Uncertainty-Aware Design Optimization with the DAKOTA Toolkit

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Sandia National Laboratories
Optimization and Uncertainty Quantification

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Outline

Design Analysis Kit for Optimization and Terascale Applications (DAKOTA)
is an SNL toolkit for optimization, uncertainty quantification, and sensitivity analysis with large-scale computational models.
`http://www.cs.sandia.gov/DAKOTA`

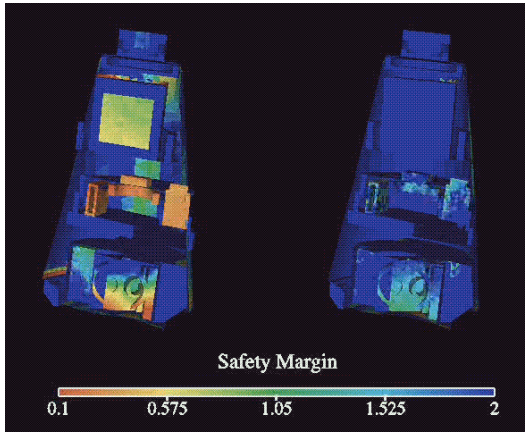
- **The DAKOTA framework and its key capabilities**
- **Uncertainty and reliability analysis techniques**
- **Reliability-based design optimization for micro-electro-mechanical system (MEMS) design**

Thanks to Barron Bichon, Mike Eldred, and Laura Swiler for slide content.

DAKOTA Motivation

Goal: perform iterative analysis on (potentially massively parallel) simulations to answer fundamental engineering questions:

- **What is the best performing design?**
- **How safe/reliable/robust is it?**
- **How much confidence do I have in my answer?**



Nominal **Optimized**

DAKOTA
optimization, sensitivity analysis, parameter estimation, uncertainty quantification

parameters
(design, UC, state)

Computational Model (simulation)
- **Black box:** nearly any Sandia or commercial simulation code
- **Semi-intrusive:** Matlab, ModelCenter, Python SIERRA multi-physics, SALINAS, Xyce

response metrics

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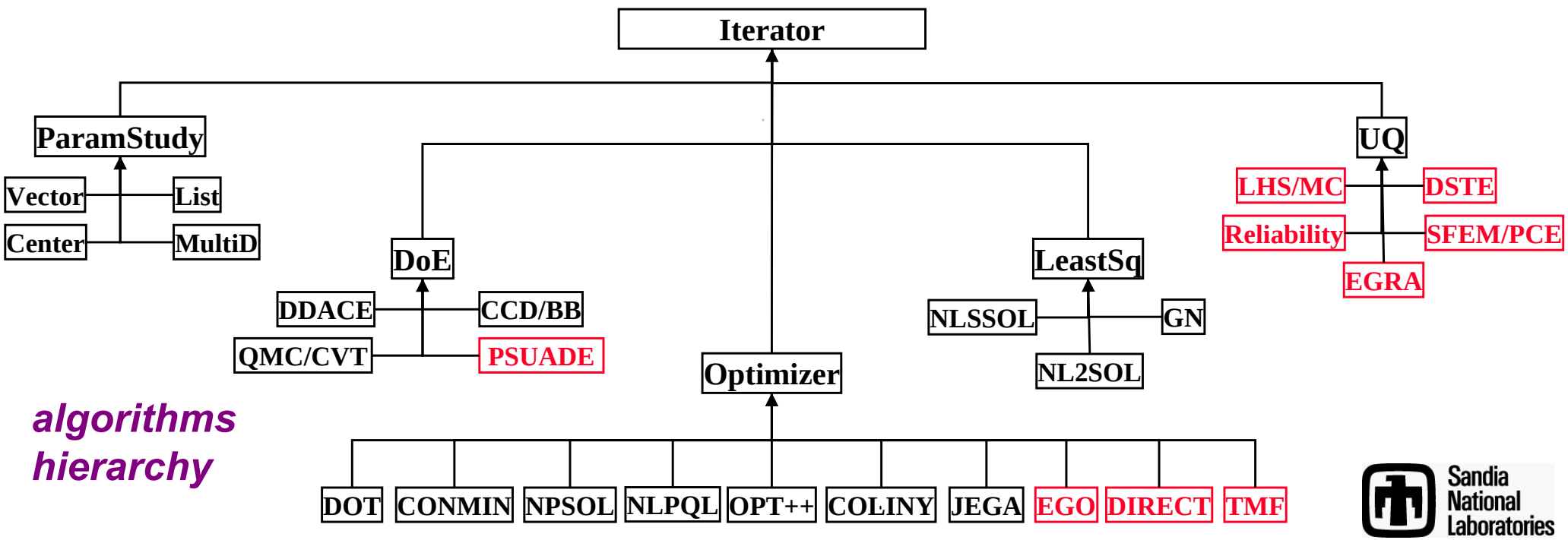
DAKOTA C++/OO Framework Goals

- **Unified software infrastructure:** reuse tools and common interfaces; *integrate commercial, open-source, and research algorithms*
- **Enable algorithm R&D**, e.g., for non-smooth/discontinuous/multimodal responses, probabilistic analysis and design, mixed variables, unreliable gradients, costly simulation failures
- **Facilitate scalable parallelism:** ASCI-scale applications and architectures; *4 nested levels of parallelism possible*
- **Impact:** tool for DOE labs and external partners; broad application deployment; *free via GNU GPL* (>3000 download registrations)



algorithms hierarchy

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Flexibility with Models & Strategies

DAKOTA models map inputs to response metrics of interest:

variables/parameters

- **design: continuous, discrete**
- **uncertain: (log)normal, (log)uniform, interval, triangular, histogram, beta/gamma, EV I, II, III**
- **state: continuous, discrete**

→

user application
(simulation)
system, fork, direct, grid

optional approximation (surrogate)

- **global (polynomial 1/2/3, neural net, kriging, MARS, RBF)**
- **local (Taylor); multipoint (TANA/3)**
- **hierarchical, multi-fidelity**

→

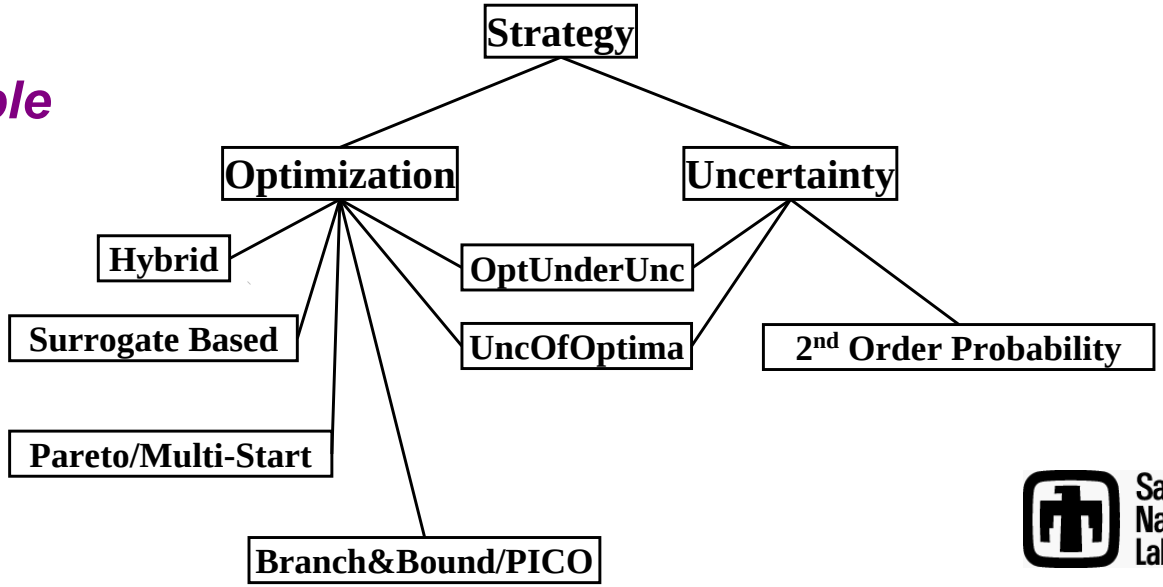
responses

- **functions: objectives, constraints, LSQ residuals, generic**
- **gradients: numerical, analytic**
- **Hessians: numerical, analytic, quasi**

app-specific: users often need initial help to ID key parameters, script, extract metrics

DAKOTA strategies enable flexible combination of multiple models and algorithms.

- ***nested***
- ***layered***
- ***cascaded***
- ***concurrent***
- ***adaptive / interactive***



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Sample Algorithm Combinations

In addition to allowing rapid selection of single optimization algorithms, DAKOTA enables advanced strategies, e.g.:

- **Global/local optimization:** perform (1) sampling, parameter study, or global optimization; then (2) local (gradient or non-gradient) optimization at each promising point.
- **Surrogate (meta-model)-based optimization:** use global surrogates or local surrogates with trust region management to reduce objective evaluation cost.
- **Efficient Global Reliability Analysis (EGRA):** reliability analysis through combination of Gaussian Process surrogate, DIRECT optimizer, and multi-modal adaptive importance sampling
- **Forthcoming example:**

  Optimization under uncertainty for MEMS

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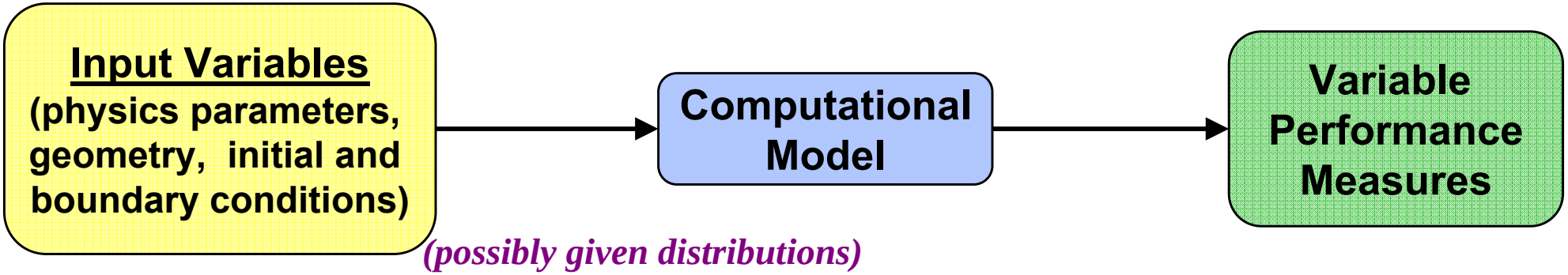
Uncertainty Quantification

Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output



Potential Goals:

- based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)
- identify parameter correlations/local sensitivities, robust optima
- identify inputs whose variances contribute most to output variance (global sensitivity analysis)
- quantify uncertainty when using calibrated model to *predict*

Methods:

- Aleatoric/irreducible: sampling (Monte Carlo, LHS, CVT), reliability analysis (mean value, FORM, algorithmic variants)
- Epistemic/reducible: 2nd order probability, Dempster-Shafer Theory of Evidence

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DAKOTA UQ Methods

Active UQ development in DAKOTA (new, developing, planned)

- **Parameter studies and study design (DoE, DACE, factorial, OA)**
- **Sampling:** LHS/MC, Quasi-MC/CVT, Bootstrap/Importance/Jackknife
  trustworthy and robust, often too costly in high dimension
- **Reliability:** Evaluate probability of attaining specified outputs / failure
  MVFOSM, x/u AMV, x/u AMV+, FORM (RIA/PMA mappings),
  MVSOSM, x/u AMV^2, x/u AMV^2+, TANA, SORM (RIA/PMA)
- **SFE:** Polynomial chaos expansions (quadrature/cubature extensions).
- **Epistemic:** Dempster-Schafer: basic probability assignment (intervals);
  Bayesian; 2nd-order probability: combines epistemic and aleatory;

Metrics: Importance factors, partial correlations, main effects, and variance-based decomposition.

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Analytic Reliability Methods

- **Define limit state function *g(x)* for response metric (model output, e.g., F_{min}) of interest, where x are uncertain variables.**
- **Reliability methods either**
  - **map specified response levels $g(x) = \bar{z}$ (perhaps corr. to a failure condition) to reliability index *β* or probability *p*; or**
  - **map specified probability or reliability levels to the corresponding response levels.**

Mean Value (first order, second moment – MVFOSM)

determine mean and variance of limit state, translate to from p, β:

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

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

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

simple approx., but widely used by analysts; also second order formulations

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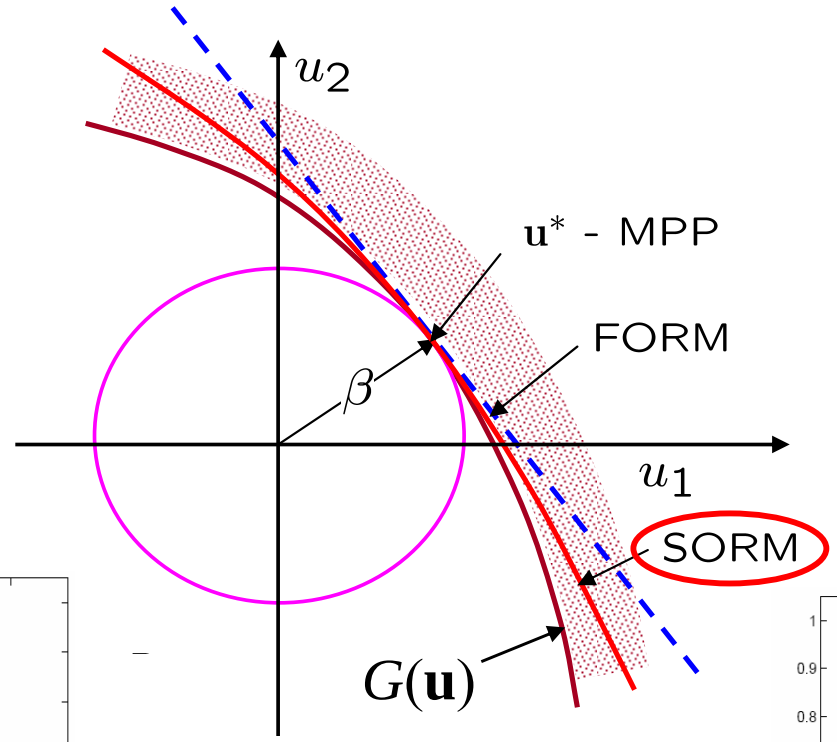
Analytic Reliability: MPP Search

Perform optimization **in u-space (std normal space corr. to uncertain x-space) to determine Most Probable Point (of response or failure occurring)**

Reliability Index Approach (RIA)

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

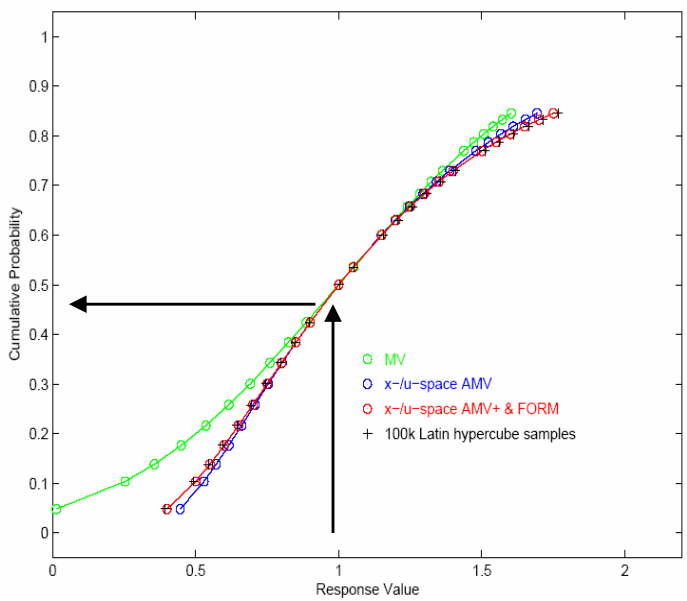
Find minimum distance to *G(u)* level curve; used for forward map *z* → *p or* β



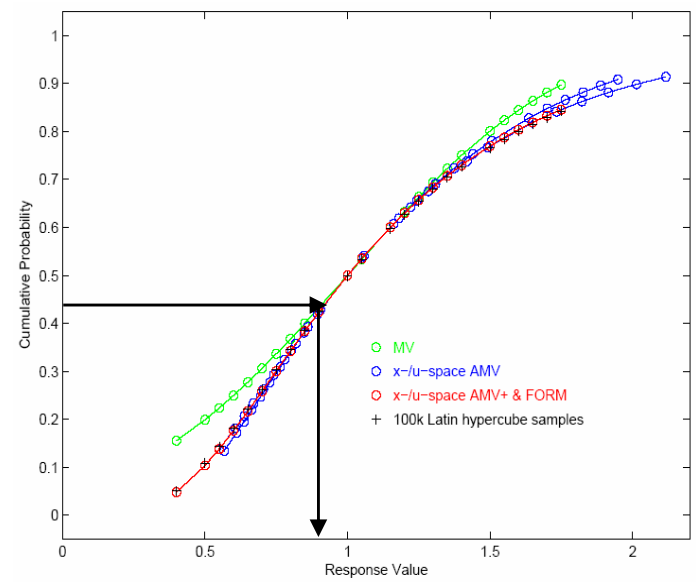
Performance Measure Approach (PMA)

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

Find minimum *G(u)* for specified β radius; used for inverse map *p* or β → *z*



...should yield better estimates of reliability than Mean Value methods



Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

- **<u>Limit state linearizations</u>: use a local surrogate for the limit state *G(u)* during optimization in u-space (or x-space):**

$$\text{u-space AMV:} \quad G(\mathbf{u}) = G(\mu_\mathbf{u}) + \nabla_u G(\mu_\mathbf{u})^T(\mathbf{u} - \mu_\mathbf{u})$$

$$\text{u-space AMV+:} \quad G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*)$$

$$\boxed{\text{u-space AMV}^2\text{+:} \quad G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*) + \tfrac{1}{2}(\mathbf{u} - \mathbf{u}^*)^T \nabla_u^2 G(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*)}$$

(could use analytic, finite difference, or quasi-Newton (BFGS, SR1) Hessians in approximation/optimization – results here mostly use SR1 quasi-Hessians.)

- **<u>Integrations (in u-space to determine probabilities)</u>: may need higher order for nonlinear limit states**

$$1^{\text{st}}\text{-order:} \left\{ \begin{array}{lcl} p(g \le z) & = & \Phi(-\beta_{cdf}) \\ p(g > z) & = & \Phi(-\beta_{ccdf}) \end{array} \right. \qquad 2^{\text{nd}}\text{-order:} \left\{ p = \Phi(-\beta) \underbrace{\prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta\kappa_i}}}_{\text{curvature correction}} \right.$$

- **MPP search algorithm:** Sequential Quadratic Prog. (SQP) vs. Nonlinear Interior Point (NIP)
- **Warm starting (for linearizations, initial iterate for MPP searches):** speeds convergence when increments made in: approximation, statistics requested, design variables

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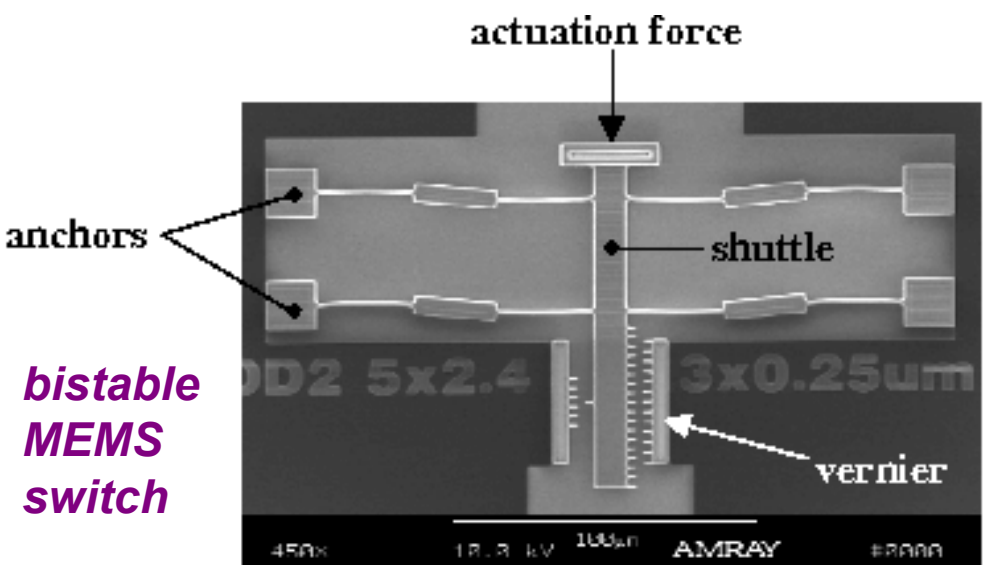
- **The DAKOTA framework and its key capabilities**
- **Uncertainty and reliability analysis techniques**
- ***Reliability-based design optimization for micro-electro-mechanical system (MEMS) design***

Shape Optimization of Compliant MEMS

- **Micro-electromechanical system (MEMS):** typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- **MEMS designs are subject to substantial variability** and lack historical knowledge base. Materials and micromachining, photo lithography, etching processes all yield uncertainty.
- Resulting part yields can be low or have poor cycle durability
- **Goal: shape optimize finite element model of bistable switch to…**
  - **Achieve prescribed reliability** in actuation force
  - Minimize sensitivity to uncertainties **(robustness)**



bistable MEMS switch

uncertainties to be considered (edge bias and residual stress)

variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

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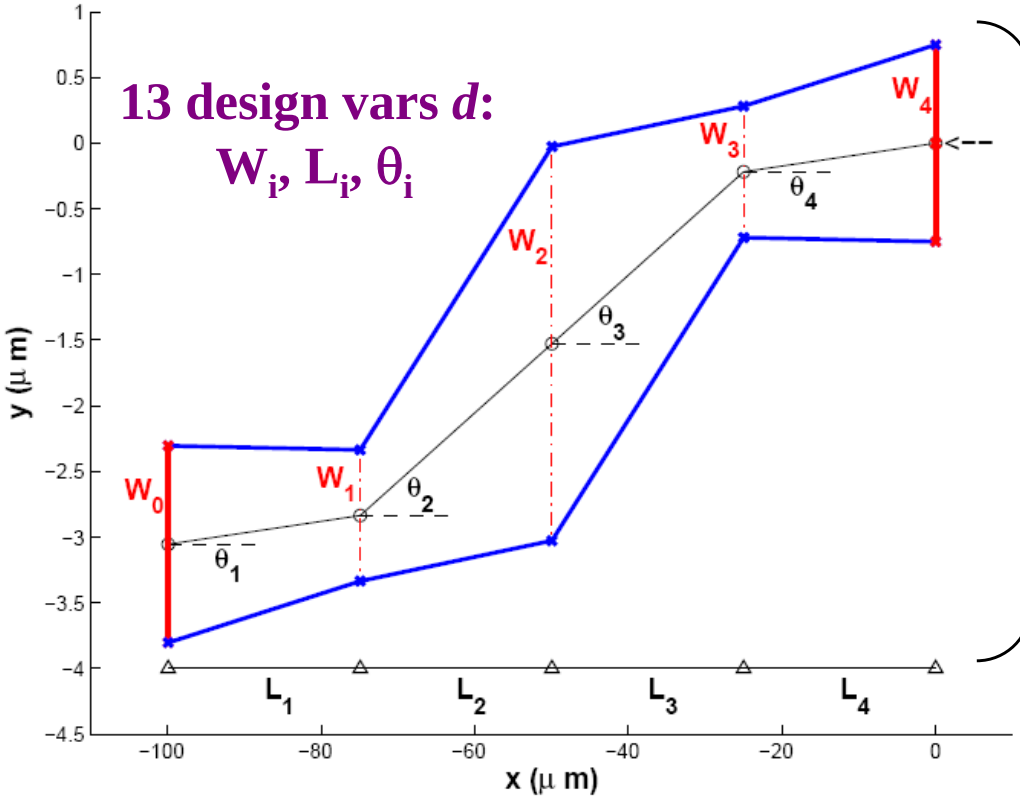
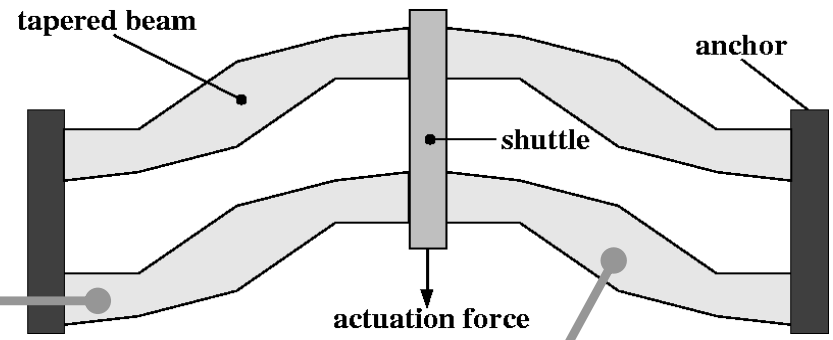
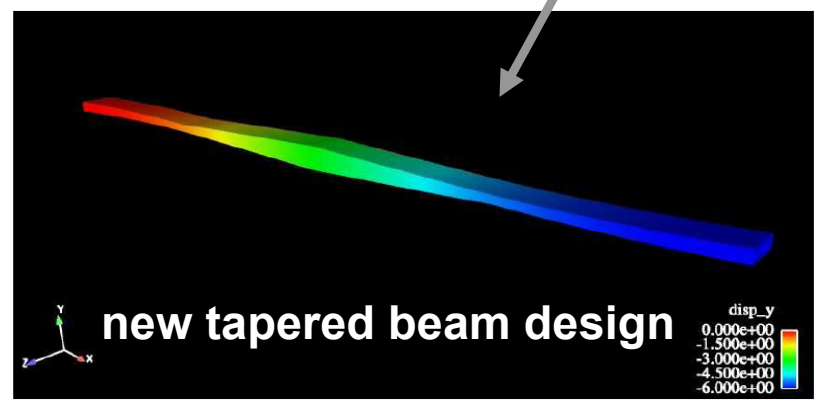
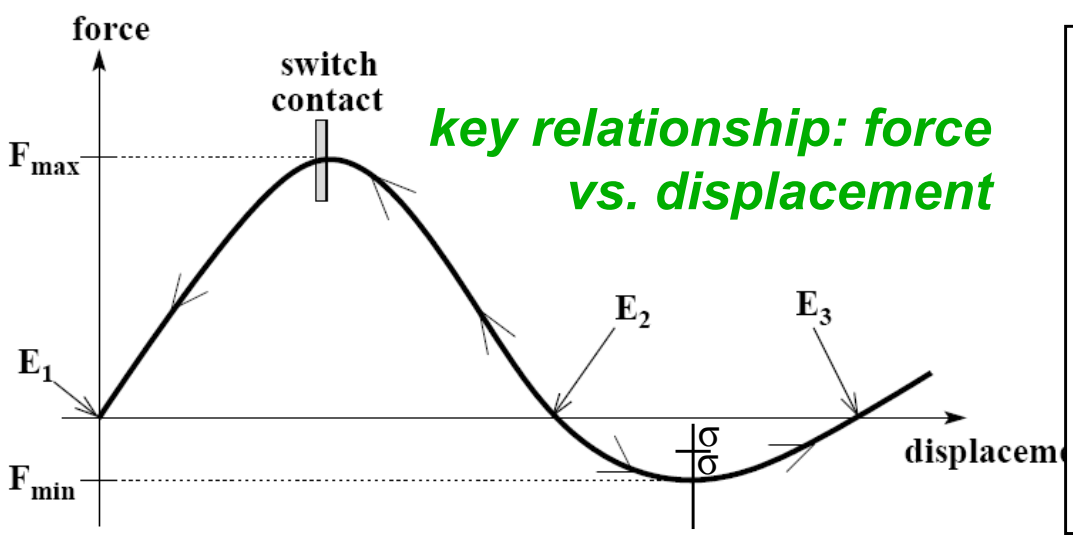
Tapered Beam Bistable Switch: Performance Metrics









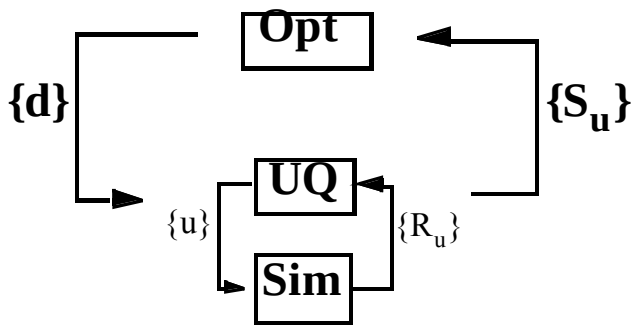
key relationship: force vs. displacement

Typical design specifications:

- **actuation force F_{min} reliably 5 μN**
- **bistable ($F_{max} > 0$, $F_{min} < 0$)**
- **maximum force: $50 < F_{max} < 150$**
- **equilibrium E2 < 8 μm**
- **maximum stress < 1200 MPa**

Optimization Under Uncertainty

Rather than design and then post-process to evaluate uncertainty…
actively design optimize while accounting for uncertainty/reliability metrics $s_u(d)$, e.g., mean, variance, reliability, probability:



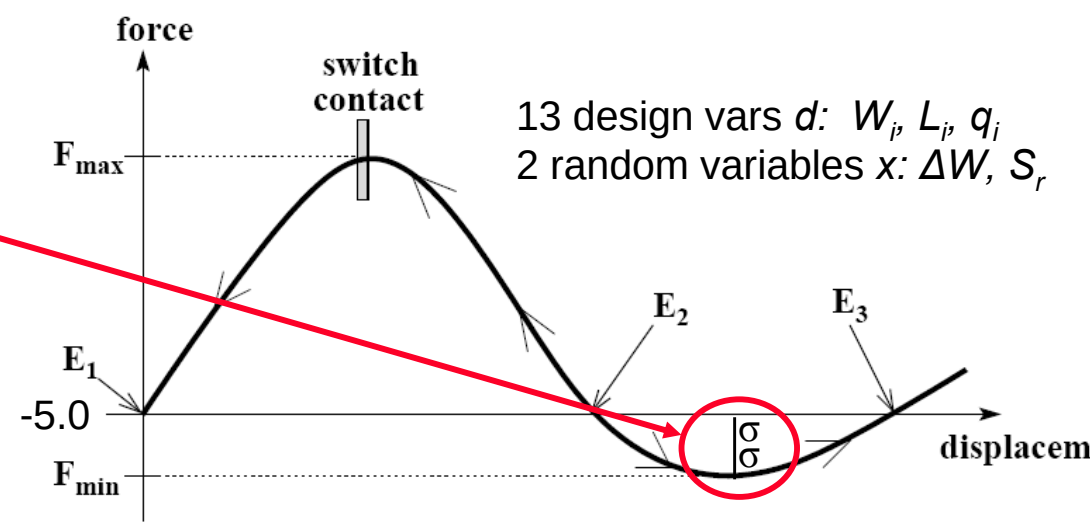
(nested paradigm)

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

Bistable switch problem formulation (Reliability-Based Design Optimization):

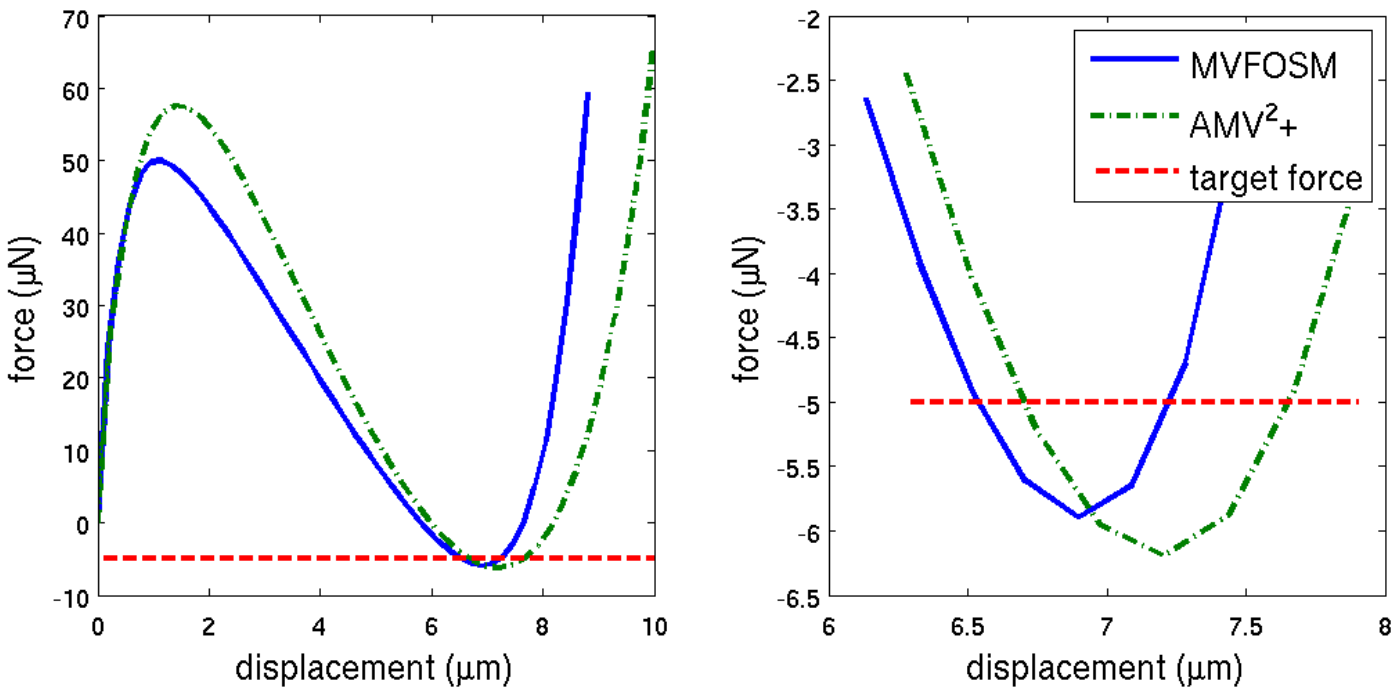
simultaneously reliable and robust designs

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



13 design vars *d:* W_i, L_i, q_i
2 random variables *x:* ΔW, S_r

RBDO Finds Optimal & Robust Design



Close-coupled results: DIRECT / CONMIN + reliability method yield optimal and reliable/robust design:

metric				MVFOSM	AMV^2+	FORM
l.b.	name	u.b.	initial $\mathbf{d}^0$	optimal $\mathbf{d}^*_M$	optimal $\mathbf{d}^*_A$	optimal $\mathbf{d}^*_F$
	E $[F_{min}]$ (μN)		-26.29	-5.896	-6.188	-6.292
2	β		5.376	2.000	1.998	1.999
50	E $[F_{max}]$ (μN)	150	68.69	50.01	57.67	57.33
	E $[E_2]$ (μm)	8	4.010	5.804	5.990	6.008
	E $[S_{max}]$ (MPa)	1200	470	1563	1333	1329
	AMV^2+ verified β		3.771	1.804	-	-
	FORM verified β		3.771	1.707	1.784	-

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Summary

- The DAKOTA toolkit includes algorithms for massively parallel uncertainty quantification and optimization with large-scale computational models.
- DAKOTA strategies enable efficient combination of algorithms, use of surrogates, and warm-starting.
- Uncertainty-aware design optimization is helpful in MEMS design where robust and/or reliable designs are essential.
- DAKOTA is a research framework for novel capability such as EGRA, an algorithm which closely couples several other algorithms to perform effective reliability analysis.

Thank you for your attention!

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Extra Slides

UQ Challenge: Nonlinear/Multimodal Limit States

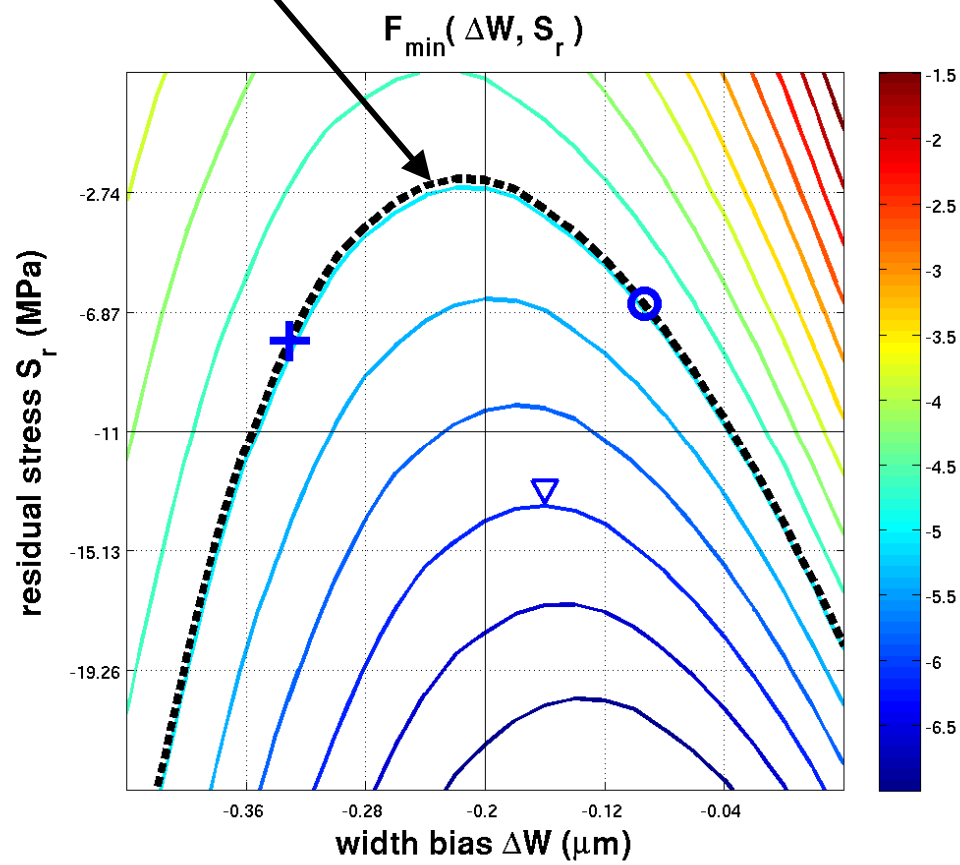
- **Calculating β requires solving nonlinear equality-constrained sub-problem in probability space**

$$\begin{cases} \min \ x^T x \\ \text{s.t.} \ g(x) = \bar{z} = -5.0 \end{cases}$$

- **Methods AMV²+ and FORM converge to different MPPs (+ and O respectively)**

- **Challenge: limit states with multiple legitimate candidates for most probable point of failure *(need all optima)***

- **Challenge: local first order probability integrations may not be accurate enough for nonlinear limit state**



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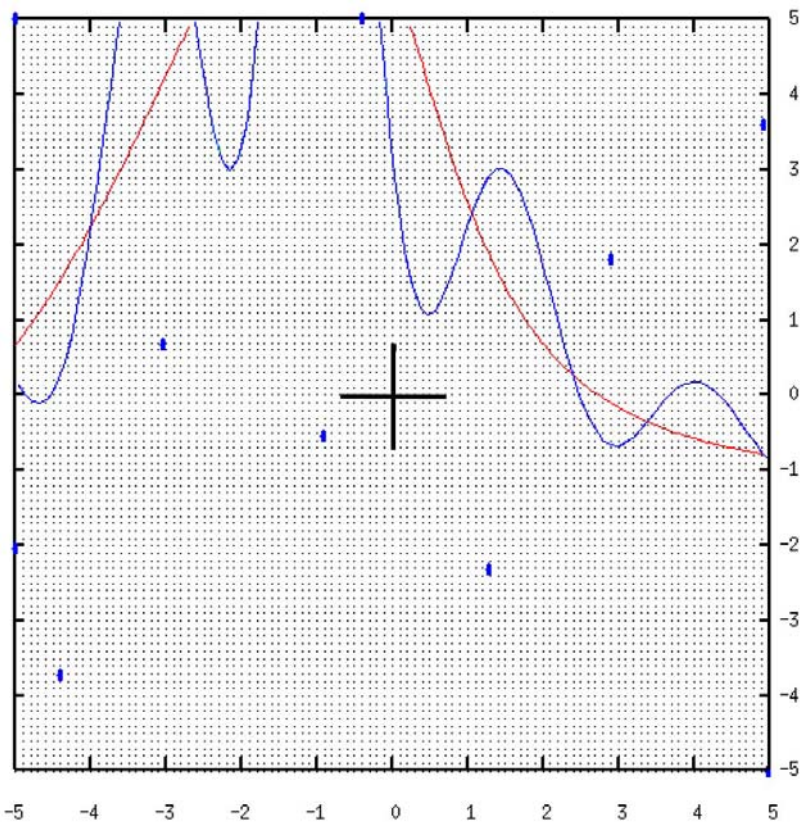
Efficient Global Reliability Analysis

- **EGRA (B.J. Bichon) performs reliability analysis with EGO (Gaussian Process surrogate and NCSU DIRECT optimizer) coupled with Multimodal adaptive importance sampling for probability calculation.**

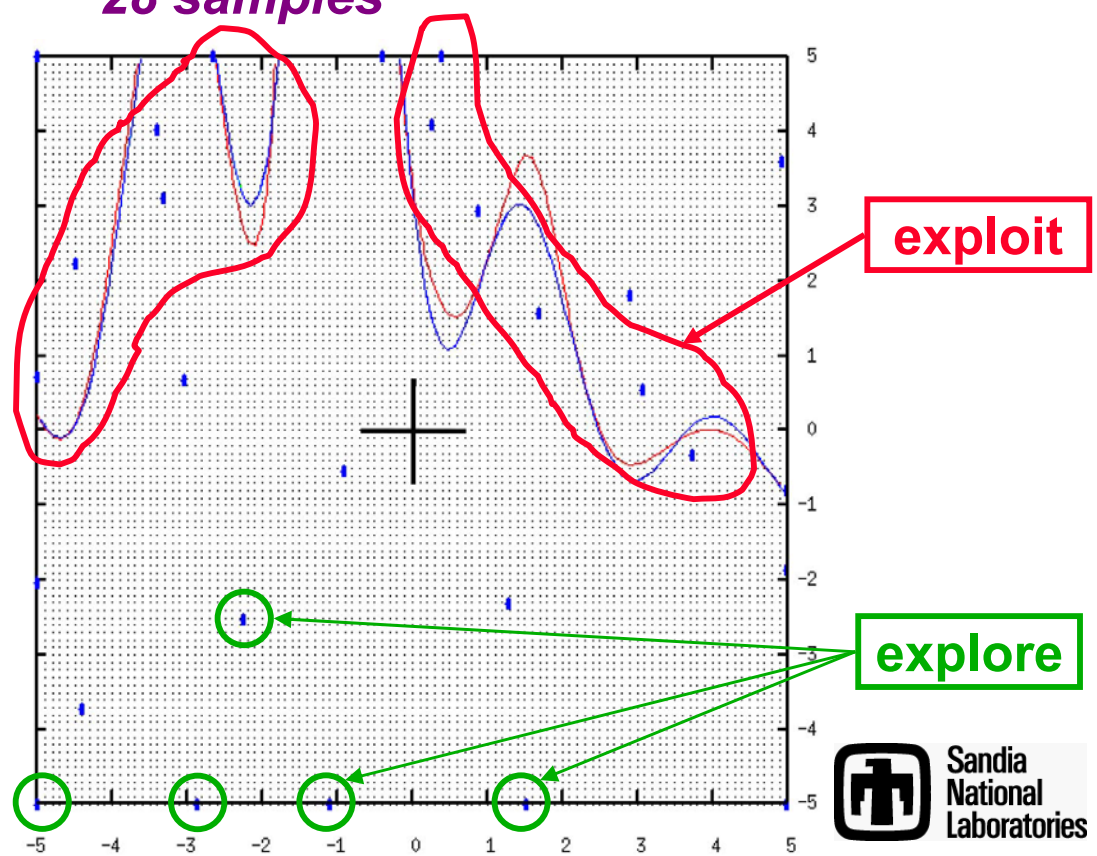
- **Created to address nonlinear and/or multi-model limit states in MPP searches.**

Gaussian process model of reliability limit state with

10 samples



28 samples



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DAKOTA/EGRA: Superior Performer

Reliability Method	Function Evaluations	First-Order p_f (% Error)	Second-Order p_f (% Error)	Sampling p_f (% Error, Avg. Error)
No Approximation	66	0.11798 (276.3%)	0.02516 (-19.7%)	—
x-space AMV^2+	26	0.11798 (276.3%)	0.02516 (-19.7%)	—
u-space AMV^2+	26	0.11798 (276.3%)	0.02516 (-19.7%)	—
x-space TANA	506	0.08642 (175.7%)	0.08716 (178.0%)	—
u-space TANA	131	0.11798 (276.3%)	0.02516 (-19.7%)	—
x-space EGO	50.4	—	—	0.03127 (0.233%, 0.929%)
u-space EGO	49.4	—	—	0.03136 (0.033%, 0.787%)
True LHS solution	1M	—	—	0.03135 (0.000%, 0.328%)

- **Most accurate local method under-predicts p_f by ~20%**
- **EGO-based method accurately quantifies probability of failure within 1% with similar number of function evaluations.**
- **Pro: LHS accuracy + MPP efficiency without gradients, good tail probability resolution**
- **Con: Exploratory samples wasteful, GP can break down for large number of samples or independent variables**

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