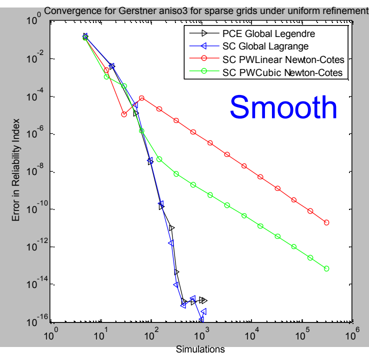

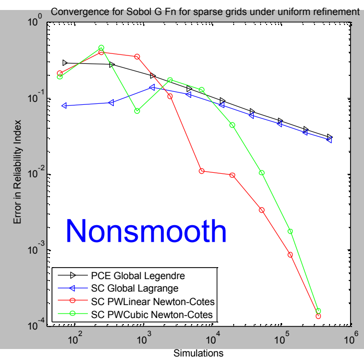

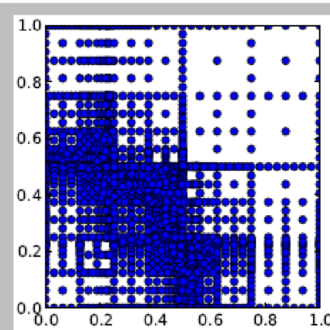

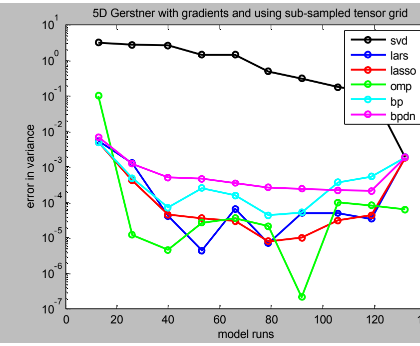

Scalable Uncertainty Quantification Methods

Michael S. Eldred, John D. Jakeman, Timothy M. Wildey

Sandia National Laboratories, Albuquerque, NM

Leo W.T. Ng

Massachusetts Institute of Technology

U.S. DEPARTMENT OF ENERGY   NNSA National Nuclear Security Administration

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Introduction
Scalable Methods for High-Dimensional UQ

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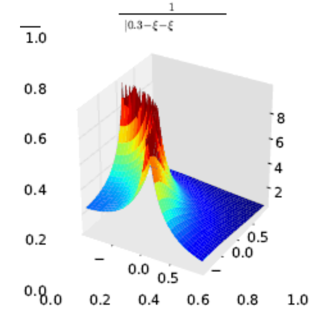
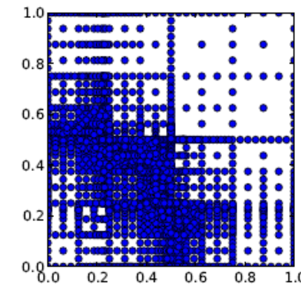
Key Challenges:

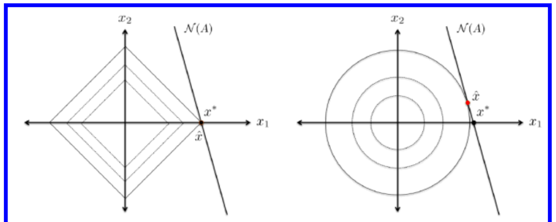
- Severe simulation budget constraints (e.g., a handful of HF runs)
- Moderate to high-dimensional in random variables: $O(10^1)$ to $O(10^2)$
- Compounding effects:
  - Mixed aleatory-epistemic uncertainties (→ nested iteration)
  - Requirement to evaluate probability of rare events (e.g., safety criteria)
  - Nonsmooth responses (→ difficulty with global basis spectral methods)





Algorithmic Capabilities:

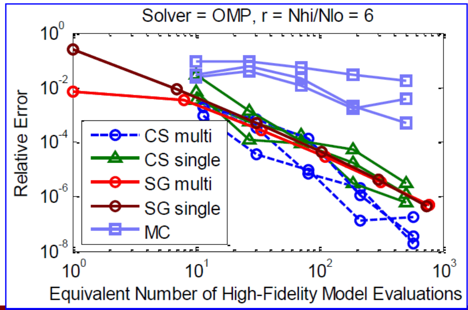
- Compute dominant uncertainty effects despite key challenges above
- Scalable UQ foundation
  - Adaptivity, Adjoints, Sparsity
- Leverage foundation within higher-level studies
  - Model form uncertainty, Multifidelity UQ, Bayesian inference



(a) CS methodology (ℓ_1 objective) (b) Pseudo-inverse (ℓ_2 objective)

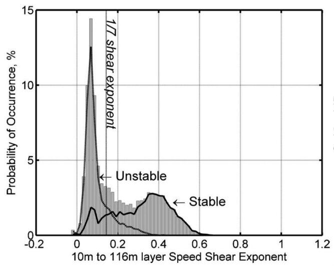
Mission Relevancy:

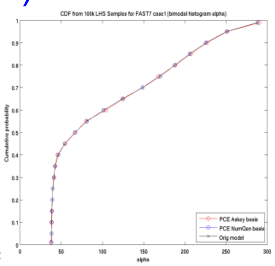
- NNSA: ASC abnormal environments
- Offices of science/energy: ASCR, SciDAC-3, CASL, CSSEF
- 2013 deployments of new UQ capabilities: Dakota v5.3, v5.3.1

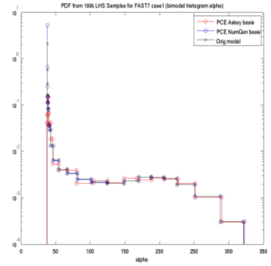


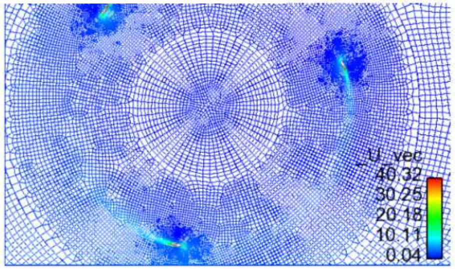
Offices of Science/Energy Examples

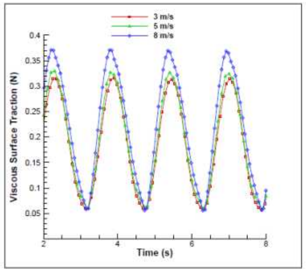
Wind energy (ASCR)



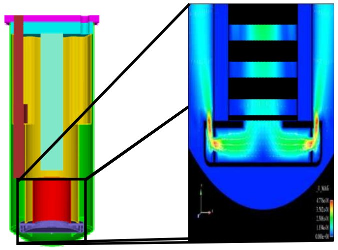


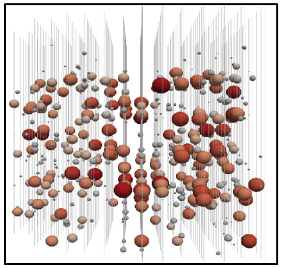




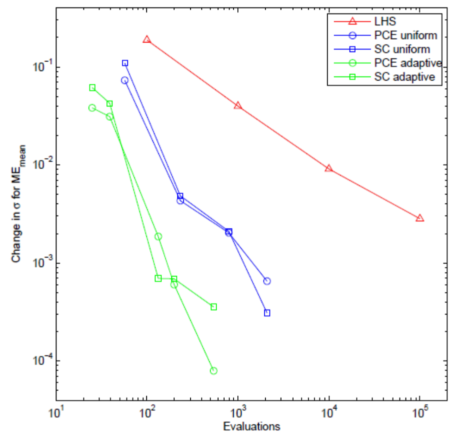


Nuclear reactors (CASL, NEAMS)



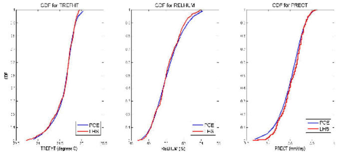


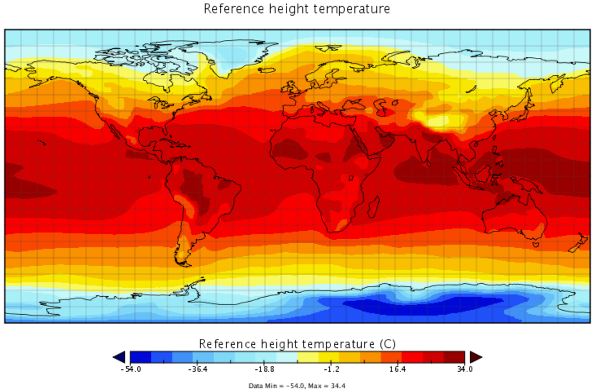
Adaptive refinement for CRUD



CSSEF: UQ w/ CAM4 (land, ocean, atmosphere)

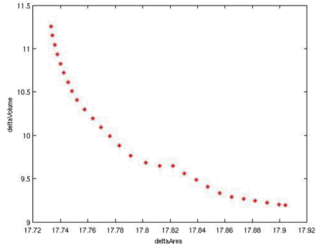
	RHMINL	RHMINH	ALFA	TAU	CZERO	KE
TREFHT	0.33	-0.06	-0.05	0.83	-0.04	0.04
T	0.58	-0.46	-0.35	-0.39	-0.05	0.19
U	-0.17	-0.37	0.07	0.82	-0.01	0.02
PS	0.79	-0.10	0.01	0.62	-0.04	0.03
RELHUM	0.05	0.58	-0.20	-0.74	-0.03	0.15
LHFLX	-0.30	0.31	0.10	0.82	0.01	-0.17
LWCF	-0.23	-0.72	-0.14	-0.59	-0.02	0.12
SWCF	0.92	0.31	0.04	0.21	-0.01	-0.03
PRECT	-0.40	0.38	0.05	0.71	0.03	-0.22
RADBAL	0.97	0.16	-0.03	-0.05	-0.02	0.01





SciDAC-3: QUEST, PISCEES

CISM Pareto set calibration



CISM global sensitivity (PCE)

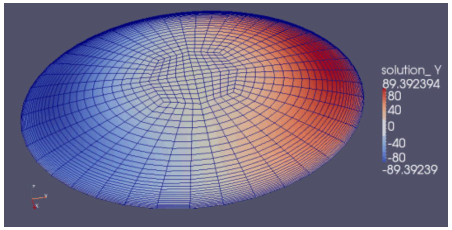
deltaArea Sobol indices:

Main	Total	
4.7513765309e-02	6.7248544556e-02	geothermal_flux
9.1650860584e-01	9.3781166646e-01	flow_factor
7.9696945177e-03	2.6872229178e-02	basal_exponent
Interaction		
9.1053996720e-03	geothermal_flux flow_factor	
6.7048737120e-03	geothermal_flux basal_exponent	
8.2731550851e-03	flow_factor basal_exponent	
3.9245058634e-03	geothermal_flux flow_factor basal_exponent	

deltaVolume Sobol indices:

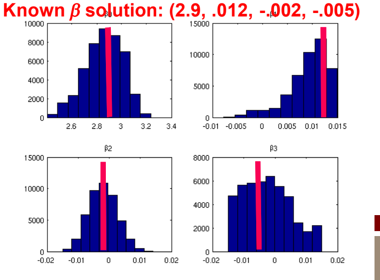
Main	Total	
2.3075148007e-04	5.8457999638e-04	geothermal_flux
9.9465232748e-01	9.9546169642e-01	flow_factor
4.2442002665e-03	4.9154442300e-03	basal_exponent
Interaction		
2.0147681120e-04	geothermal_flux flow_factor	
6.3351832896e-05	geothermal_flux basal_exponent	
5.1889225839e-04	flow_factor basal_exponent	
8.8999872203e-05	geothermal_flux flow_factor basal_exponent	

Bayesian calibration with FELIX ice dome



$$\beta(x,y) = \beta_0 + \beta_1 x + \beta_2 y + \beta_3 r$$

Known β solution: (2.9, .012, -.002, -.005)



Research in Scalable UQ Methods

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For production UQ analyses, we prefer fast converging global methods:

- Local approximate methods (reliability methods, moment-based methods) exhibit significant errors in presence of multimodal/nonsmooth/highly nonlinear responses
- MC/LHS are robust with dim.-independent conv., but rates can be unacceptably slow

Spectral methods (e.g., PCE) provide a more effective balance of robustness and efficiency, especially when solution smoothness can be exploited

- Exponential growth in expansion cardinality with n and p
- Collocation requirements are generally on the order of the number of terms

To mitigate the curse of dimensionality:

- *A priori* model reduction methods (e.g., POD, Karhunen-Loeve)
- Goal-oriented adaptive refinement to reduce effective dimension
- Adjoint techniques [given n (random dimension) > m (response QoI)]
- Sparsity detection methods: compressive sensing, least interpolation

Primary focus is stochastic exp., but other adaptive sampling efforts are related (and will be leveraged within an abstract adaptive framework):

- Reliability: EGRA, GPAIS, POF darts (Bichon, Dalbey, Ebeida, et al.)
- Topology-guided: Morse-Smale complexes (Maljovec et al.)

Non-Intrusive Stochastic Expansions:
Polynomial Chaos and Stochastic Collocation

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Polynomial chaos: spectral projection using orthogonal polynomial basis fns

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

using

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

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

- Estimate α_j using regression or numerical integration: sampling, tensor quadrature, sparse grids, or cubature

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

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

Stochastic collocation: instead of estimating coefficients for known basis functions, form interpolants for known coefficients

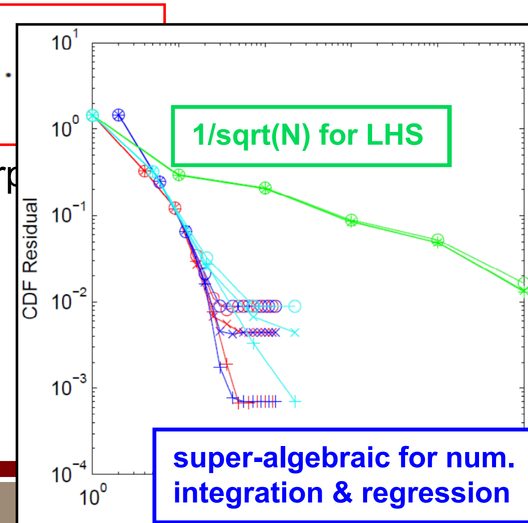
$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

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

$$L_i = \prod_{\substack{j=1\\ j\neq i}}^{m} \frac{x - x_j}{x_i - x_j} \Rightarrow R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right)\left(L_{j_1}^{i_1} \otimes \cdots\right.$$

Sparse interpolants formed using Σ of tensor interp

- Tailor expansion form:
  - p-refinement: anisotropic tensor/sparse, generalized sparse
  - h-refinement: local bases with dimension & local refinement
- Method selection: fault tolerance, decay, sparsity, error est.



Approaches for forming PCE/SC Expansions

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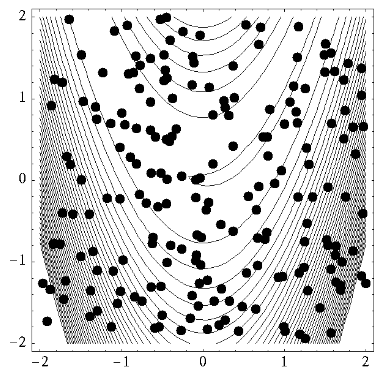
Random sampling: PCE

Expectation (sampling):

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

Least squares regression:

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



$$\Psi \alpha = R$$

Compressive sensing

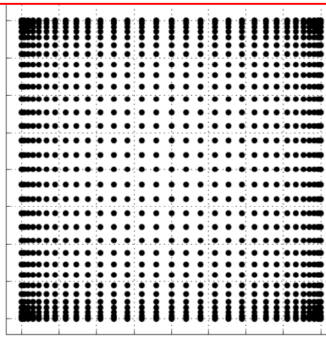
- Underdetermined systems: sparse basis pursuit for with L1 regularization

Tensor-product quadrature: PCE/SC

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

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

- **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 2*p*, select *m* = *p* + *1***

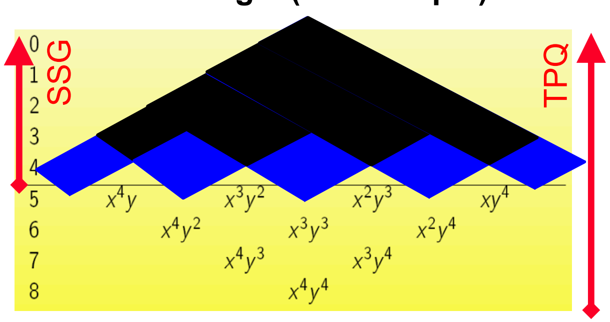


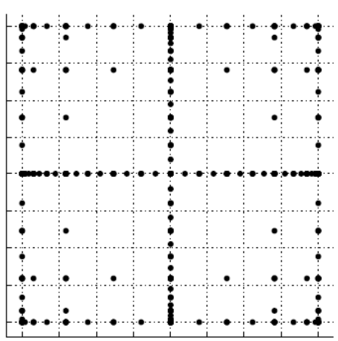
Sparse Grid: PCE/SC

$$\mathscr{A}(\mathrm{w}, n) = \sum_{|\mathbf{i}| \le \mathrm{w}+n} (\Delta^{i_1} \otimes \cdots \otimes \Delta^{i_n})$$

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

Pascal's triangle (2D example):



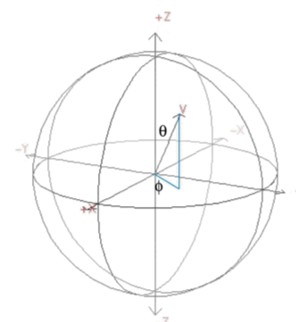


Cubature: PCE

Stroud and extensions (Xiu, Cools)

→ Low order PCE

→ global SA, anisotropy detection



Gaussian i = 2 → p = 1

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

Arbitrary PDF

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

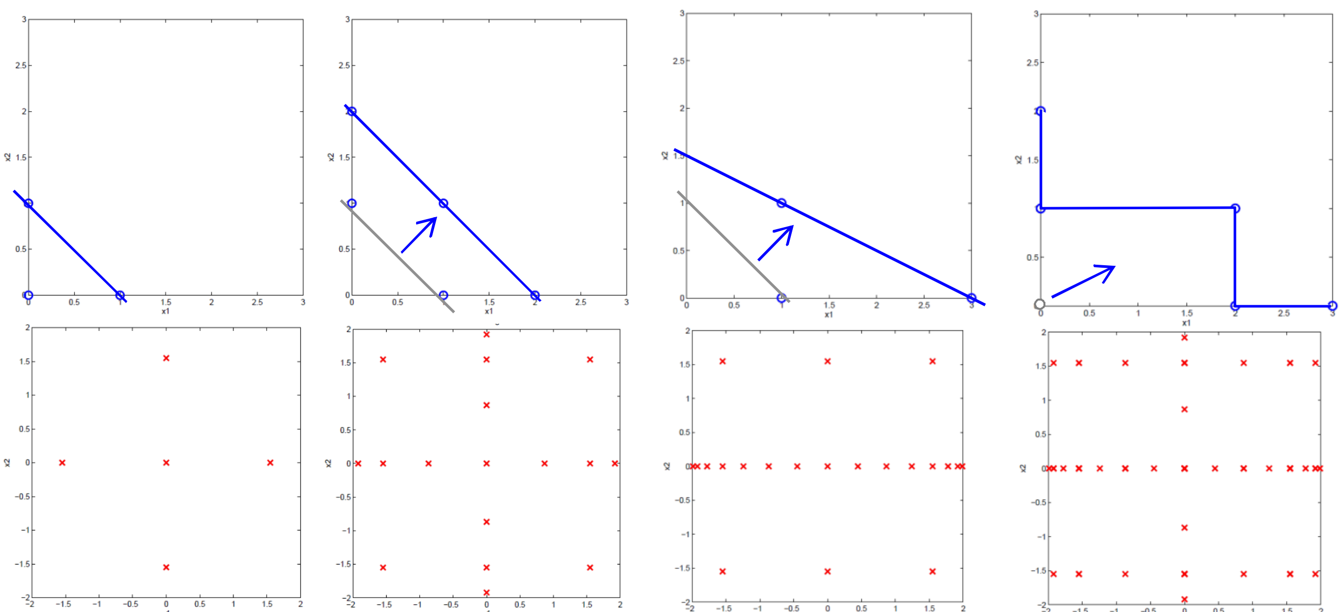
Adaptive Collocation Methods

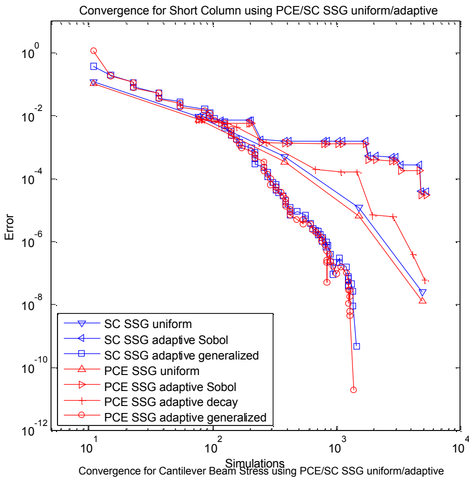
Polynomial order (p-) refinement approaches:

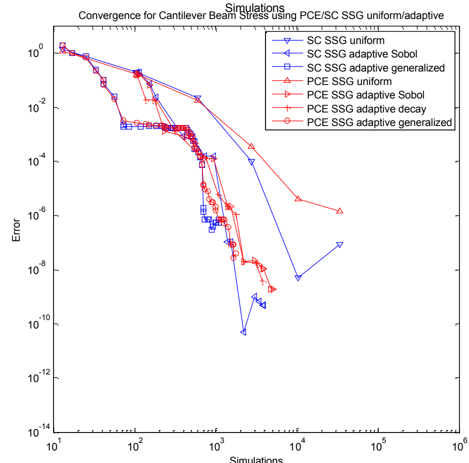
- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted/nested)
  - *Assess convergence:* L^2 change in response covariance
- **Adaptive:** *anisotropic* tensor/sparse grids

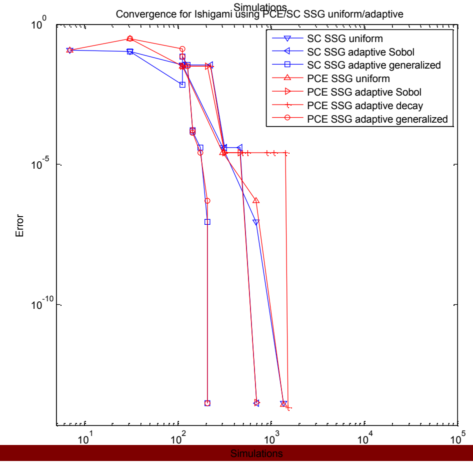
$$\underline{\mathrm{w}\gamma} < \mathbf{i} \cdot \gamma \le \underline{\mathrm{w}\gamma} + |\gamma|$$

  - **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy
  - **PCE:** spectral coefficient decay rates → anisotropy
- **Goal-oriented adaptive:** *generalized* sparse grids
  - **PCE/SC:** change in QOI induced by trial index sets on active front
  - Fine-grained control: frontier not limited by index set constraint









Adaptive Collocation Methods: Generalized Sparse Grids

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Polynomial order (p-) refinement approaches:

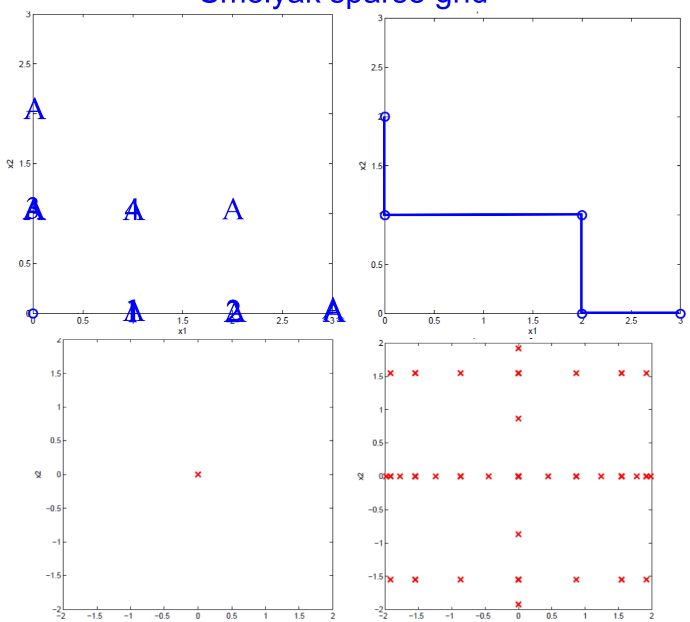
- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted growth in nested rules)
  - *Assess convergence:* L^2 change in response covariance
- **Dimension-adaptive:** *anisotropic* tensor/sparse grids

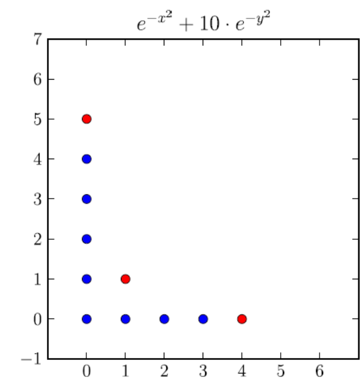
$$w\underline{\gamma} < \mathbf{i}\cdot\gamma \le w\underline{\gamma} + |\gamma|$$

  - **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

(Adjoint) Derivative-Enhancement

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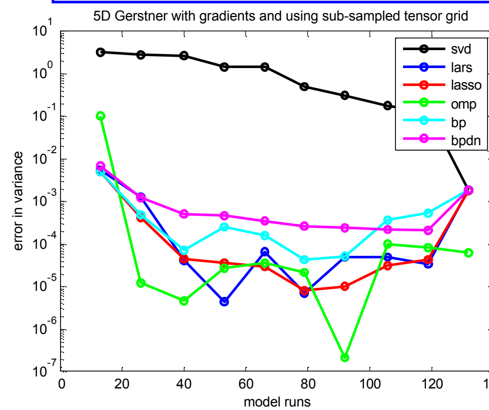
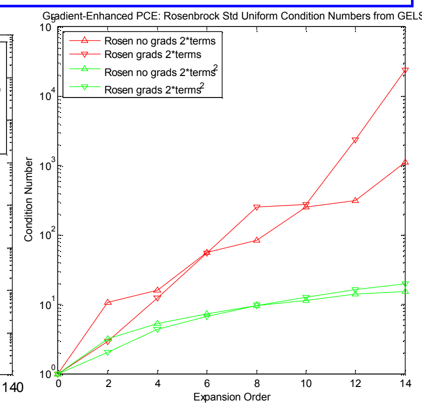
PCE:

- **Linear regression including derivatives**
  - **Gradients/Hessians → addtnl. eqns.**
  - **Over-determined: SVD, eq-constrained LS**
  - **Under-determined: compressive sensing**

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



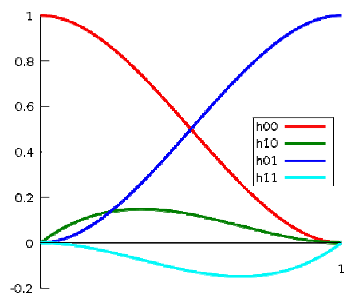


SC:

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

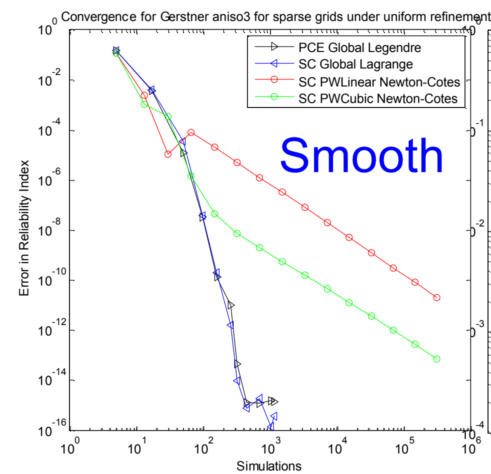
$$f = \sum_{i=1}^{N} f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3)$$

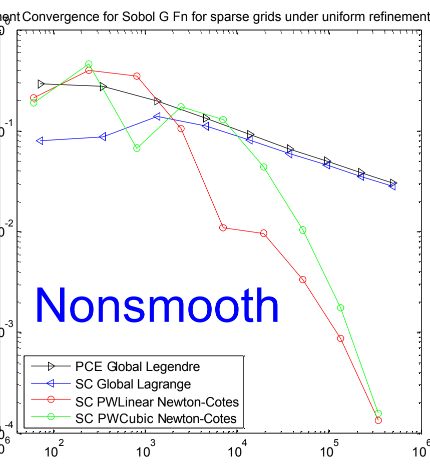
Cubic shape fns: type 1 (value) & type 2 (gradient)



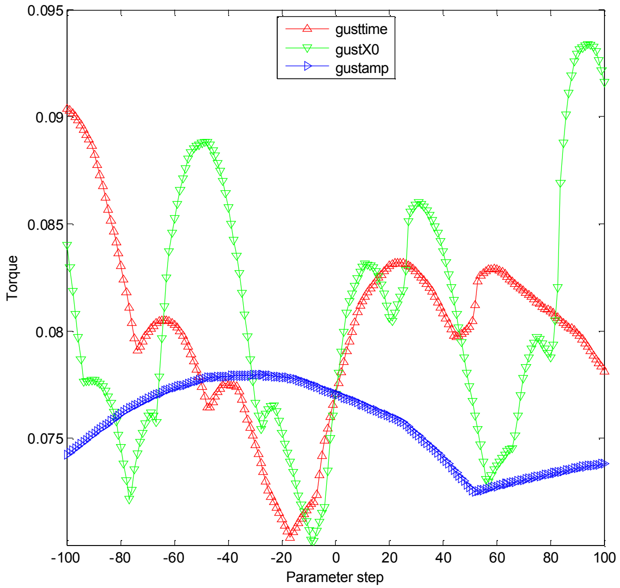
$$\mu = \sum_{i=1}^{N} f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)}$$

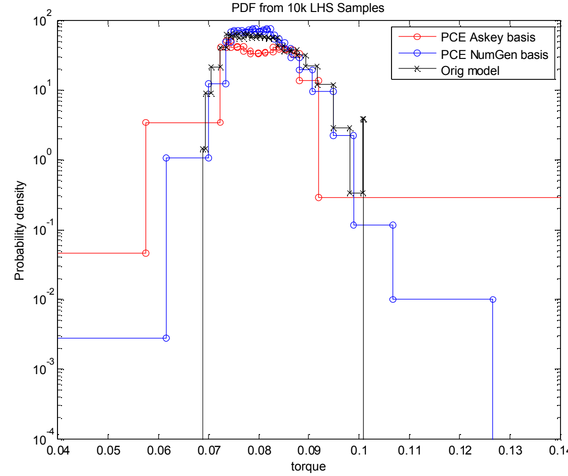
and similar for higher-order moments

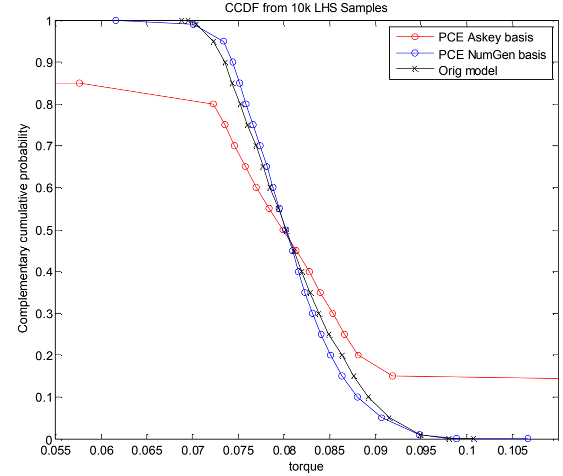


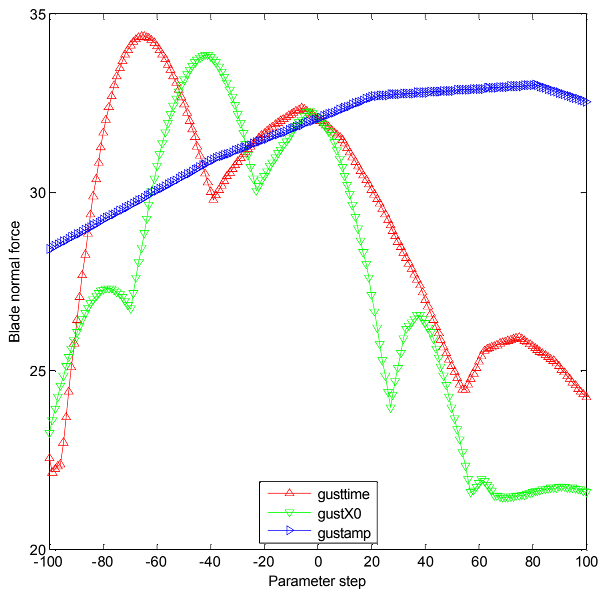


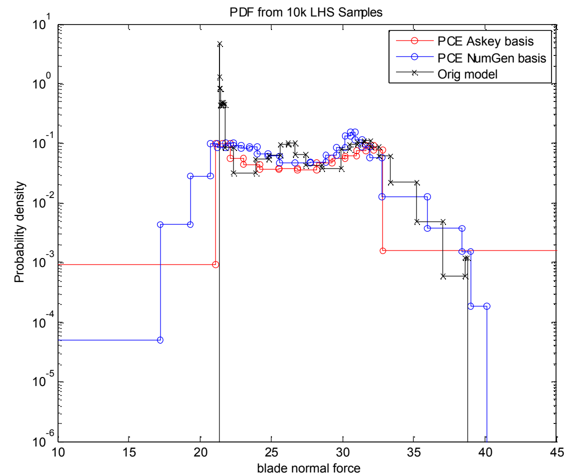
ASCR: VAWT with Uncertain Gust Loading

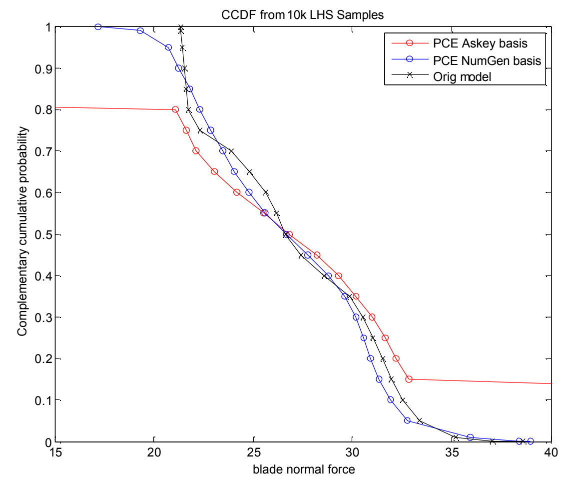








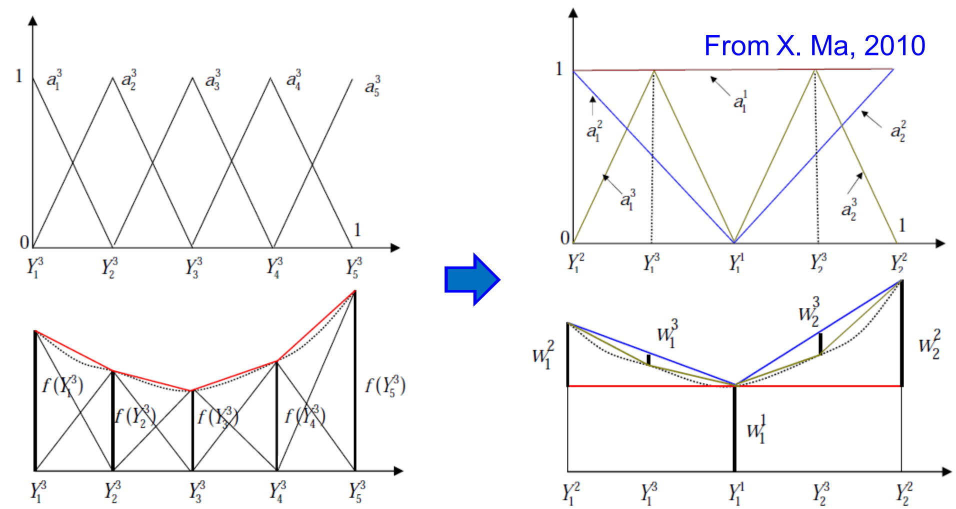




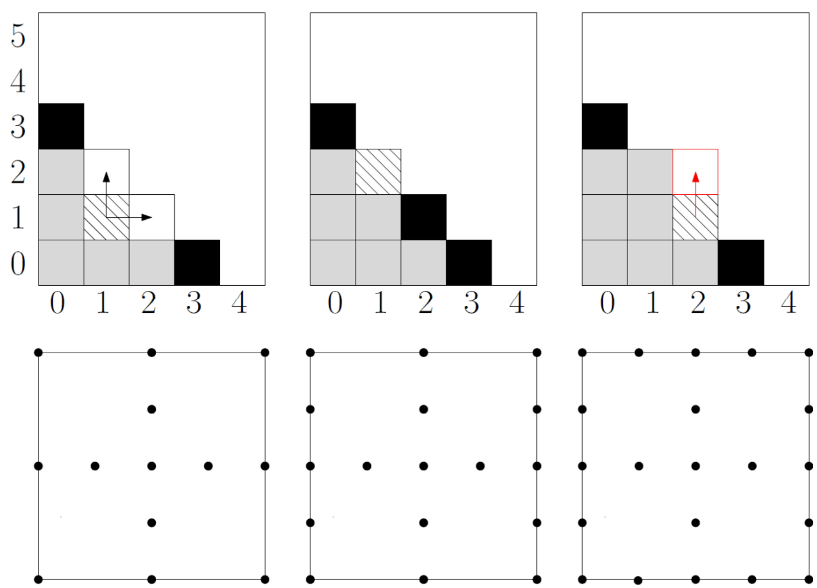
Local Error Estimation with Hierarchical Surpluses

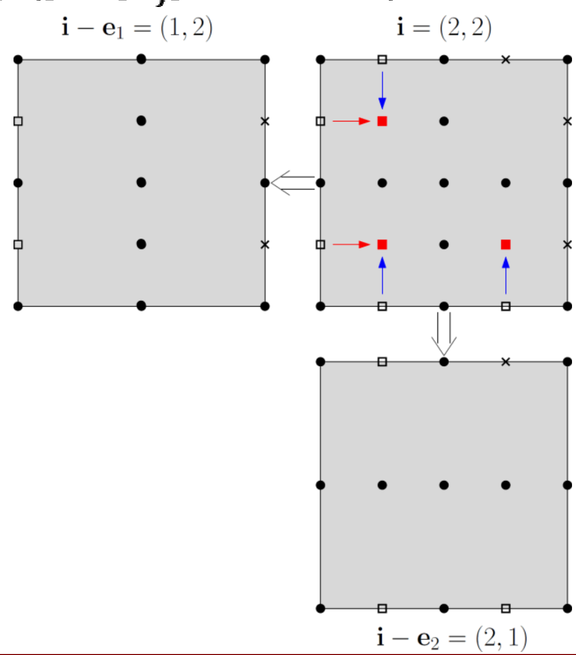
Hierarchical basis:

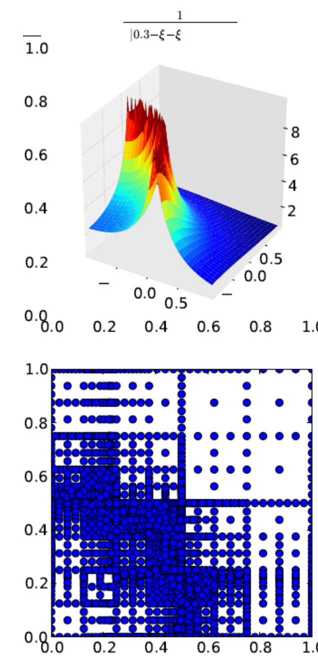
- *Improved precision* in QoI increments
- Surpluses provide error estimates for *local refinement* using local/global hierarchical interpolants
- New error indicators under development that leverage both *value and gradient surpluses*



$$\Delta\Sigma_{ij} = \Delta E[R_i R_j] - \mu_{R_i}\,\Delta E[R_j] - \mu_{R_j}\,\Delta E[R_i] - \Delta E[R_i]\Delta E[R_j] \;\rightarrow\; \Delta\sigma, \Delta\beta$$







L1 Regularized Regression: Compressive Sensing

$$\begin{bmatrix} f(\mathbf{x}^{(1)}) \\ f(\mathbf{x}^{(2)}) \\ \vdots \\ f(\mathbf{x}^{(N)}) \end{bmatrix} = \begin{bmatrix} 1 & \Phi_2(\mathbf{x}^{(1)}) & \Phi_2(\mathbf{x}^{(1)}) & \dots & \Phi_P(\mathbf{x}^{(1)}) \\ 1 & \Phi_1(\mathbf{x}^{(2)}) & \Phi_2(\mathbf{x}^{(2)}) & \dots & \Phi_P(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \Phi_1(\mathbf{x}^{(N)}) & \Phi_2(\mathbf{x}^{(N)}) & \dots & \Phi_P(\mathbf{x}^{(N)}) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_P \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{bmatrix}$$

or in matrix notation

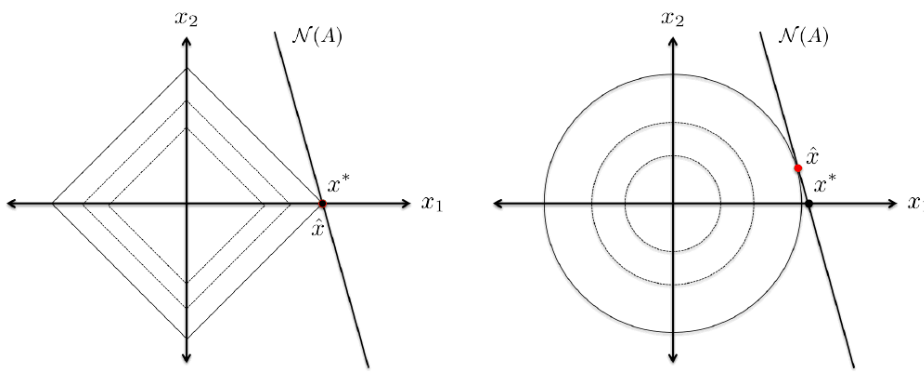
$$\mathbf{b} = \mathbf{A}\mathbf{x} + \varepsilon$$

and find the minimum norm solution

$$\min_{\mathbf{x}} \quad \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$$

or (more recently) find a sparse solution

$$\min_{\mathbf{x}} \ \|\mathbf{x}\|_1 \quad \text{such that} \quad \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 \leq \varepsilon$$



(a) CS methodology (ℓ_1 objective) (b) Pseudo-inverse (ℓ_2 objective)

BP

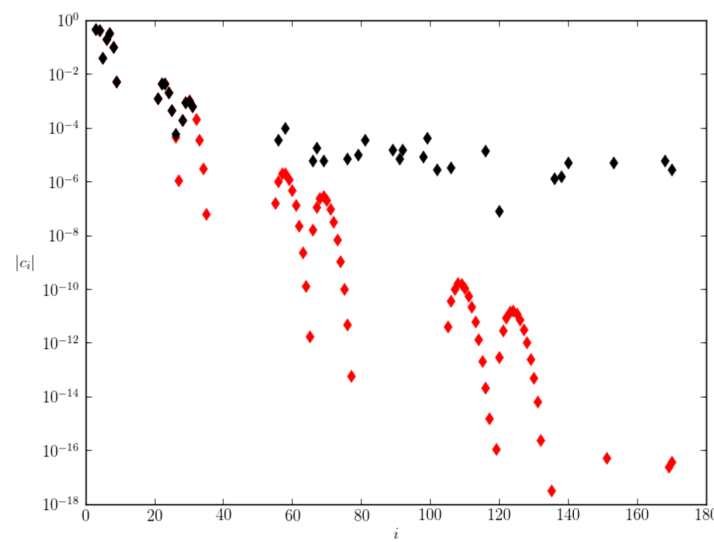
$$\mathbf{c} = \arg\min \ \|\mathbf{c}\|_{\ell^1} \quad \text{such that} \quad \mathbf{\Phi}\mathbf{c} = \mathbf{y}$$

BPDN and OMP

$$\mathbf{c} = \arg\min \ \|\mathbf{c}\|_{\ell^1} \quad \text{such that} \quad \|\mathbf{\Phi}\mathbf{c} - \mathbf{y}\|_{\ell^2} \leq \varepsilon$$

LASSO and LARS

$$\mathbf{c} = \arg\min \ \|\mathbf{\Phi}\mathbf{c} - \mathbf{y}\|_{\ell^2}^2 \quad \text{such that} \|\mathbf{x}\|_{\ell^1} \leq \tau$$



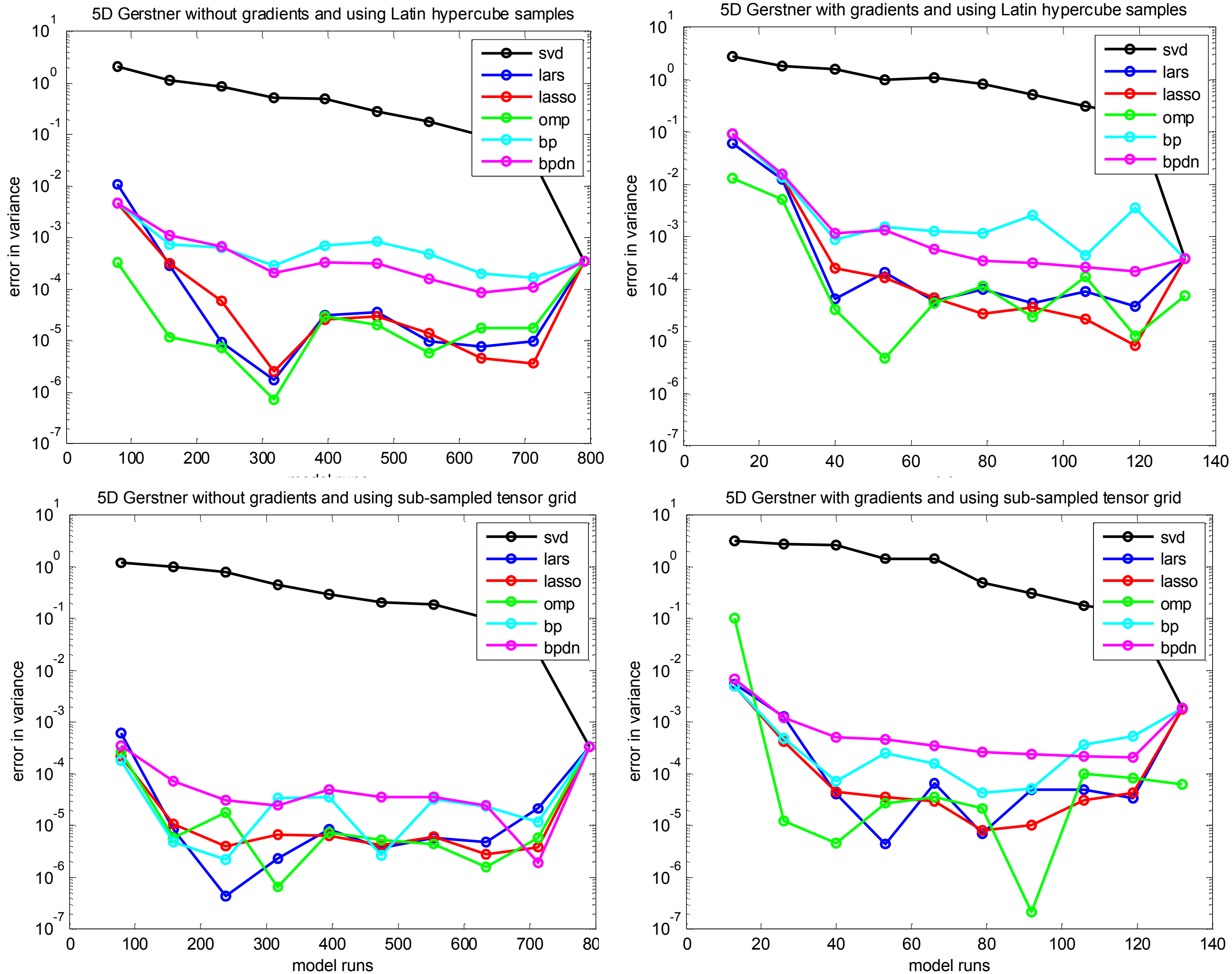
Comparison of CS with SVD for under-determined PCE

5D Gerstner test, convergence in variance

Value-based | **Gradient-enhanced**

Unstructured
(LHS on random variable PDFs)

Structured
(uniform sub-sampling of tensor quadrature multi-index)



Production ASC UQ Example:
Deploy Advanced UQ, Part 1

Traditional approach: MVFOSM with central finite differences (2n+1 evaluations, linear Taylor series)

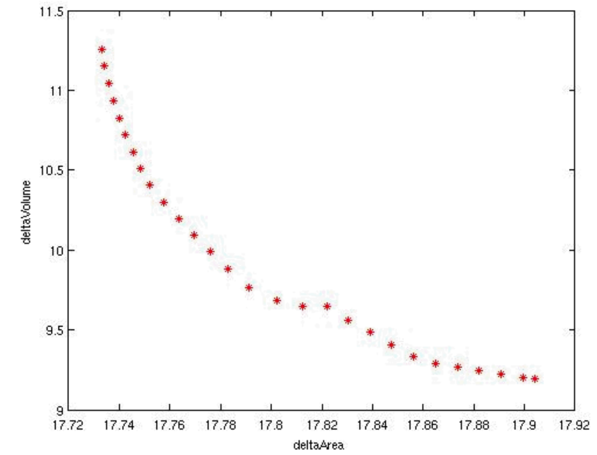
- Compare to level 1 sparse grid PCE: captures nonlinear main effects and nonlinear sensitivity analysis
  - 2n+1 evaluations at Gauss points → second order main effects, no interactions
  - First set of active indices within a generalized sparse grid approach
  - Naturally leads to subsequent refinement, as budget allows
    - Index set(s) with greatest influence on QoI → higher-order main + interaction effects

Traditional approach: LHS with coarse sampling (N samples, 1/ sqrt(N) convergence rate)

- Post-process unstructured data using regression PCE
  - Standard SVD for over-determined low-order expansions
  - Compressive sensing for under-determined higher-order expansions
  - K-fold cross-validation → expansion order, noise tolerance

SciDAC-3 Case Study: CISM LHS data for PISCEES

- Calibration with (weighted) NLS and MOGA
  - GP fit w/ 100 LHS pts → surrogate-based calibration
  - Unweighted, variance weighted, & single-objective
  - Exhaustive multi-objective GA on GP → Pareto frontier



- UQ with regression PCE: moments, VBD, PDF, CDF

deltaArea Sobol indices:

Main	Total	
4.7513765309e-02	6.7248544556e-02	geothermal_flux
9.1650860584e-01	9.3781166646e-01	flow_factor
7.9696945177e-03	2.6872229178e-02	basal_exponent

Interaction

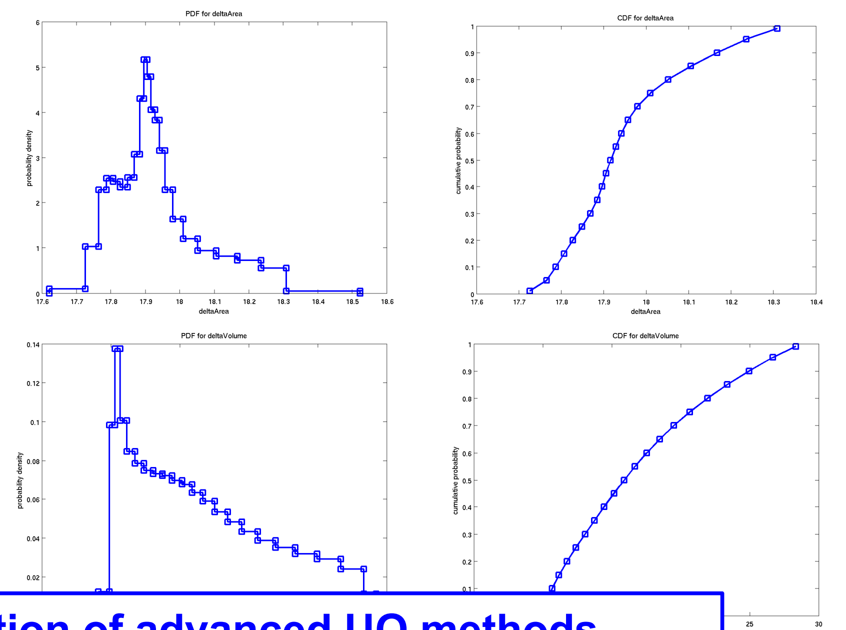
9.1053996720e-03 geothermal_flux flow_factor
6.7048737120e-03 geothermal_flux basal_exponent
8.2731550851e-03 flow_factor basal_exponent
3.9245058634e-03 geothermal_flux flow_factor basal_exponent

deltaVolume Sobol indices:

Main	Total	
2.3075148007e-04	5.8457999638e-04	geothermal_flux
9.9465232748e-01	9.9546169642e-01	flow_factor
4.2442002665e-03	4.9154442300e-03	basal_exponent

Interaction

2.0147681120e-04 geothermal_flux flow_factor
6.3351832896e-05 geothermal_flux basal_exponent

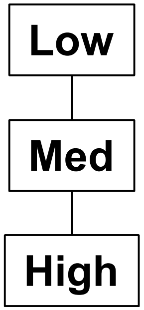


In many cases, the bar is low for adoption of advanced UQ methods – often we can post-process existing data to generate new / improved results.

Multiple Model Forms in UQ

Discrete model choices, same physics (additional dimensions for multi-{physics,scale})

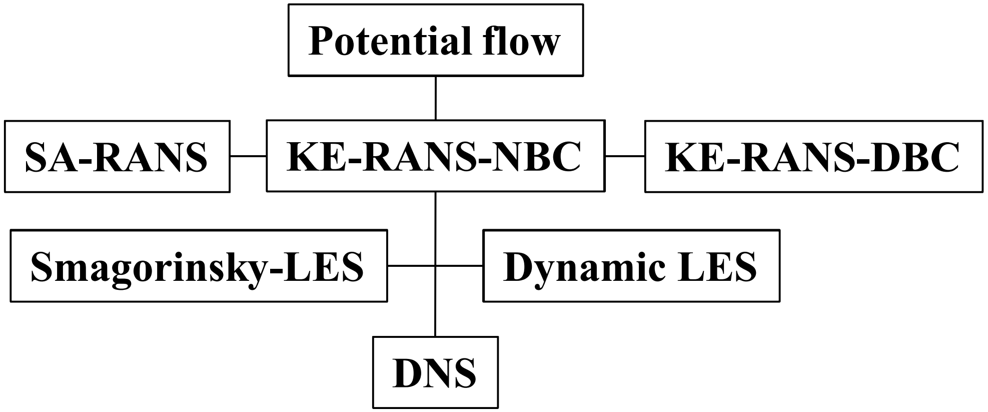
- A clear hierarchy of fidelity (low to high)



- An ensemble of models that are all credible (lacking a clear preference structure)

  - With data: Bayesian model selection
  - *Without (adequate) data:* epistemic model form uncertainty propagation

- Both



Multifidelity UQ using Stochastic Expansions

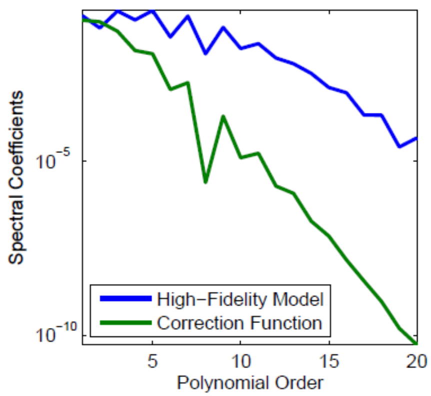
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity “design” codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

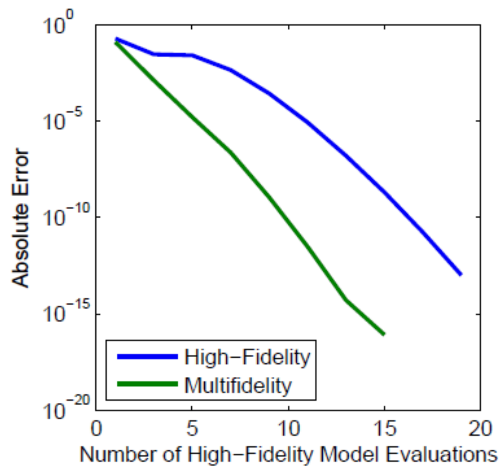
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

$$N_{lo} >> N_{hi}$$

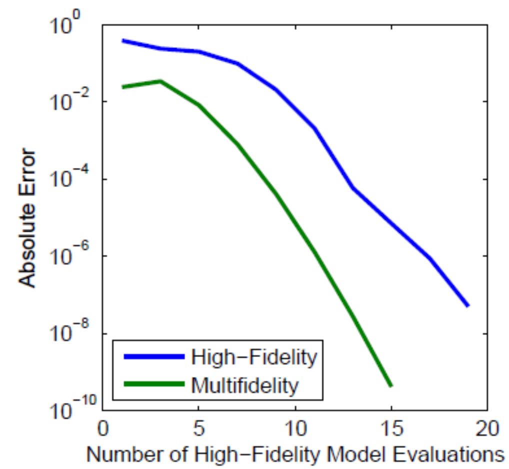
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5 e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

$$R_{\text{low}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi,$$





(a) Error in mean



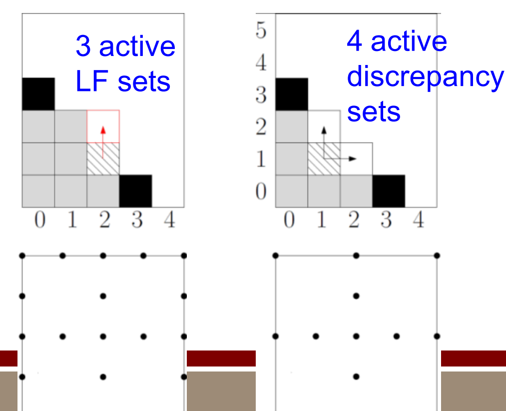
(b) Error in standard deviation

Adaptive sparse grid multifidelity algorithm:

- Generalized SG for LF & discrepancy levels
- Greedy selection from grids: max ΔQoI/ΔCost
- Refine discrepancy where LF is less predictive

Compressive sensing multifidelity algorithm:

- Target sparsity within the model discrepancy



Elliptic PDE with Finite Elements

$$-\frac{d}{dx}\left[\kappa(x,\omega)\frac{du(x,\omega)}{dx}\right] = 1, \qquad x \in (0,1), \qquad u(0,\omega) = u(1,\omega) = 0$$

$$\kappa(x,\omega) = 0.1 + 0.03\sum_{k=1}^{10}\sqrt{\lambda_k}\phi_k(x)Y_k(\omega), \qquad Y_k \sim \text{Uniform}[-1,1]$$

$$C_{\kappa\kappa}(x,x') = \exp\left[-\left(\frac{x-x'}{0.2}\right)^2\right]$$

QoI is u(0.5, ω).

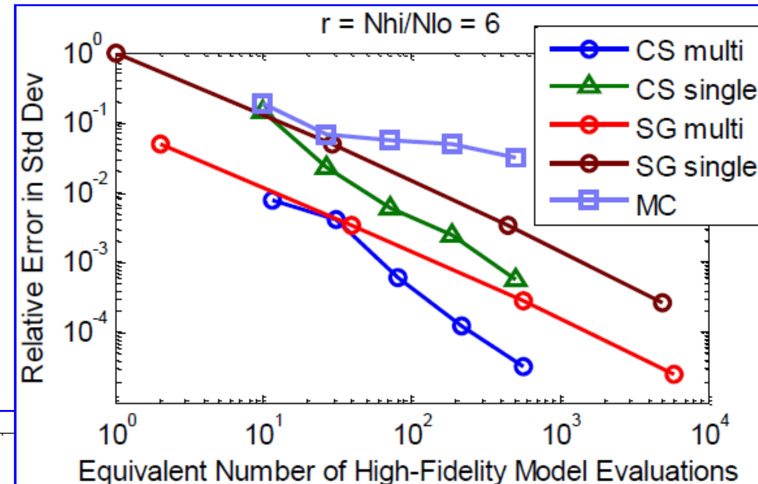
LF = coarse spatial grid with 50 states.

HF = fine spatial grid with 500 states.

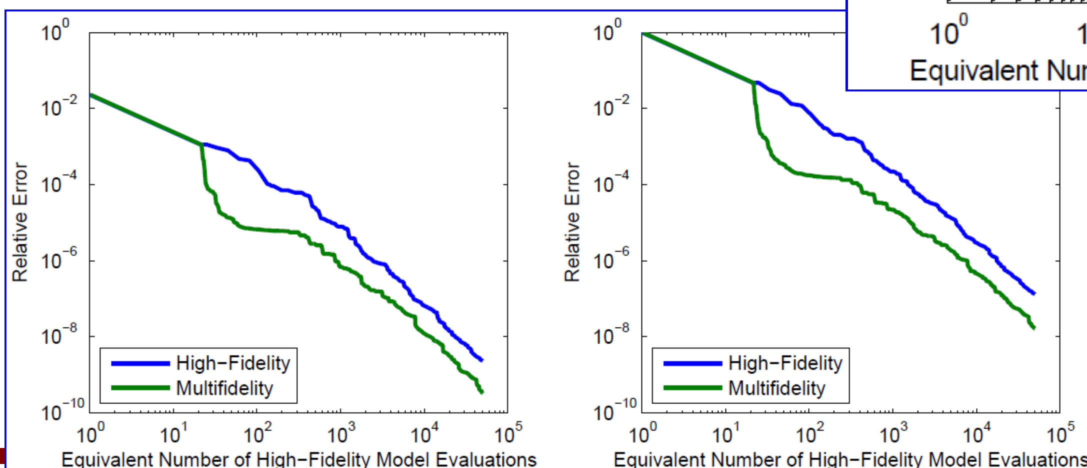
Expense ratio = 40.

Static offset & uniform refinement

Static offset level = 1	Relative Error in Mean	Relative Error in Std Deviation	High-Fidelity Evaluations	Low-Fidelity Evaluations
Single-Fidelity ($q = 3$)	5.3×10^{-6}	2.7×10^{-4}	1981	–
Single-Fidelity ($q = 4$)	4.1×10^{-7}	2.3×10^{-5}	12,981	–
Multifidelity ($q = 4$, $r = 1$)	4.7×10^{-7}	2.6×10^{-5}	1981	12,981



Adaptive



(a) Error in mean (b) Error in standard deviation

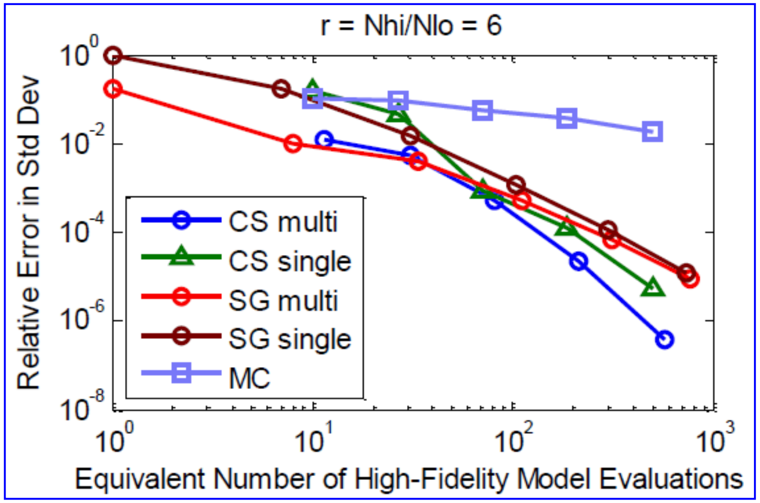
High-Order Sparse Discrepancy using CS

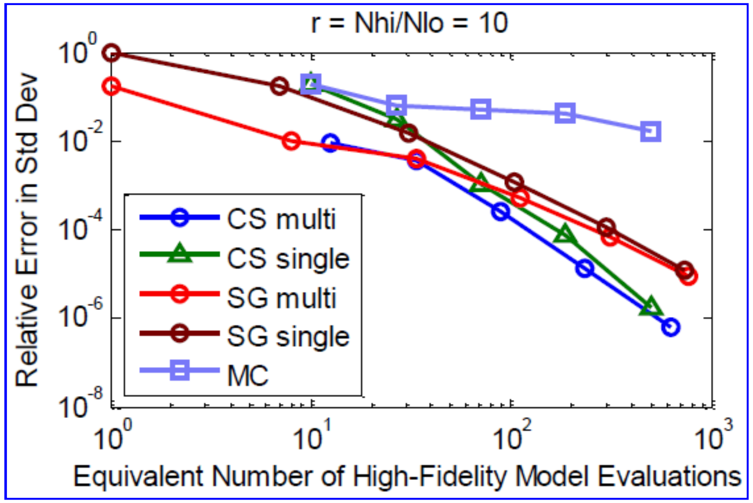
r = 6

r = 10

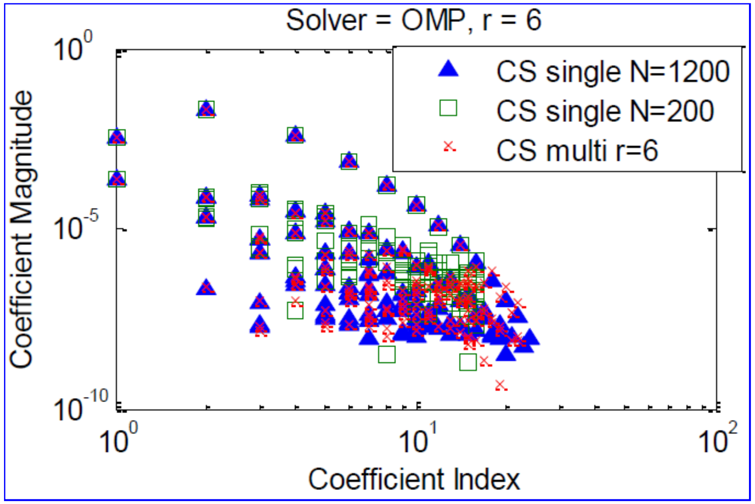
Std Deviation

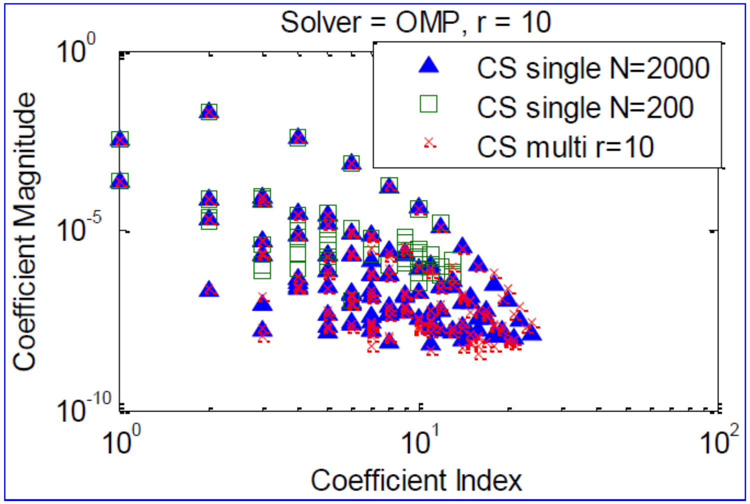
MC and CS results averaged over 10 runs





Sparse coefficients





Production ASC UQ Example:
Deploy Advanced UQ, Part 2

Challenges:

- severe evaluation budget restrictions
- characterization of very low probability events
- mixed aleatory-epistemic uncertainties (epistemic interval on aleatory tail probability)

Current approach: exhaustive sampling of a very low fidelity model, calibrated to HF at means

- Single HF evaluation, but low confidence in tail probabilities

Investigate rigorous multifidelity UQ

- Sparse grids or compressive sensing for LF and model discrepancy
- Uniform (CS) or adaptive refinement (SG) of model discrepancy for statistical QoI
- Targeted use of a handful of HF evaluations

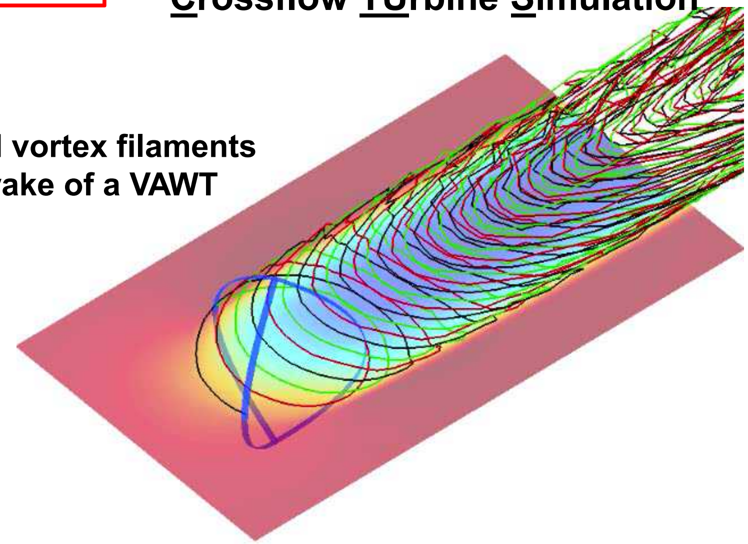
ASCR MF UQ example: VAWT CFD/FSI Modeling

Vertical-axis Wind Turbine (VAWT)

Low fidelity

CACTUS: Code for Axial and Crossflow TUrbine Simulation

Computed vortex filaments in the wake of a VAWT



High fidelity: DG formulation for LES

Multiple Model Forms in UQ

Current directions

Epistemic model form uncertainty propagation

- Mixed aleatory-epistemic UQ with discrete model forms
- MINLP at outer loop for epistemic intervals

Bayesian model selection

- Posterior PDF for model M_k

$$p(\boldsymbol{\theta_k}|D, M_k) = \frac{p(D|\boldsymbol{\theta_k}, M_k)p(\boldsymbol{\theta_k}|M_k)}{p(D|M_k)}$$

- Model evidence

$$p(D|M_k) = \int p(D|\boldsymbol{\theta_k}, M_k)p(\boldsymbol{\theta_k}|M_k)d\boldsymbol{\theta_k}$$

Multifidelity Bayesian inference

- Multiple levels of discrepancy including data

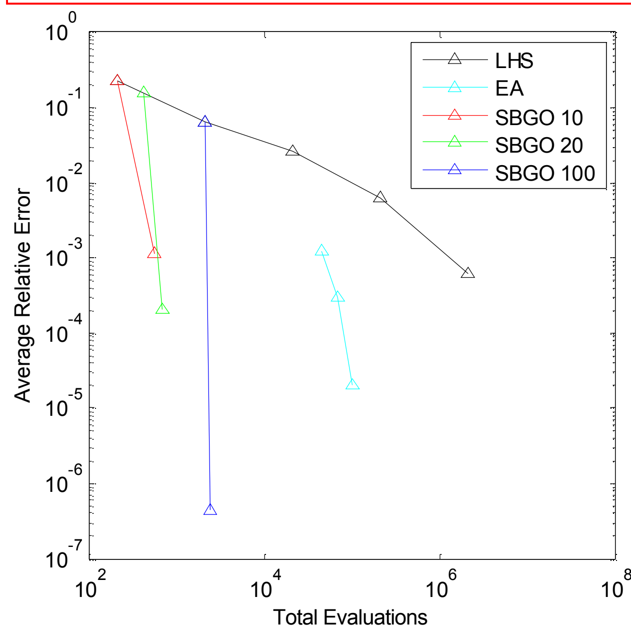
$$\hat{q}_{truth}(\boldsymbol{\xi}) = q_l(\boldsymbol{\theta_s}, \boldsymbol{\theta_l}, \boldsymbol{\xi}) + \delta_{lm}(\boldsymbol{\theta_s}, \boldsymbol{\theta_m}, \boldsymbol{\xi}) + \delta_{mh}(\boldsymbol{\theta_s}, \boldsymbol{\theta_h}, \boldsymbol{\xi}) + \delta_{hd}(\boldsymbol{\xi}) + \epsilon$$

- Stochastic surrogates for reversible-jump MCMC

$$\hat{q}_{truth}(\boldsymbol{\xi}) = \sum_{j=1}^{N_l} q_{l_j} \boldsymbol{L}_j(\boldsymbol{\theta_s}, \boldsymbol{\theta_l}, \boldsymbol{\xi}) + \sum_{j=1}^{N_m} \delta_{lm_j} \boldsymbol{L}_j(\boldsymbol{\theta_s}, \boldsymbol{\theta_m}, \boldsymbol{\xi}) + \sum_{j=1}^{N_h} \delta_{mh_j} \boldsymbol{L}_j(\boldsymbol{\theta_s}, \boldsymbol{\theta_h}, \boldsymbol{\xi}) + \sum_{j=1}^{N_d} \delta_{hd_j} \boldsymbol{L}_j(\boldsymbol{\xi})$$

Rosenbrock

$$\text{Form 1}: \quad f_1 = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$
$$\text{Form 2}: \quad f_2 = 100(x_2 - x_1^2 + .2)^2 + (0.8 - x_1)^2$$



Epistemic vars: 1 discrete model form (2 values), 2 continuous defining interval means for 2 aleatory vars

Eldred, M.S. and Wildey, T.M., "Propagation of Model Form Uncertainty for Thermal Hydraulics using RANS Turbulence Models in Drekar," Sandia Technical Report 2012-5845, July 2012.

Summary

UQ deployment faces a number of key challenges

- Severe simulation budget constraints and moderate to high random dimensionality
- Compounded by mixed uncertainties, nonsmoothness, rare events

Investments in scalable UQ R&D

- We are targeting a broad suite of scalable and robust core UQ methods
- Within the highlighted area of stochastic expansions:
  - Uniform, dimension-adaptive, and local adaptive p-/h-refinement with QoI goal orientation
  - Sparsity detection with compressed sensing
  - Matrix of formulations: local / global, value / gradient, structured / unstructured, nodal / hierarchical
- We are building on this foundation
  - Multifidelity UQ, Mixed UQ including model form, Bayesian model selection & multifidelity inference

Impact and deployment

- UQ tools deployed through DAKOTA (v5.3 released 1/31/13, v5.3.1 released 5/15/13)
- Impact with NNSA and Offices of Science/Nuclear Energy/Renewable Energy