Advances in UQ Algorithms for Wind Energy Applications

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Research in Scalable UQ Methods

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

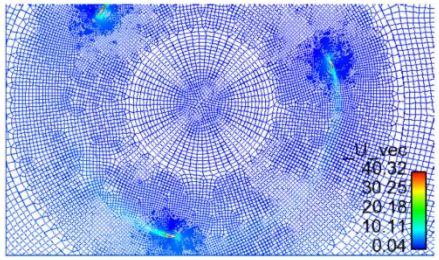
- Local approximate methods (reliability methods, moment-based methods) exhibit significant errors in presence of multimodal/nonsmooth/highly nonlinear responses
- MC/LHS are robust with dimension-independent conv., but rates can be unacceptably slow

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 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



Build on this foundation:

- Error balancing framework
- Multiple model forms
  - Model hierarchy → multifidelity UQ (LF: EOLO, FAST, CACTUS; HF: URANS, DG LES)
  - Epistemic model form → mixed aleatory-epistemic/continuous-discrete UQ

Non-Intrusive Stochastic Expansions: Polynomial Chaos and Stochastic Collocation

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 <u>interpolants</u> 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

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

Sparse interpolants formed using Σ of tensor interpolants

- 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.

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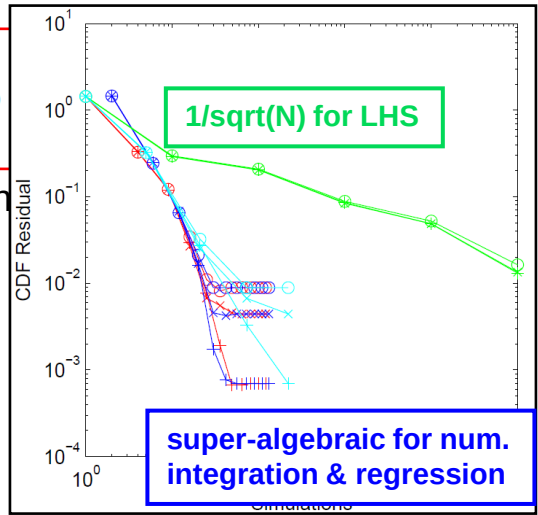
Sparse interpolants formed using Σ of tensor in



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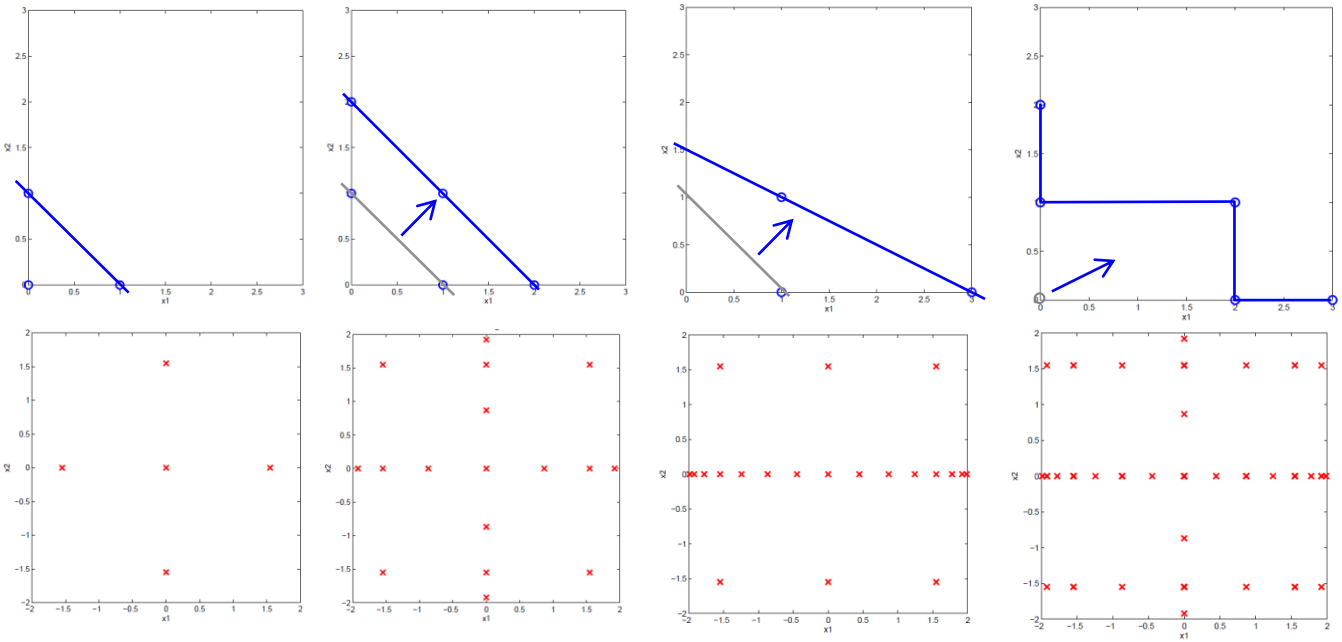
Stochastic Expansions on Structured Grids:
Adaptive Collocation Methods

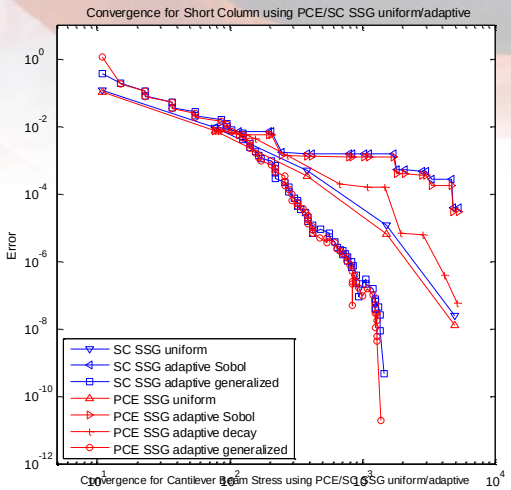
Polynomial order (p-) refinement approaches:

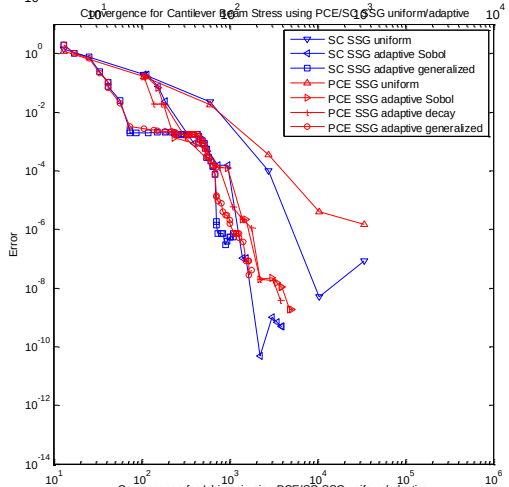
- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted/nested)
  - *Assess convergence:* L^2 change in response covariance
- **Adaptive:** *anisotropic* tensor/sparse grids

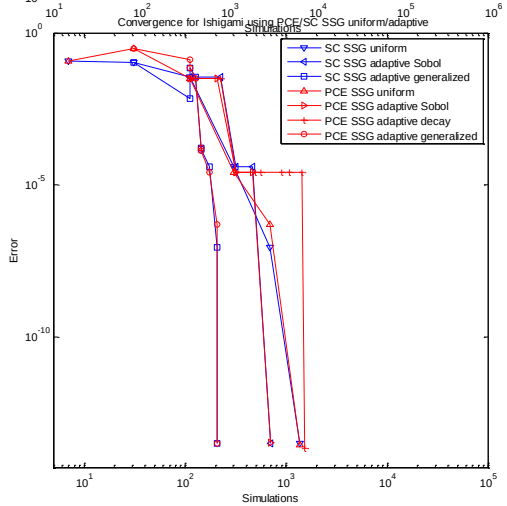
$$w\underline{\alpha} - |\alpha| < \sum_{n=1}^{d}(i_n - 1)\alpha_n \leq w\underline{\alpha}$$

  - **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









Extend Scalability: (Adjoint) Derivative-Enhancement

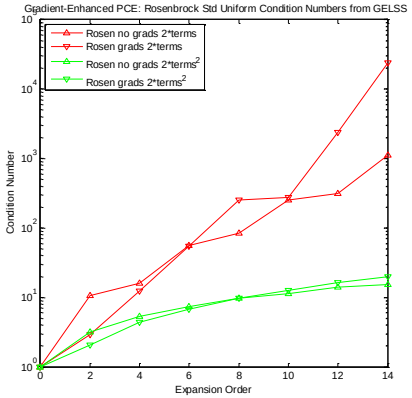
$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i)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

PCE:

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

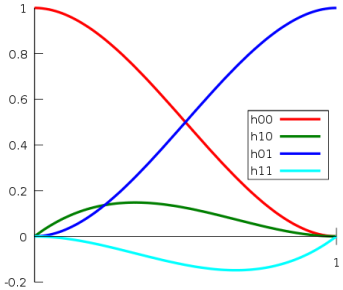
SC:

- **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)

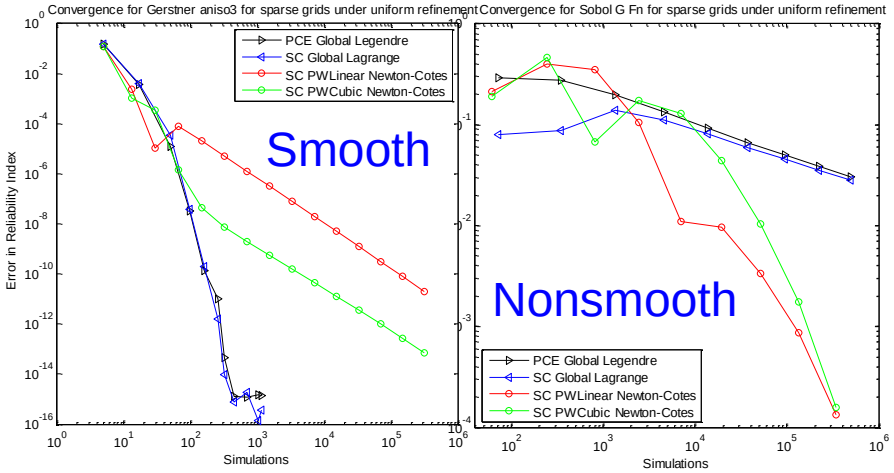


$$\mu = \sum_{i=1}^{N} f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)}$$

and similar for higher-order moments

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

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



Stochastic Expansions on Unstructured Grids:
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

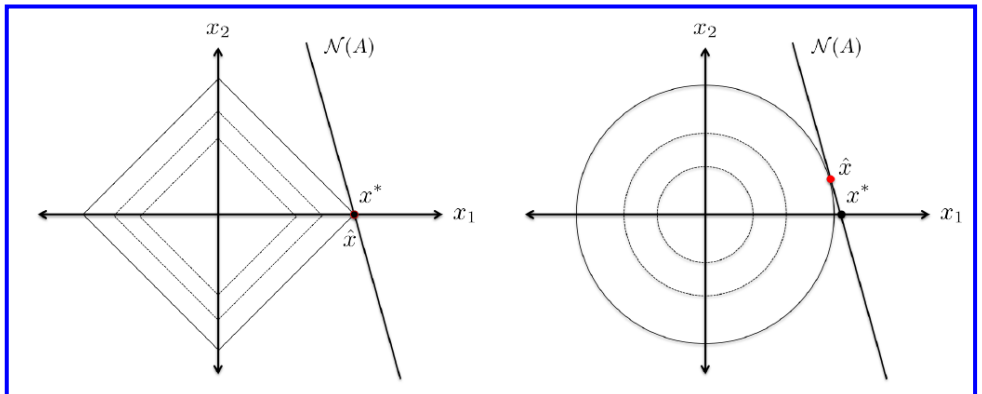
$$\mathbf{b} = \mathbf{A}\mathbf{x} + \varepsilon$$

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

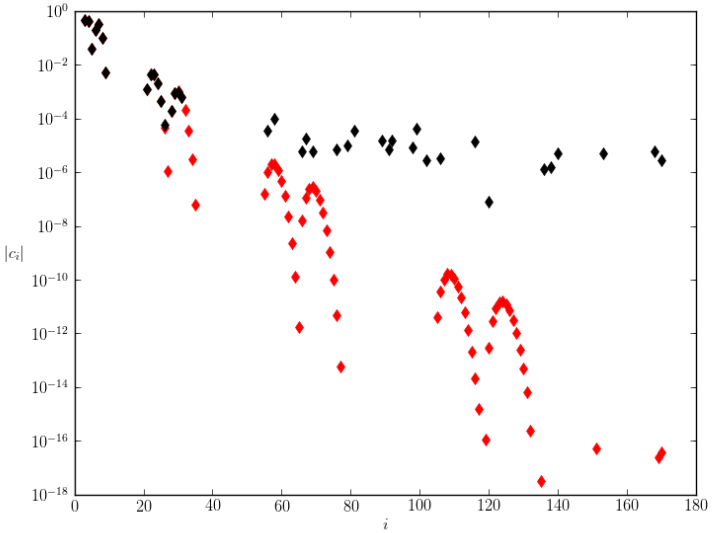
$$\mathbf{c} = \arg\min \ \|\mathbf{c}\|_{\ell^1} \quad \text{such that} \quad \mathbf{\Phi}\mathbf{c} = \mathbf{y}$$

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

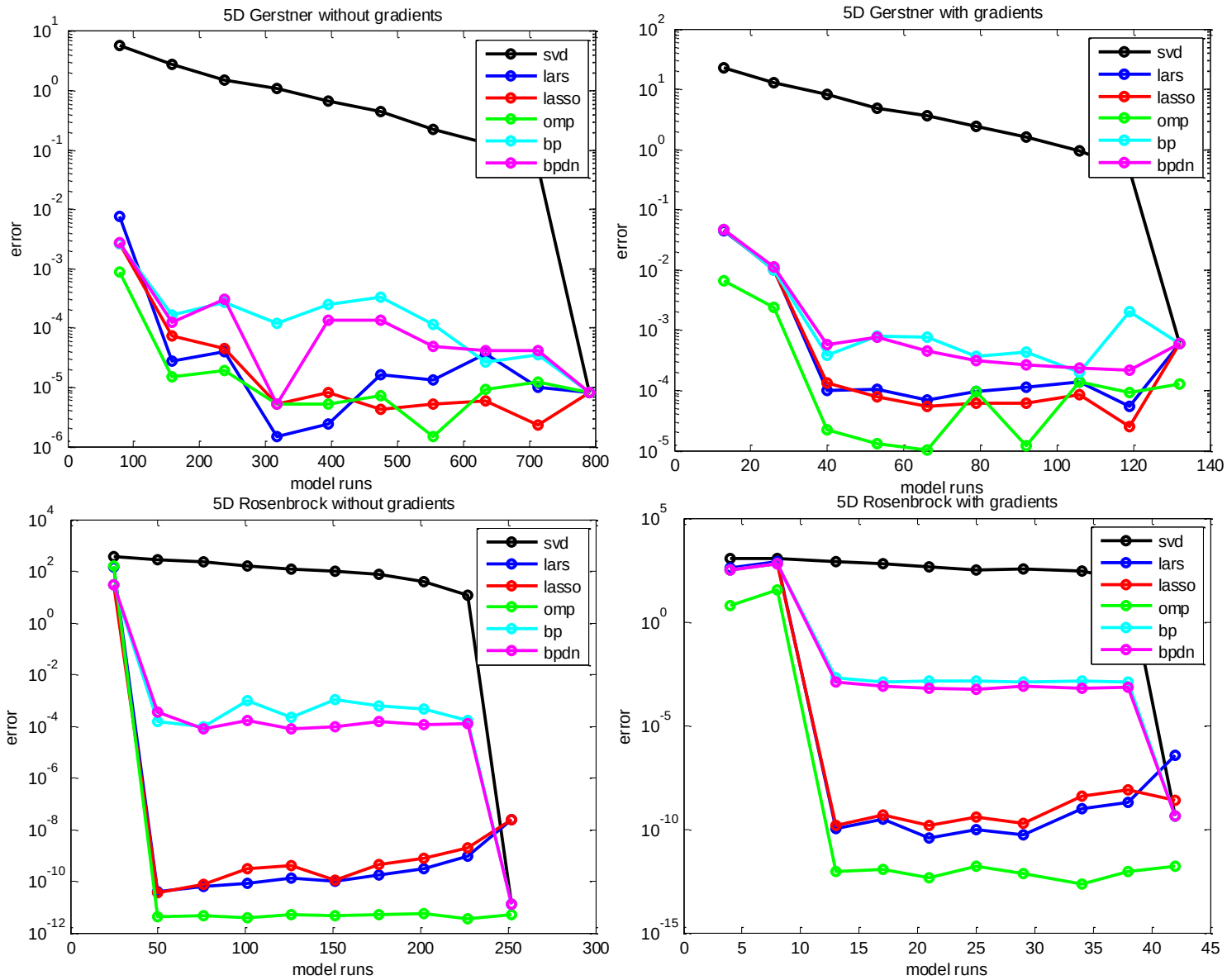
$$\mathbf{c} = \arg\min \ \|\mathbf{\Phi}\mathbf{c} - \mathbf{y}\|_{\ell^2}^2 \quad \text{such that} \|\mathbf{x}\|_{\ell^1} \leq \tau$$



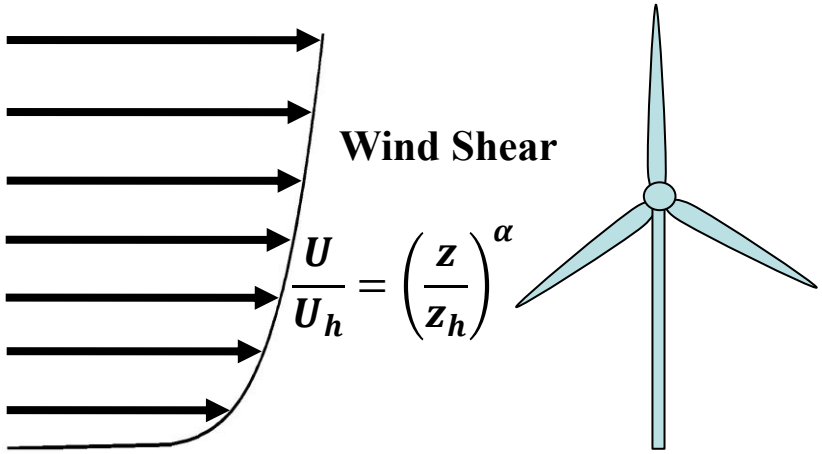
Comparison of CS Methods with SVD for under-determined PCE

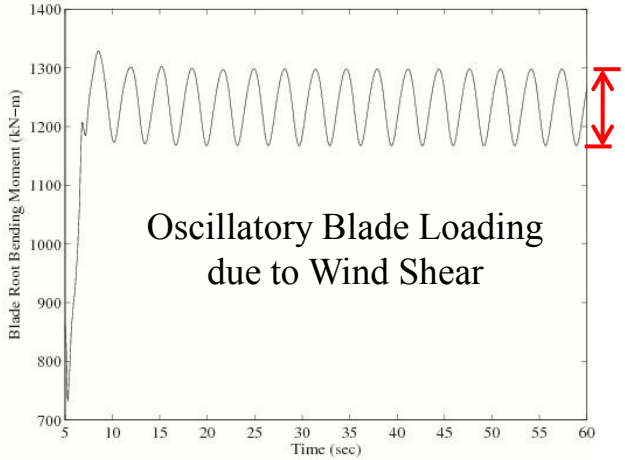
5D Gerstner without/with gradients

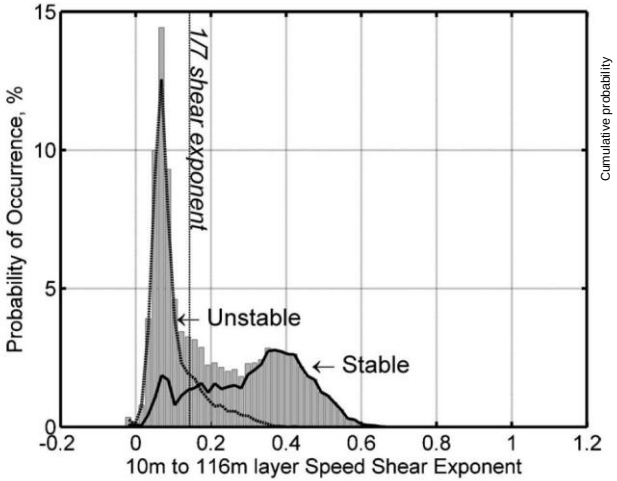
5D Rosenbrock without/with gradients

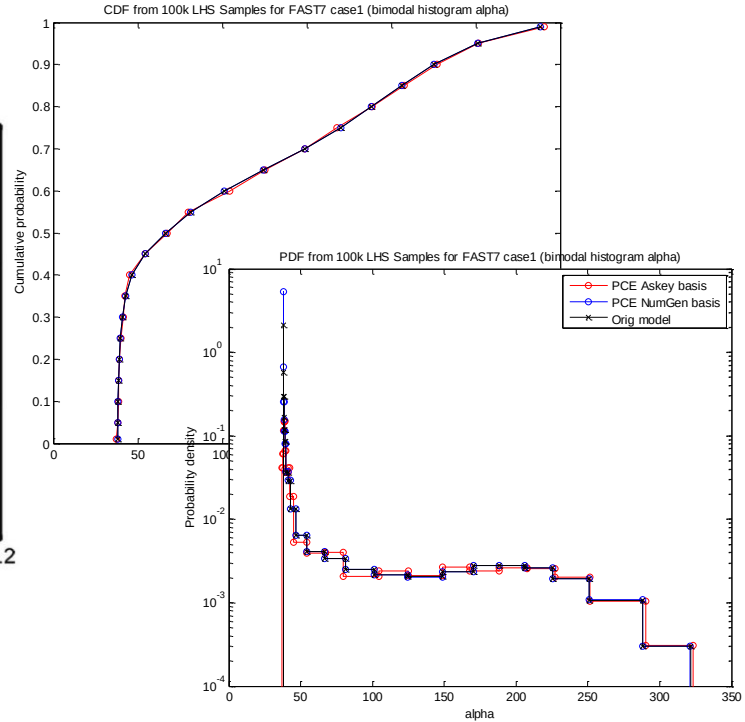


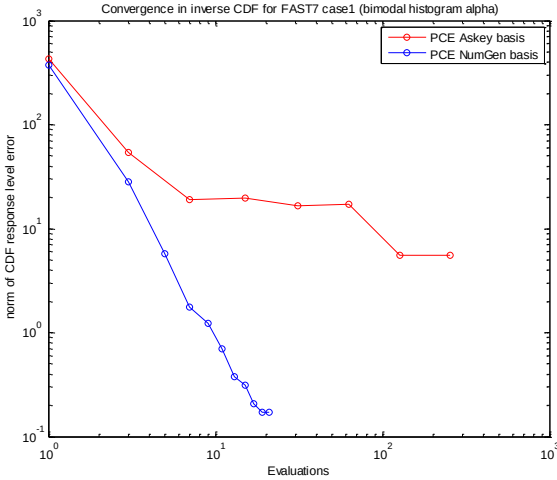
FAST: HAWT Loads due to Uncertain Wind Shear











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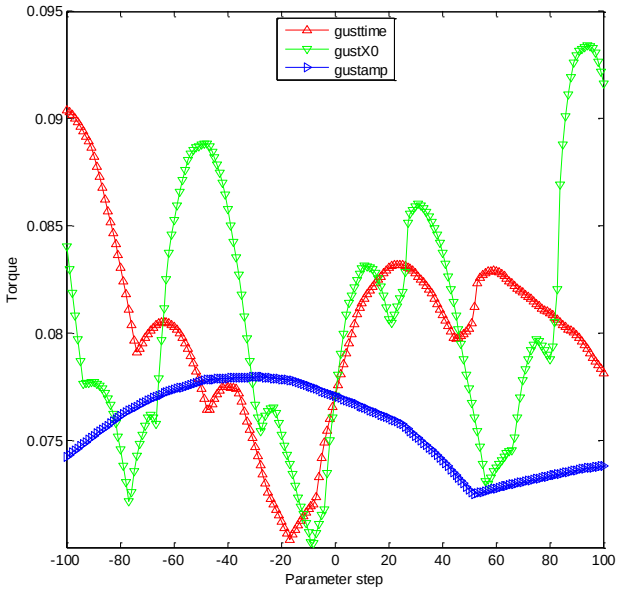
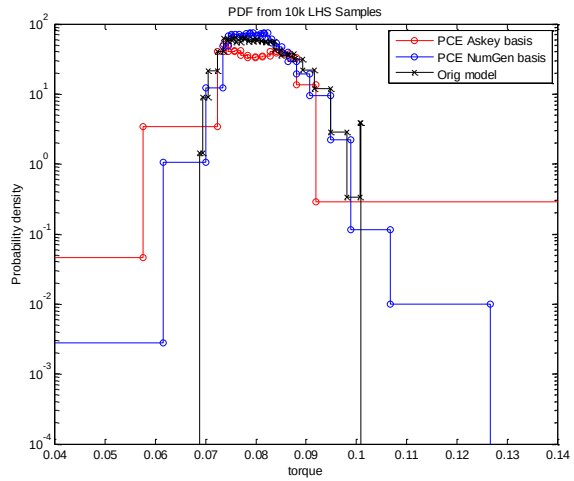
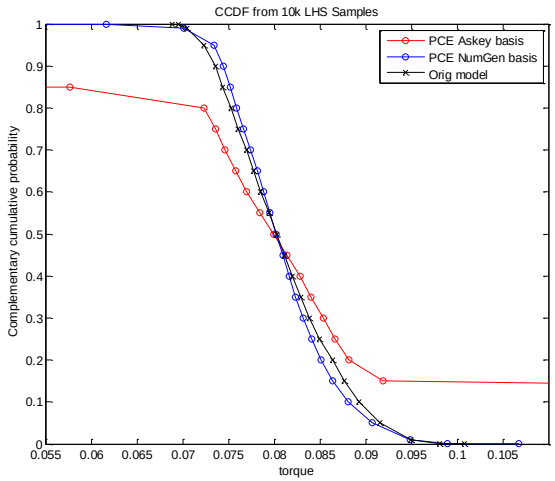
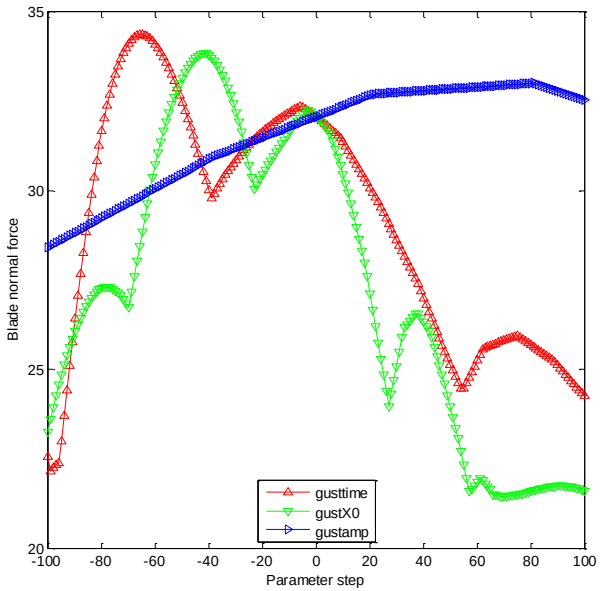
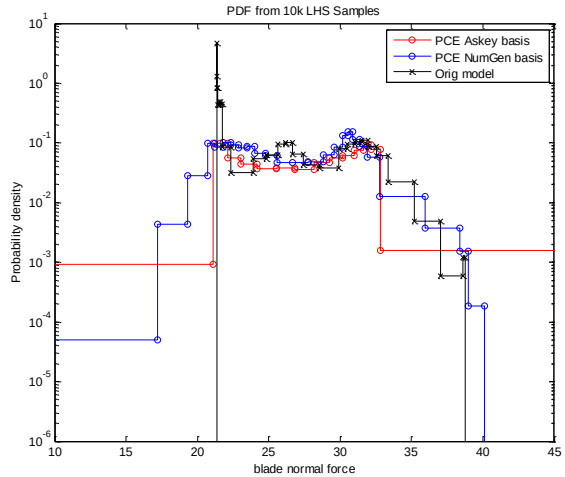
CACTUS: VAWT with Uncertain Gust Loading (V1)

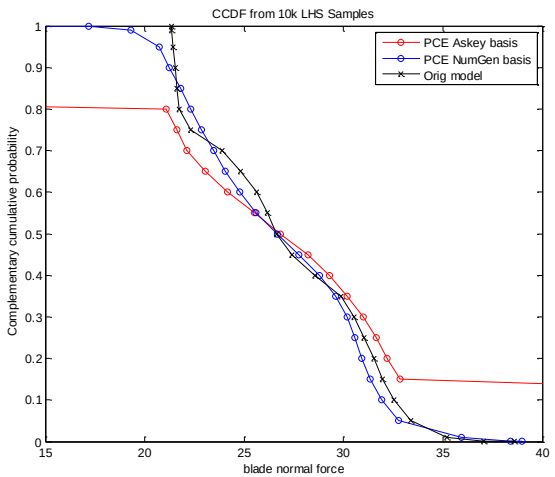












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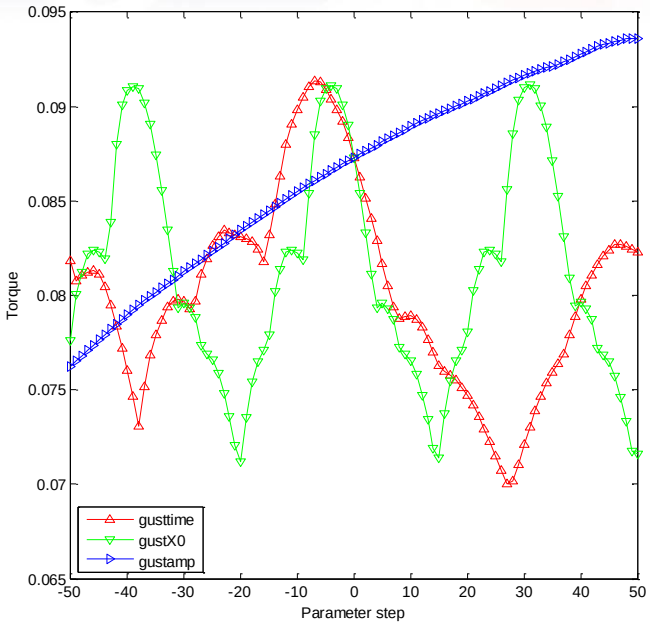
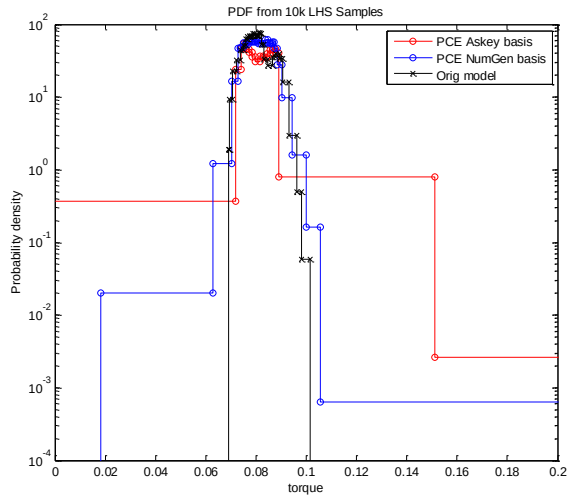
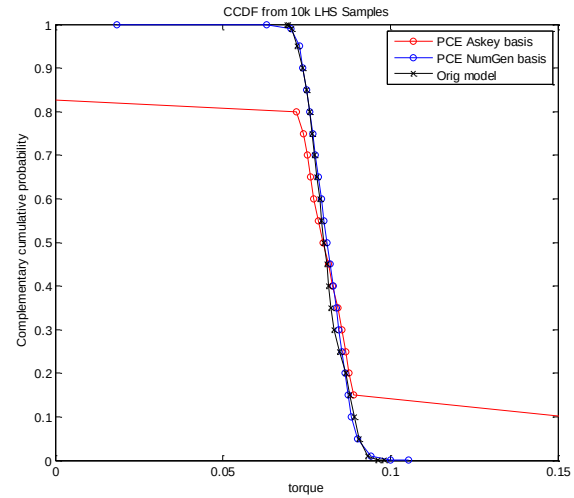
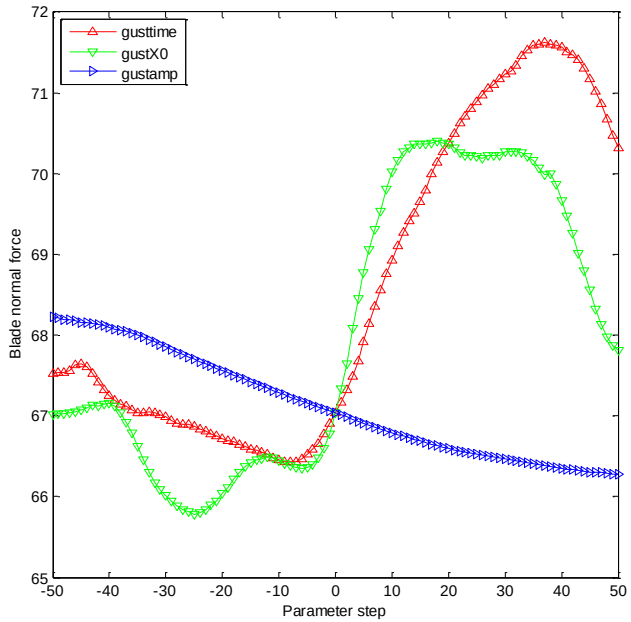
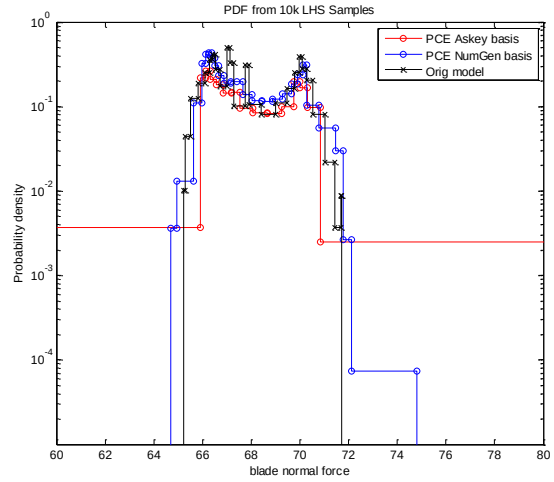
CACTUS: VAWT Loads due to Uncertain Gust (V2)

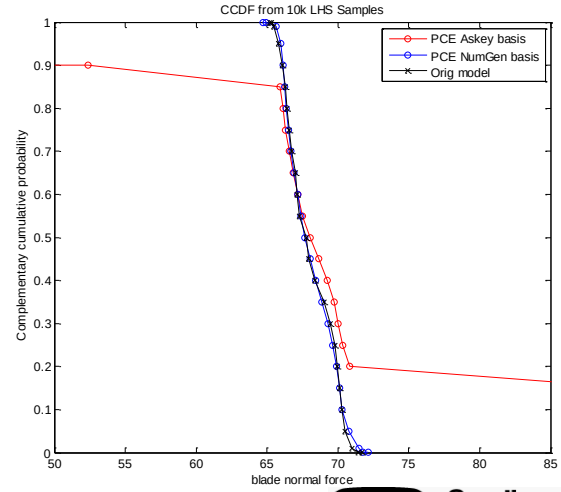












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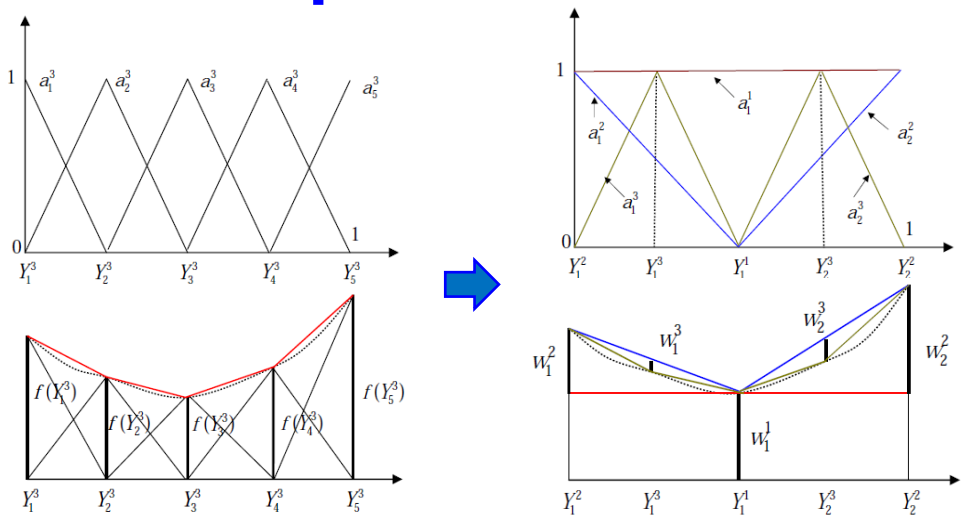
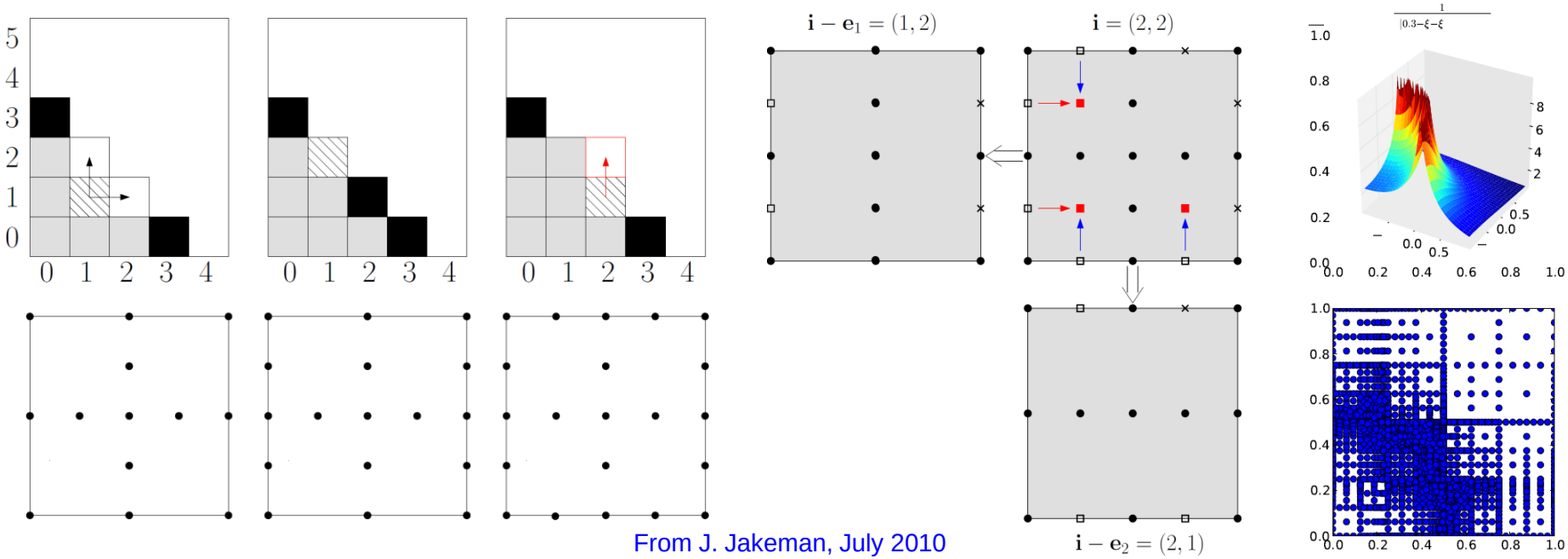
Local Error Estimation with Hierarchical Value/Gradient Surpluses

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*



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



From J. Jakeman, July 2010

Error budgets

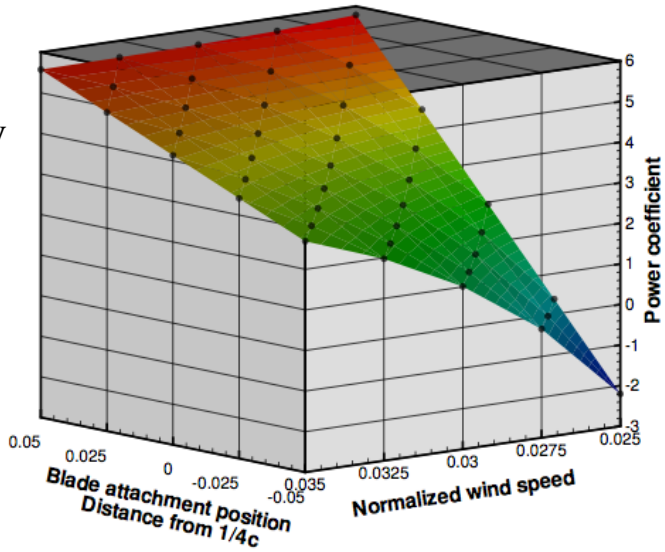
Two uncertain parameters:
Blade attachment point, freestream velocity
Objective function: Mean power produced

Given an accuracy requirement (e.g. confidence in power prediction), need to budget sources of errors and uncertainties

Consider contribution of each simplex element to total variability

$$\varepsilon_\mu \lessapprox \sum_{j=1}^{n_e} \bar{\Omega}_j (\varepsilon_{\mathrm{AUQ}_j} + \varepsilon_{\mathrm{EUQ}_j} + \varepsilon_{\Delta \mathrm{x}_j})$$

- Aleatory propagation/error estimation: Simplex SSC
- Numerical discretization error: Adjoints (space + time)
- Epistemic uncertainties: turbulence model perturbation



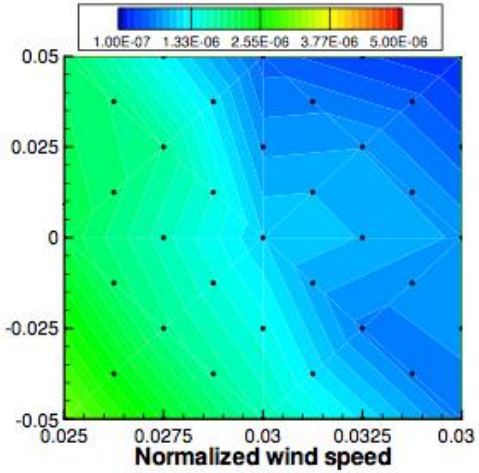


Figure : Stochastic

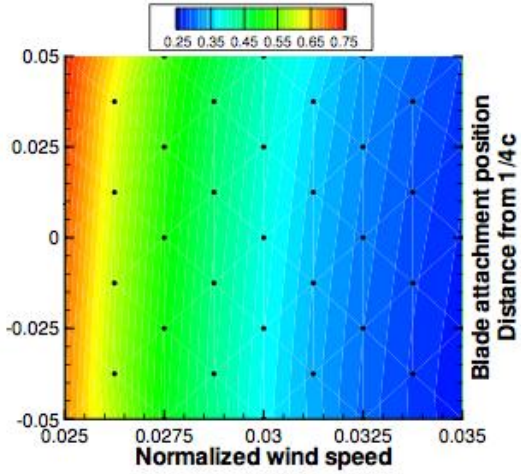


Figure : Spatial error

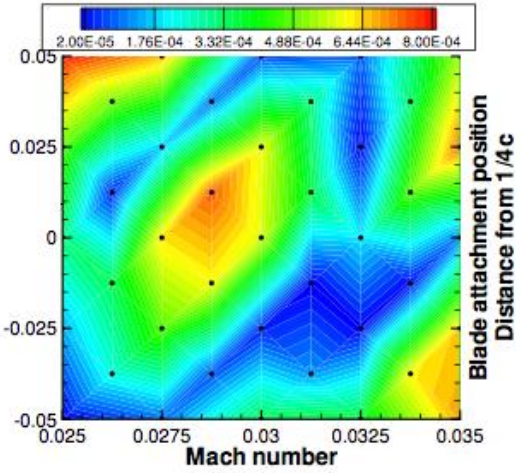
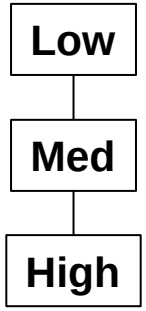


Figure : Temporal error

Core-Enabled UQ: Multiple Model Forms

Same physics: (multiphysics, multi-scale provide additional dimensions in model "tree")

- A clear hierarchy of fidelity (low to high) → multifidelity UQ
  - Leverage concepts from provably-convergent multifidelity surrogate-based opt.



- An ensemble of models that could all be credible (lacking a clear preference structure)
  - model form uncertainty (inadequate data) → extend mixed aleatory-epistemic UQ capabilities to include categorical model forms

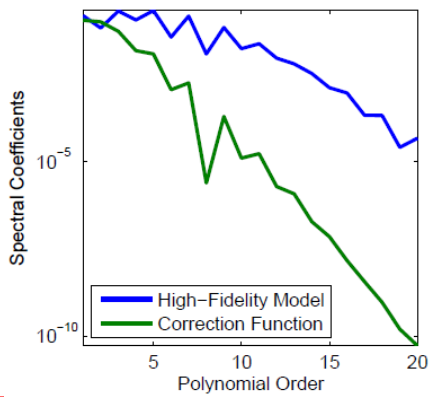
Multifidelity UQ

Multifidelity UQ through stochastic expansion of model discrepancy:

- Extension of multifidelity opt methods that converge to local HF optimum based on local corrections
- Converge to global HF statistics based on global corrections (0th/1st consistency @HF collocation pts)

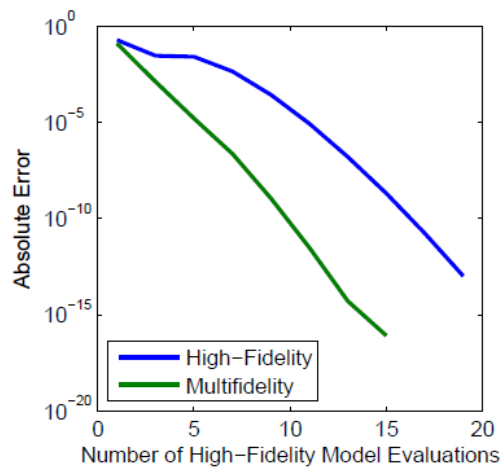
$$\hat{f}_{hi}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

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

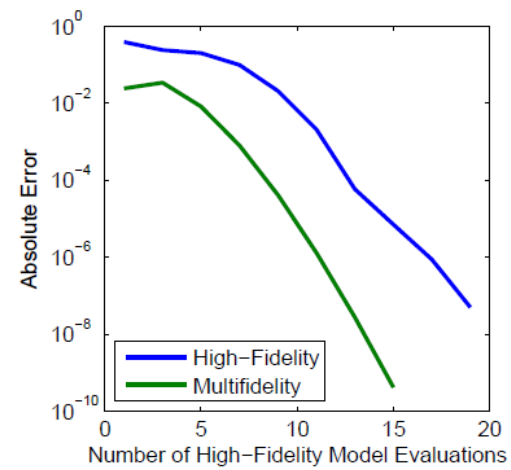


$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi - 0.5 e^{-0.02(\xi-5)^2}$$

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



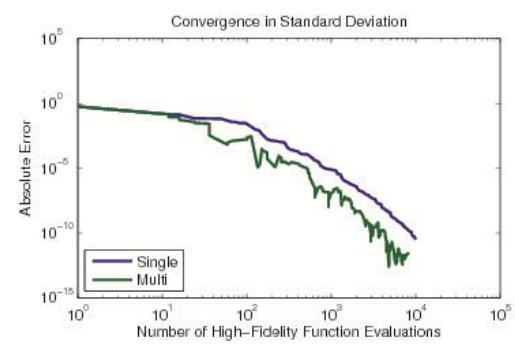
(a) Error in mean



(b) Error in standard deviation

Adaptive algorithm balances LF/HF cost and targets regions where LF predictive capabilities break down:

- Greedy selection of index sets for LF *or* model discrepancy based on ΔQOI/ΔCost



Elliptic PDE with FEM

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

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

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

QoI is u(0.5, ω).

LF = coarse spatial grid with 50 states.

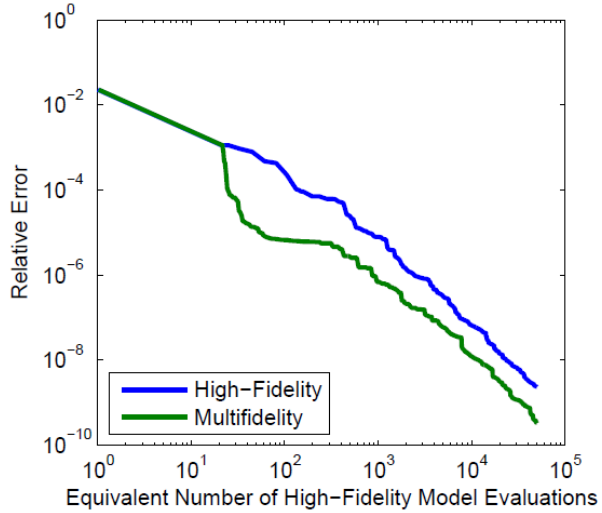
HF = fine spatial grid with 500 states.

r_{work} = 40.

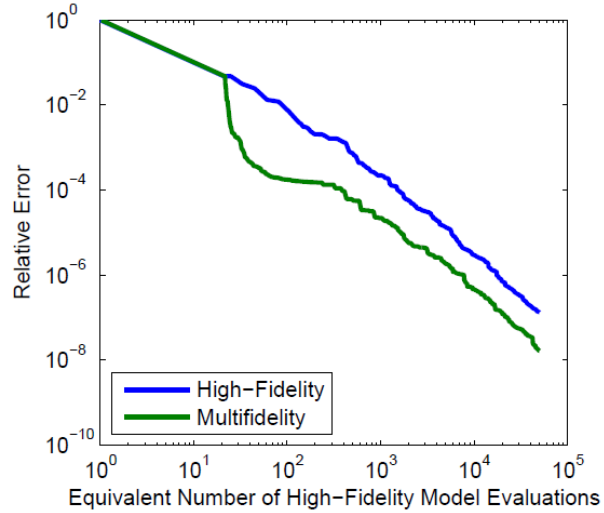
Defined offset

	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

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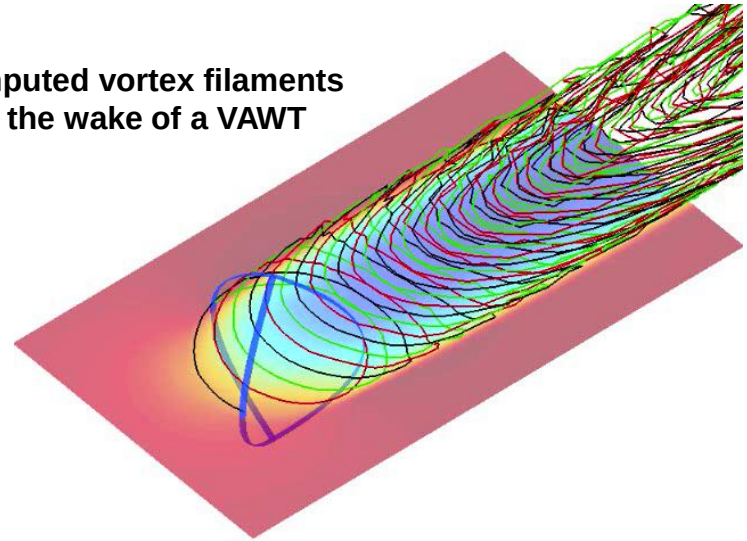
Current Focus: VAWT Performance Modeling

Vertical-axis Wind Turbine (VAWT)

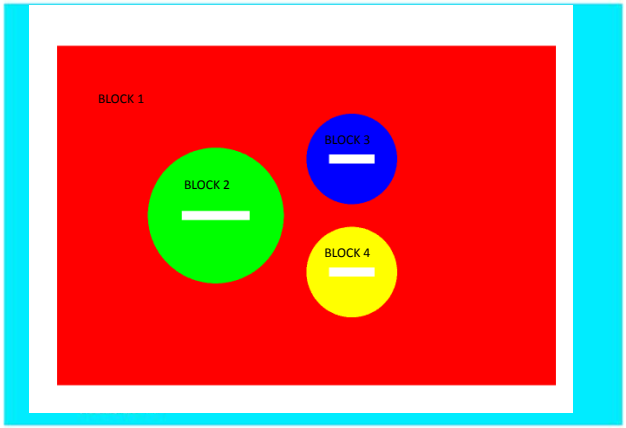
Low fidelity

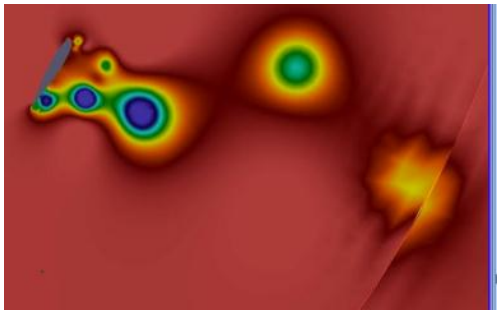
CACTUS: Code for Axial and Crossflow TUrbine Simulation

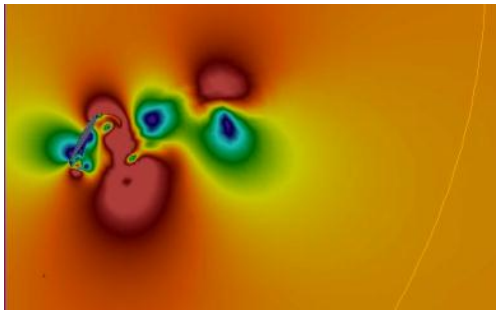
Computed vortex filaments in the wake of a VAWT



High fidelity: DG formulation for LES







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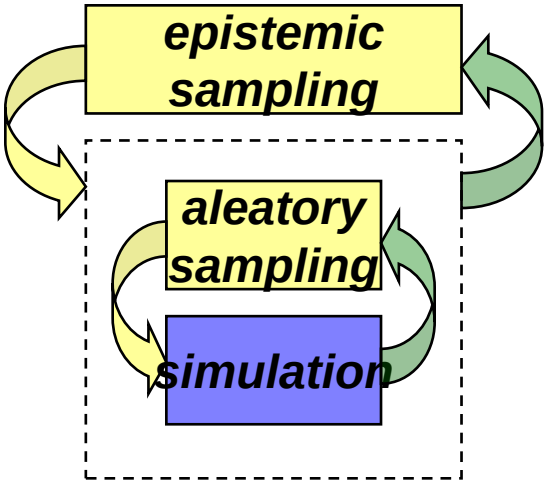
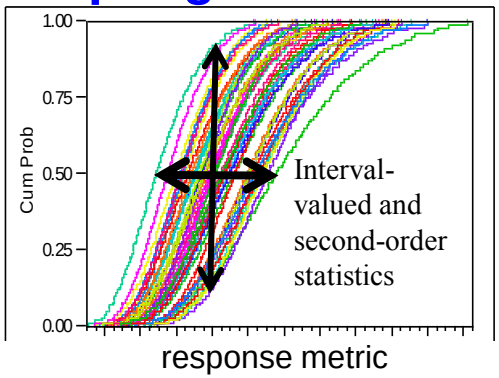
Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

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

Increasing epistemic structure (stronger assumptions)

Address accuracy and efficiency

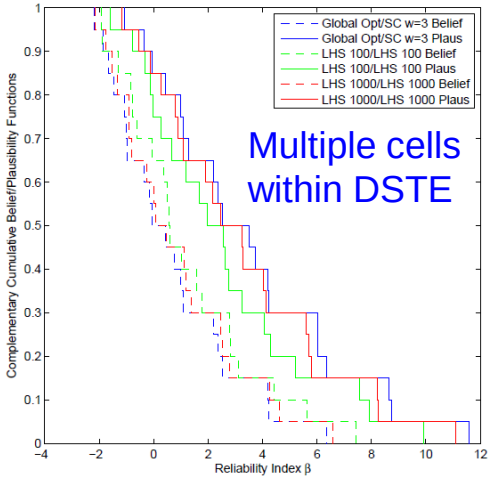
- Inner loop: stochastic exp. that are epistemic-aware (aleatory, combined)
- Outer loop:
  - IVP, DSTE: opt-based interval estimation, global (EGO) or local (NLP)
  - SOP: nested stochastic exp. (nested expectation is only post-processing in special cases)

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

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

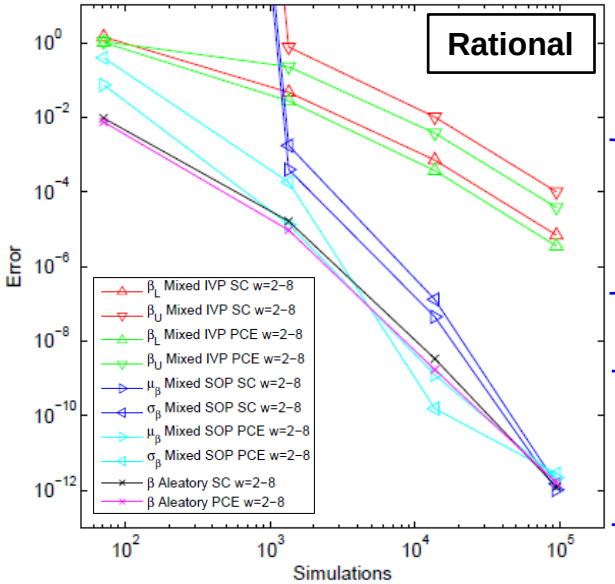
Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals					
EGO	SC SSG w = 1	Aleatory	(84/91, 0/0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(372/403, 0/0)	[75.0002, 374.999]	[-2.18735, 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]



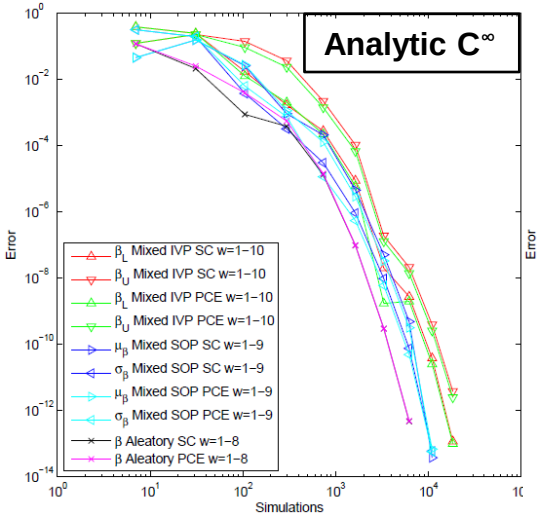
Multiple cells within DSTE

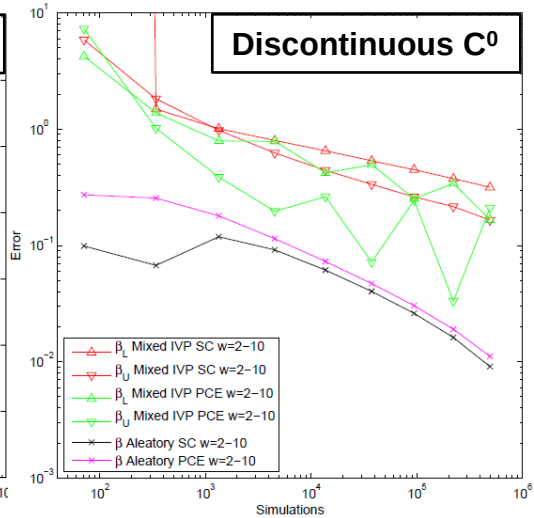
Convergence rates for combined expansions



L^∞ metrics: IVP mixed, DSTE mixed

L^2 metrics: Aleatory, SOP mixed





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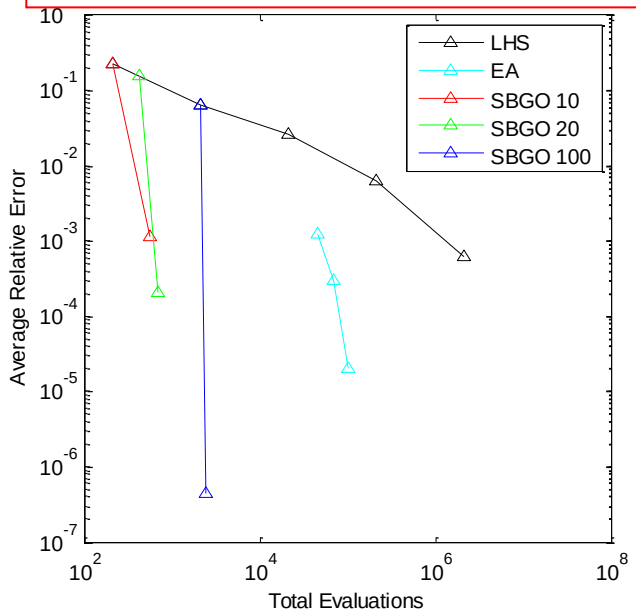
Addition of Discrete Epistemic Model Form

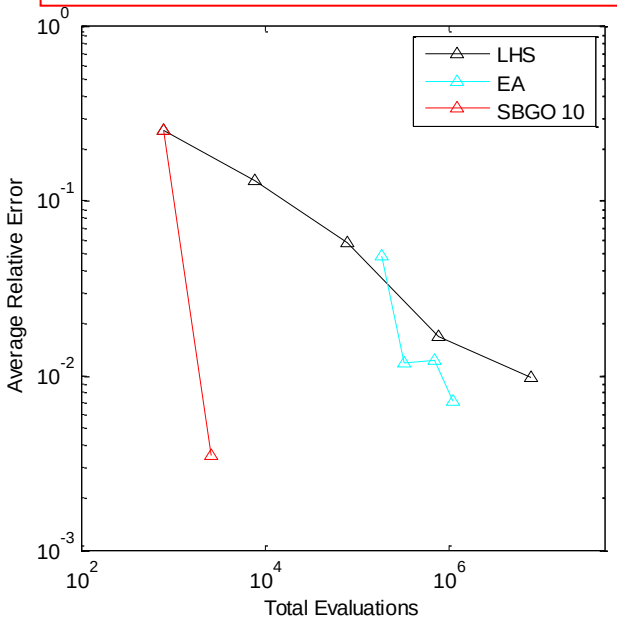
MINLP interval estimation approaches

- Latin hypercube sampling (LHS)
- Evolutionary algorithm (EA)
- Surrogate-based global optimization (SBGO)

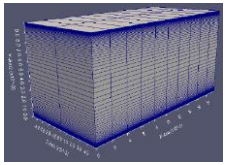
$$\text{Form 1}: \quad f_1 = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$
$$\text{Form 2}: \quad f_2 = 100(x_2 - x_1^2 + .2)^2 + (0.8 - x_1)^2$$

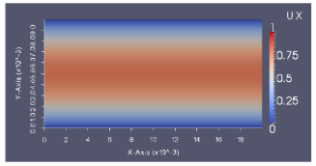


$$\text{Form 1}: \quad f_1 = 1 - \frac{4M}{bh^2Y} - \left(\frac{P}{bhY}\right)^2$$
$$\text{Form 2}: \quad f_2 = 1 - \frac{4P}{bh^2Y} - \left(\frac{P}{bhY}\right)^2$$
$$\text{Form 3}: \quad f_3 = 1 - \frac{4M}{bh^2Y} - \left(\frac{M}{bhY}\right)^2$$
$$\text{Form 4}: \quad f_4 = 1 - \frac{4M}{bh^2Y} - \left(\frac{P}{bhY}\right)^2 - \frac{4(P-M)}{bhY}$$



Drekar RANS turbulence: Spalart-Allmaras, k-ε





Method	Outer Evals	Total Evals	μ_{ux}	$\mu_{pressure}$
LHS	10	250	[0.727604, 2.78150]	[32.6109, 282.237]
SBGO	17	425	[0.622869, 4.44624]	[21.7321, 297.957]

Summary

Remarks on UQ

- We are developing a broad suite of scalable and robust core UQ methods
  - adaptive refinement, adjoint enhancement, & sparsity detection on structured & unstructured grids
  - framework for balancing errors among deterministic and stochastic sources
- We are now building on this foundation with multifidelity and model form UQ

Remarks on wind turbine simulation

- We have deployed UQ methodologies to current production wind simulation tools
  - Design codes from NREL and SNL: FAST, EOLO, CACTUS
  - LF tools have exhibited nonsmooth behavior, particularly when modeling turbulent in-flows and gust loading, motivating an increased emphasis on algorithmic robustness (local h-refinement)
- HF simulation tools (e.g., DG LES) are coming online
  - assess reliability in design limiting environments
  - anchor low fidelity results in the multifidelity setting

Impact and deployment

- UQ tools deployed through DAKOTA (v5.3 releasing 1/31/13)
- NREL systems analysis tool is leveraging OpenMDAO and DAKOTA
- Sandia: DAKOTA is being deployed to Sandia-led efforts in EERE's Wind Power Program

Directions

- Leadership-class CFD (towards exascale) for complex configurations & multiple turbines
  - leveraging low fidelity design codes in a rigorous manner
- Exploring partnership opportunities to strengthen ties of UQ/OUU R&D to wind energy