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 $\rightarrow$ multifidelity UQ (LF: EOLO, FAST, CACTUS; HF: URANS, DG LES)
  - Epistemic model form $\rightarrow$ mixed aleatory-epistemic/continuous-discrete UQ
Non-Intrusive Stochastic Expansions: Polynomial Chaos and Stochastic Collocation

**Polynomial Chaos:** spectral projection using orthogonal polynomial basis functions

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

- Estimate \( \alpha_j \) using regression or numerical integration: sampling, tensor quadrature, sparse grids, or cubature

**Stochastic Collocation:** 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

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

Sparse interpolants formed using \( \sum \) 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.
Non-Intrusive Stochastic Stochastic Expansions: Polynomial Chaos and Stochastic Collocation

**Polynomial chaos:** spectral projection using orthogonal polynomial basis functions

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

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

- 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.
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
  - **PCE/SC:** variance-based decomp. $\rightarrow$ total Sobol’ indices $\rightarrow$ anisotropy
  - **PCE:** spectral coefficient decay rates $\rightarrow$ 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

**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

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

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

and similar for higher-order moments

\[
e^{-10x^2-5y^2}
\]
Stochastic Expansions on Unstructured Grids: Compressive Sensing

\[
\begin{bmatrix}
    f(x^{(1)}) \\
    f(x^{(2)}) \\
    \vdots \\
    f(x^{(N)}) \\
\end{bmatrix} = 
\begin{bmatrix}
    1 & \phi_2(x^{(1)}) & \phi_2(x^{(1)}) & \cdots & \phi_P(x^{(1)}) \\
    1 & \phi_1(x^{(2)}) & \phi_2(x^{(2)}) & \cdots & \phi_P(x^{(2)}) \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    1 & \phi_1(x^{(N)}) & \phi_2(x^{(N)}) & \cdots & \phi_P(x^{(N)}) \\
\end{bmatrix} \begin{bmatrix}
    c_0 \\
    c_1 \\
    c_2 \\
    \vdots \\
    c_P \\
\end{bmatrix} + 
\begin{bmatrix}
    \varepsilon_1 \\
    \varepsilon_2 \\
    \vdots \\
    \varepsilon_N \\
\end{bmatrix}
\]

or in matrix notation

\[\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{\varepsilon}\]

and find the minimum norm solution

\[
\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2
\]

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 ($\ell_1$ objective)  (b) Pseudo-inverse ($\ell_2$ objective)

BP

\[\mathbf{c} = \arg \min \|\mathbf{c}\|_{\ell_1} \quad \text{such that} \quad \Phi\mathbf{c} = \mathbf{y}\]

BPDN and OMP

\[\mathbf{c} = \arg \min \|\mathbf{c}\|_{\ell_1} \quad \text{such that} \quad \|\Phi\mathbf{c} - \mathbf{y}\|_{\ell_2} \leq \varepsilon\]

LASSO and LARS

\[\mathbf{c} = \arg \min \|\Phi\mathbf{c} - \mathbf{y}\|_{\ell_2}^2 \quad \text{such that} \quad \|\mathbf{x}\|_{\ell_1} \leq \tau\]
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

Wind Shear

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

Oscillatory Blade Loading due to Wind Shear

CDF from 100k LHS Samples for FAST7 case1 (bimodal histogram alpha)

PDF from 100k LHS Samples for FAST7 case1 (bimodal histogram alpha)

Convergence in inverse CDF for FAST7 case1 (bimodal histogram alpha)
CACTUS: VAWT with Uncertain Gust Loading (V1)
CACTUS: VAWT Loads due to Uncertain Gust (V2)
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
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

$$\varepsilon_\mu \approx \sum_{j=1}^{n_e} \Omega_j (\varepsilon_{AUQ_j} + \varepsilon_{EUQ_j} + \varepsilon_{\Delta x_j})$$

- Aleatory propagation/error estimation: Simplex SSC
- Numerical discretization error: Adjoint perturbation (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

```
Low
  Med
  High
```

```
SA-RANS   KE-RANS-NBC   KE-RANS-DBC
```
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)

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

\[ N_{lo} \gg N_{hi} \]

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 \( \Delta \text{QOI}/\Delta \text{Cost} \)
Elliptic PDE with FEM

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

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

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

QoI is \(u(0.5, \omega)\).

LF = coarse spatial grid with 50 states.
HF = fine spatial grid with 500 states.
\(r_{\text{work}} = 40\).

<table>
<thead>
<tr>
<th>Defined offset</th>
<th>Relative Error in Mean</th>
<th>Relative Error in Std Deviation</th>
<th>High-Fidelity Evaluations</th>
<th>Low-Fidelity Evaluations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-Fidelity ((q = 3))</td>
<td>(5.3 \times 10^{-6})</td>
<td>(2.7 \times 10^{-4})</td>
<td>1981</td>
<td>–</td>
</tr>
<tr>
<td>Single-Fidelity ((q = 4))</td>
<td>(4.1 \times 10^{-7})</td>
<td>(2.3 \times 10^{-5})</td>
<td>12,981</td>
<td>–</td>
</tr>
<tr>
<td>Multifidelity ((q = 4, r = 1))</td>
<td>(4.7 \times 10^{-7})</td>
<td>(2.6 \times 10^{-5})</td>
<td>1981</td>
<td>12,981</td>
</tr>
</tbody>
</table>

Adaptive

(a) Error in mean

(b) Error in standard deviation
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
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 $\rightarrow$ under-resolved sampling (especially @ outer loop)
- Under-prediction of credible outcomes

Algorithmic approaches

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

Address accuracy and efficiency

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

<table>
<thead>
<tr>
<th>Interv Est Approach</th>
<th>UQ Approach</th>
<th>Expansion Variables</th>
<th>Evaluations (F_n, Grad)</th>
<th>Area</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>EGO SC SSG w = 1</td>
<td>Aleatory</td>
<td>(84/91, 0/0)</td>
<td>75.0002, 374.999</td>
<td>-2.26264, 11.8623</td>
<td></td>
</tr>
<tr>
<td>EGO SC SSG w = 2</td>
<td>Aleatory</td>
<td>(372/403, 0/0)</td>
<td>75.0002, 374.999</td>
<td>-2.18735, 11.5900</td>
<td></td>
</tr>
<tr>
<td>EGO SC SSG w = 3</td>
<td>Aleatory</td>
<td>(1260/1365, 0/0)</td>
<td>75.0002, 374.999</td>
<td>-2.18732, 11.5900</td>
<td></td>
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<tr>
<td>EGO SC SSG w = 4</td>
<td>Aleatory</td>
<td>(3564/3861, 0/0)</td>
<td>75.0002, 374.999</td>
<td>-2.18732, 11.5900</td>
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<tr>
<td>NPSOL SC SSG w = 1</td>
<td>Aleatory</td>
<td>(21/77, 21/77)</td>
<td>75.0000, 375.000</td>
<td>-2.26264, 11.8623</td>
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<td>(93/341, 93/341)</td>
<td>75.0000, 375.000</td>
<td>-2.18735, 11.5900</td>
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</tr>
<tr>
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<td>Aleatory</td>
<td>(315/1155, 315/1155)</td>
<td>75.0000, 375.000</td>
<td>-2.18732, 11.5900</td>
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<tr>
<td>NPSOL SC SSG w = 4</td>
<td>Aleatory</td>
<td>(891/3267, 891/3267)</td>
<td>75.0000, 375.000</td>
<td>-2.18732, 11.5900</td>
<td></td>
</tr>
</tbody>
</table>

IVP SC SSG Aleatory: \( \beta \) interval converged to 5-6 digits by 300-400 evals

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

Fully converged area interval = [75., 375.], \( \beta \) interval = [-2.18732, 11.5900]

Multiple cells within DSTE

Convergence rates for combined expansions

- \( L^\infty \) metrics: IVP mixed, DSTE mixed
- \( L^2 \) metrics: Aleatory, SOP mixed

Analytic \( C^\infty \)

Discontinuous \( C^0 \)
**Addition of Discrete Epistemic Model Form**

**MINLP interval estimation approaches**
- Latin hypercube sampling (LHS)
- Evolutionary algorithm (EA)
- Surrogate-based global optimization (SBGO)

\[
\begin{align*}
\text{Form 1: } f_1 &= 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \\
\text{Form 2: } f_2 &= 100(x_2 - x_1^2 + .2)^2 + (0.8 - x_1)^2
\end{align*}
\]

---

**Drekar RANS turbulence:** Spalart-Allmaras, k-\(\varepsilon\)

<table>
<thead>
<tr>
<th>Method</th>
<th>Outer Evals</th>
<th>Total Evals</th>
<th>(\mu_{ux})</th>
<th>(\mu_{pressure})</th>
</tr>
</thead>
<tbody>
<tr>
<td>LHS</td>
<td>10</td>
<td>250</td>
<td>[0.727604, 2.78150]</td>
<td>[32.6109, 282.237]</td>
</tr>
<tr>
<td>SBGO</td>
<td>17</td>
<td>425</td>
<td>[0.622869, 4.44624]</td>
<td>[21.7321, 297.957]</td>
</tr>
</tbody>
</table>
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