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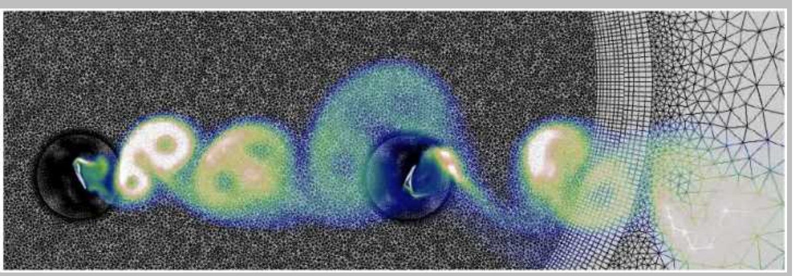

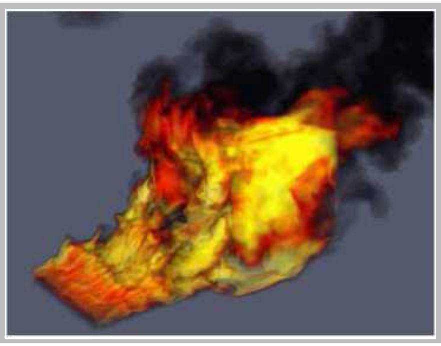

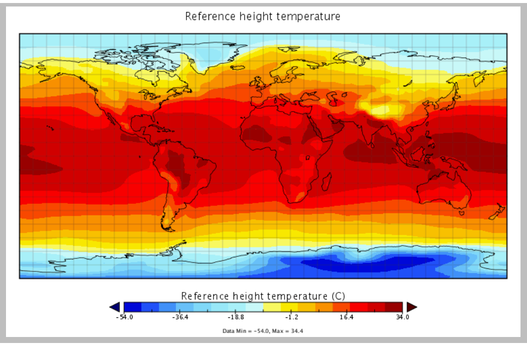

Building on the Foundation: Optimization Under Uncertainty and Related Topics

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Optimization Under Uncertainty

Standard NLP

$$\begin{aligned} \min \quad & f(d) \\ \text{s.t.} \quad & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \end{aligned}$$

optimize, accounting for uncertainty metrics

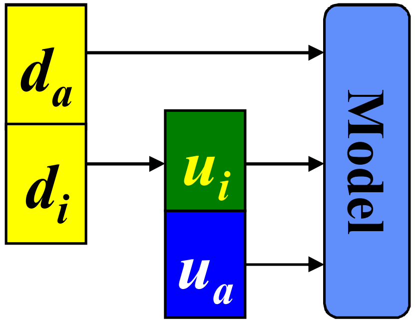
(using any UQ method)

Add resp stats s_u $(\mu, \sigma, z/\beta/p)$

$$\begin{aligned} \min \quad & f(d) + W s_u(d) \\ \text{s.t.} \quad & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \\ & a_l \le A_i s_u(d) \le a_u \\ & A_e s_u(d) = a_t \end{aligned}$$

Input design parameterization

- **Design vars may augment uncertain vars in simulation**
- **Inserted design vars: an optimization design var may be a parameter of an uncertain dist, e.g., the mean of a normal**



Control response statistics to design for…

…robustness:

min/constrain moments μ, σ^2, or $z(\beta)$ range

…reliability:

min/max/constrain p/β (tail stats, failure)

…combined/other:

Pareto, inversion/model calibration under uncertainty

Epistemic/Mixed

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	Adaptive 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, tensor, sparse)	Dimension-adaptive p-/h-refinement, grad-enhancement, sparsity detection	Local adapt refinement, adjoint EE, discrete vars	Stanford, Utah
Epistemic & Mixed UQ	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

UQ with Sampling Methods

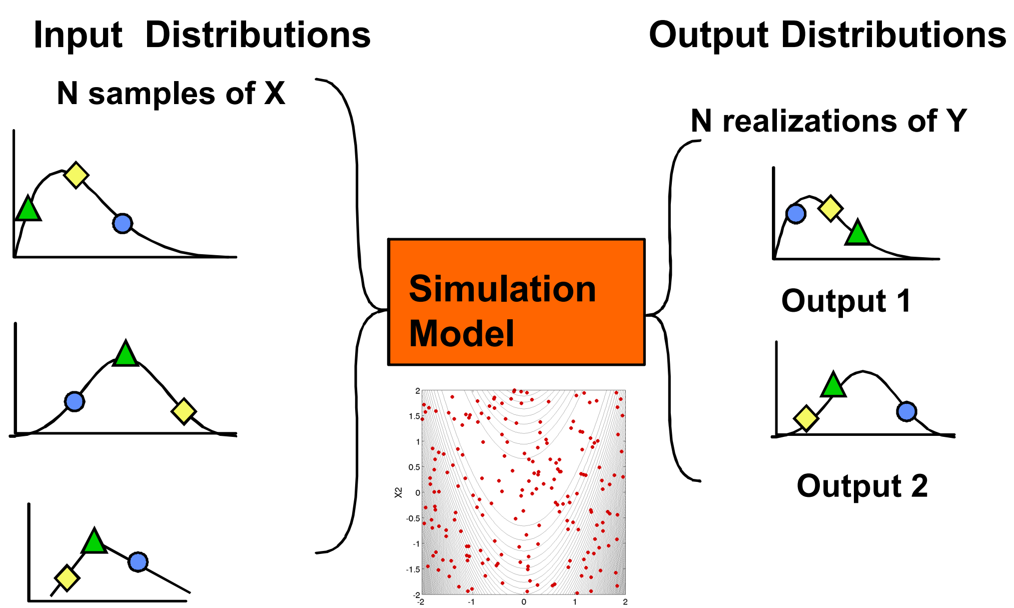
Starting from distributions on the uncertain input values, draw observations from each distribution, pair samples, and execute the model for each pairing

→ ensemble of results yields distributions of the outputs

- Monte Carlo: **basic random sampling**
- Pseudo Monte Carlo: **Latin Hypercube Sampling (LHS)**
- Quasi Monte Carlo: **Halton, Hammersley, Sobol sequences**
- Orthogonal arrays, Centroidal Voronoi Tesselation (CVT), Importance Sampling

Advantage: **Sampling is easy to implement, robust, and transparent.**

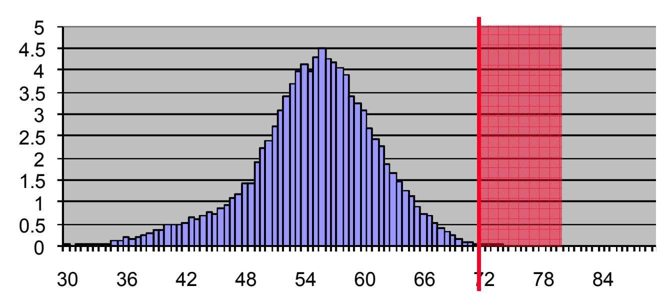
Disadvantage: **$N^{-1/2}$ convergence, often impractical for p_{fail}, stats nonsmooth over d**



- **sample mean and variance**

$$\bar{T} = \frac{1}{N}\sum_{i=1}^{N} T(u^i) \qquad T_{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}\left[T(u^i) - \bar{T}\right]^2$$

- **full PDF(probabilities)**

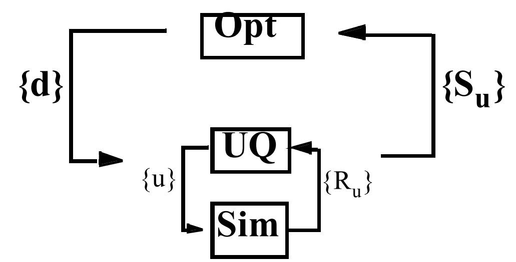


Optimization under Uncertainty with Surrogates

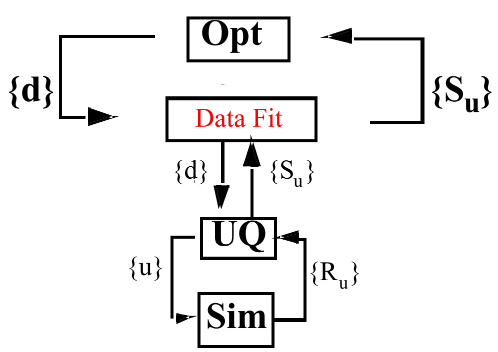
SBOUU: employ ***surrogate models*** for interpolation of noisy data and approximation of expensive simulations and/or statistics.

- Data fit (global, local, multipoint)
- Multifidelity
- Reduced-order models (ROM)

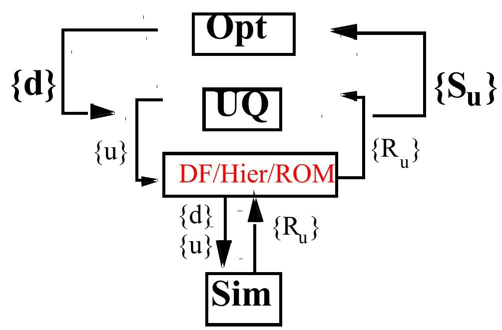
Rely on ***truth models*** for surrogate construction, updating, and step verification



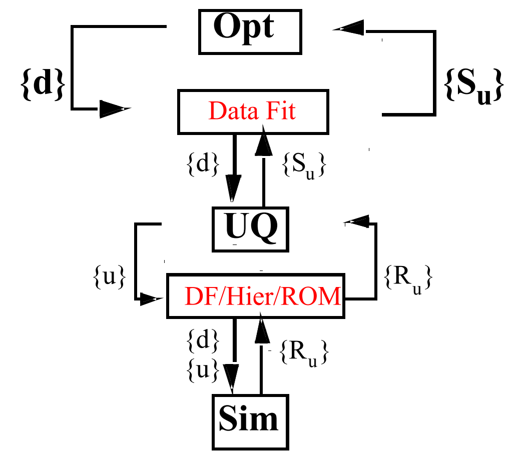
Formulation 1:
Nested (no surrogate)



Formulation 2:
Design Surrogate



Formulation 3:
UQ Surrogate



Formulation 4:
Design and UQ Surrogates

Formulations 2 & 4 amenable to trust-region approaches

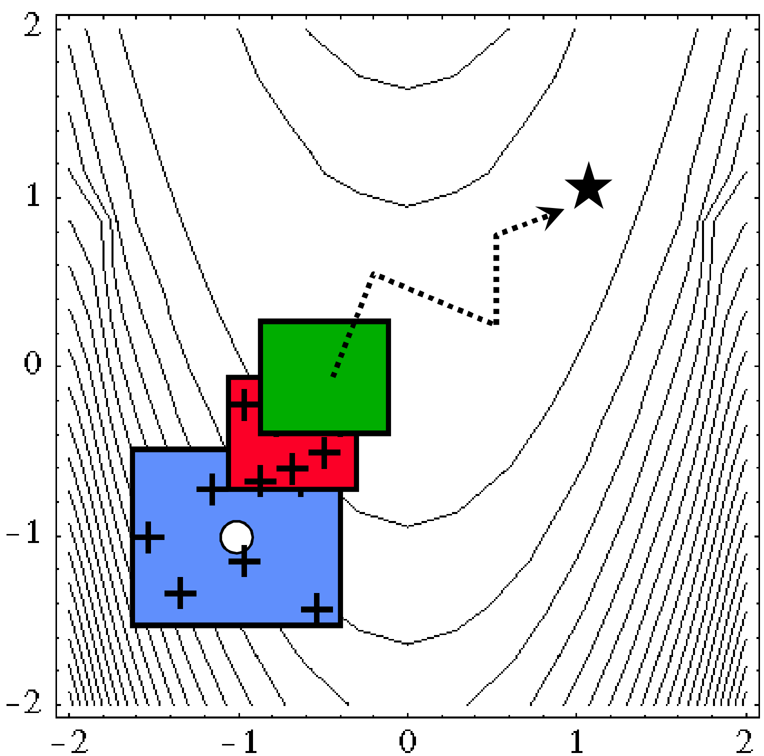
Goals: **maintain quality of results, provable convergence (for a selected confidence level)**

Trust Region Surrogate-Based Optimization (SBO) – Data Fit Case

Data fit surrogates:

- *Global:* polynomial resp surf, NN, splines, kriging/GP, radial basis fn
- *Local:* 1st/2nd-order Taylor series
- *Multipoint*: two-point exponential approx (TPEA), two-point adaptive nonlinearity approx (TANA)

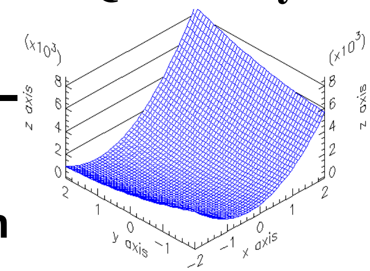
Sequence of trust regions



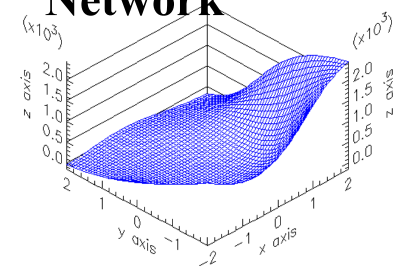
(Global) data fits in SBO:

- Smoothing: extract desired global trend from noisy data
- DACE: number of design variables limited to $O(10^1)$
- Local consistency must be balanced with global accuracy
  - Constrained LLS
  - TS w/ global Hessian estimation

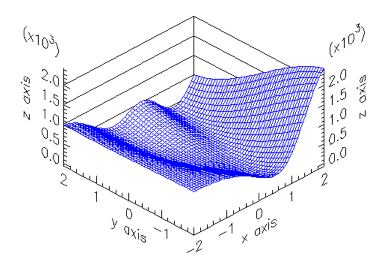
Quad Poly



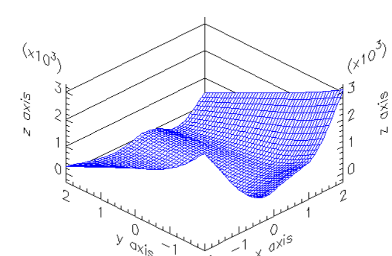
Neural Network



Kriging

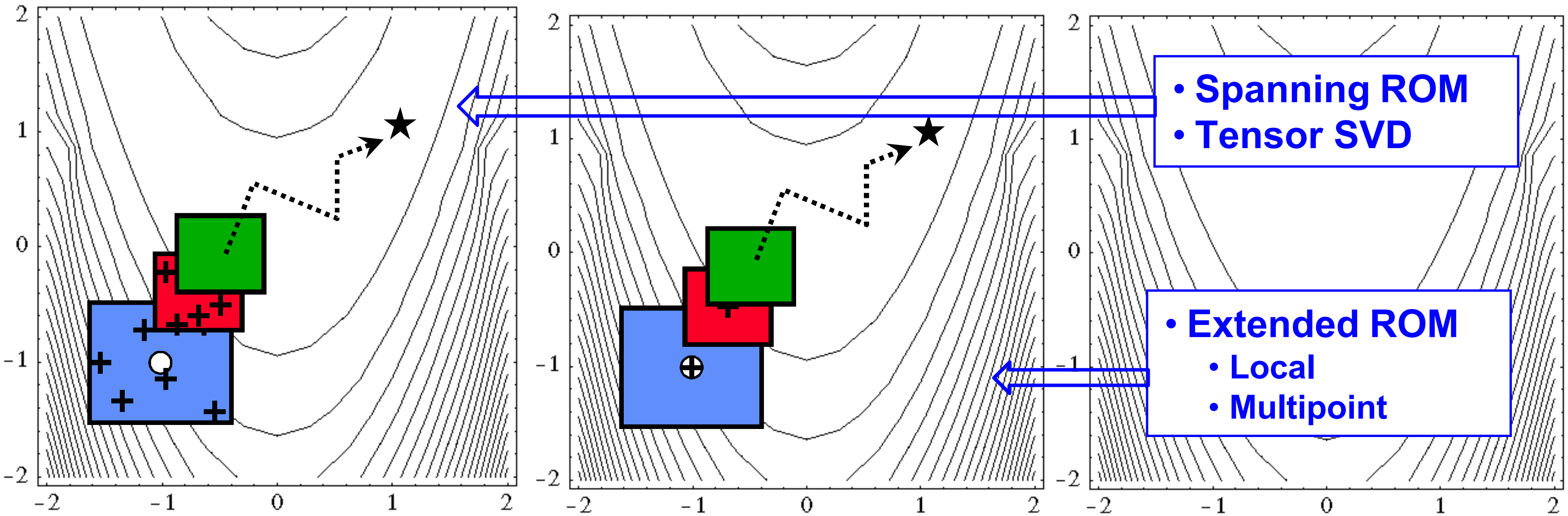


Splines



Trust-Region Surrogate-Based Optimization

Data Fit → *Multifidelity* → *ROM*



Data fit surrogates:

- Global: polynomial regress., splines, neural net, kriging/GP, radial basis fn
- Local: 1st/2nd-order Taylor
- Multipoint: TPEA, TANA, …

Data fits in SBO

- Smoothing: extract global trend
- DACE: number of des. vars. limited
- Local consistency must be balanced with global accuracy

Multifidelity surrogates:

- Coarser discretizations, looser conv. tols., reduced element order
- Omitted physics: e.g., Euler CFD, panel methods

Multifidelity SBO

- HF evals scale better w/ des. vars.
- Requires smooth LF model
- May require design vect. mapping
- Correction quality is ***crucial***

ROM surrogates:

- Spectral decomposition (str. dynamics)
- POD/PCA w/ SVD (CFD, image analysis)
- KL/PCE (random fields, stoch. proc.)

ROMs in SBO

- Key issue: capture parameter changes
  - E- ROM, S-ROM, tensor SVD
- Some simulation intrusion to re-project
- TR progressions resemble local, multipoint, or global

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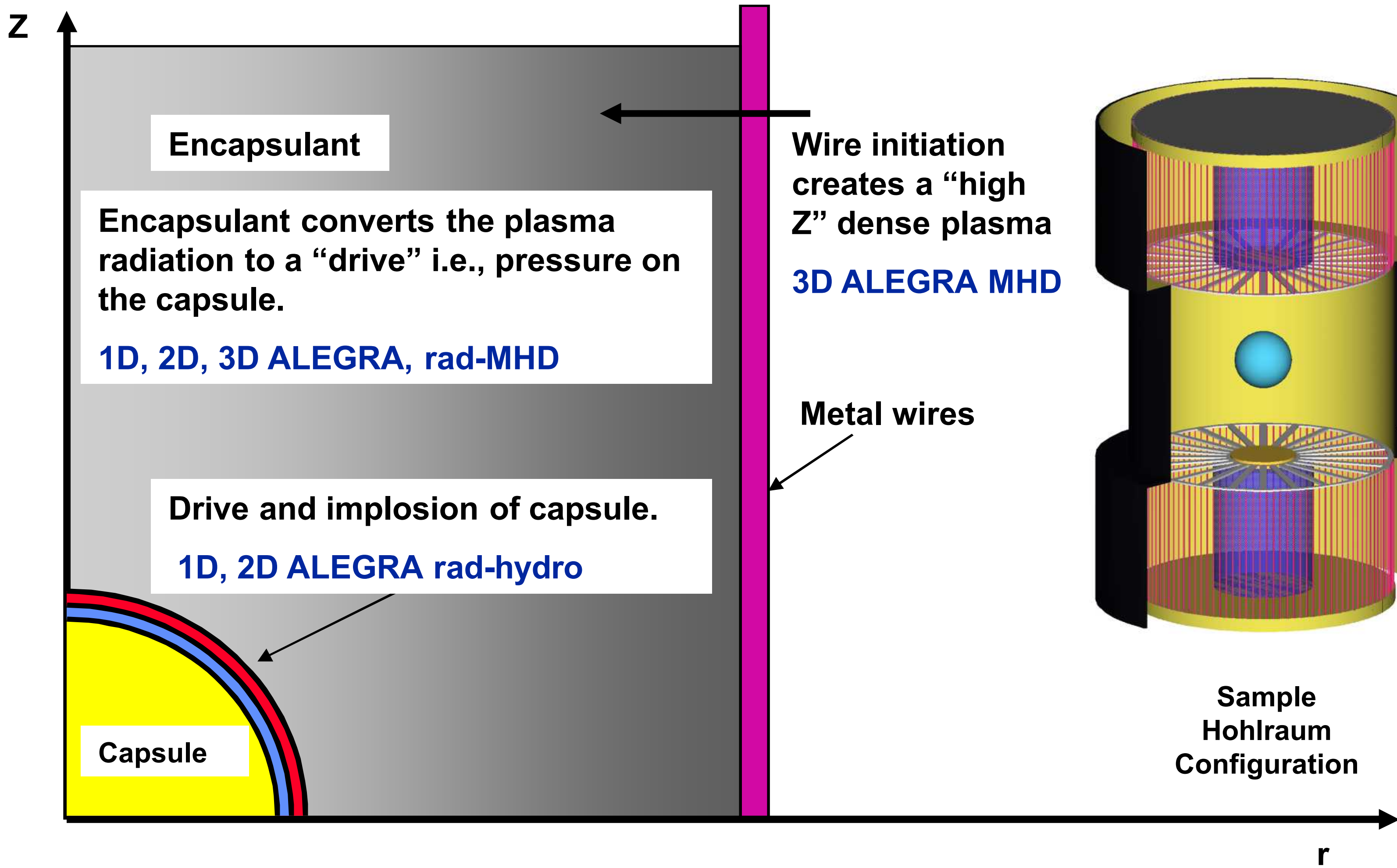
TR-SBOUU Benchmark Results

- **Direct nested OUU is expensive and requires seed reuse**
- **SBOUU expense much lower (up to 100x), but unreliable.**
- **TR-SBOUU maintains quality of results and reduces expense ~10x**
  - **Ex. 1: formulation 4 with TR 5-7x less expensive than direct nesting**
  - **Ex. 2: formulation 4 with TR 8-12x less expensive than direct nesting**
  - **ICF Ex.: formulations 2/4 with TR locate vicinity of a min in a single cycle**
- **Greater algorithmic robustness:**
  - **Navigation of nonsmooth engineering problems**
  - **Less sensitive to seed reuse: variable patterns OK and often helpful, possibility of exploitation of poor sample design is reduced**
  - **Less sensitive to starting point: data fit SBO provides some global identification**
- **Primary weakness:**
  - **Resolution of statistics with (under-resolved) sampling → best for moments & their projections**

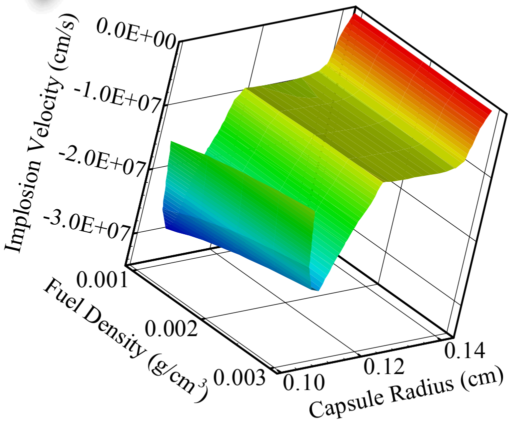
2002-2003 conference papers (AIAA MA&O, SIAM CS&E, USNCCM): Eldred, M.S., Giunta, A.A., Wojtkiewicz, S.F., Jr., and Trucano, T.G., "Formulations for Surrogate-Based Optimization Under Uncertainty."

Robust Hohlraum Design for Inertial Confinement Fusion



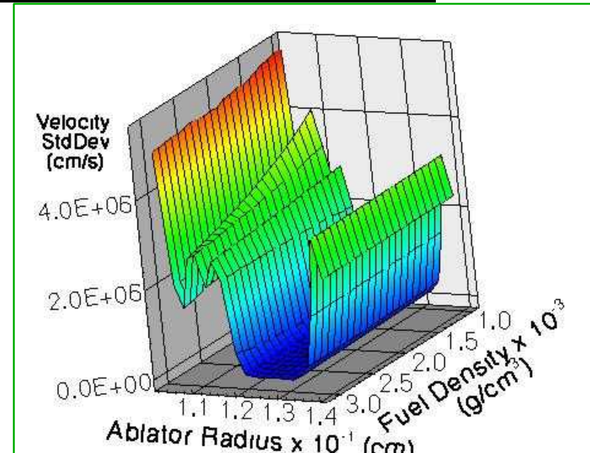
Uncertainties in: plasma, drive, and capsule characteristics

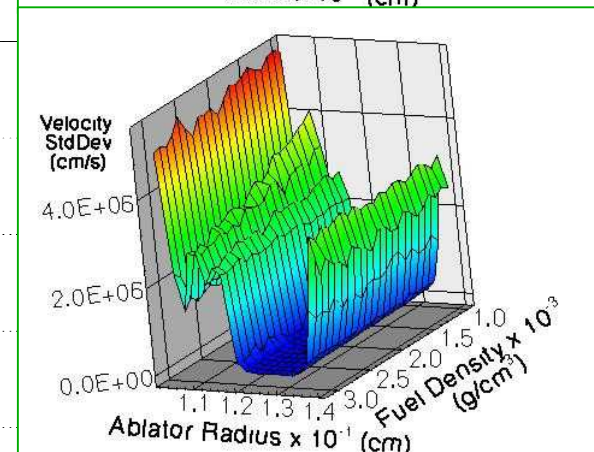
ICF Capsule Design
2D Optimization

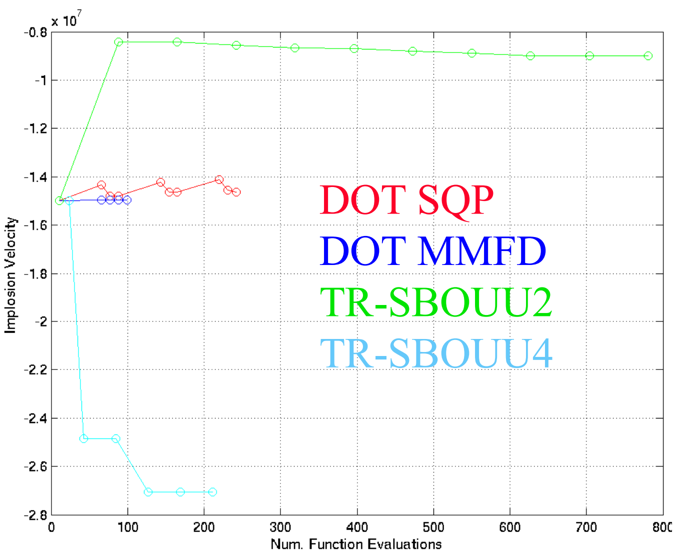


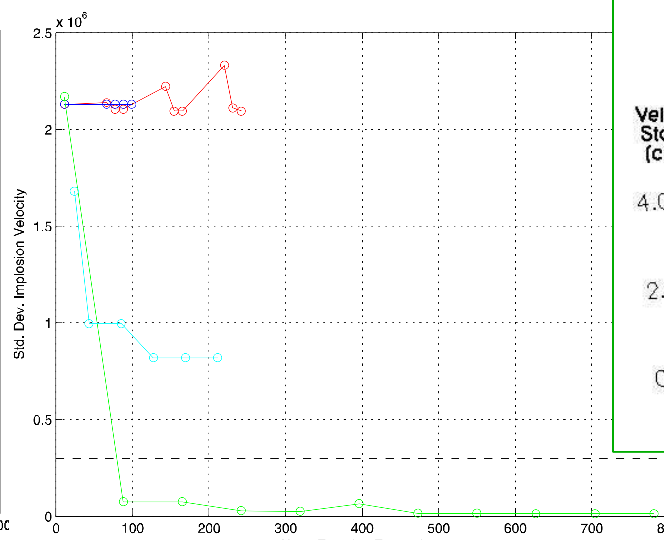
$$\underset{\mu_r,\mu_P}{\text{Maximize}} \; -V$$

s.t.
$$\sigma_V \le 3.e{+}5 \text{ cm/s}$$
$$0.103 \text{ cm} \le \mu_r \le 0.14 \text{ cm}$$
$$0.001 \text{ g/cc} \le \mu_\rho \le 0.003 \text{ g/cc}$$
$$R = \mathrm{U}[\mu_r - 2.5\text{e-}3,\ \mu_r + 2.5\text{e-}3]$$
$$P = \mathrm{U}[\mu_\rho - 2.5\text{e-}5,\ \mu_\rho + 2.5\text{e-}5]$$









- Nested OUU stalls
- TR-SBOUU finds solution vicinity in a single cycle, effectively stepping over nonmoothness in $V(r)$, $\sigma_V(r)$ (objective/constraint are multimodal → min dependent on initial TR)
- Less sensitive to seed reuse and starting point

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UQ with Reliability Methods

Mean Value Method

$$\mu_g = g(\mu_{\mathbf{x}})$$

$$\sigma_g = \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})$$

$$\bar{z} \rightarrow p, \beta \begin{cases} \beta_{cdf} = \dfrac{\mu_g - \bar{z}}{\sigma_g} \\ \beta_{ccdf} = \dfrac{\bar{z} - \mu_g}{\sigma_g} \end{cases}$$

$$\bar{p}, \bar{\beta} \rightarrow z \begin{cases} z = \mu_g - \sigma_g \bar{\beta}_{cdf} \\ z = \mu_g + \sigma_g \bar{\beta}_{ccdf} \end{cases}$$

Rough statistics

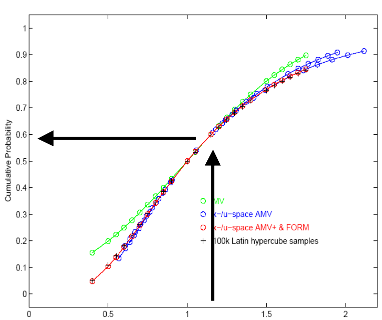
MPP search methods

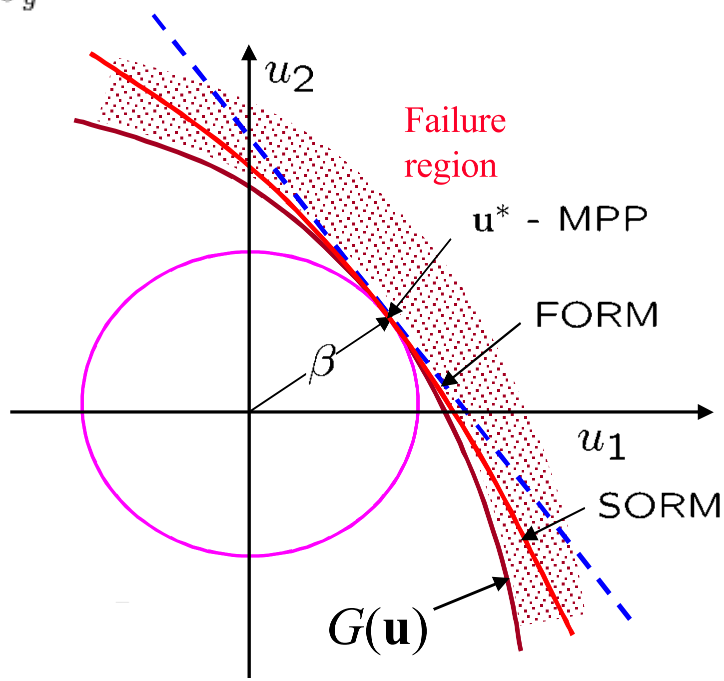
Reliability Index Approach (RIA)

$$\text{minimize} \quad \mathbf{u}^T\mathbf{u}$$
$$\text{subject to} \quad G(\mathbf{u}) = \bar{z}$$

Find min dist to G level curve

Used for fwd map $z \rightarrow p/\beta$





Nataf x → u: $\Phi(z_i) = F(x_i)$

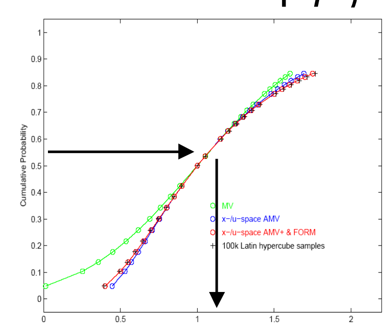
$\mathbf{z} = \mathbf{L}\mathbf{u}$

Performance Measure Approach (PMA)

$$\text{minimize} \quad \pm G(\mathbf{u})$$
$$\text{subject to} \quad \mathbf{u}^T\mathbf{u} = \bar{\beta}^2$$

Find min G at β radius

Used for inv map $p/\beta \rightarrow z$



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RBDO Algorithms

Bi-level/Nested RBDO

- **Constrain RIA *z* → *p/β* result**
- **Constrain PMA *p/β* → *z* result**

RIA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \\ \text{or} & p \leq \bar{p} \end{cases}$$

PMA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Analytic Bi-level RBDO

- **Analytic reliability sensitivities avoid numerical differencing at design level**

$$\begin{cases} \nabla_{\mathbf{d}} z = \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} \beta_{cdf} = \dfrac{1}{\| \nabla_{\mathbf{u}} G \|} \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} p_{cdf} = -\phi(-\beta_{cdf}) \nabla_{\mathbf{d}} \beta_{cdf} \end{cases}$$
(1st order)

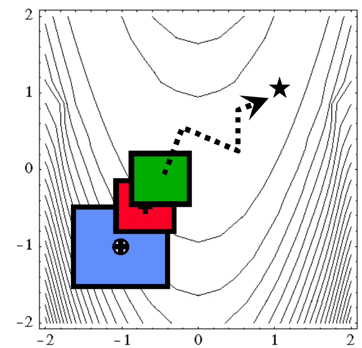
If $\mathbf{d}$ = distr param, then expand
$$\nabla_{\mathbf{d}} g = \nabla_{\mathbf{d}} \mathbf{x} \nabla_{\mathbf{x}} g$$

Sequential/Surrogate-based RBDO:

- **Break nesting: iterate between opt & UQ until target is met. Trust-region surrogate-based approach is non-heuristic.**

$$\begin{array}{ll} \text{minimize} & f(\mathbf{d}_c) + \nabla_d f(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \\ \text{subject to} & \beta(\mathbf{d}_c) + \nabla_d \beta(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \geq \bar{\beta} \\ \text{or} & p(\mathbf{d}_c) + \nabla_d p(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \leq \bar{p} \\ & \| \mathbf{d} - \mathbf{d}_c \|_\infty \leq \Delta^k \end{array}$$

1^{st}-order (also 2^{nd}-order w/ QN)



Unilevel RBDO:

- **All at once: apply KKT conditions of MPP search as equality constraints**
  - Opt. increases in scale (***d***,***u***)
  - Requires 2nd-order info for derivatives of 1st-order KKT

$$\begin{array}{rl} \min\limits_{\mathbf{d}_{aug}=(\mathbf{d},\mathbf{u}_1,..,\mathbf{u}_{N_{hard}})} & : f(\mathbf{d}, \mathbf{p}, \mathbf{y}(\mathbf{d}, \mathbf{p})) \\ \text{s. t.} & : G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_{allowed} - \beta_i \geq 0 \\ & \|\mathbf{u}_i\| \, \|\nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta)\| + \mathbf{u}_i^T \nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_i = \|\mathbf{u}_i\| \\ & \mathbf{d}^l \leq \mathbf{d} \leq \mathbf{d}^u \end{array}$$

KKT of MPP

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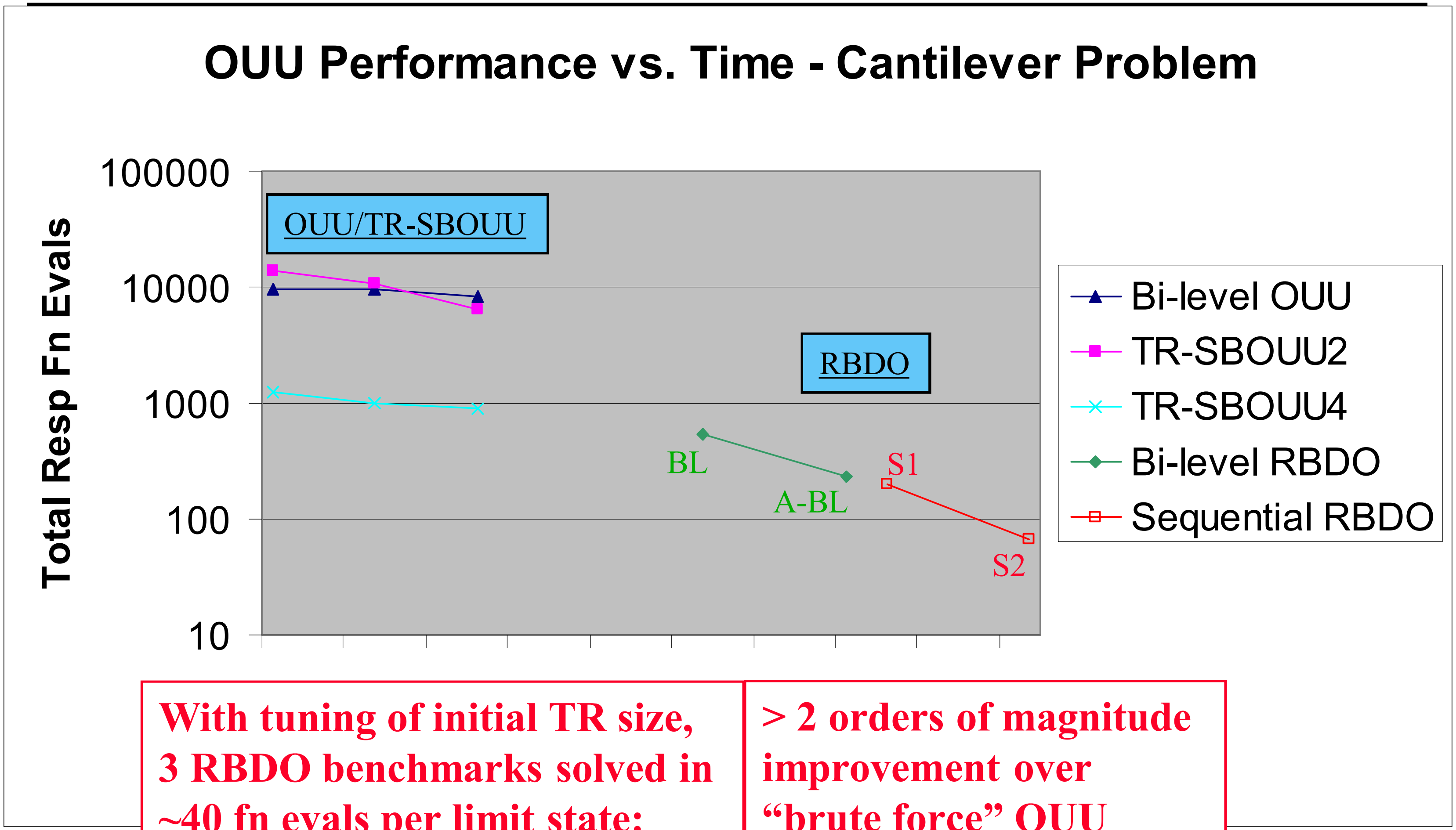
OUU Progress (2002-2005)



With tuning of initial TR size, 3 RBDO benchmarks solved in ~40 fn evals per limit state:

- 35 for 1 limit state in short column
- 75 for 2 limit states in cantilever
- 45 for 1 limit state in steel column

> 2 orders of magnitude improvement over "brute force" OUU

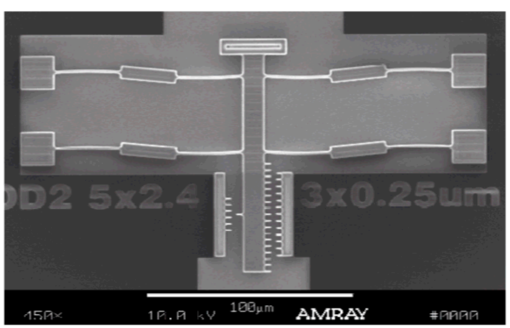
Shape Optimization of Compliant MEMS

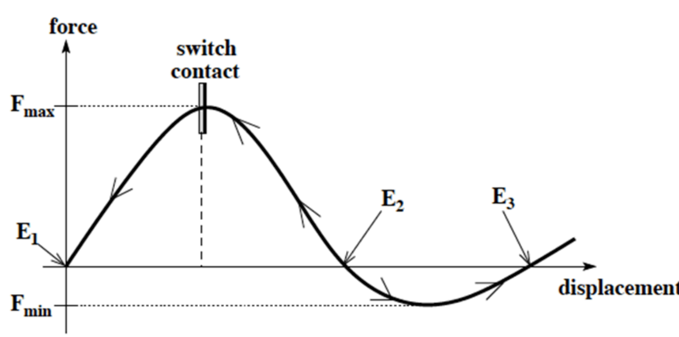
- **MEMS subject to substantial variabilities & lack historical knowledge base**
- **Sources of uncertainty**
  - **Material properties, manufactured geometries, residual stresses**
  - **Data can be obtained → aleatoric uncertainty, probabilistic approaches**
- **Resulting part yields can be low or have poor cycle durability**

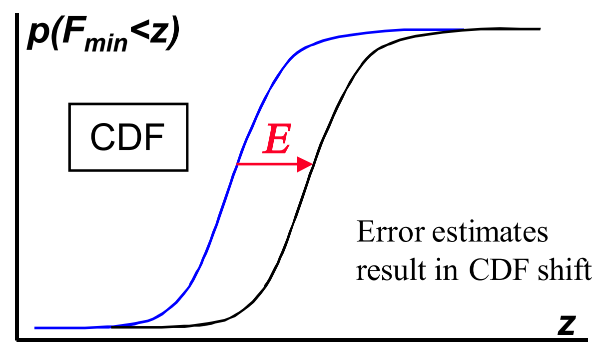
ASC Milestone: Solution-Verified Reliability Analysis & Design of MEMS

- **Account for both manufacturing uncertainties and simulation errors in MEMS design**
- **Integrate UQ/RBDO (DAKOTA), ZZ/QOI error est (Coda), adapt (SIERRA), nonlin mech (Aria)**
- **Goals: On-line soln verification → project UQ/OUU results to fully converged mesh; Achieve prescribed reliability; Minimize sensitivity to uncertainties (robustness)**

Bi-stable MEMS Switch

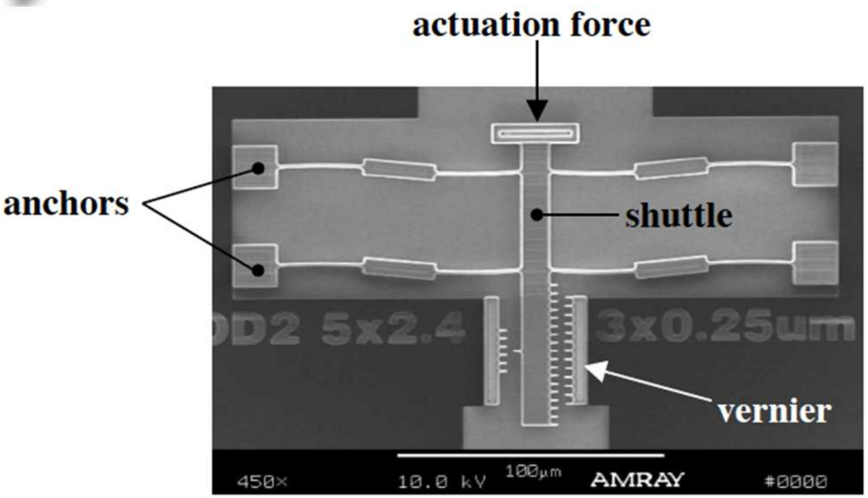


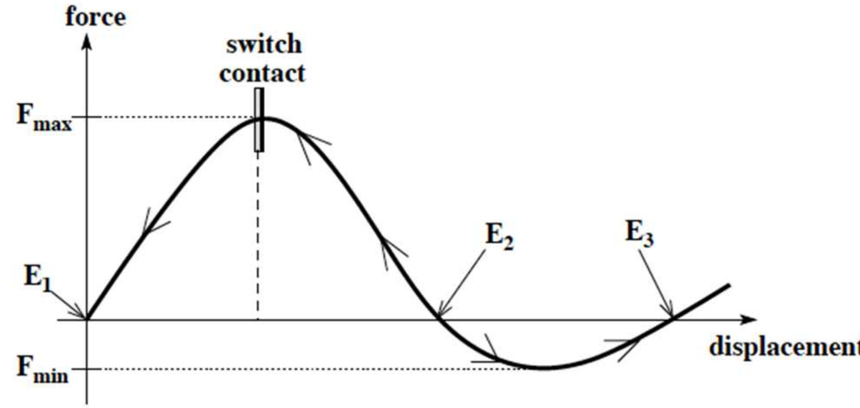


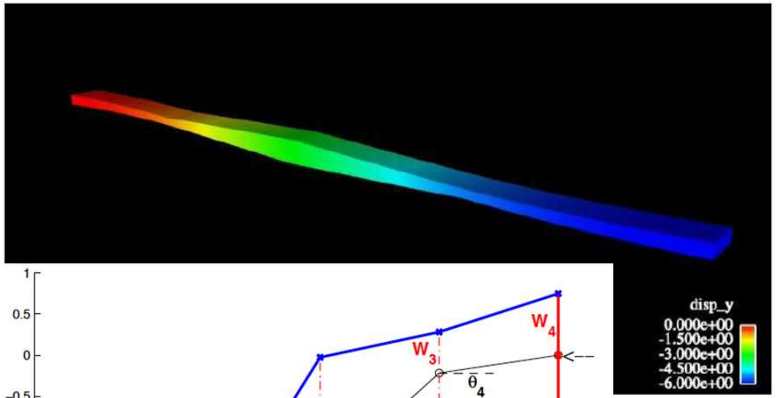


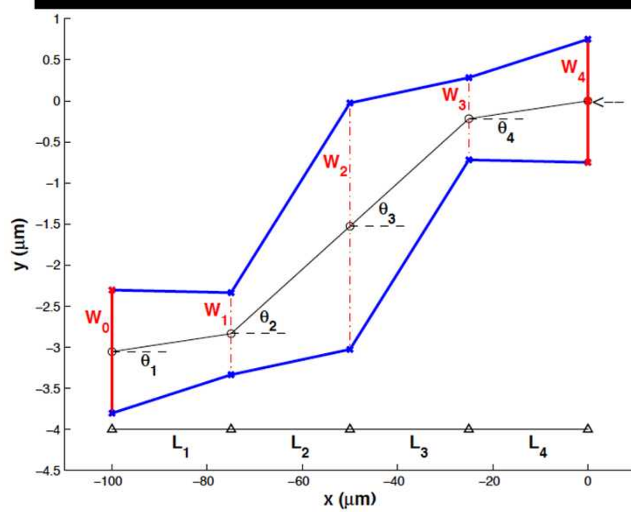
- ***Error-corrected*: EE as analysis correction factors**
- ***Error-informed*: EE as indicators for uniform/adaptive refinement (tight tols: eliminate correction)**
- ***Combined*: control error levels (loose tols: assure correction accuracy) & use correction factors**

Bi-Stable Switch: Problem Formulation









13 design vars: W_i, L_i, θ_i

2 random vars:

variable	mean (μ)	std. dev.	distribution
ΔW (width bias)	-0.2 μm	0.08	normal
S_r (residual stress)	-11 Mpa	4.13	normal

$$
\begin{array}{llcll}
\max & & \mathrm{E}\left[F_{min}(\mathbf{d},\mathbf{x})\right] & & \\
\text{s.t.} & 2 \leq & \beta_{ccdf}(\mathbf{d}) & & \\
 & 50 \leq & \mathrm{E}\left[F_{max}(\mathbf{d},\mathbf{x})\right] & \leq & 150 \\
 & & \mathrm{E}\left[E_2(\mathbf{d},\mathbf{x})\right] & \leq & 8 \\
 & & \mathrm{E}\left[S_{max}(\mathbf{d},\mathbf{x})\right] & \leq & 3000
\end{array}
$$

→ reliable + robust

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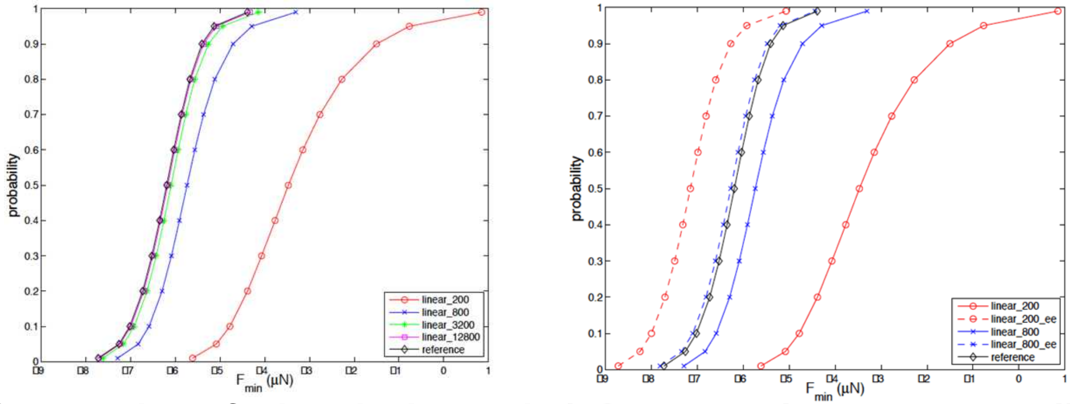
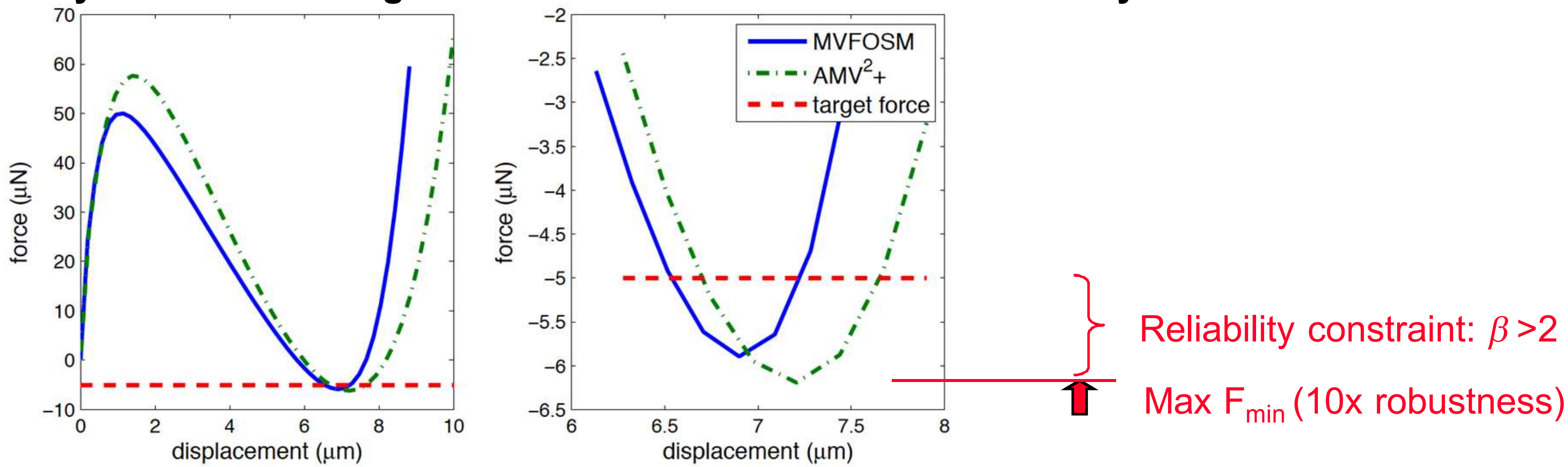
Milestone Results:
Solution-Verified Reliability Analysis and Design

- **Reliability analysis: compute error-corrected CDFs and assess accuracy/efficiency**



- **RBDO: carry best fwd to design switch for max robustness s.t. reliability constraint**



Conclusions: **UQ/OUU with error corrected/informed approaches can be:**

- **more accurate:** controlling/correcting errors leads to higher confidence in UQ/RBDO results
- **less expensive:** `Linear800+EE` analysis above < 10% cost of fully converged reference
- **more reliable:** on-line approach accounts for any parameter dependence (esp. shape vars)
- **more convenient:** can eliminate need for manual *a priori* convergence studies

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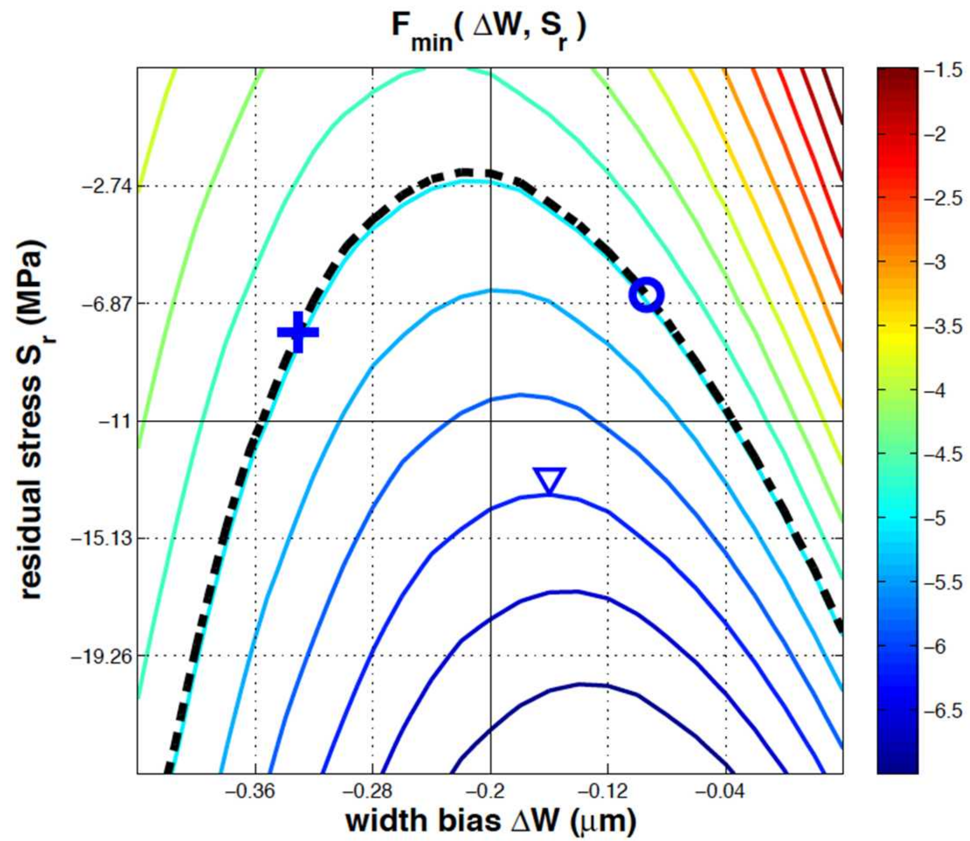
Issues with RBDO

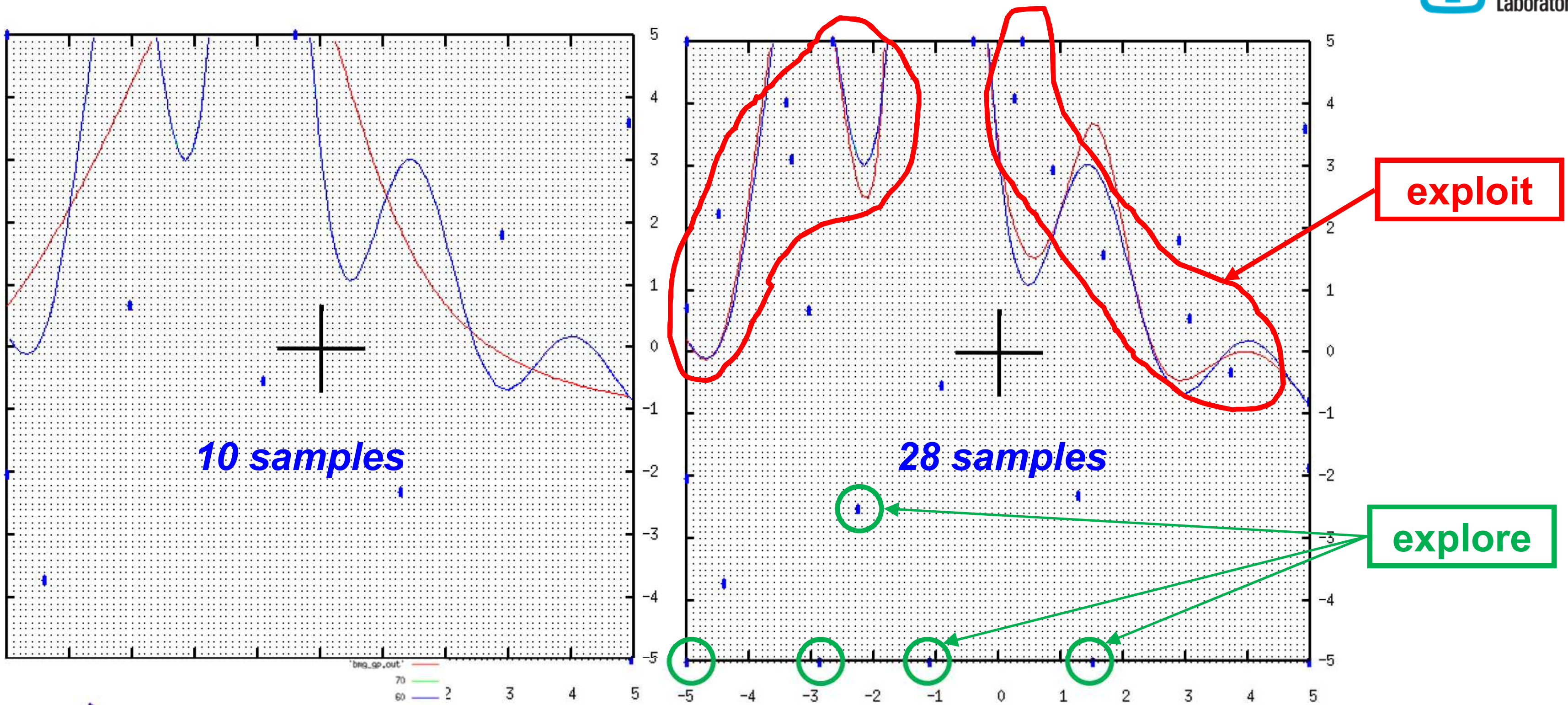
Insight from parameter study over 3σ uncertain variable range for fixed design variables d_M*. *Dashed black line denotes $g(x) = F_{min}(x) = -5.0$.*

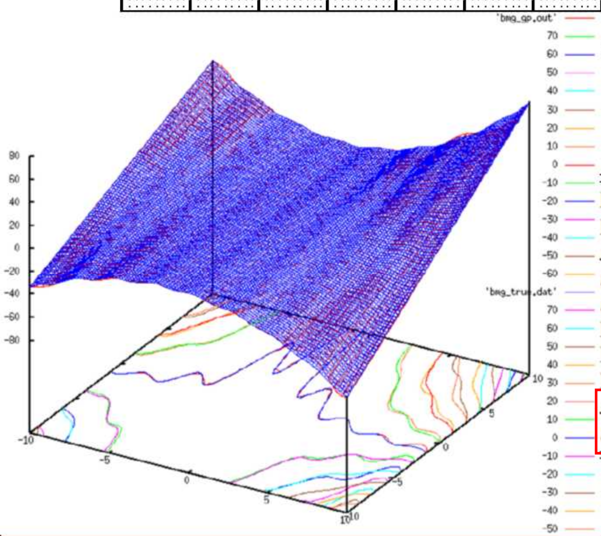
- **AMV²+ and FORM converge to different MPPs (+ and O respectively)**
- **Issue: high nonlinearity leading to multiple legitimate MPP solns.**
- **Challenge: design optimization may tend to seek out regions encircled by the failure domain. 1st-order and even 2nd-order probability integrations can experience difficulty with this degree of nonlinearity.**



As for UQ, need to achieve a more effective balance in robustness / efficiency

Efficient Global Reliability Analysis





Reliability method	Function evaluations	First-order p_f (% error)	Second-order p_f (% error)	Sampling p_f (% error, avg. error)
No approximation	70	0.11797 (277.0%)	0.02516 (−19.6%)	——
x space AMV^2+	26	0.11797 (277.0%)	0.02516 (−19.6%)	——
u space AMV^2+	26	0.11777 (277.0%)	0.02516 (−19.6%)	——
u space TANA	131	0.11797 (277.0%)	0.02516 (−19.6%)	——
LHS solution	10 k	——	——	0.03117 (0.385%, 2.847%)
LHS solution	100 k	——	——	0.03126 (0.085%, 1.397%)
LHS solution	1 M	——	——	0.03129 (truth, 0.339%)
x space EGRA	35.1	——	——	0.03134 (0.155%, 0.433%)
u space EGRA	35.2	——	——	0.03133 (0.136%, 0.296%)

EGRA-based OUU

Bi-level / Nested: opt outer loop, UQ inner loop

- Separate GPs (Uncertain approx):
  - EGO over **d**; For each **d**, EGRA resolves g(**u**)
  - No data leveraging among UQ runs for nearby **d**
- Single GP (Combined approx):
  - EGRA resolves g(**d**, **u**) using a single GP; EGO post-processes this GP for p(**d**)
  - Leverages data but may resolve g in regions of **d** that are not important for optimization

Reliability:

$$\begin{array}{ll} \text{minimize} & f(\mathbf{d}) \\ \text{subject to} & P\left[g(\mathbf{d},\mathbf{x}) \geq \bar{z}\right] \leq \bar{p}_f \end{array}$$

Sequential: break nesting → iterate between opt & UQ by updating approximate constraint

- Combined GP for g(**d**, **u**) with refinement
- After each approx design cycle, perform EGRA at **d*** → updates g(**d**, **u**); iterate until conv.
- Leverages data and avoids resolving g in unimportant regions of **d**

Table 1. Results for the short column RBDO example.

Design/Reliability Methods	Avg. Obj. Fn (Best Feasible)	Avg. β^* Value (# violations)	Avg. g Evals (Best Feasible)	
Nested NIPS/AMV^2+	216.2	2.500	1190	FD gradients
Sequential NIPS/AMV^2+	216.2	2.500	757	FD gradients
Nested EGO/Separate EGRA	216.4 (216.1)	2.502 (3)	333.3 (260)	
Nested EGO/Single EGRA	218.5 (217.4)	2.505 (3)	134.1 (144)	
Sequential EGO/EGRA	216.9 (216.5)	2.514 (1)	148.7 (163)	

Bichon, B.J., Eldred, M.S., and Mahadevan, S., "Efficient Global Surrogate Modeling for Reliability-Based Design Optimization," (to appear) *ASME Journal of Mechanical Design*.

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

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

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

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

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.

Stochastic Sensitivity Analysis

- **PCE/SC have convenient analytic features**
  - Expansions readily differentiated w.r.t. ξ
  - Analytic moment expressions
- **Augment w/ nonprobabilistic dimensions *s***
  - Design, epistemic uncertain

$$R \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}) \qquad R(\boldsymbol{\xi}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

$$\begin{cases} \mu_R = \alpha_0 \\ \sigma_R^2 = \sum_{j=1}^{P} \alpha_j^2 \langle \Psi_j^2 \rangle \end{cases} \qquad \begin{cases} \mu_R = \sum_{j=1}^{N_p} r_j w_j \\ \sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2 \end{cases}$$

- **Approach 1: PCE/SC over prob. vars for each set of nonprobabilistic vars**

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

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{k=1}^{N_p} r_k(\boldsymbol{s}) \boldsymbol{L}_k(\boldsymbol{\xi})$$

⇒ Moment sensitivity = expectation of response sensitivity

$$\begin{cases} \frac{d\mu}{ds} = \langle \frac{dR}{ds} \rangle \\ \frac{d\sigma^2}{ds} = 2\sum_{k=1}^{P} \alpha_k \langle \frac{dR}{ds}, \Psi_k \rangle \end{cases} \qquad \begin{cases} \frac{d\mu}{ds} = \sum_{k=1}^{N_p} w_k \frac{dr_k}{ds} \\ \frac{d\sigma^2}{ds} = \sum_{k=1}^{N_p} 2 w_k (r_k - \mu) \frac{dr_k}{ds} \end{cases}$$

→Additional data requirements (*dR/ds*), but no additional dimensions

- **Approach 2: PCE/SC over all variables**

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \qquad R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s})$$

Moment sensitivity = expectations over ξ + differentiation of remaining polynomial in *s*

⇒

$$\mu_R(s) = \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}}$$

$$\sigma_R^2(s)$$

$$\mu_R(s) = \sum_{j=1}^{N_p} r_j \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}}$$

$$\sigma_R^2(s) = \sum_{j=1}^{N_p} \sum_{k=1}^{N_p} \ldots (\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} - \mu_R^2(s)$$

→ Additional dimensions, but no additional data requirements

PCE-based and SC-based OUU

Analytic Bi-level:

- **Analytic moment/reliability sensitivities *(*avoid numerical derivs. at design level)**
- **Uncertain or Combined expansions**

Reliability:

$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \end{cases}$$

(β initially based on moment proj)

Robustness:

$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \sigma^2 \leq \bar{\sigma}^2 \end{cases}$$

Sequential/Surrogate-based:

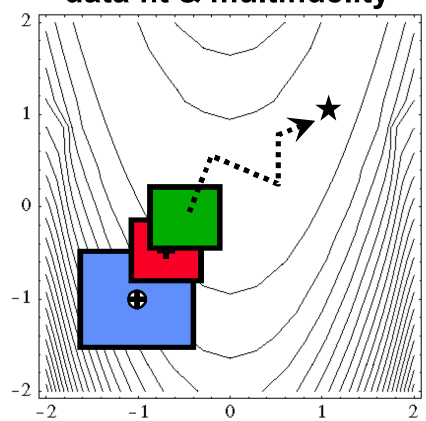
- **Break nesting: iterate between opt & UQ w/ (surrogate) linkage**
- **Uncertain expansions**

$$\begin{cases} \text{minimize} & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} & \beta(\mathbf{s}_c) + \nabla_s \beta(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \geq \bar{\beta} \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} & \sigma^2(\mathbf{s}_c) + \nabla_s \sigma^2(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \leq \bar{\sigma}^2 \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

- 1st-order
- Also QN 2nd-order

TR-SBO with local data fit & multifidelity



Multifidelity (focused on UQ fidelity):

- **Optimize corrected LF UQ model over TR**
  - **LF = Combined expansion (over *s*), MVFOSM**
  - **HF = Uncertain expansion (at single design pt)**
- **Additive corrections enforce LF/HF consistency**
  - **1st order & QN 2nd-order**

$$\hat{\beta_{hi}}(\mathbf{s}) = \beta_{lo}(\mathbf{s}) + \alpha_\beta(\mathbf{s})$$

$$\hat{\sigma_{hi}}^2(\mathbf{s}) = \sigma_{lo}^2(\mathbf{s}) + \alpha_{\sigma^2}(\mathbf{s})$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\beta_{hi}}(\mathbf{s}) \geq \bar{\beta} \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\sigma_{hi}}^2(\mathbf{s}) \leq \bar{\sigma}^2 \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

Unilevel approach (sim residuals @ collocation pts)

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Computational Results: PCE-/SC-based OUU

Typical result:

short column

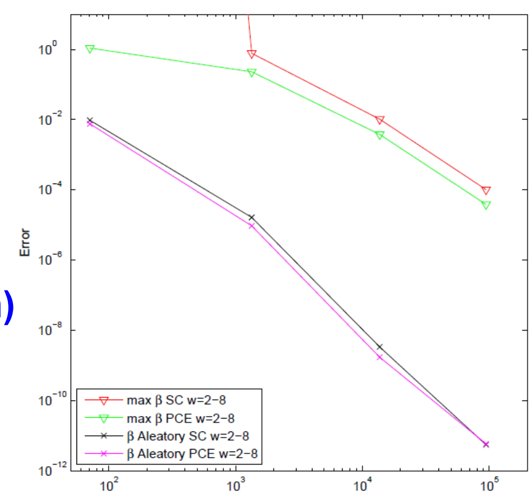
$$\begin{aligned} \min \quad & bh \\ \text{s.t.} \quad & \beta \geq 2.5 \\ & 5.0 \leq b \leq 15.0 \\ & 15.0 \leq h \leq 25.0 \end{aligned}$$

Design approach	Expansion variables	Integration approach	Evaluations (Fn, Grad)	Area	β_{CDF}
PCE/SC Bilevel	Uncertain	SSG w = 2	(465, 465)	202.87	2.5001
PCE/SC Bilevel	Combined	SSG w = 3	(341, 0)	201.67/199.46	2.5000
PCE/SC Sequential 1	Uncertain	SSG w = 2	(372, 186)	202.86	2.5000
PCE/SC Sequential Q2	Uncertain	SSG w = 2	(341, 186)	202.86	2.5000
PCE/SC {Comb, Unc} Multifidelity 1	{Comb, Unc}	SSG {w = 3, w = 2}	(992/1333, 155)	202.86	2.5000
PCE/SC {MV, Unc} Multifidelity 1	Uncertain	SSG w = 2	(281, 188)	202.86	2.5000

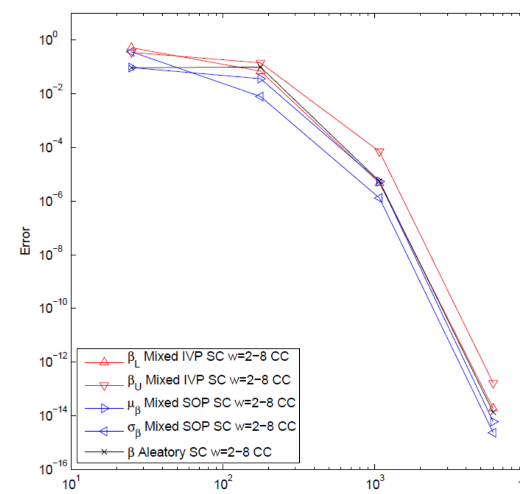
Fully converged solution is (b, h) = (8.1147, 25.000) with Area = 202.87

- 1st-order uncertain locally accurate & reliable: effective in bi-level & sequential
- 0th-order combined can be more efficient but optima not as precise
- Sequential is competitive; quasi-2nd-order linkage assists convergence
- Multifidelity coerces LF UQ results to HF optimum; top performer with cheapest LF (Mean Value)

Rational functions (Short column, Cantilever beam)



Smooth C∞ (Ishigami)



Eldred, M.S., "Design Under Uncertainty Employing Stochastic Expansion Methods," *Intl Journal for UQ*, Vol. 1, No. 2, Feb. 2011, pp. 119-146.

Summary

Strengths, Weaknesses, Research needs

Sampling (nongradient-based)

- ***UQ Strengths:*** Simple and reliable, convergence rate is dimension-independent
- ***UQ Weaknesses:*** $N^{-1/2}$ convergence → expensive for accurate tail statistics
- ***OUU:*** smoothing with surrogates, TR-SBOUU 10x reduction with improved algorithmic robustness

Local reliability (gradient-based)

- ***Strengths:*** computationally efficient, widely used, scalable to large *n* (w/ efficient derivs.)
- ***Weaknesses:*** algorithmic failures for nonsmooth, multimodal, highly nonlinear limit states
- ***OUU:*** exploits analytic design grads, additional 10x reduction with analytic bi-level and sequential; but optimizers tend to exploit weaknesses above

Global reliability (typically nongradient-based)

- ***Strengths:*** handles multimodal and/or highly nonlinear limit states
- ***Weaknesses:*** conditioning, nonsmoothness (ensemble emulation); scaling to large *n* (adjoint enhancement)
- ***OUU:*** global nongradient at both levels; sequential reuses GP data while avoiding unimportant ***d*** regions

Stochastic expansions (typically nongradient-based)

- ***Strengths:*** functional representation, exponential conv rates for smooth problems
- ***Weaknesses:*** nonsmoothness (h-refinement), scaling to large *n* (adaptivity, adjoints)
- ***OUU:*** SSA enables gradient-based NLP or gradient-enhanced global opt.; bi-level, sequential, and multifidelity approaches

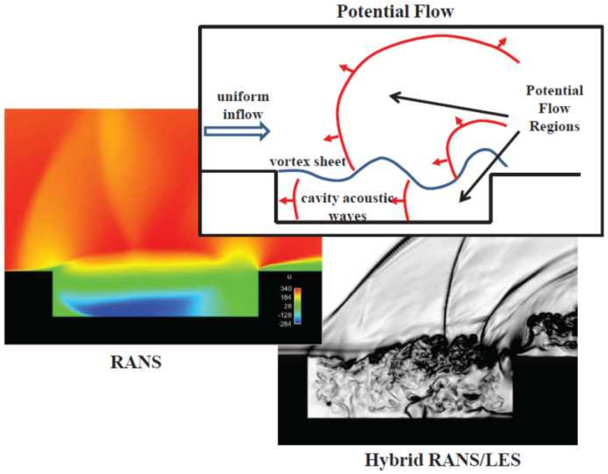
Related topics

- Epistemic & mixed UQ, including discrete epistemic model forms
- MCUU & Bayesian calibration

Multiple Model Forms in UQ

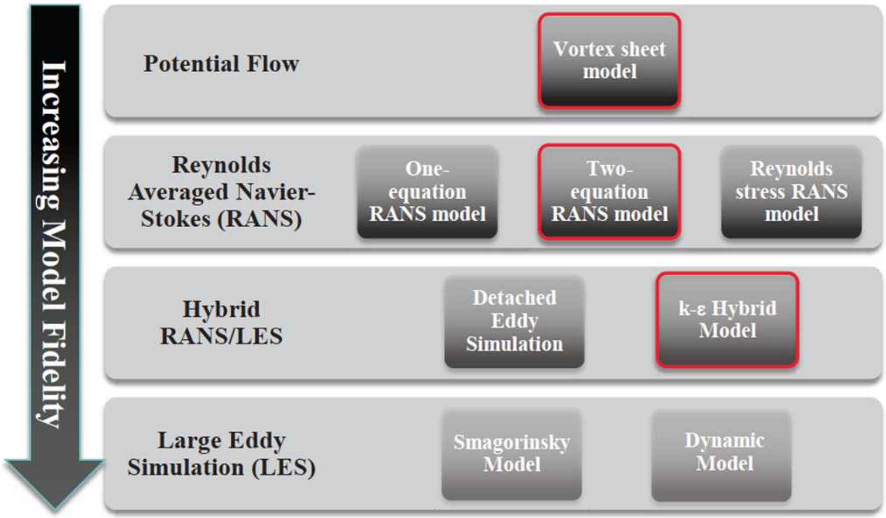
Discrete model choices, same physics (additional dimensions for multi-{physics,scale})

- A clear hierarchy of fidelity (from low to high)
  - *Multifidelity UQ methods:* generate statistics for truth model leveraging less expensive models
  - *Multifidelity inference:* calibration enables resolution of low complexity discrepancies



- 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
  - Combine model selection and multifidelity inference processes



Multifidelity UQ using Stochastic Expansions

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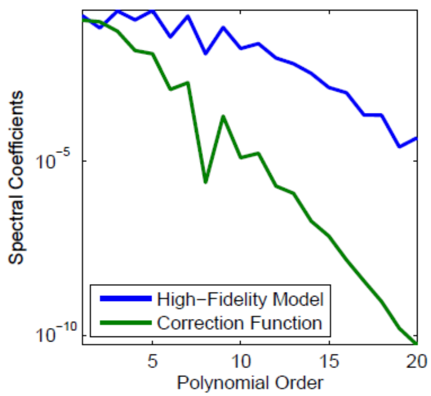
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

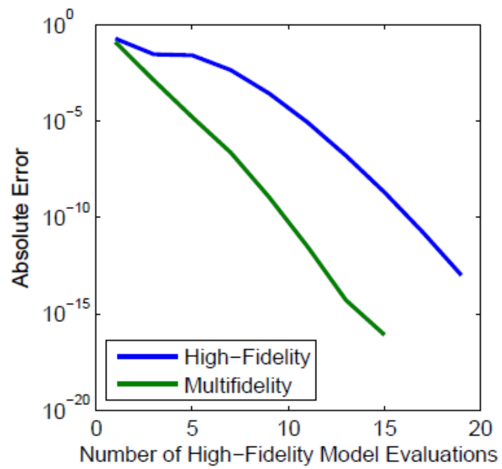
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

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

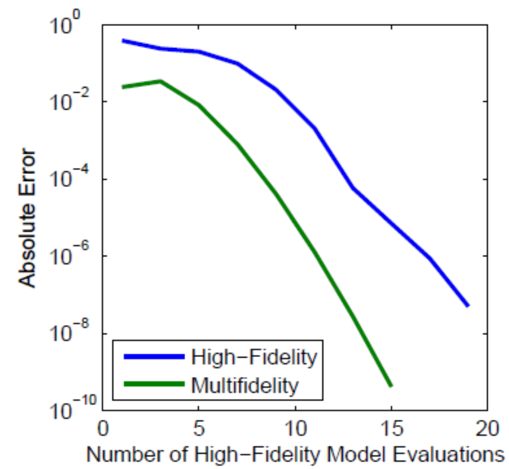
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

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





(a) Error in mean



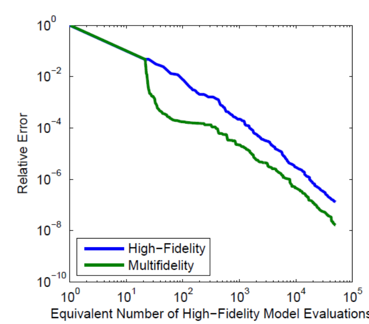
(b) Error in standard deviation

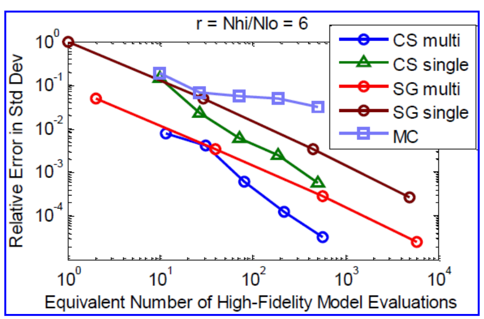
Adaptive sparse grid multifidelity algorithm:

- 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





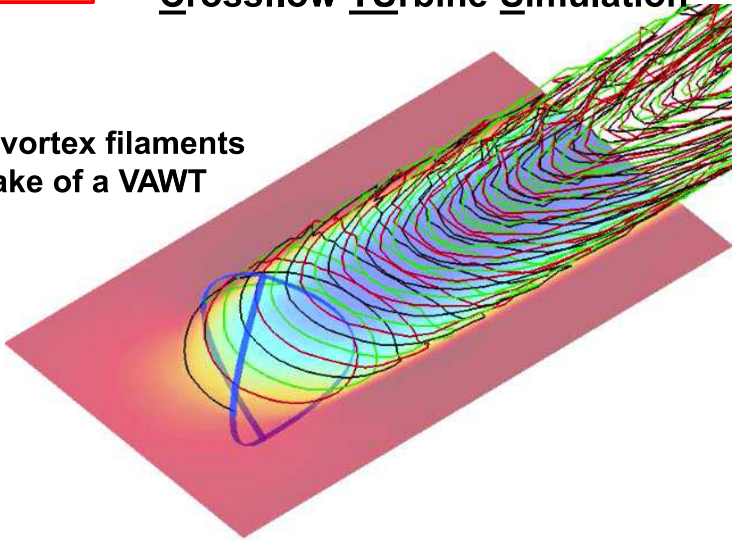
ASCR MF UQ example: VAWT Gust Response

Vertical-axis Wind Turbine (VAWT)

Low fidelity

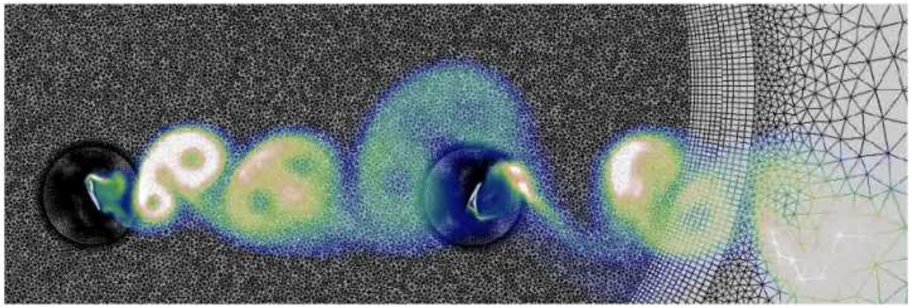
CACTUS: Code for Axial and Crossflow TUrbine Simulation

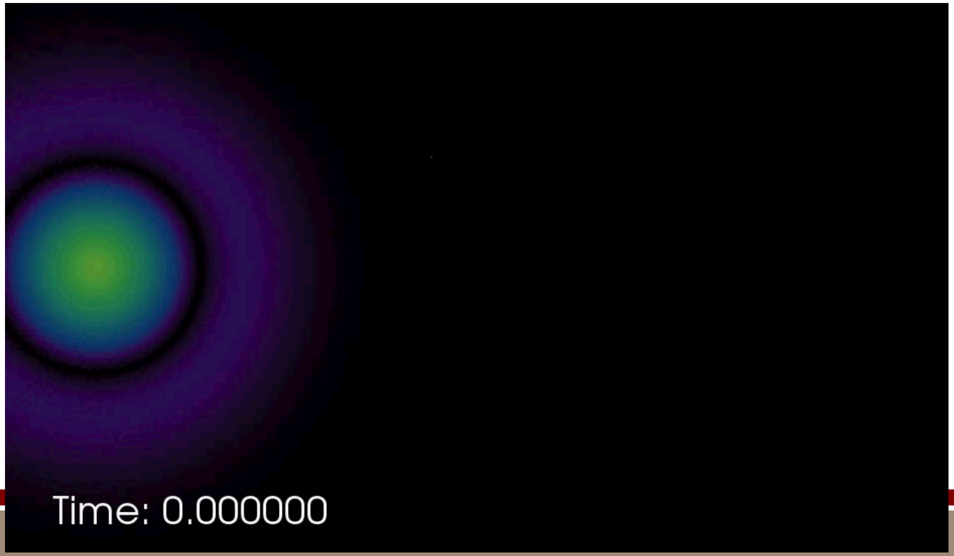
Computed vortex filaments in the wake of a VAWT



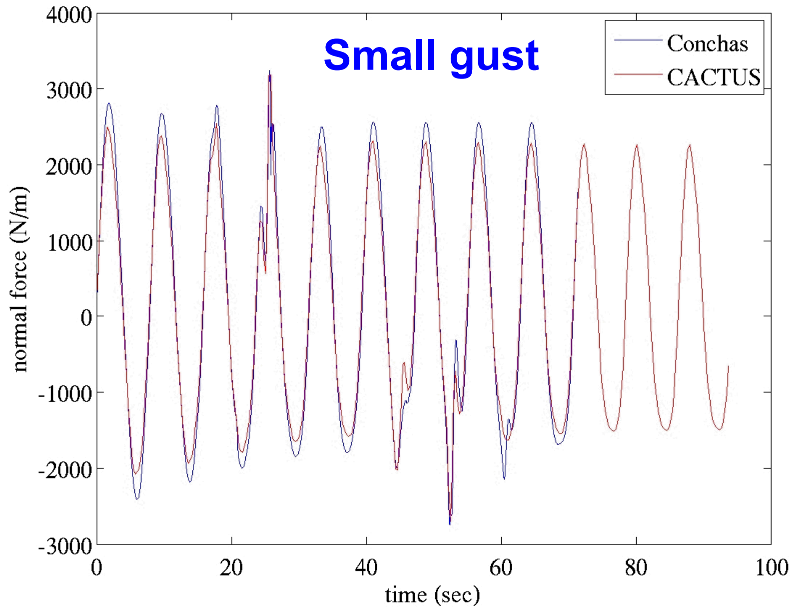
High fidelity

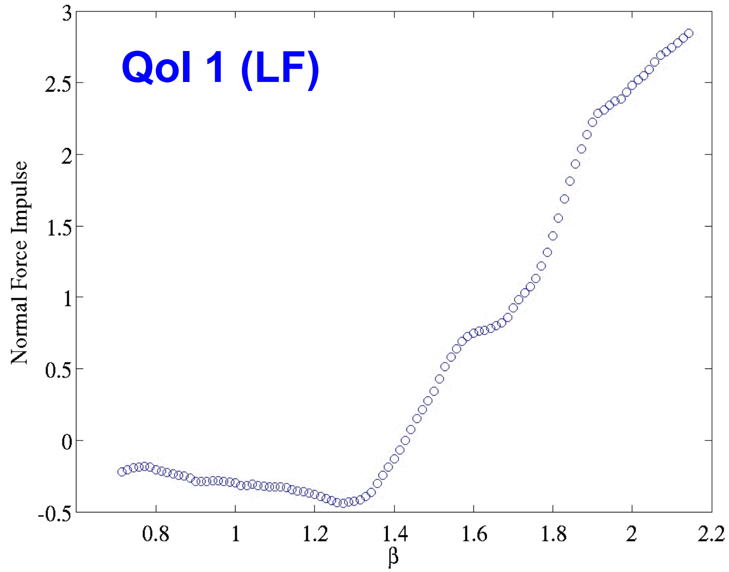
Conchas: DG formulation for LES

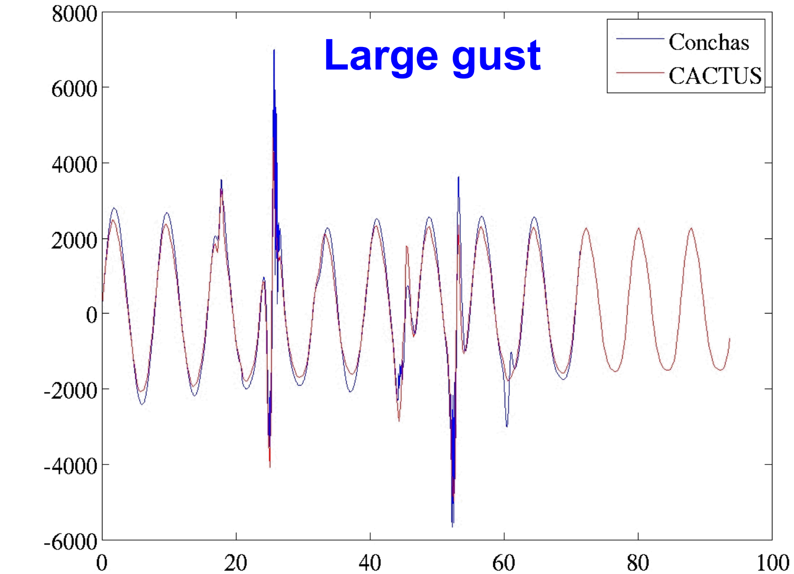


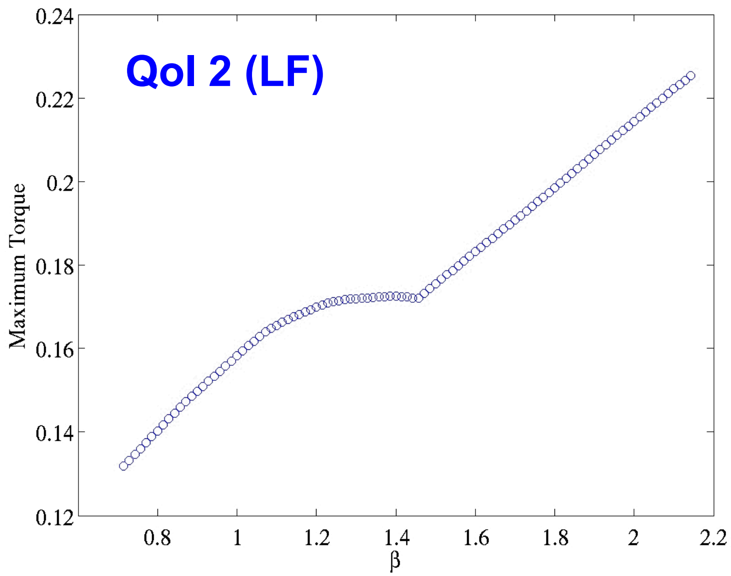


LF/HF simulation comparison







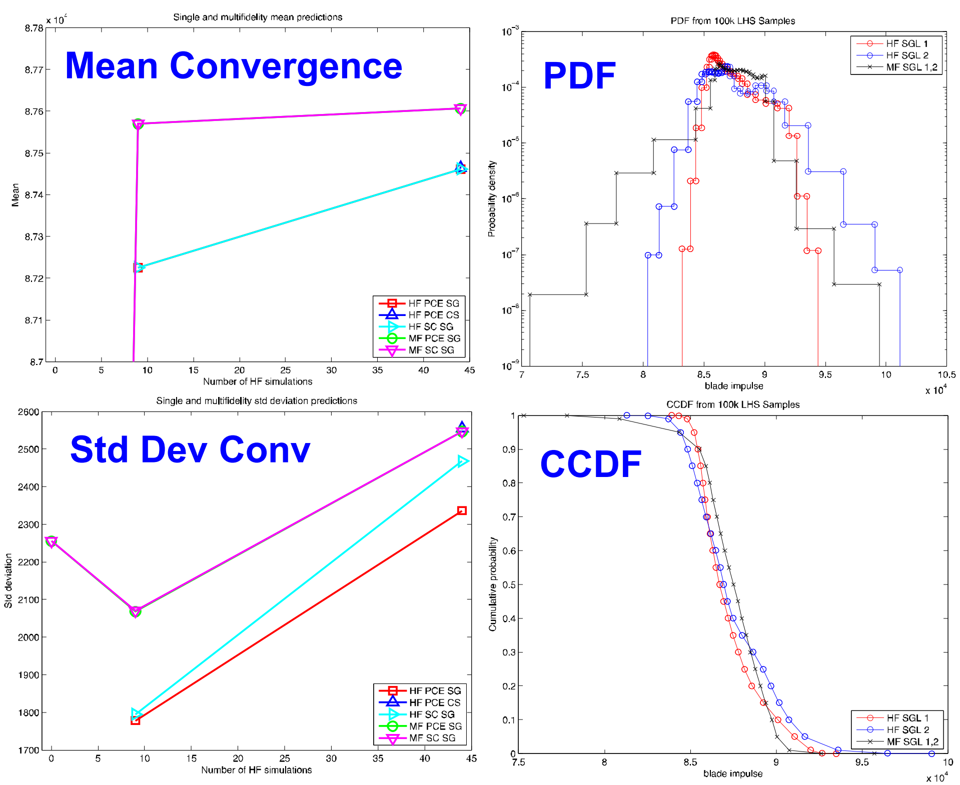


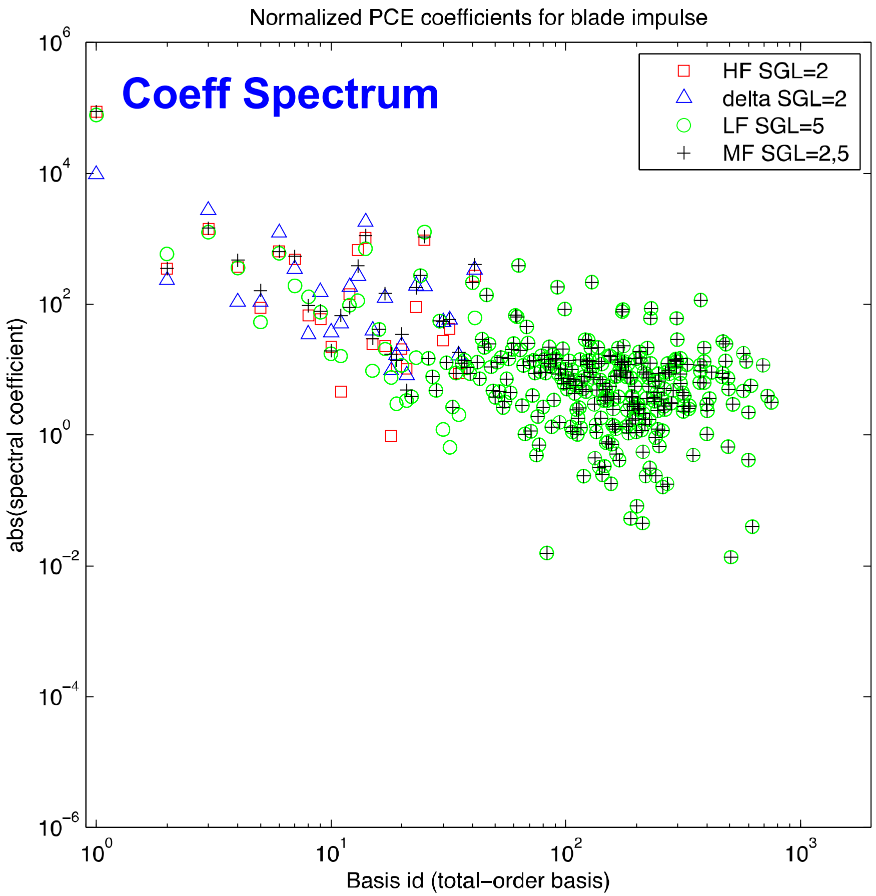
Numerical studies – Level 2,5 sparse grid case

3 random vars: vortex radius (~ bnd normal), position (~ uniform), amplitude (~ gumbel)

- Multifidelity sparse grid using isotropic grids with default growth rules
  - LF = level 5 (1099 Cactus simulations), Δ = level 2 (44 HF LES simulations)

Blade impulse



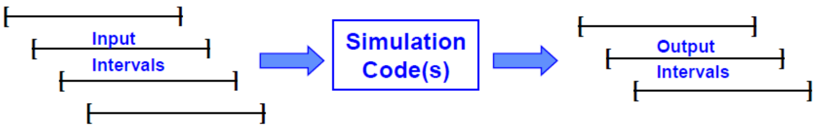


Epistemic UQ

Epistemic UQ: one does not know enough to specify probability distributions

Sometimes referred to as subjective, reducible, or lack of knowledge uncertainty

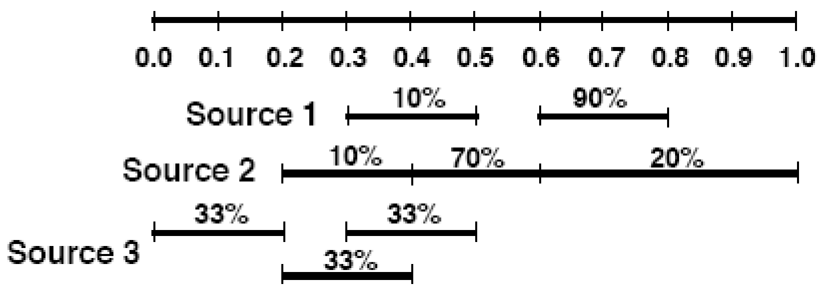
Interval analysis

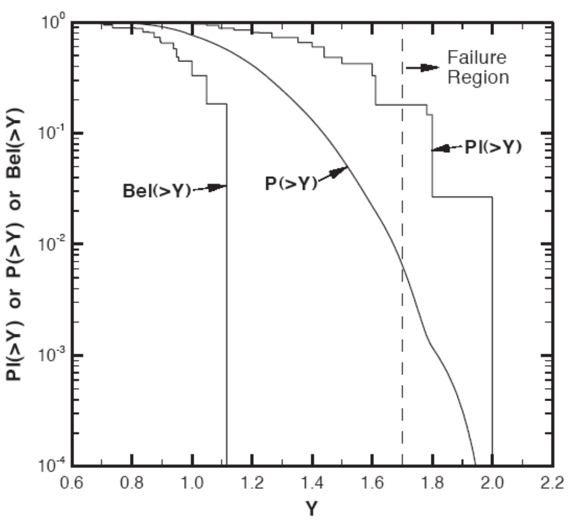


- Propagate input intervals to output intervals
- Intrusive interval methods (operation by operation propagation) have been investigated for several decades, but have not become mainstream (key issue: interval growth)
- Sampling methods (+ surrogate models if expensive evals) are commonly used
- Optimization methods are promising and some variants exploit data reuse

Dempster-Shafer theory of evidence

- Basic probability assignment (interval-based)
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals





Imprecise probability (p-boxes), Info gap, …

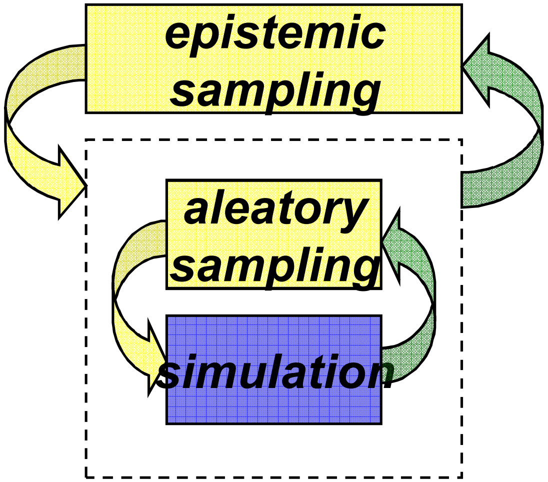
Notes on Rigorous Separation

Taking your set of uncertain variables and drop each one in one bucket or another based on your confidence of its characterization:

- Not really the right approach, IMO
- Advocate an approach that separates reducible parts from irreducible parts
  - Provides a natural interpretation of mixed aleatory-epistemic results!
- For example there may an imprecisely known random excitation, but you know there is an excitation → separate what reducible from irreducible and model the reducible part as best you can (conservatism may be appropriate)
  - For example, assume an aleatory Gaussian input w/ epistemic moments…
  - Or posit a range of possible distributions….
- If we don't perform this separation rigourously and mix reducible and irreducible uncertainy, then what is the impact?
  - Generally speaking results become difficult to interpret (some argue that aggregate p-box is still representative, but…)
  - Specifically, aleatory results represent a partial view of the true irreducible variability.
  - Example: mock transient thermal simulator

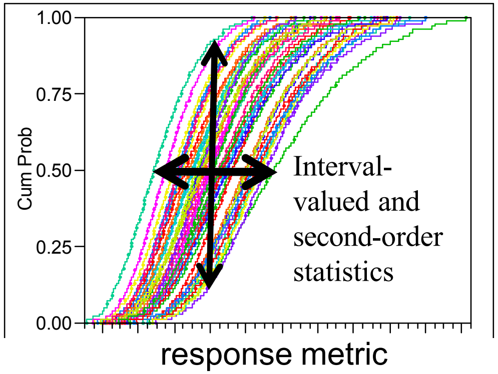
Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

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)

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

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

Mixed Aleatory-Epistemic UQ: IVP, SOP, and DSTE

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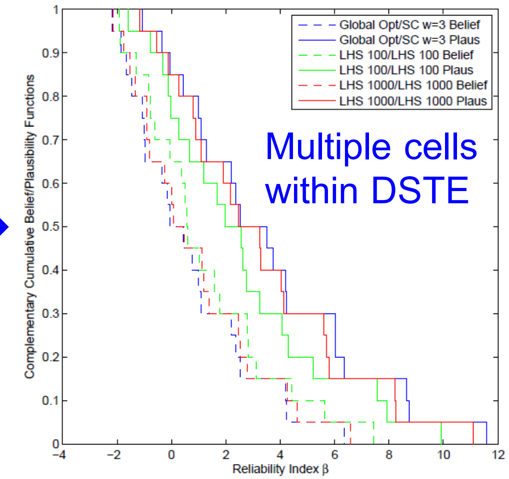
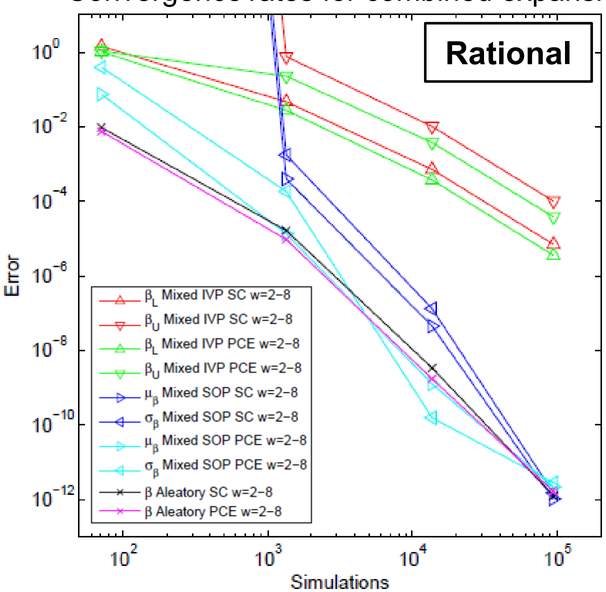
Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals					
EGO	SC SSG w = 1	Aleatory	(84/91, 0/0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(372/403, 0/0)	[75.0002, 374.999]	[-2.18735,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



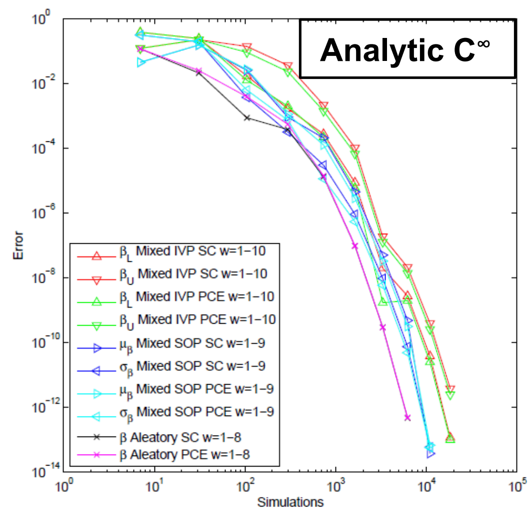
Multiple cells within DSTE

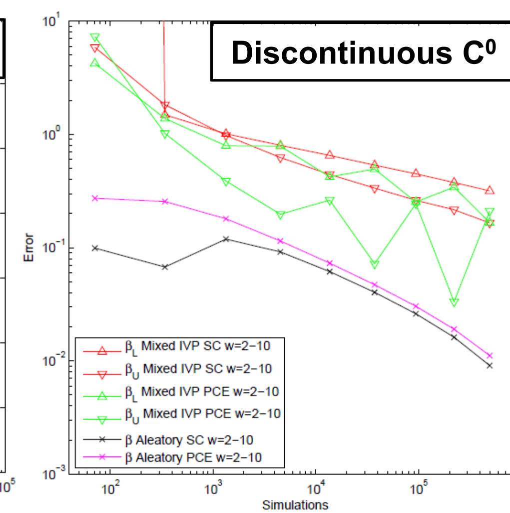
Convergence rates for combined expansions



L^∞ metrics: IVP mixed, DSTE mixed

L^2 metrics: Aleatory, SOP mixed





Eldred, M.S., Swiler, L.P., and Tang, G., "Mixed Aleatory-Epistemic Uncertainty Quantification with Stochastic Expansions and Optimization-Based Interval Estimation," *RESS*, Vol. 96, No. 9, Sept. 2011, pp. 1092-1113.

Performance Results for Algebraic Test Problems

Mixed-integer global optimization approaches for interval estimation

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

Short column

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

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

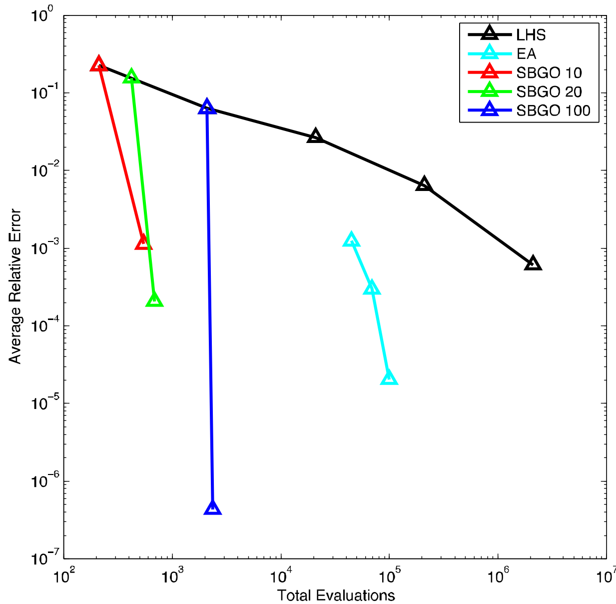
$$\text{Form 3}: \quad f_3 = 1 - \frac{4M}{bh^2Y} - \left(\frac{M}{bhY}\right)^2$$

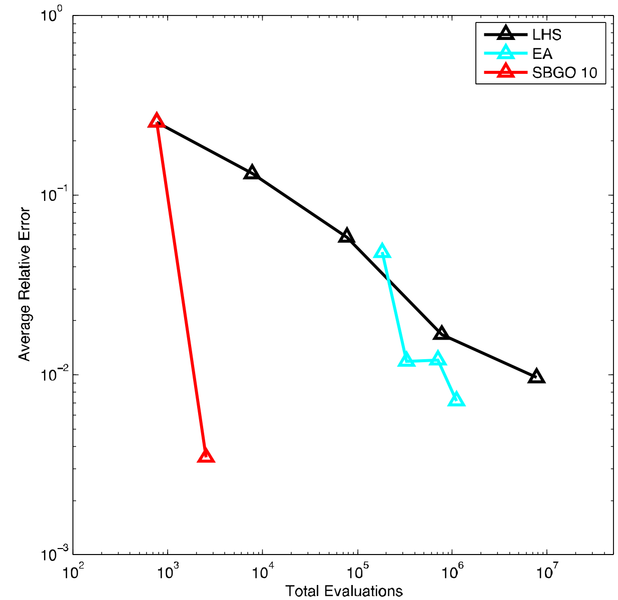
$$\text{Form 4}: \quad f_4 = 1 - \frac{4M}{bh^2Y} - \left(\frac{P}{bhY}\right)^2 - \frac{4(P-M)}{bhY}$$

Rosenbrock

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

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





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

Epistemic vars: 1 discrete model form (4 values), 3 continuous defining interval means within 5 aleatory vars

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

Results for Thermal-Hydraulics with Drekar

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

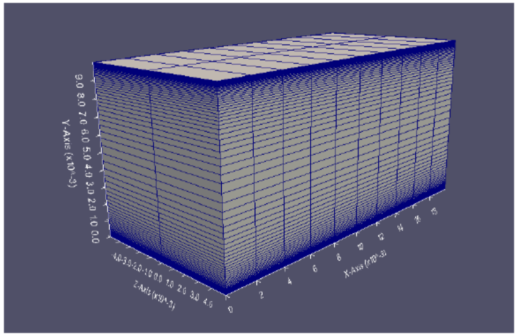


Figure 4. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

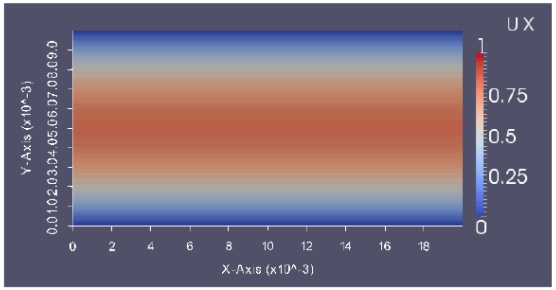


Figure 5. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

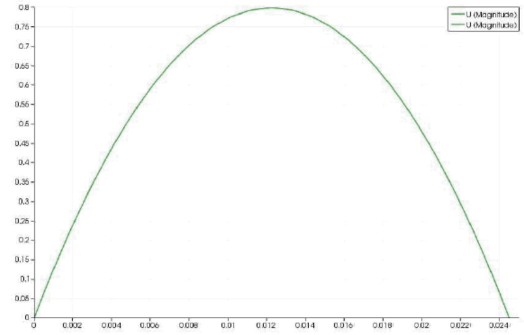


Figure 6. The profile of of the steady-state x-velocity along the outflow boundary for a typical realization computed using a RANS model in Drekar.

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]

Clear benefit shown in utilizing optimization approaches relative to LHS:

- *Rosenbrock:* cost reductions of 20x for EA and 1000x for SBGO w/ comparable accuracy.
- *Short column:* EA more converged for 3 out of 4 bounds with 10x cost reduction; SBGO provided most converged results for all 4 bounds with 3000x reduction in cost.
- *Drekar:* SBGO provided significant refinement in all 4 bounds (intervals broadened by 86% for m_{ux} and 11% for $m_{pressure}$) using only 7 additional outer loop evaluations.

Summary Points

Address key UQ challenges

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

Impact DOE missions

- NNSA (ASC) & Offices of Science/Energy (ASCR, SciDAC-3, CSSEF, NE/CASL, EERE)

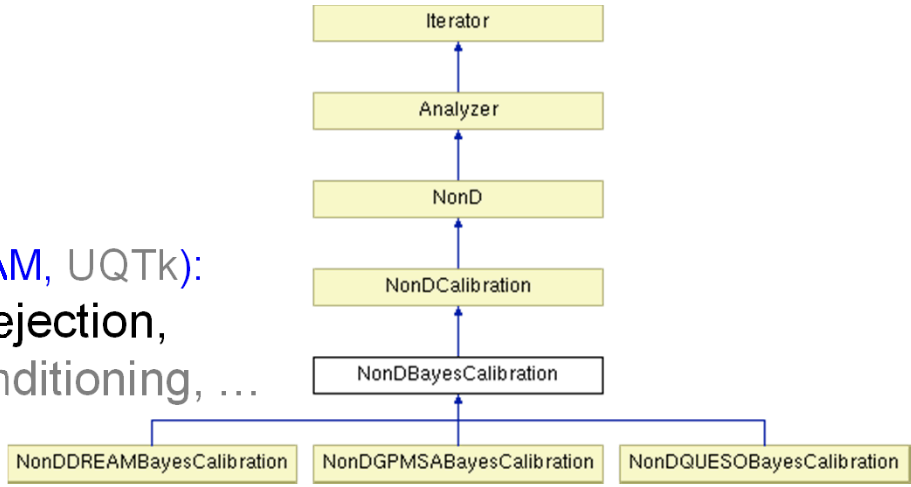
Investments in scalable UQ R&D

- Developing a broad suite of scalable and robust core UQ methods:
  - Sampling, reliability, stochastic expansion, epistemic
  - Goal-oriented adaptive refinement, (Adjoint) gradient-enhancement, Sparsity detection
- Building on this foundation (address complexities, compound efficiencies)
  - Design under uncertainty: SBOUU, RBDO, PCBDO, et al.
  - Multifidelity UQ, Mixed aleatory-epistemic UQ, emulator-based Bayesian inference

Extra Slides

Bayesian Methods

Inference and Model Selection

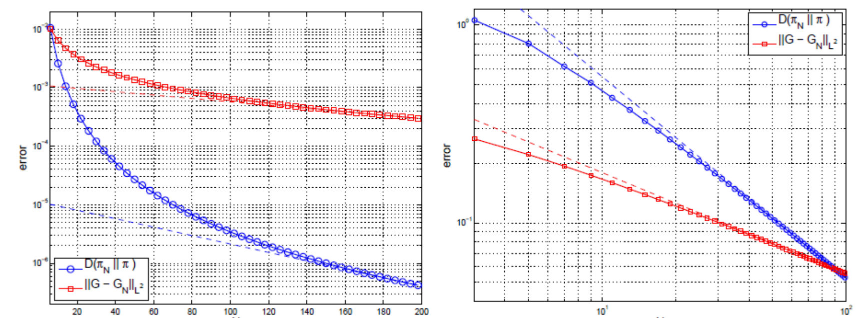


Likelihoods: Gaussian (with management of functional data, replicates, etc.)

Posterior evaluators (QUESO, GPMSA, DREAM, UQTk): MCMC with Metropolis-Hastings, delayed rejection, differential evolution, parallel chains, preconditioning, …

Emulators (Pecos/Surfpack): built over support of prior; for posterior sampling

- No emulator
- Stochastic expansions (PCE/SC)
- Gaussian processes
- Multifidelity models



From Marzouk & Xiu, 2009

(a) Smooth problem: exponential convergence. (b) Discontinuous problem: algebraic convergence.

Advanced topics:

- discrepancy modeling and multifidelity inference
- PCE/KLE coefficient inference
- model averaging and selection

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

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

Moderate dimensional KLE Random Field Model

Bayesian inference of Basal sliding field for Greenland

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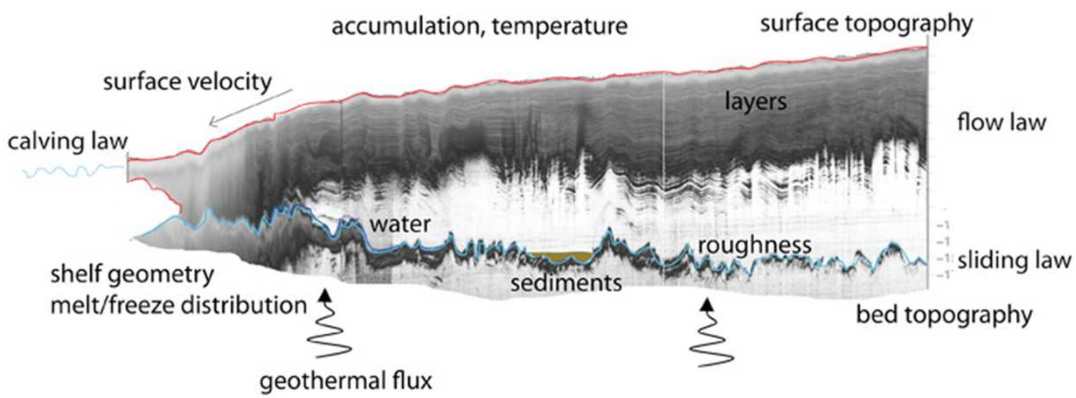
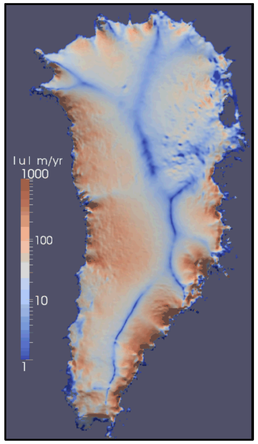


Figure 1: Schematic of observations, boundary conditions, and processes affecting ice sheet initialization.



Greenland surface ice velocity

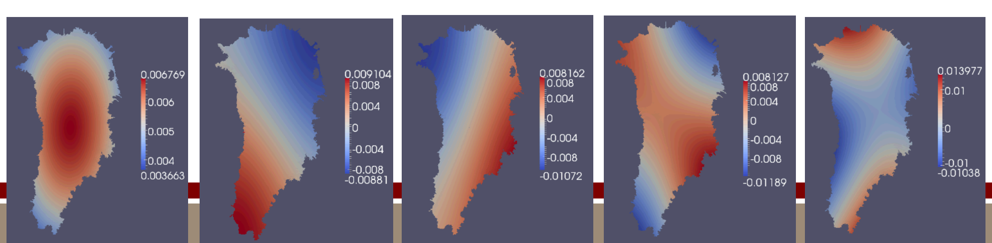
Karhunen-Loeve expansion (KLE):

Assume analytic spatial covariance kernel (squared exponential) for random field

$$C(r_1, r_2) = e^{-(r_1 - r_2)^2 / L^2}$$

and integrate over domain for modes. Length scale (L) balances feature resolution vs. # KLE modes (and may require iteration for inference).

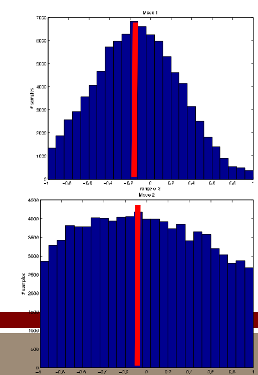
KLE modes (5 capture 95% energy):

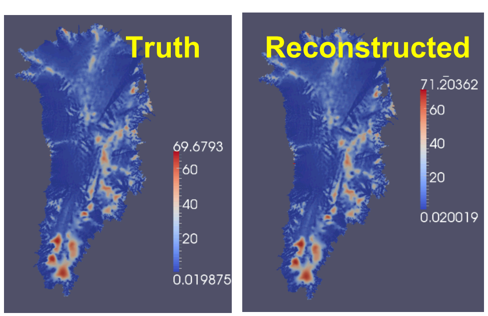


Dimension reduced inference of KLE coeffs:

- Mismatch = sum sq of surface velocity discrepancy
- PCE formed for mismatch over uniform prior distributions for isotropic sparse grid lev = 3
- MCMC on PCE with 100k samples, 1st 10k discarded

Posterior coeffs 1,2





OUU Formulation Issues (probabilistic)

Augment with response statistics $\mathbf{s}_u$ **(e.g., μ, σ, z/β/p)** *using linear mapping:*

$$
\begin{aligned}
\text{Minimize} \quad & f(\mathbf{d}) + \mathbf{W}\mathbf{s}_u(\mathbf{d}) \\
\text{Subject to} \quad & \mathbf{g}_l \le \mathbf{g}(\mathbf{d}) \le \mathbf{g}_u \\
& \mathbf{h}(\mathbf{d}) = \mathbf{h}_t \\
& \mathbf{a}_l \le \mathbf{A}_i\mathbf{s}_u(\mathbf{d}) \le \mathbf{a}_u \\
& \mathbf{A}_e\mathbf{s}_u(\mathbf{d}) = \mathbf{a}_t \\
& \mathbf{d}_l \le \mathbf{d} \le \mathbf{d}_u
\end{aligned}
$$

Nonlinear mappings **(σ^2, σ/μ)** *via AMPL*

Input design parameterization:

- **Augmented design variables**
- **Inserted design variables**
  - **Native distribution params may be sufficient**
  - **Extended parameterizations → location, scale**

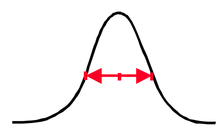
E.g., triangular distribution:

$$f(x) = \frac{2(x - L_T)}{(U_T - L_T)(M_T - L_T)}$$

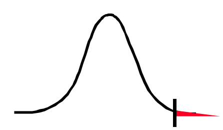
if $L_T \le x \le M_T$

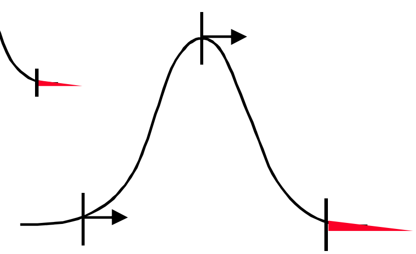
Output metric characterization:

- **Robustness metrics → min/constrain σ^2**
  - **awk for reliability → use G(β) range**



- **Reliability metrics → max/constrain *p*/β**
  - **awk for sampling (by binning) → projected *p*/β, IS**



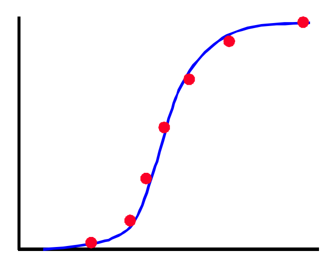


- **Combination →**
  - **Also Pareto opt., …**

$$
\begin{aligned}
\text{Maximize} \quad & \mu_r \text{ or } r\ (\beta = -2) \\
\text{subject to} \quad & 2 \le \beta\ (r > r_{crit})
\end{aligned}
$$

- **Inversion** (model calibration) **under uncertainty**
  - **NLS with output PDF/CDF**

$$
\begin{aligned}
\textbf{Minimize} \quad & f(\mathbf{x}) = \sum_{i=1}^{n} [T_i(\mathbf{x})]^2 \\
\textbf{where} \quad & T_i(\mathbf{x}) = R_i(\mathbf{x}) - \overline{R}_i
\end{aligned}
$$



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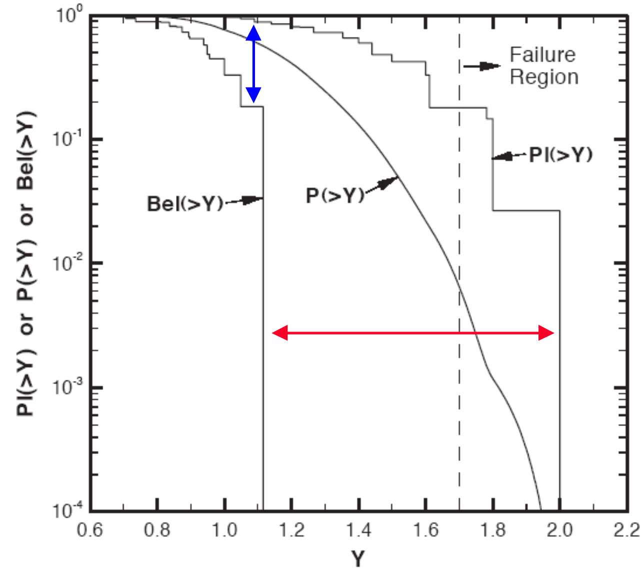
OUU Formulation Issues (nonprobabilistic)

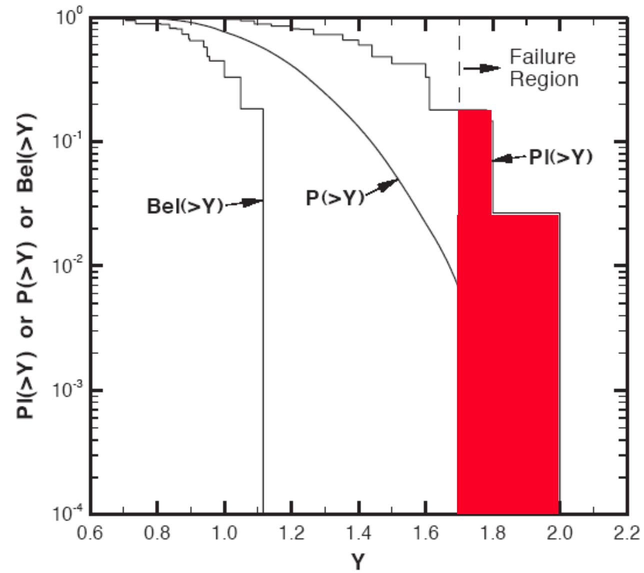
Input design parameterization:

- Augmented design variables
- Inserted design variables
  - As for uniform PDF → need locn, scale for BPAs

Output metric characterization:

- Robustness
  - insensitivity to epistemic uncertainties
  - minimize/constrain response interval
  - Pl – Bel for Y^* → $[p_{bel}, p_{pl}]$ or p^* → $[Y_{bel}, Y_{pl}]$
- Reliability
  - Minimize/constrain appropriate interval bound
  - Pl(Y) or Bel(Y), depending on failure sense
- Combination

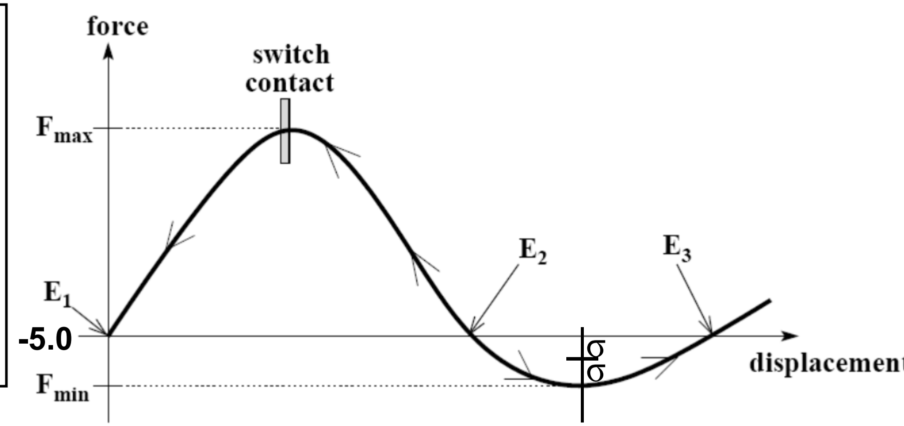




Bistable Switch: Problem Formulation

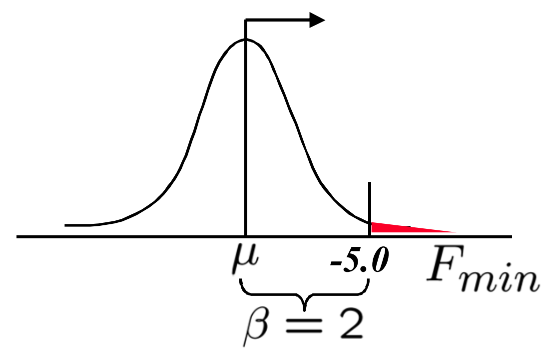
Typical design specifications:

- **actuation force F_{min} reliably < target (-5 μN)**
- **bistable ($F_{max} > 0$, $F_{min} < 0$)**
- **maximum force: $50 < F_{max} < 150$**
- **equilibrium $E_2 < 8$ μm**
- **maximum stress < 1200 MPa**



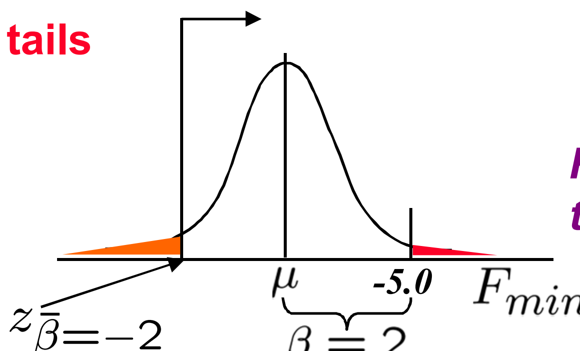
simultaneously reliable and robust designs

$$
\begin{array}{llcl}
\text{max} & & & \text{E}\left[F_{min}(\mathbf{d},\mathbf{x})\right] \\
\text{s.t.} & 2 & \leq & \beta_{ccdf}(\mathbf{d}) \\
 & 50 & \leq & \text{E}\left[F_{max}(\mathbf{d},\mathbf{x})\right] \leq 150 \\
 & & & \text{E}\left[E_2(\mathbf{d},\mathbf{x})\right] \leq 8 \\
 & & & \text{E}\left[S_{max}(\mathbf{d},\mathbf{x})\right] \leq 3000
\end{array}
$$



combined RIA/PMA to control both tails (reliable/robust):

$$
\begin{array}{llcl}
\text{max} & & & z_{\bar{\beta}=-2}(\mathbf{d}) \\
\text{s.t.} & 2 & \leq & \beta_{ccdf}(\mathbf{d}) \\
 & & & \textit{nln. constr.}
\end{array}
$$



RIA/PMA combination: twice the cost

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