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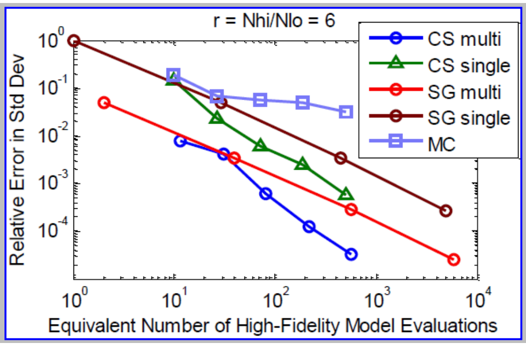

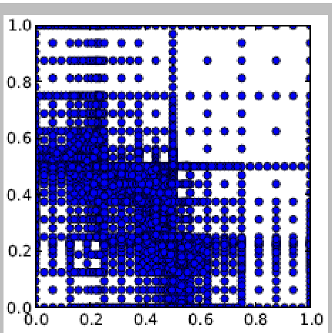

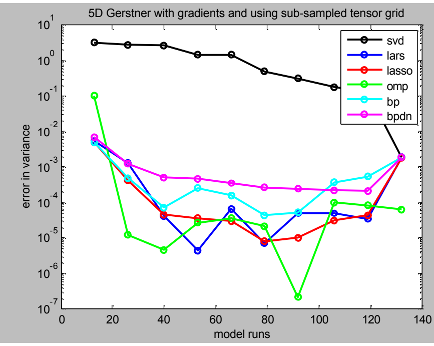

Deployment of Scalable UQ Methods for High-Fidelity Simulation-based Applications within the DOE

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

Sandia National Laboratories, Albuquerque, NM

DAKOTA: Research, development, & deployment of advanced iterative algorithms for simulation-based assessment and design

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DAKOTA
- **Optimization**
- **Uncertainty Quant.**
- **Parameter Est.**
- **Sensitivity Analysis**

Model Parameters

Black box:
- **Sandia simulation codes**
- **Commercial simulation codes**

Library mode (semi-intrusive):
- **ALEGRA (shock physics), Xyce (circuits), Sage (CFD), Albany/TriKota (Trilinos-based), MATLAB, Python, ModelCenter, SIERRA (multiphysics)**

Design Metrics

Iterative systems analysis

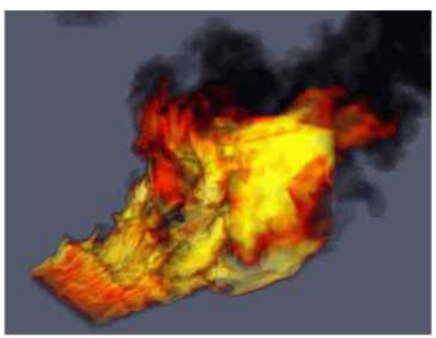
Multilevel parallel computing

Simulation management

Impact across a variety of DOE mission areas

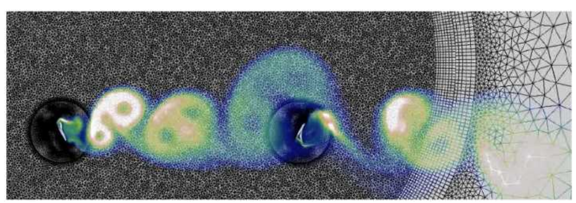
Stockpile (NNSA ASC)

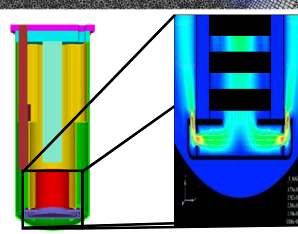
Abnormal environments



Energy (ASCR, EERE, NE)

Wind turbines, nuclear reactors





Climate (SciDAC, CSSEF)

Ice sheet modeling, CISM, CESM, ISSM

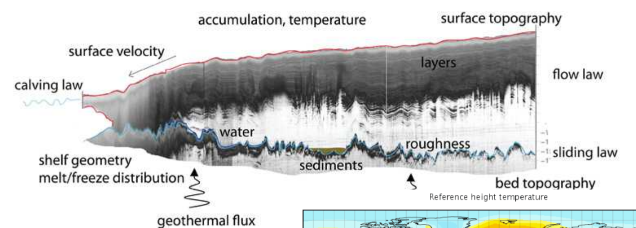
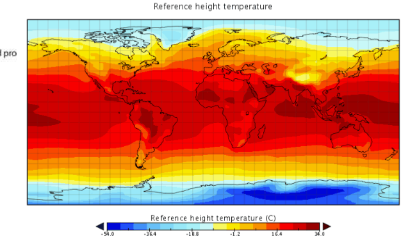


Figure 1: Schematic of observations, boundary conditions, and pro



Emphasis on Scalable Methods for High-fidelity UQ on HPC

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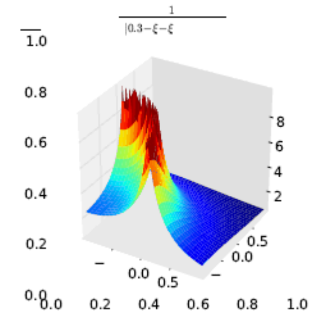
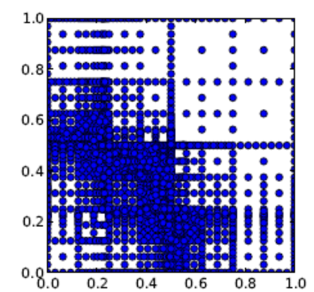
Key Challenges:

- 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) [post KLE]
- Compounding effects:
  - Mixed aleatory-epistemic uncertainties (→ nested iteration)
  - Requirement to evaluate probability of rare events (e.g., safety criteria)
  - Nonsmooth responses (→ difficulty with fast converging spectral methods)



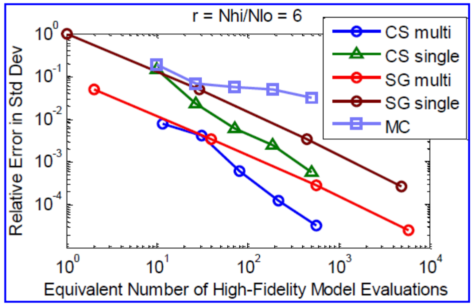
Core UQ Capabilities:

- Sampling methods: LHS, MC, QMC, incremental
- Reliability methods: local (MV, AMV+, FORM, …), global (EGRA, GPAIS, POFDarts)
- Stochastic expansion methods: polynomial chaos, stochastic collocation
- Epistemic methods: interval estimation, Dempster-Shafer evidence



Research Thrusts:

- Compute dominant uncertainty effects despite key challenges above
- Scalable UQ foundation
  - Adaptive refinement, Adjoint enhancement, Sparsity detection
- Leverage his foundation within component-based meta-iteration
  - Mixed UQ incl. model form, Multifidelity UQ, Bayesian methods



Uncertainty Quantification Algorithms in DAKOTA: New methods bridge robustness/efficiency gap

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	Traditional (at Sandia)	Production	Recently released	Under dev Planned	Collabs.
Sampling	**Latin Hypercube, Monte Carlo**	**Incremental**	**Importance**	**Bootstrap, Jackknife**	**FSU**
Reliability	***Local:* Mean Value, 1st- & 2nd-order reliability (AMV+, FORM, SORM)**	**Global reliability methods (EGRA)**	**GPAIS, POFDarts, GPs with gradient-enhancement**	**Recursive emulation, TGP**	***Local:* Notre Dame, *Global:* Vanderbilt**
Stochastic expansion		**Polynomial chaos, stoch collocation (regression,**	**Dimension-adaptive p-/h-refinement, grad-enhancement, sparsity detection**	**Local adapt refinement, adjoint EE, discrete vars**	**Stanford, Utah**
Epistemic	**Interval-valued/ 2nd-order prob. w/nested sampling**		**Opt-based interval est, Dempster-Shafer, discrete model forms**	**Discrete GPs, Imprec. probability**	**Arizona St**
Bayesian			**Emulator based MCMC with QUESO, GPMSA**	**model selection, multifidelity**	**LANL, UT Austin**
Other			**Efficient subspace method, Morris-Smale topology**	**Rand fields / stoch proc, Moment meth**	**NCSU, Utah, Cornell, Maryland**

Research: Scalability, Robustness, Goal-orientation

Adv. Deployment Fills Gaps

Solution-Verified Reliability Analysis and Design of MEMS

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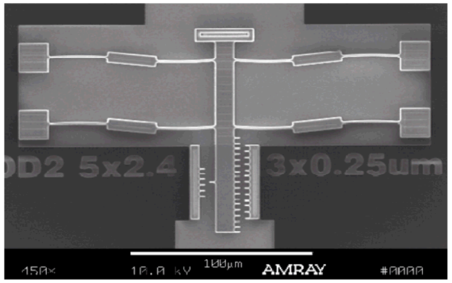
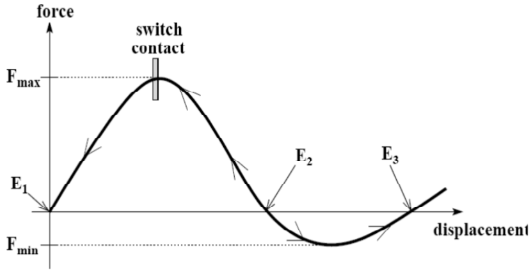
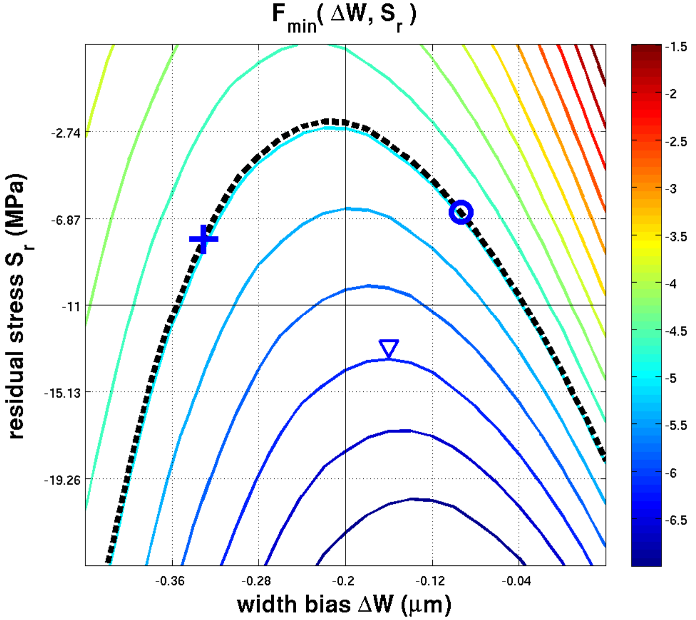
- Problem: MEMS subject to substantial variabilities
  - Material properties, manufactured geometry, residual stresses
  - Part yields can be low or have poor durability
  - Data can be obtained → aleatory UQ → probabilistic methods
- Goal: account for both uncertainties and errors in design
  - Integrate UQ/OUU (DAKOTA), ZZ/QOI error estimation (Encore), adaptivity (SIERRA), nonlin mech (Aria) → MESA application
  - Perform soln verification in automated, parameter-adaptive way
  - Generate fully converged UQ/OUU results at lower cost





- **AMV^2+ and FORM converge to different MPPs (+ and o, respectively)**
- **Issue: high nonlinearity leading to multiple legitimate MPP solns.**
- **Challenge: design optimization may tend to seek out regions encircled by the failure domain. 1st-order and even 2nd-order probability integrations can experience difficulty with this degree of nonlinearity. Optimizers can/will exploit this model weakness.**



Parameter study over 3σ uncertain variable range for fixed design variables d_M*. ***Dashed black line denotes $g(x) = F_{min}(x) = -5.0$.***

Non-Intrusive Stochastic Expansions:
Polynomial Chaos and Stochastic Collocation

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Polynomial chaos: spectral projection using orthogonal polynomial basis fns

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

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

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

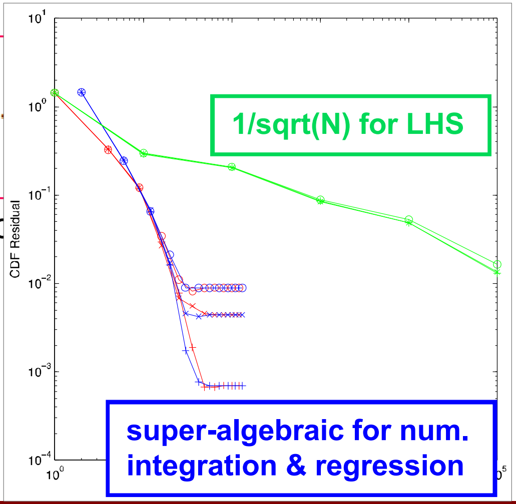
Stochastic collocation: instead of estimating coefficients for known basis functions, form interpolants for known coefficients

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

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

$$L_j = \prod_{\substack{k=1 \\ k \neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k} \;\Rightarrow\; R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots\right.$$

Sparse interpolants formed using Σ of tensor interpo



- 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.

Adaptive Collocation Methods: Generalized Sparse Grids

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.

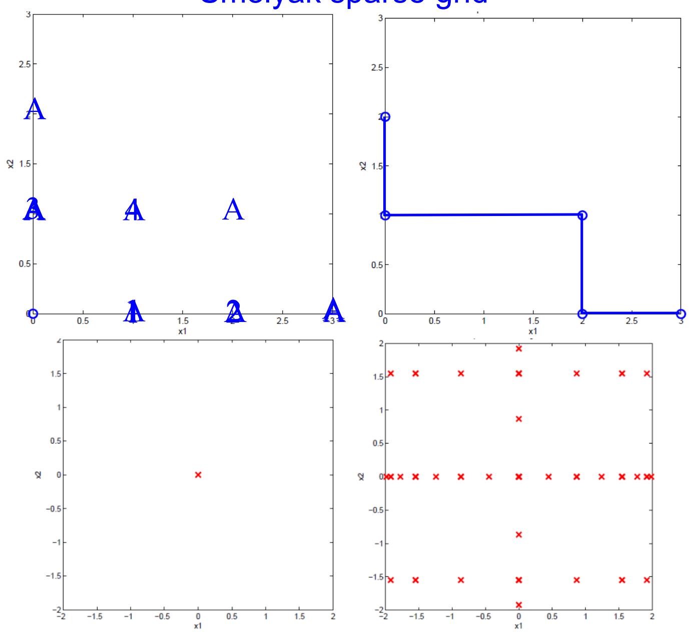
2. ***Trial set evaluation:*** For each trial index set, evaluate tensor grid, form tensor expansion, update combinatorial coefficients, and combine with reference expansion. Perform necessary bookkeeping to allow efficient restoration.

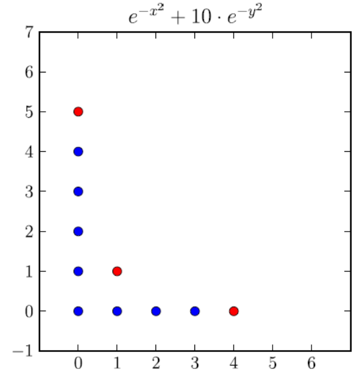
3. ***Trial set selection:*** Select trial index set that induces largest change in statistical QOI.

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

Extend Scalability: (Adjoint) Derivative-Enhancement

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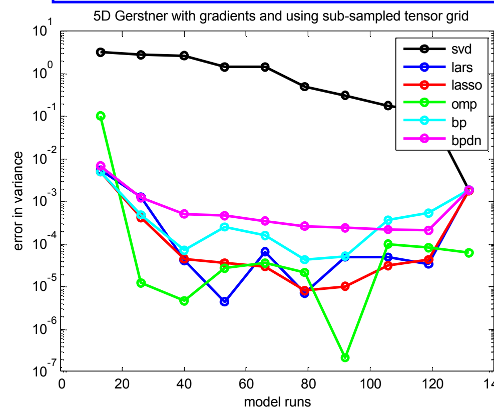
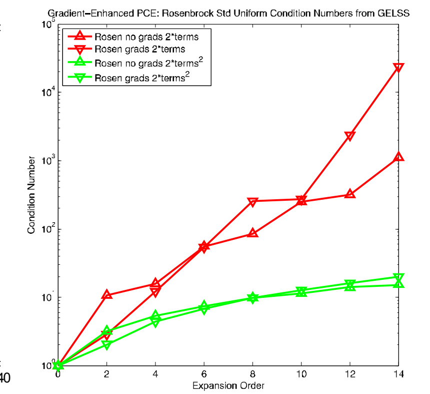
PCE:

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

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



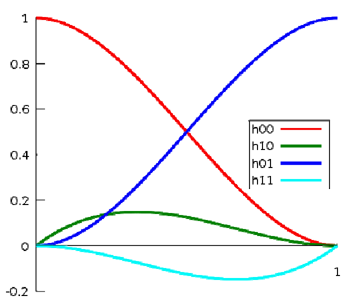


SC:

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

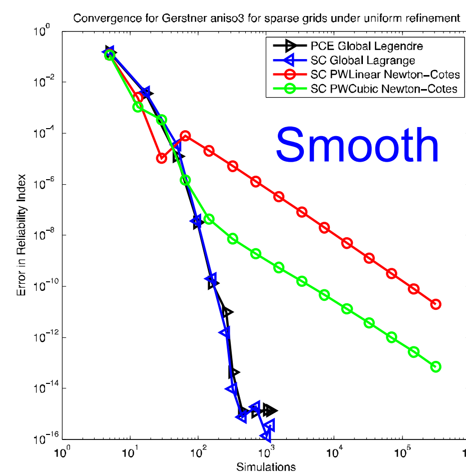
$$
f = \sum_{i=1}^{N} f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3)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

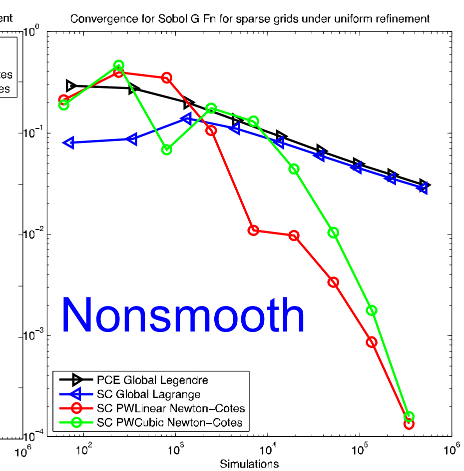
Cubic shape fns: type 1 (value) & type 2 (gradient)



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

and similar for higher-order moments





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

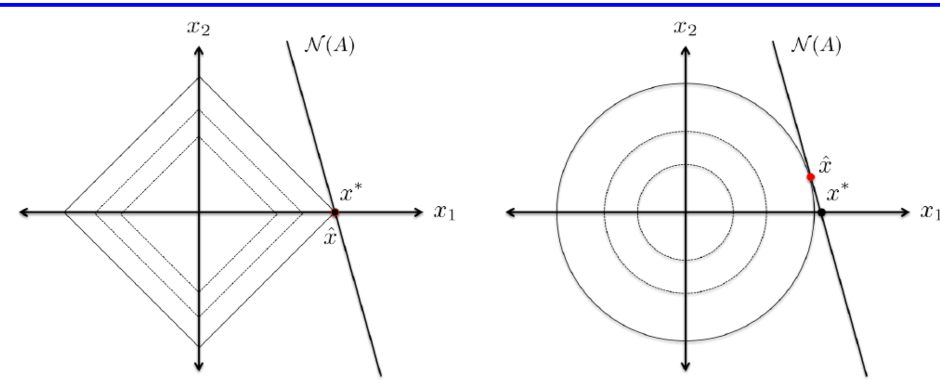
$$\mathbf{b} = \mathbf{Ax} + \varepsilon$$

and find the minimum norm solution

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

or (more recently) find a sparse solution

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



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

BP

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

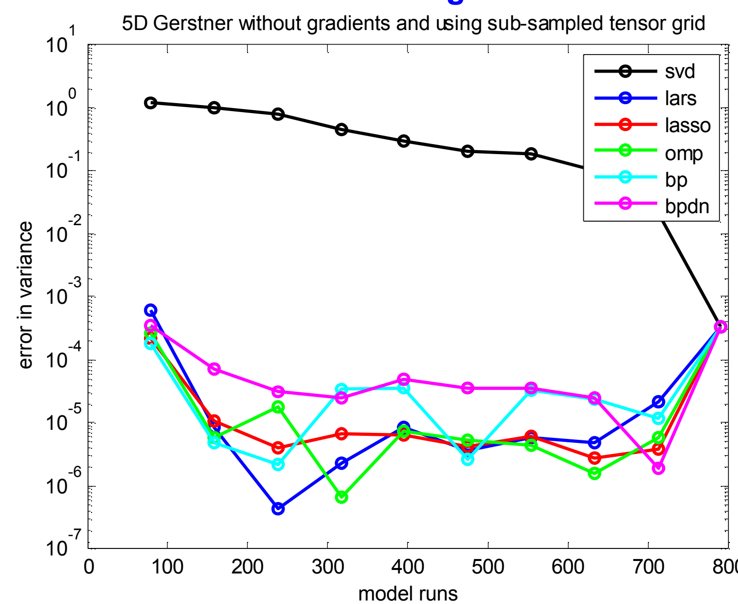
BPDN and OMP

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

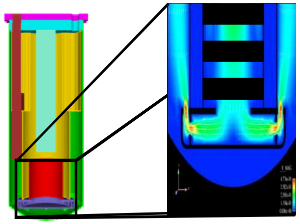
LASSO and LARS

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

Structured or unstructured grids
Value-based or gradient-enhanced



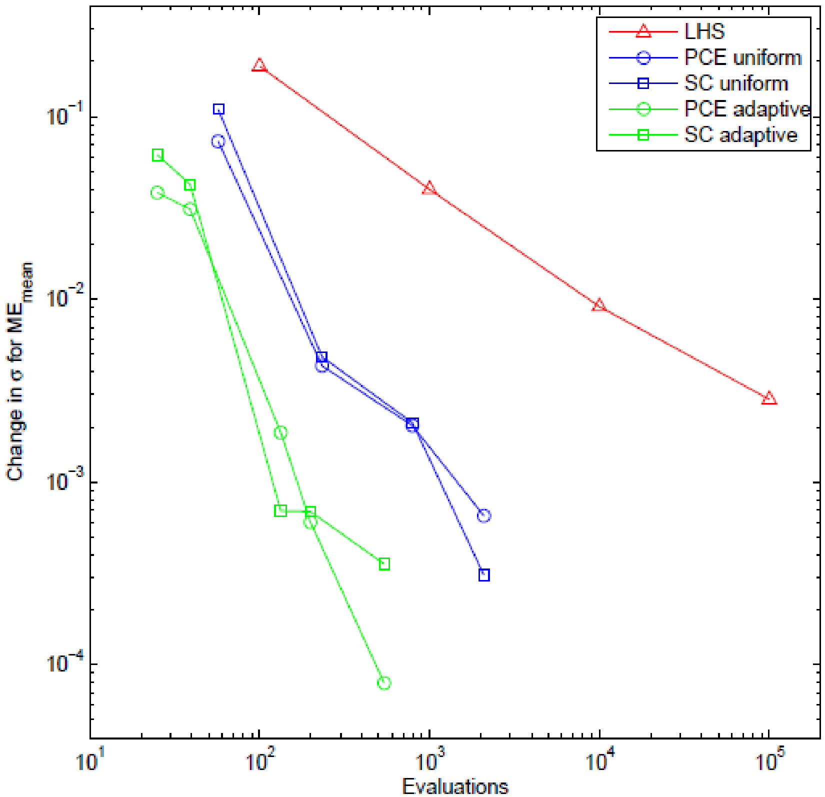
Application Deployment (CASL)



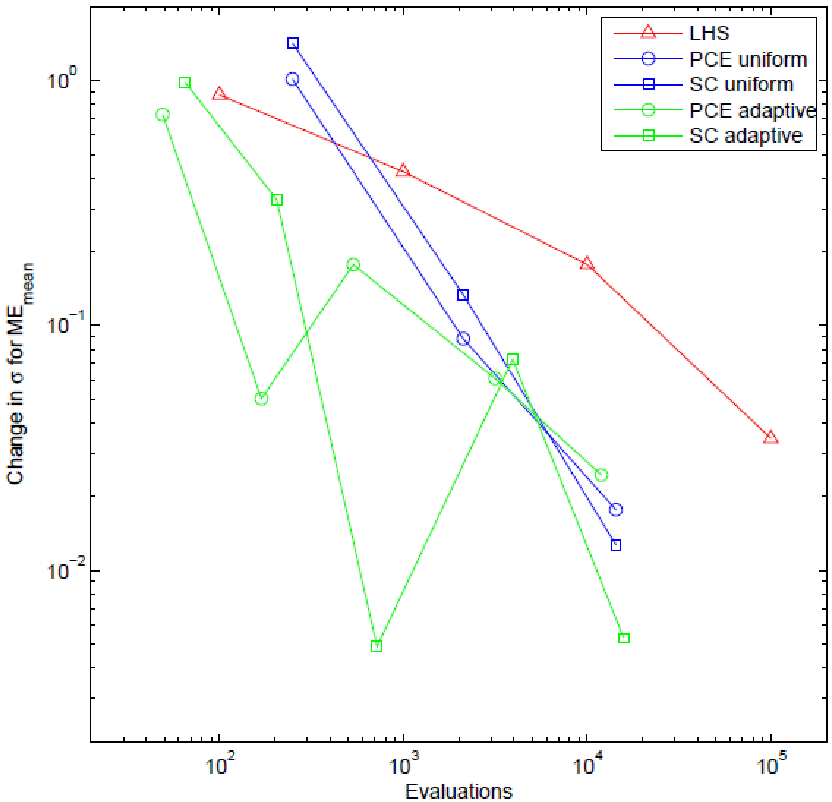
Application: Nuclear reactor cores experience localized boiling, which leads to CRUD (Chalk River Unidentified Deposit). These deposits result in undesirable power shifts (CIPS) within the core. Statistics of mass evaporation (ME) rate are of interest.

Methodology: PCE/SC with uniform/adaptive refinement compared to LHS

Plant A (n=4, smooth, mild anisotropy)



Plant B (n=10, discontinuous, high anisotropy)



Local Error Estimation with Hierarchical Surpluses

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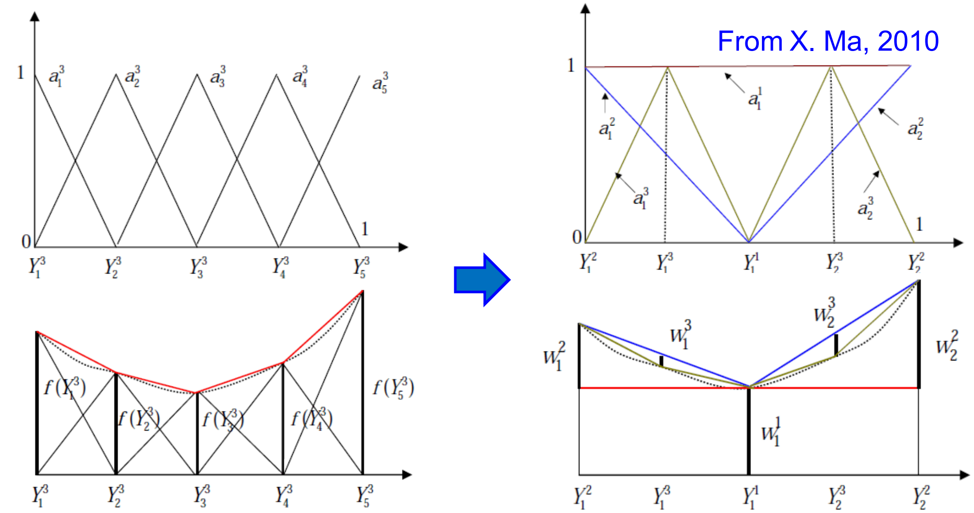
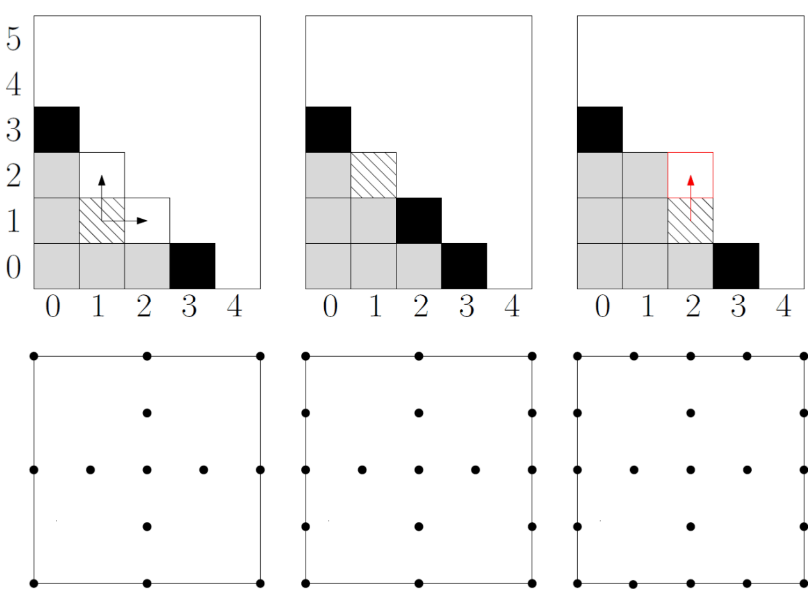
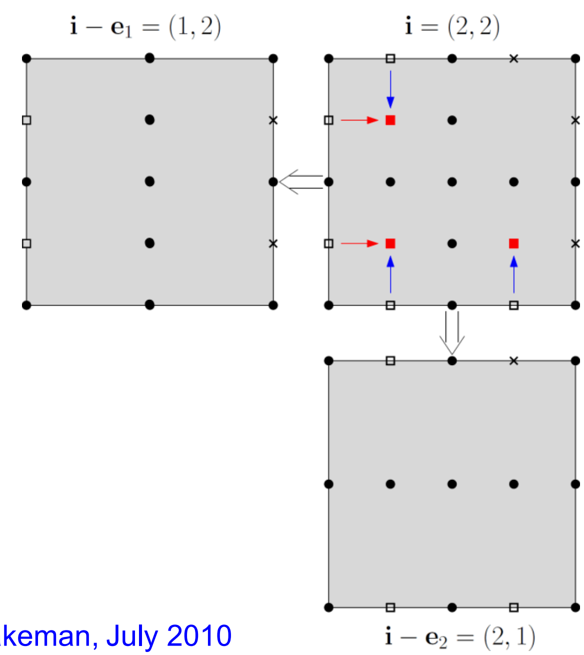
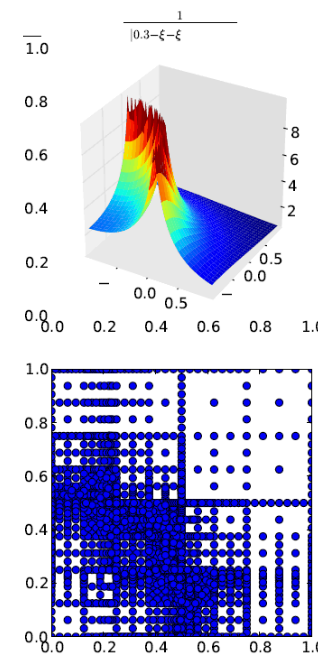
Hierarchical basis:

- *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*



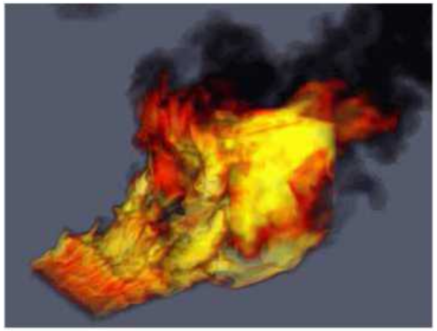






From J. Jakeman, July 2010

NNSA Example: UQ Modernization for Abnormal Thermal Environments



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

- Compared to level 1 sparse grid PCE: captures nonlinear main effects and supports nonlinear sensitivity analysis
  - 2n+1 evaluations at Gauss points → quadratic 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

→ Identified cases of mild and severe nonlinearity (MV ok, MV not ok) in thermal response

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

→ Identified N dominant main+interaction terms within candidate set, efficient global SA via VBD

Core UQ Algorithms: strengths, weaknesses, research needs

Sampling (nongradient-based)

- ***Strengths:*** Simple and reliable, convergence rate is dimension-independent
- ***Weaknesses:*** $N^{-1/2}$ convergence → expensive for accurate tail statistics

Local reliability (gradient-based)

- ***Strengths:*** computationally efficient, widely used, scalable to large *n* (w/ efficient/adjoint derivatives)
- ***Weaknesses:*** algorithmic failures for limit states with following features
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. insufficient to resolve probability at MPP

Global reliability (typically nongradient-based)

- ***Strengths:*** handles multimodal and/or highly nonlinear limit states, tailored for efficient probability estimation
- ***Weaknesses:***
  - Conditioning, nonsmoothness → ensemble emulation (recursion, discretization)
  - Scaling to large *n* → adjoint gradient-enhancement, additional refinement bias

Stochastic expansions (typically nongradient-based)

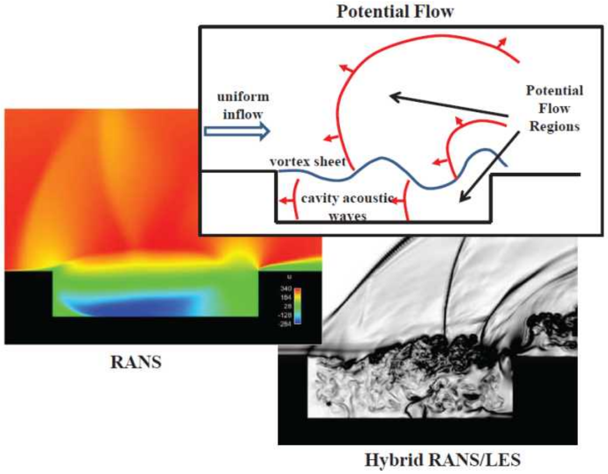
- ***Strengths:*** functional representation, exponential convergence rates for smooth problems, best for moment est.
- ***Weaknesses:***
  - Nonsmoothness → local h-refinement based on hierarchical error estimates
  - Scaling to large *n* → adaptive refinement, adjoint gradient-enhancement, sparsity detection

Epistemic methods (typically nongradient-based)

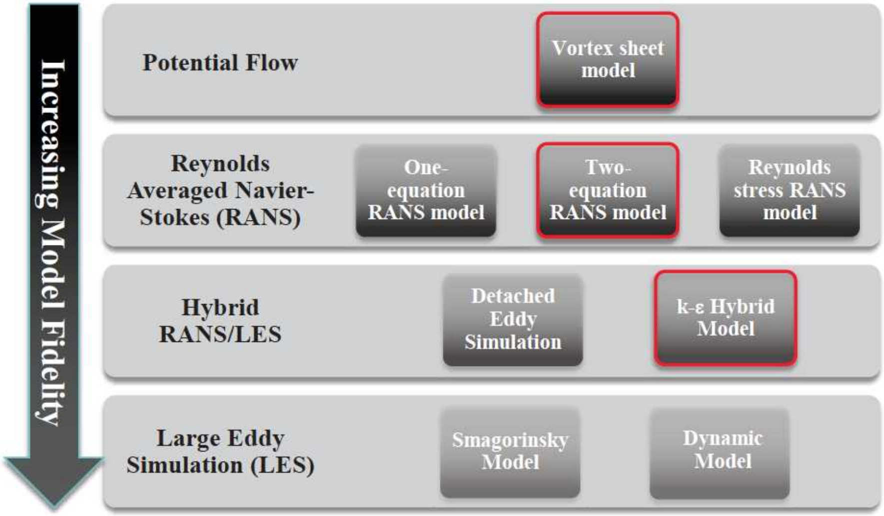
- ***Strengths:*** extrema are point solutions instead of integrated quantities
- ***Weaknesses:*** high degrees of input structure (Dempster-Shafer) require *many* extrema (bridging intervals and distributions breaks down as continuum is approached discretely)

Multiple Model Forms in UQ

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



- A clear hierarchy of fidelity (from low to high)
  - *Multifidelity UQ methods:* generate statistics for truth model leveraging less expensive models
- An ensemble of models that are all credible (lacking a clear preference structure): e.g., turbulence models
  - *Without (adequate) data:* epistemic model form uncertainty propagation
  - *With data:* Bayesian model selection
- Both hierarchy and peers
  - *Multifidelity inference:* calibration enables resolution of low complexity discrepancies



Multifidelity UQ using Stochastic Expansions

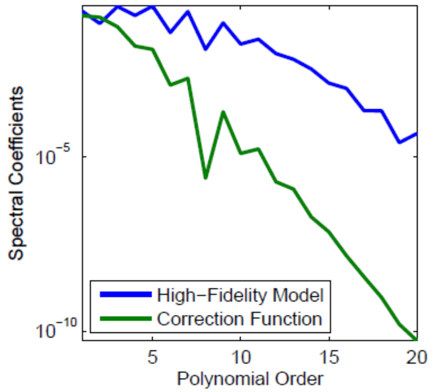
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity “design” codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

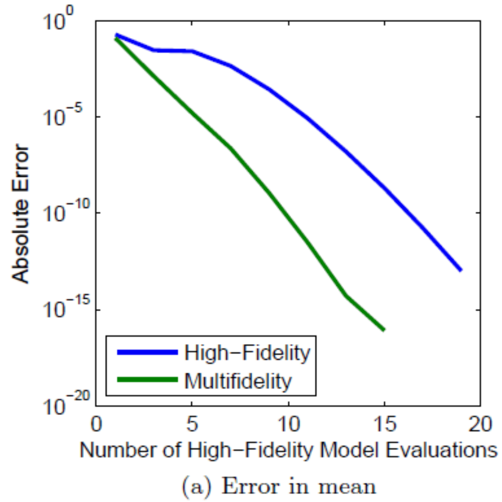
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

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

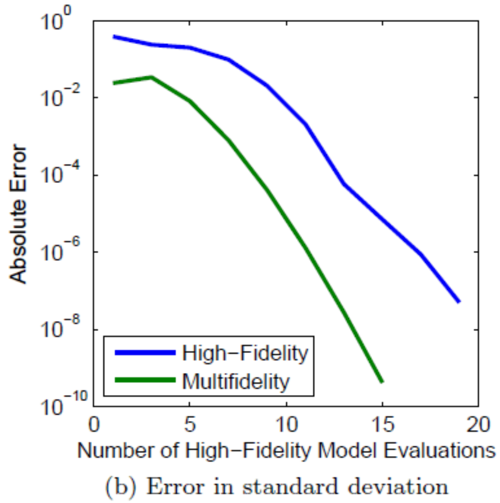
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5 e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

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





(a) Error in mean



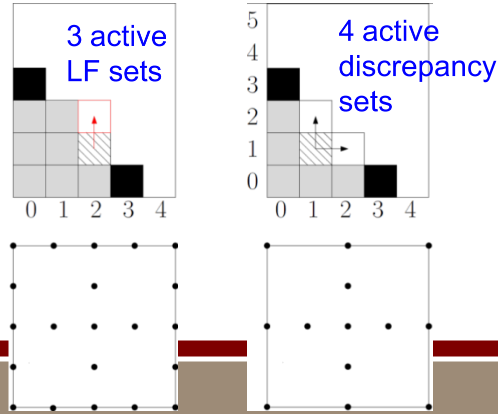
(b) Error in standard deviation

Adaptive sparse grid multifidelity algorithm:

- Generalized sparse grids for LF & each discrepancy level
- Greedy selection among multiple grids: max ΔQoI/ΔCost
- Refines discrepancy where LF is less predictive

Compressive sensing multifidelity algorithm:

- Target sparsity within the model discrepancy



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).

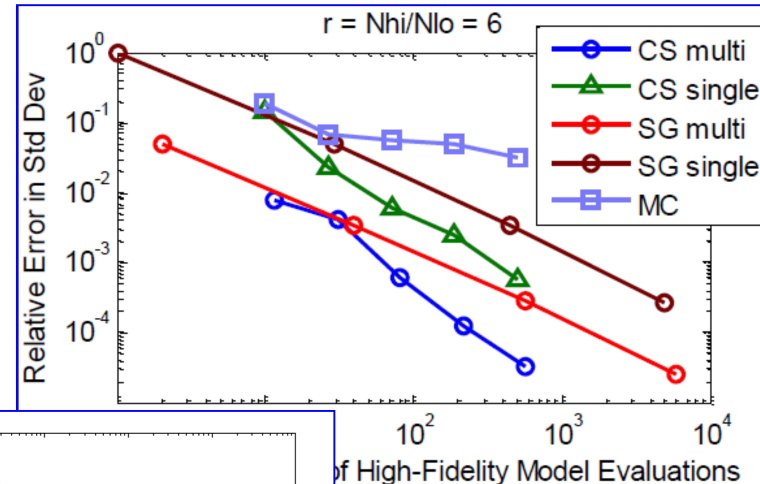
LF = coarse spatial grid with 50 states.

HF = fine spatial grid with 500 states.

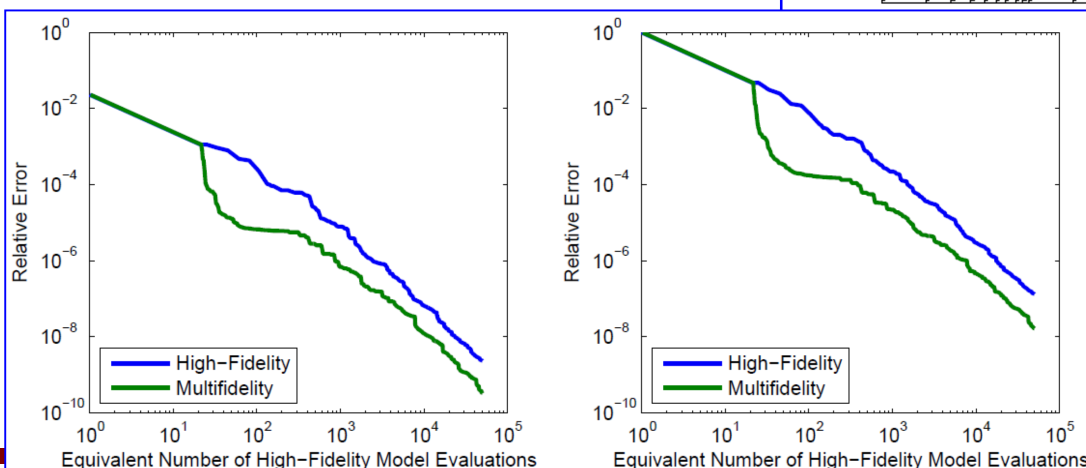
Expense ratio = 40.

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 Sparse Grid



(a) Error in mean

(b) Error in standard deviation

ASCR MF UQ example: VAWT Gust Response

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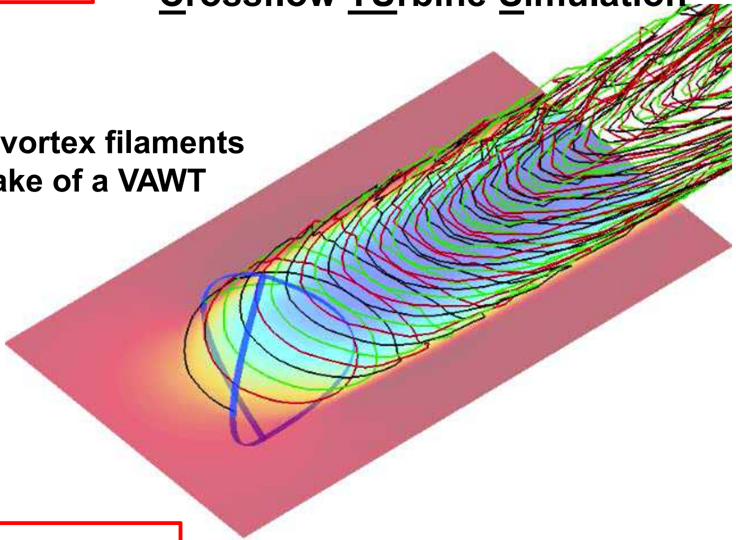
Vertical-axis Wind Turbine (VAWT)

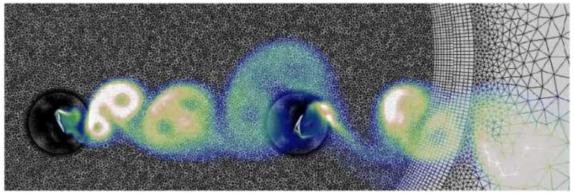
Low fidelity

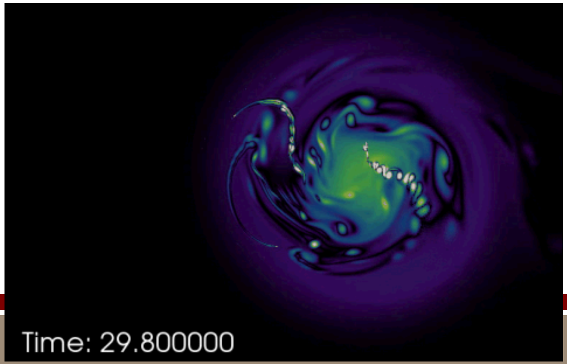
CACTUS: Code for Axial and Crossflow TUrbine Simulation

Computed vortex filaments in the wake of a VAWT



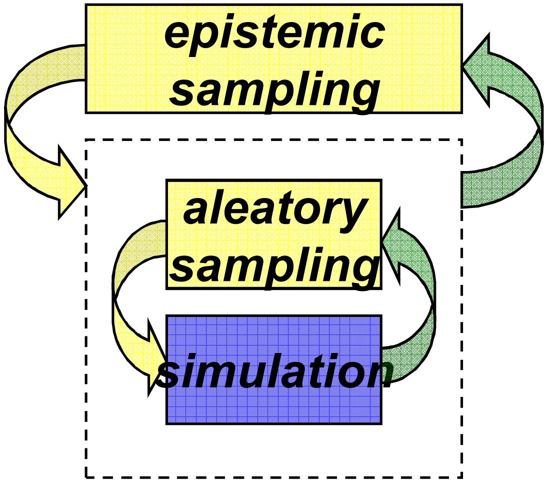
High fidelity: DG formulation for LES





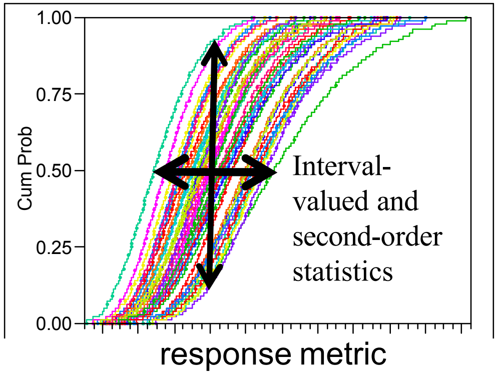
Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

Epistemic uncertainty (aka: subjective, reducible, lack of knowledge uncertainty): insufficient info to specify objective probability distributions



Traditional approach: nested sampling

- Expensive sims → 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)

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

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

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

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Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β

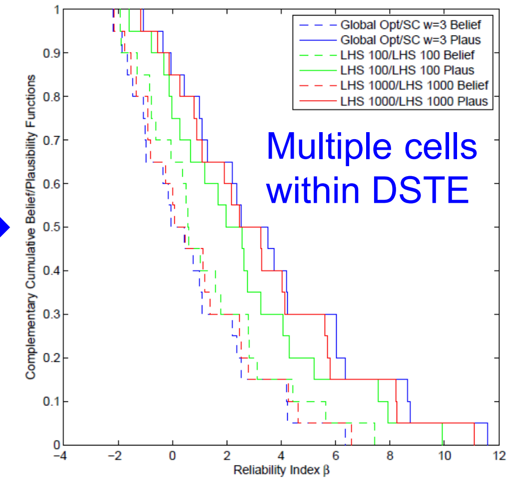
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals

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

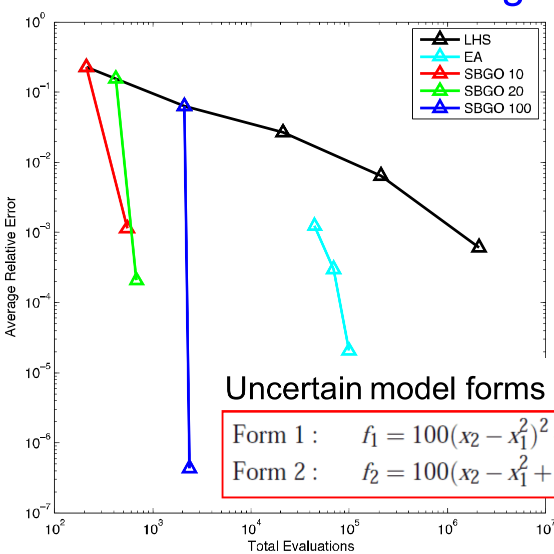
LHS 100	LHS 100	N/A	$(10^4/10^4, 0/0)$	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	$(10^6/10^6, 0/0)$	[76.5939, 368.225]	[-2.19883, 11.2353]
LHS 10^4	LHS 10^4	N/A	$(10^8/10^8, 0/0)$	[76.4755, 373.935]	[-2.16323, 11.5593]

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



Multiple cells within DSTE

Interval est w/ mixed-integer global opt



Uncertain model forms (Rosenbrock)

Form 1 : $f_1 = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

Form 2 : $f_2 = 100(x_2 - x_1^2 + .2)^2 + (0.8 - x_1)^2$

Drekar RANS turbulence: Spalart-Allmaras, k-ε with Neumann BC, k-ε with Dirichlet BC

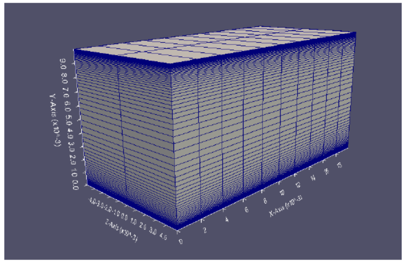


Figure 4. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

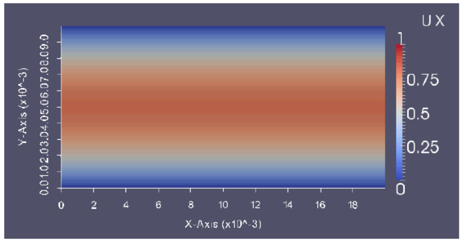


Figure 5. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

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]

Office of Science Example: SciDAC (PISCEES)

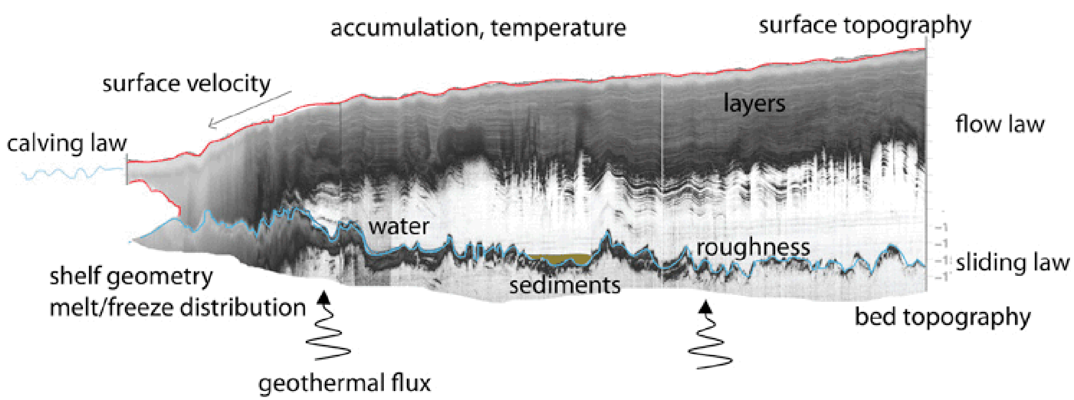
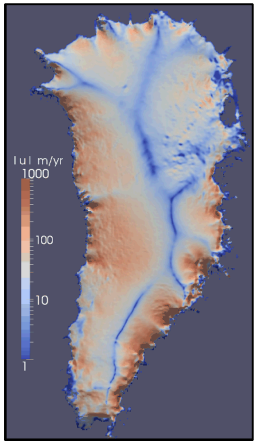
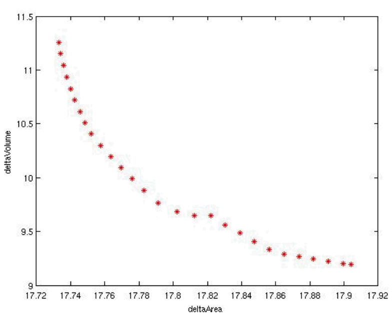


Figure 1: Schematic of observations, boundary conditions, and processes affecting ice sheet initialization.



Greenland surface ice velocity

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

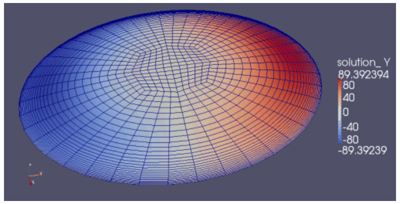
deltaVolume Sobol indices:

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

Model problem: ice dome in FELIX

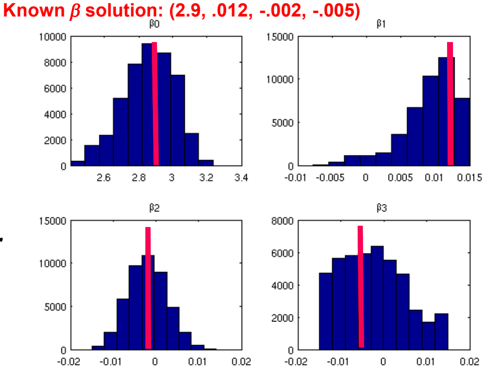


Ice sheet initialization from (synthetic) data using Bayesian calibration

Basal sliding field (4 param):

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

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



Summary

Sandia National Laboratories

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 developing a broad suite of scalable and robust core UQ methods with a focus on addressing a critical gap that has existed with popular production methods
- Within the highlighted area of stochastic expansions:
  - Adaptive refinement, adjoint enhancement, sparsity detection
  - Suite of formulations: local / global, value / gradient, structured / unstructured, nodal / hierarchical
- We are building on this foundation
  - Multifidelity UQ, Mixed UQ including model form, Bayesian inference

Impact and deployment

- UQ tools deployed through Dakota (v5.3.1 released 5/15/13, v5.4 scheduled 11/15/13)
- Impact with NNSA (stockpile), Energy (wind, nuclear), and Climate (community earth/ice