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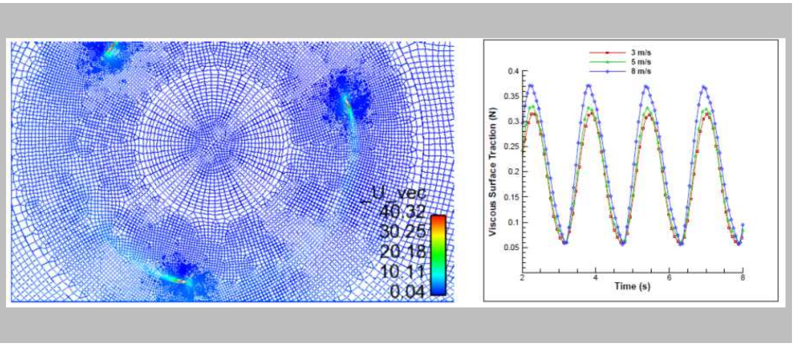

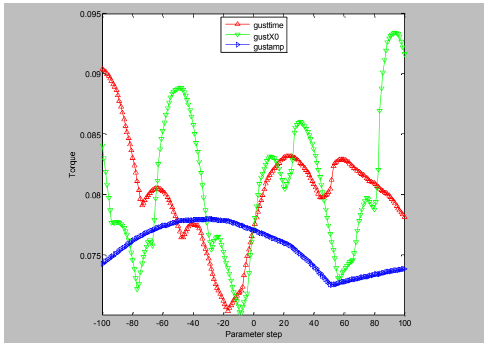

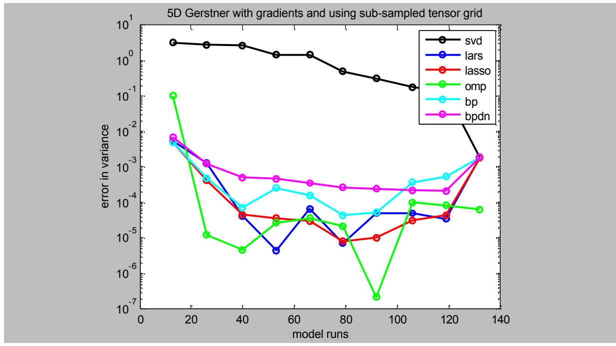

Emerging UQ Capabilities Applied to Wind Turbine Assessment

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Introduction
Scalable Methods for High-Dimensional UQ

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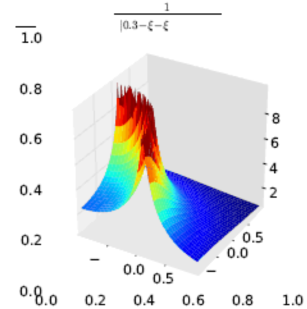
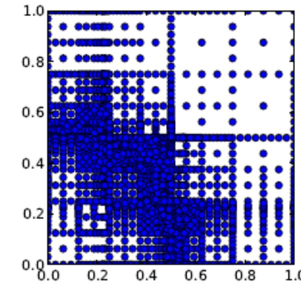
Key Challenges:

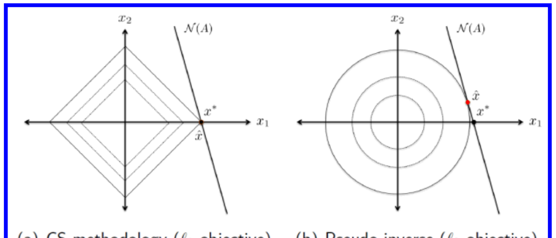
- Severe simulation budget constraints (e.g., a handful of HF runs)
- Moderate to high-dimensional in random variables: $O(10^1)$ to $O(10^2)$
- Compounding effects:
    - Mixed aleatory-epistemic uncertainties (→ nested iteration)
    - Requirement to evaluate probability of rare events (e.g., safety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





Algorithmic Capabilities:

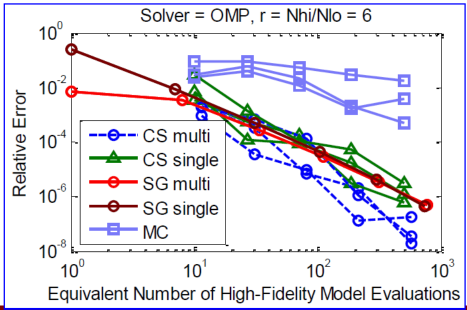
- Compute dominant uncertainty effects despite key challenges above
- Scalable UQ foundation
    - Adaptivity, Adjoints, Sparsity
- Leverage foundation within higher-level studies
    - Model form uncertainty, Multifidelity UQ, Bayesian inference



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

Mission Relevancy:

- NNSA: ASC assured safety and security (abnormal thermal / mechanical)
- Office of science: ASCR, SciDAC-3, CASL, CSSEF
- New UQ capabilities deployed in Dakota v5.3 (1/31/13) & v5.3.1 (5/15/13)



Office of Science Examples

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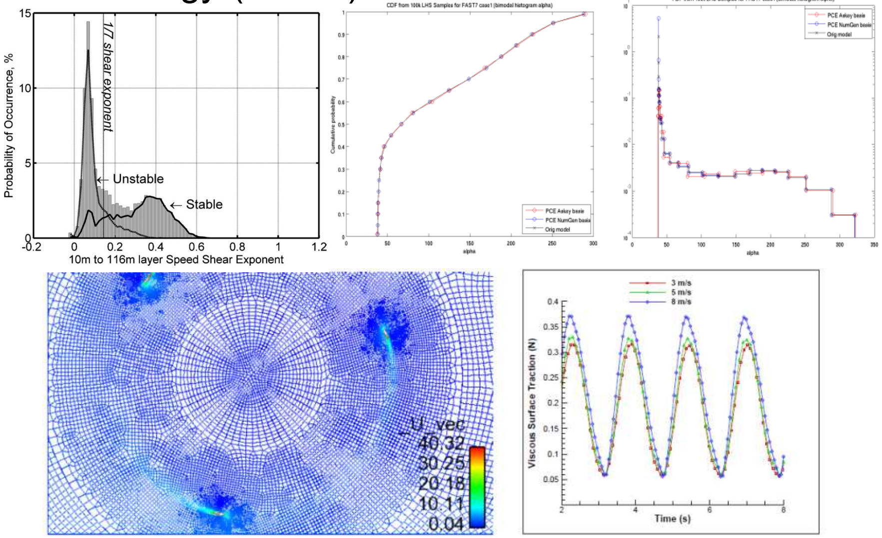
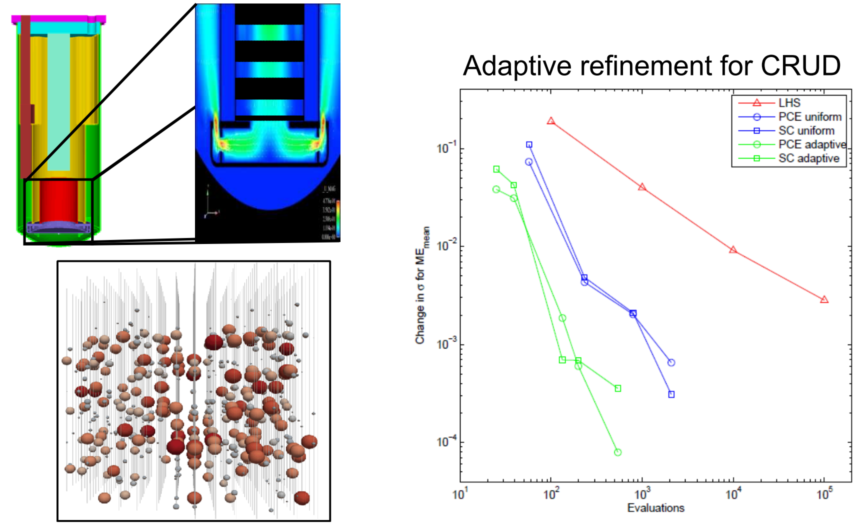
Wind energy (ASCR)

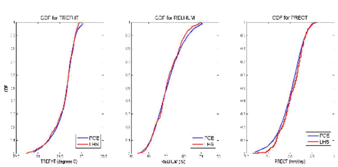


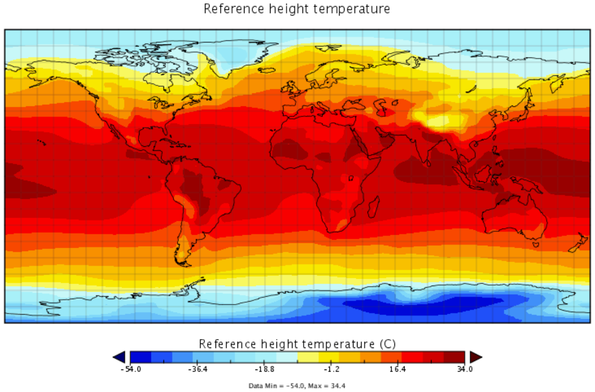
Nuclear reactors (CASL, NEAMS)



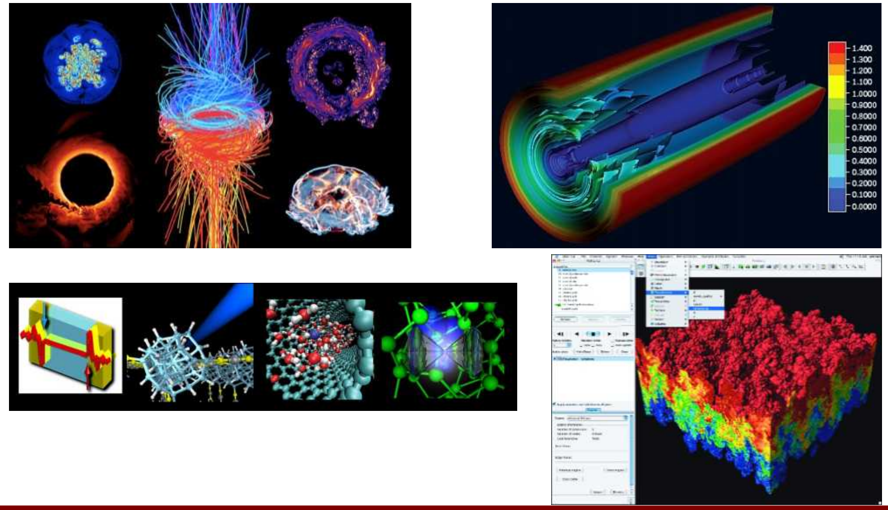
CSSEF: UQ w/ CAM4 (land, ocean, atmosphere)

	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	-0.05	-0.05	-0.02	0.01

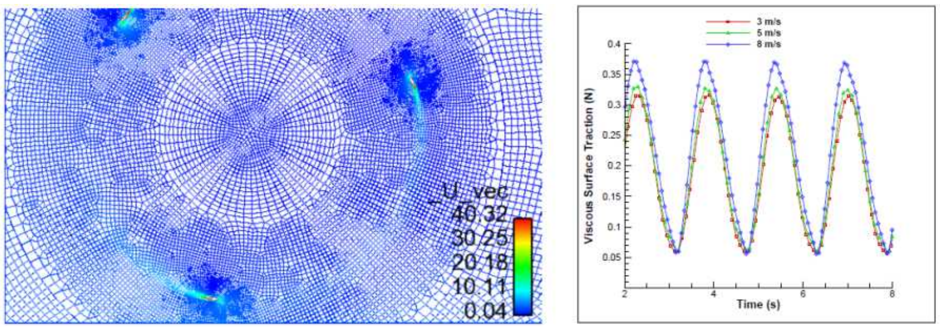




SciDAC-3: Fusion, BER, BES, nuclear, high energy



Large-Scale Uncertainty and Error Analysis for Time-dependent Fluid/Structure Interactions in Wind Turbine Applications



High fidelity simulation of SNL VAWT geometry (left) with leading edge viscous surface traction for three cross wind velocities (right).

Novel Ideas

1. **Develop adaptive collocation techniques to overcome curse of dimensionality and inaccuracy in capturing discontinuous response surfaces**
   - **Structured (sparse) grids**
   - **Unstructured (simplex) grids**
2. **Enhance scaling of global approximations though inclusion of local (adjoint) gradient information**
3. **Leverage error estimation within an error balancing framework: spatial/temporal/stochastic discretizations**
4. **Increase efficiency by blending multifidelity simulations (LF: FAST, Cactus, time spectral; HF: RANS, LES)**

Impact and Champions

IMPACT. The project seeks to develop novel algorithms to perform UQ in Wind-Energy applications

- **High-fidelity multi-physics simulations of wind turbines in the presence of uncertainty is a grand challenge for Exascale-class systems**
- **This project addresses curse-of-dimensionality and discontinuous responses – key bottlenecks in UQ – using adaptive refinement and adjoint-enhanced approximations**
- **The Wind Energy Community would benefit through improvement of design practice and certification**

Principal Investigators: J. Alonso, G. Iaccarino (Stanford), M. Eldred (Sandia), D. Xiu (Purdue)

Milestones/Dates/Status

	Scheduled	Actual
• Develop adjoint-enhanced PCE/SC on sparse/simplex grids	June 2012	June 2012
• Demonstrate use of UQ algorithms to a wind turbine multi-physics design problem	Dec 2011	completed
• Develop adjoint-based error estimation in vertical wind turbine application	Dec 2012	Dec 2012
• Demonstrate use of UQ algorithms to a wind turbine aero-elastic design problem	Sept 2011	completed
• Demonstrate multi-fidelity UQ methods on a vertical-axis wind turbine analysis problem	Sept 2012	Sept 2012

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3/25/2012

Research in Scalable UQ Methods

Commonly used UQ methods → robustness or efficiency, pick one.

- 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) are fast-converging global methods that provide a more effective balance of robustness / efficiency, especially when smoothness can be exploited. But global methods suffer from the *curse of dimensionality*:

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

To mitigate this curse:

- *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* (QoI dimension)]
- 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

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

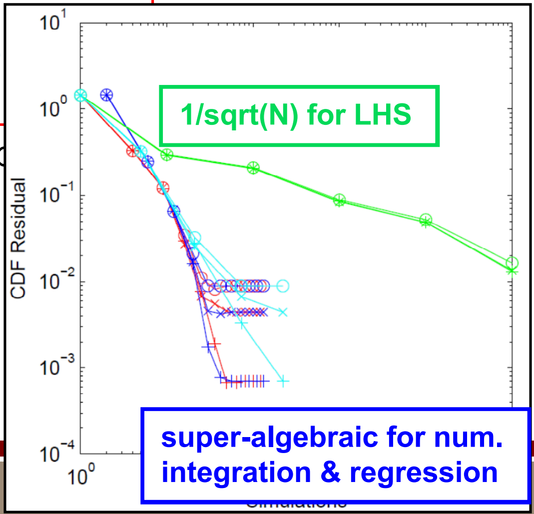
$$L_i = \prod_{\substack{j=1\\ j \neq i}}^{m} \frac{x - x_j}{x_i - x_j}$$

$$\Rightarrow$$

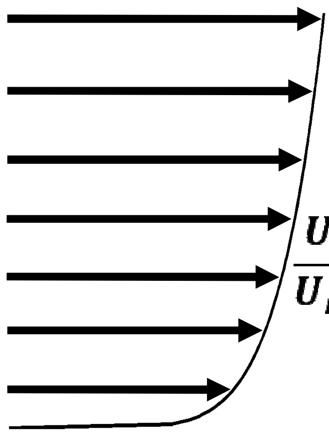
$$R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots\right.$$

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.

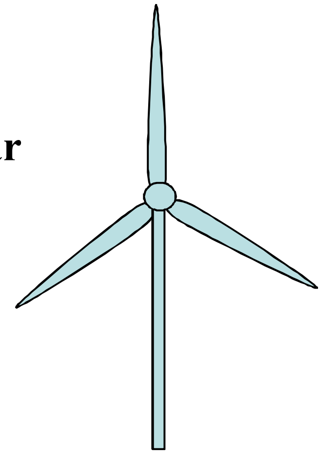


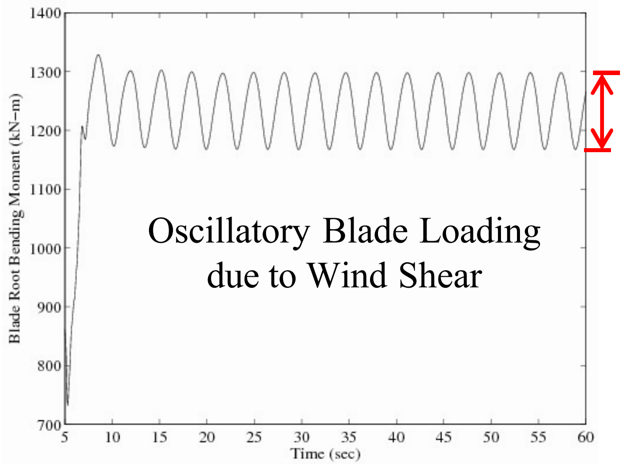
FAST: LF assessment of Wind Turbine Loads due to Uncertain Wind Shear

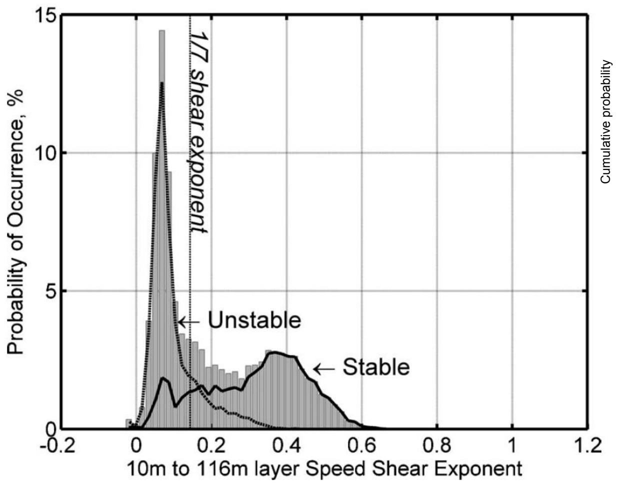


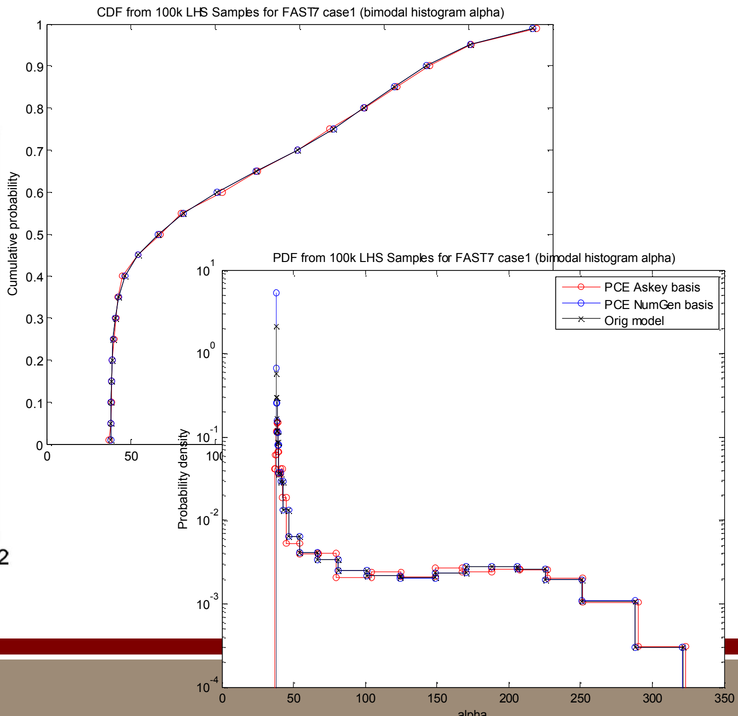
Wind Shear

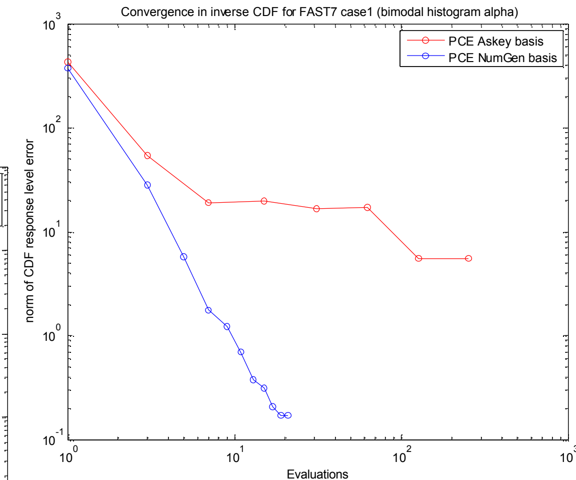
$$\frac{U}{U_h} = \left(\frac{z}{z_h}\right)^{\alpha}$$



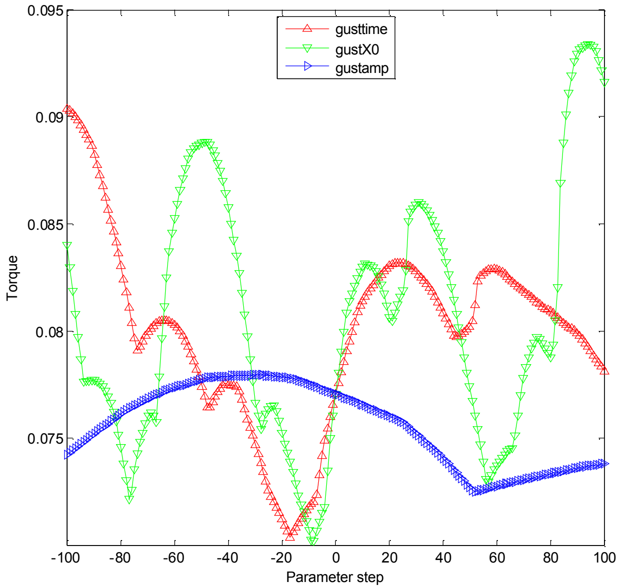


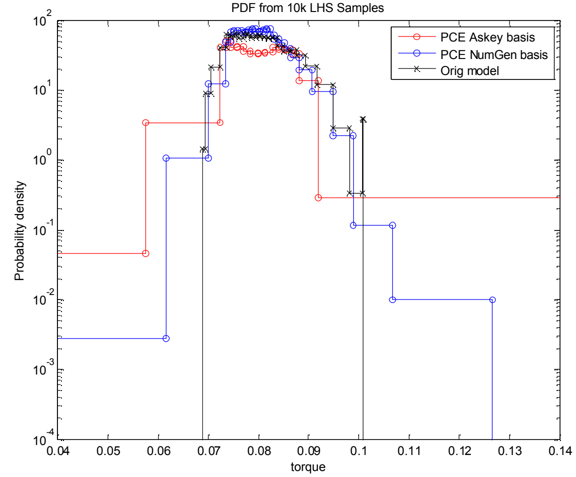


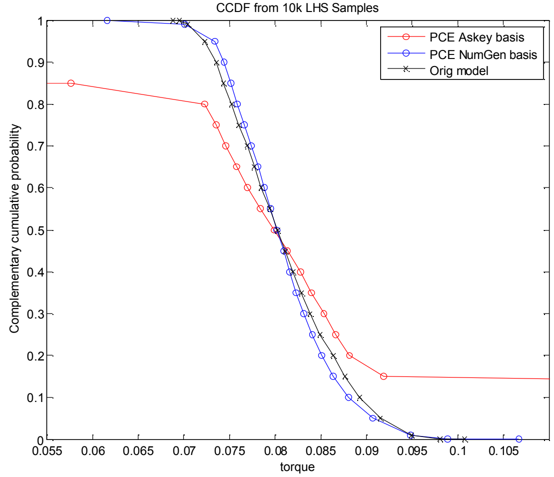


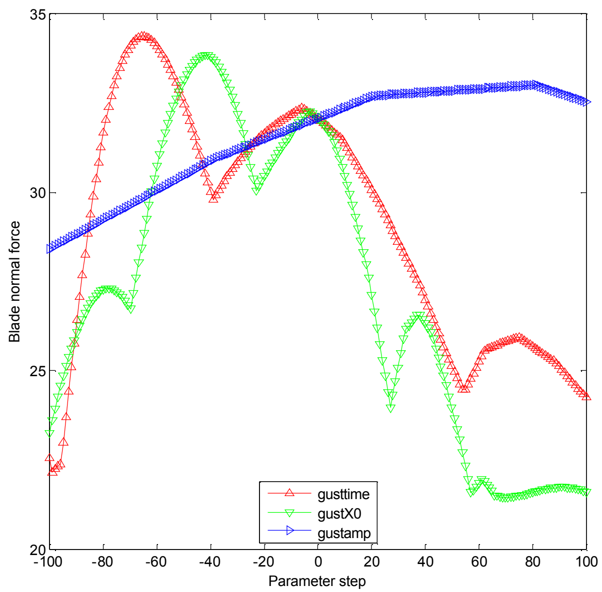


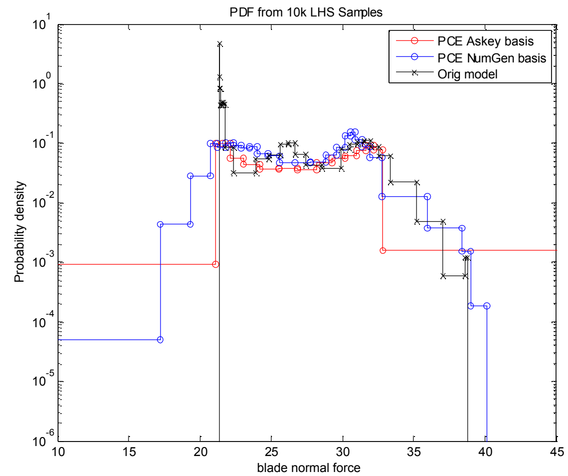
ASCR: VAWT with Uncertain Gust Loading

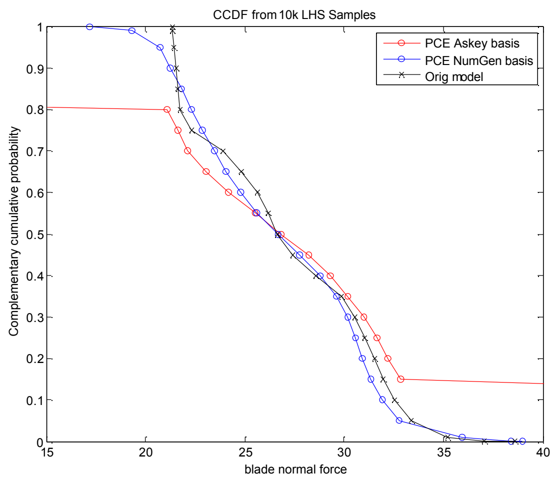








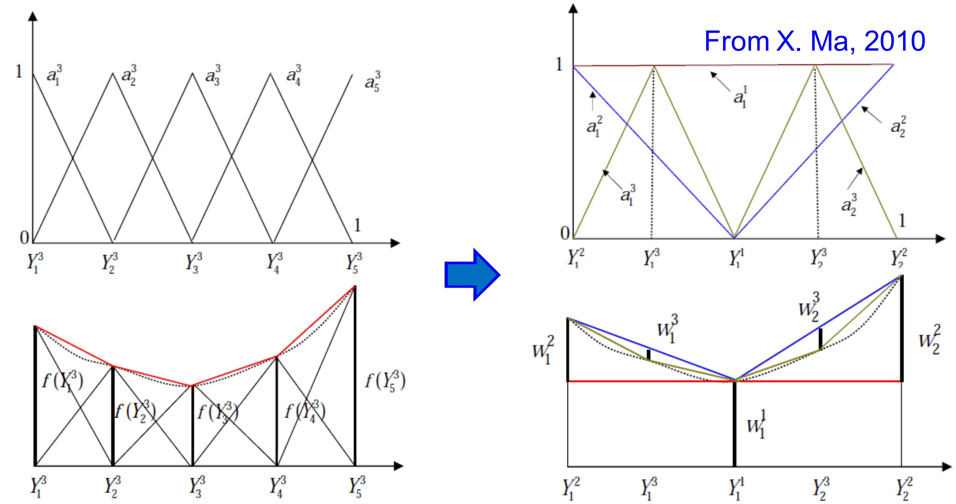




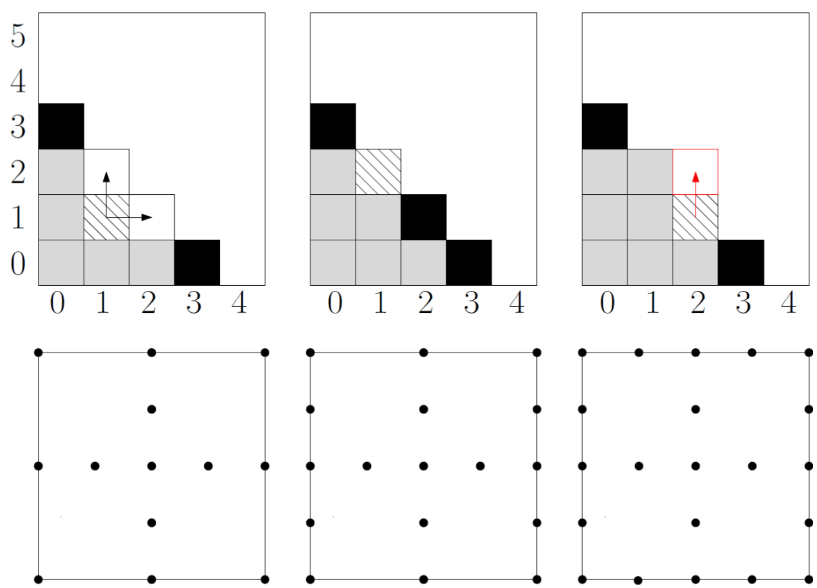
Local Error Estimation with Hierarchical Surpluses

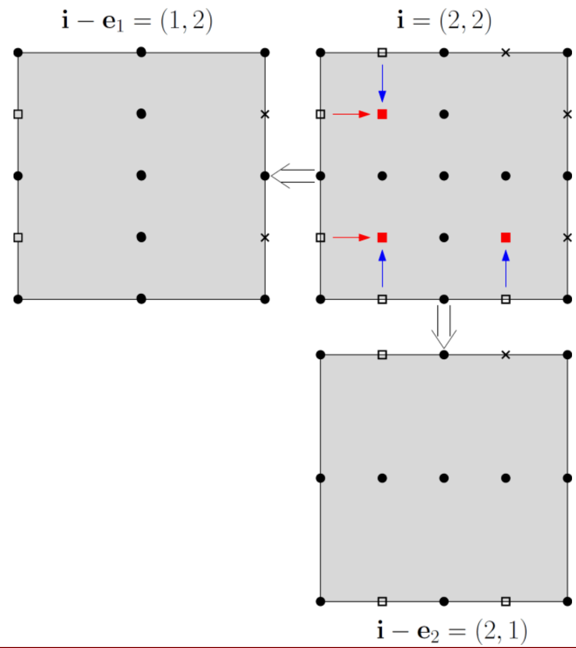
Hierarchical basis:

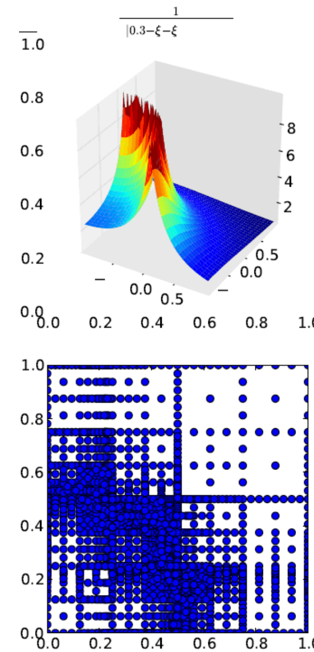
- *Improved precision* in QoI increments
- Surpluses provide error estimates for *local refinement* using local/global hierarchical interpolants
- New error indicators under development that leverage both *value and gradient surpluses*



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







Stochastic Expansions on Unstructured Grids:

Compressive Sensing

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

or in matrix notation

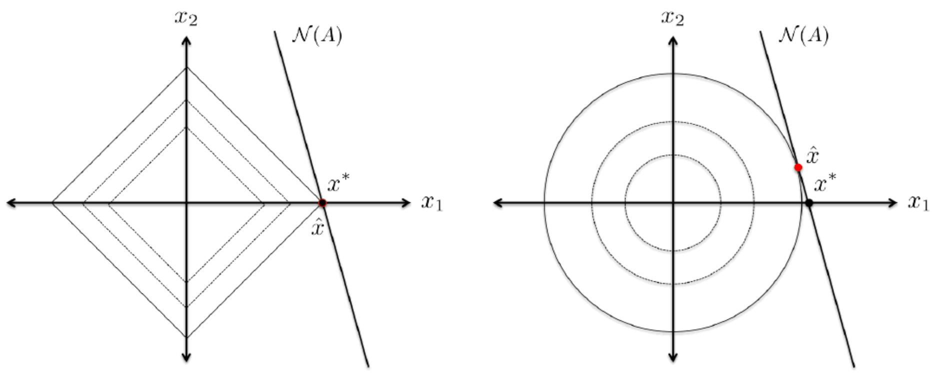
$$\mathbf{b} = \mathbf{A}\mathbf{x} + \varepsilon$$

and find the minimum norm solution

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

or (more recently) find a sparse solution

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



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

BP

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

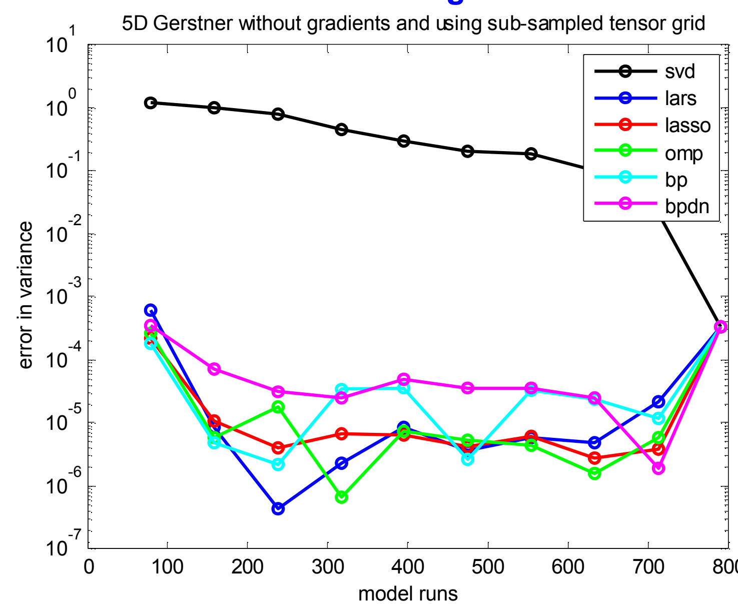
BPDN and OMP

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

LASSO and LARS

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

Structured or unstructured grids
Value-based or gradient-enhanced



Multiple Model Forms in UQ

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

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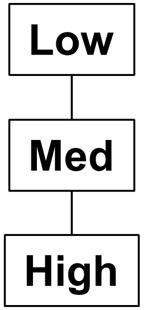
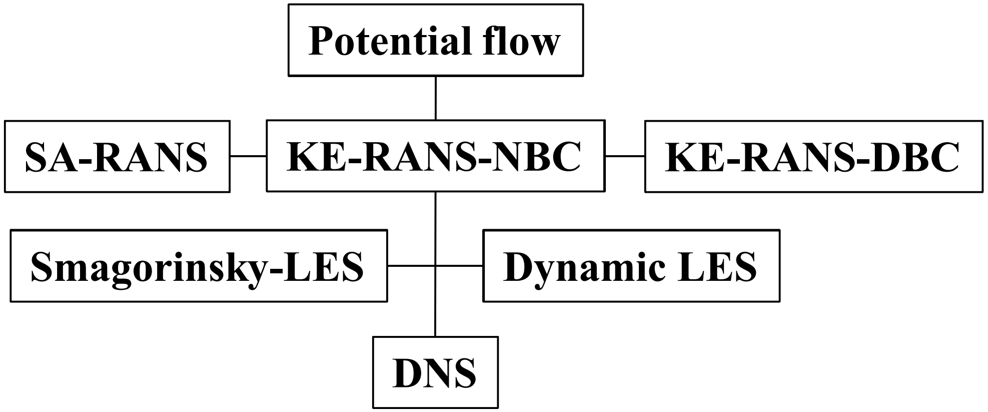
- A clear hierarchy of fidelity (low to high)



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

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

- Both



Multifidelity UQ using Stochastic Expansions

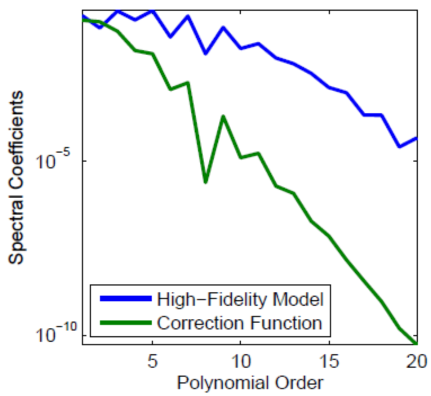
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

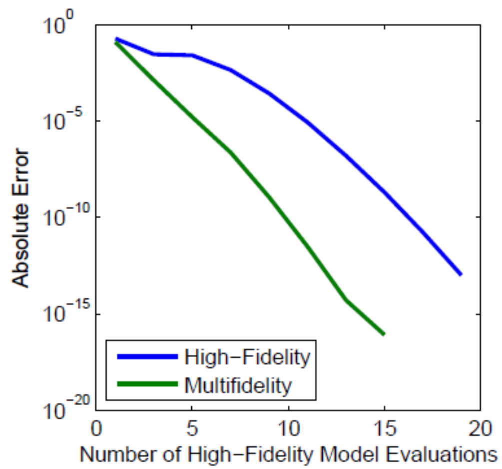
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

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

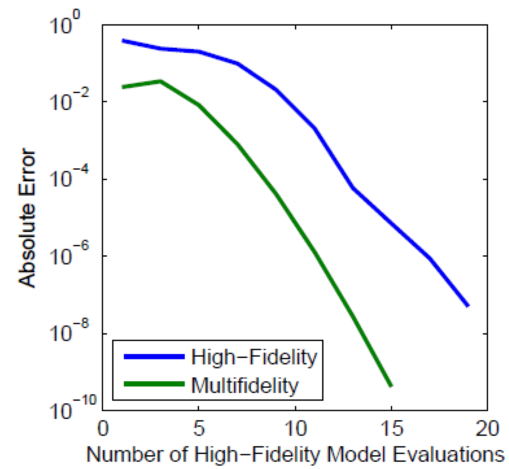
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5 e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

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





(a) Error in mean



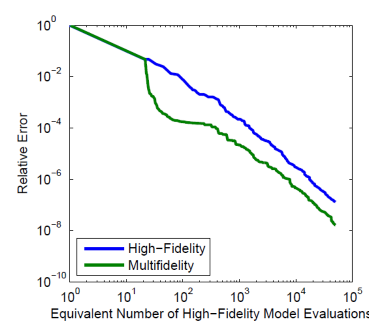
(b) Error in standard deviation

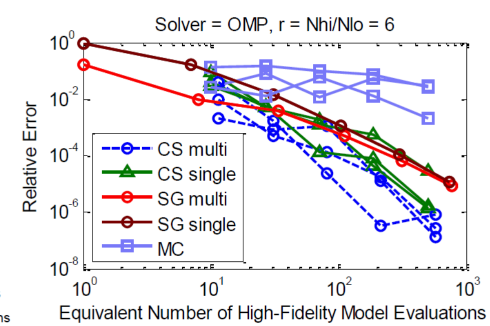
Adaptive sparse grid multifidelity algorithm:

- Gen. sparse grids 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





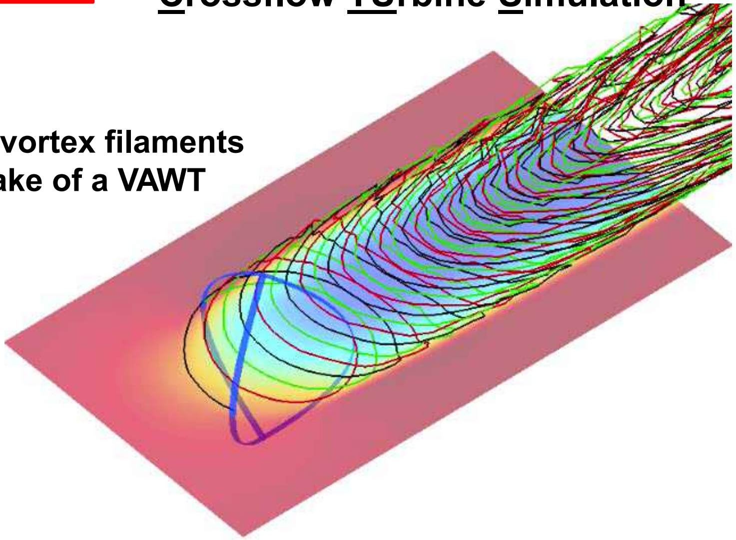
ASCR MF UQ example: VAWT CFD/FSI Modeling

Vertical-axis Wind Turbine (VAWT)

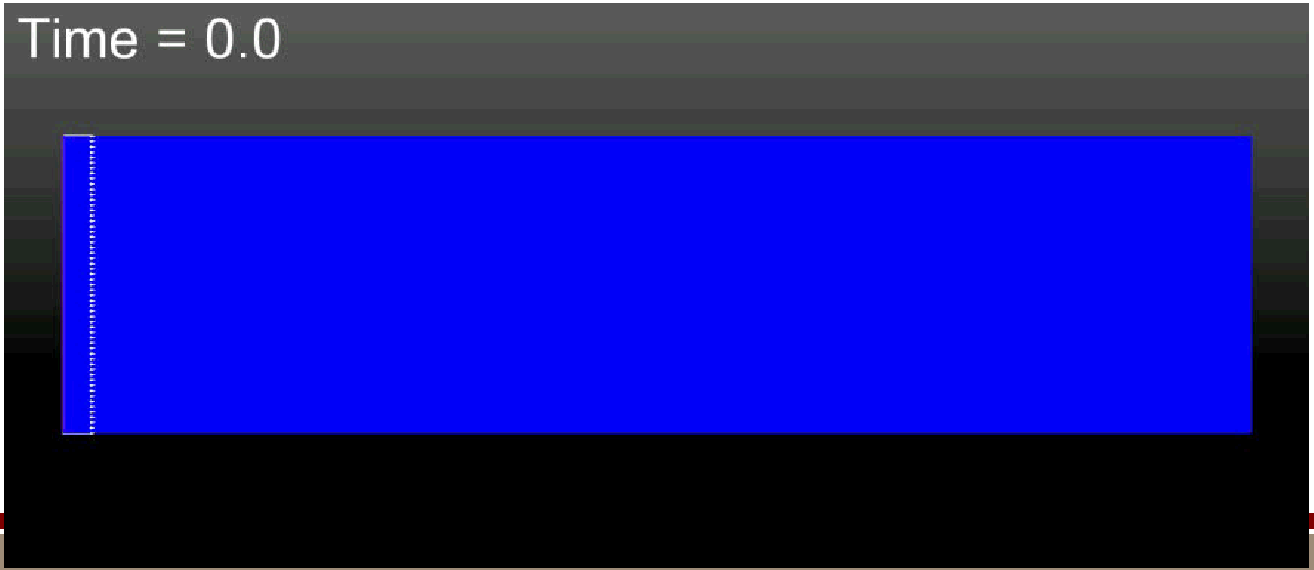
Low fidelity

CACTUS: Code for Axial and Crossflow TUrbine Simulation

Computed vortex filaments in the wake of a VAWT



High fidelity: DG formulation for LES



Impacts

Investments in scalable UQ R&D

- We are developing a broad suite of scalable and robust core UQ methods:
  - Goal-oriented adaptive refinement, (Adjoint) gradient-enhancement, Sparsity detection
- We are building on this foundation
  - Multifidelity UQ, Mixed aleatory-epistemic UQ, Bayesian inference

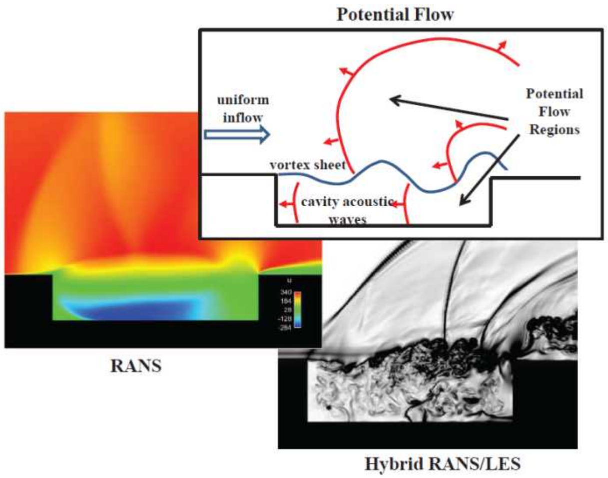
Algorithm Impacts

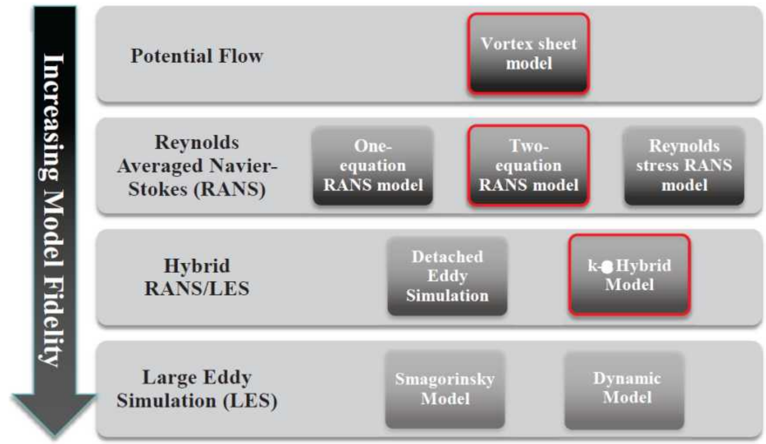
- Address key UQ challenges
  - Severe simulation budget constraints and moderate to high random dimensionality
  - Compounded by mixed uncertainties, nonsmoothness, rare events
- Algorithms deployed through Dakota (v5.3 released 1/31/13, v5.3.1 released 5/15/2013)
- Mission impact for NNSA (ASC) & Office of Science (ASCR, CASL, SciDAC-3, CSSEF)

Programmatic Impacts

- Collaborations with Stanford (Aero, Mechanical) & Purdue/Utah (Math)
- Large-scale LES investments at SNL and Stanford
- NREL:
  - Adoption of Dakota (SNL) + OpenMDAO (NASA) as basis for next gen systems analysis tools (Veers, Dykes, et al.)
- SNL:
  - Dakota is being deployed to Sandia-led efforts in EERE’s Wind Power Program (Barone et al.)
  - Campus Executive LDRD awarded for Santiago Padron (Advisor: Alonso, Mentor: Eldred), FY14-16

FY14-16 ASCR UQ Proposal:
Extreme-Scale UQ Exploiting the CFD Model Hierarchy





Example model family and multifidelity hierarchy: potential flow, RANS, hybrid RANS/LES, LES.

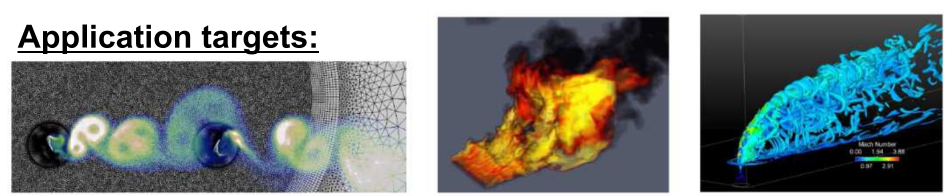
Our focus is on the development and delivery of extreme-scale (XScale) uncertainty quantification (UQ) for complex computational fluid dynamics (CFD) simulations of direct relevance to mission areas of the Office of Science. Our proposal revolves around two inter-related themes:

1. **XScale spectrum:** targeting a computational spectrum of solutions ranging from sparse UQ with the highest-fidelity XScale CFD to XScale UQ exploiting massive concurrency in reduced-fidelity CFD.
2. **CFD model ensemble:** exploiting the availability of multiple levels of fidelity to accelerate propagation and inference processes and addressing critical uncertainties due to alternative model forms.

Algorithm targets:

- Core UQ: flexible quad., adaptive collocation, sparsity detect
- XScale: Asynch parallel UQ via stoch domain decomposition
- Multifidelity: UQ, Bayesian inference
- Model form: Bayesian model selection, sequential data assimilation, intrusive uncertainty injection

Application targets:



(a) Vertical axis wind turbine application using unstructured LES and sliding mesh

(b) Hydrocarbon pool fire with turbulent reacting flow (LES)

(c) Non-reacting supersonic jet in transonic cross-flow (RANS/LES)

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