SAND2008-3204C

The DAKOTA Toolkit for Parallel Optimization and Uncertainty Analysis

Brian M. Adams
Sandia National Laboratories
Optimization and Uncertainty Quantification

May 12, 2008

Architectures for Hybrid Design Space Exploration
SIAM OP08 Mini-symposium 49
Boston, MA

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

Outline

By combining optimization, uncertainty analysis methods, and surrogate (meta-) modeling in a single framework, DAKOTA enables advanced studies with computational models.

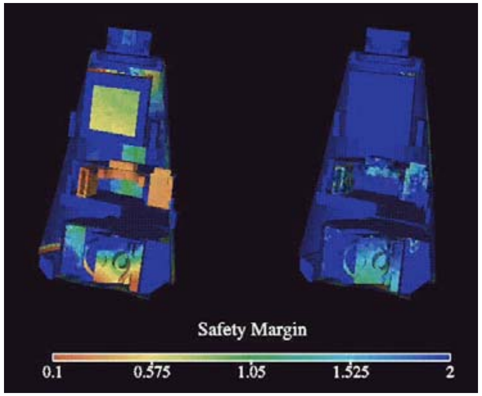
- **The DAKOTA framework and design concepts**
- **Tour of methods**
- **Strategies combining methods**
  - **Surrogate-based optimization**
  - **Optimization for uncertainty quantification**
  - **Reliability-based design (OPT+UQ)**
- **Ongoing research**

Slide (and research) credits: Mike Eldred (PI), Laura Swiler, Barron Bichon
http://www.cs.sandia.gov/DAKOTA/

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)

response metrics

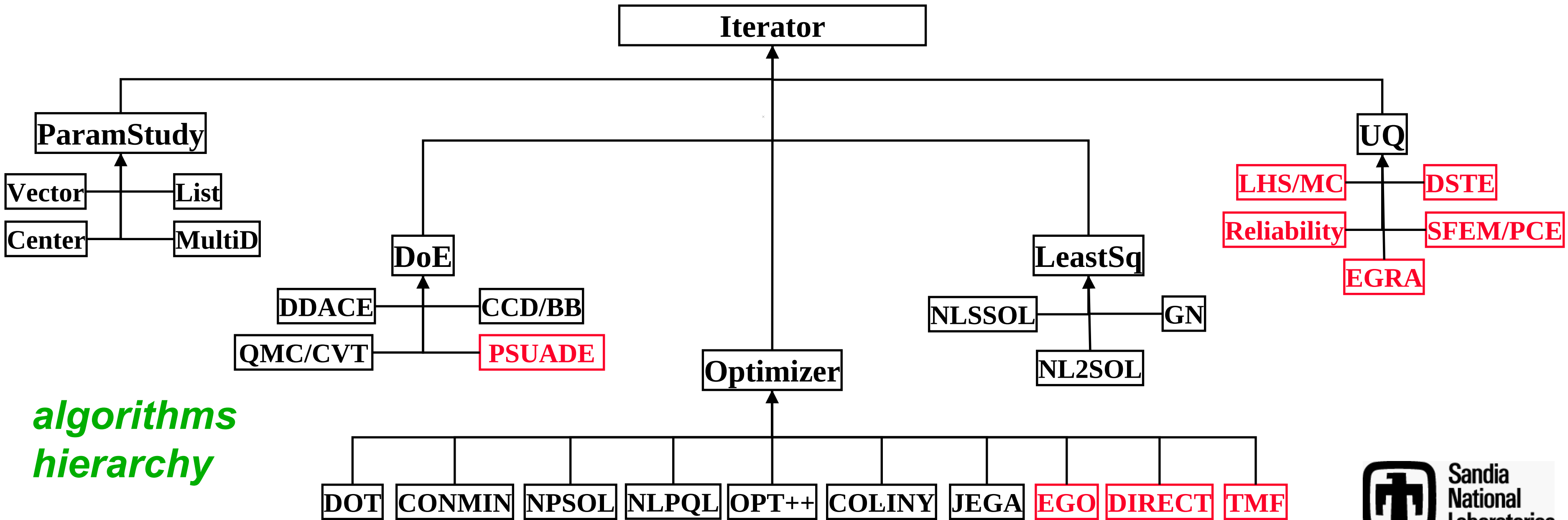
Computational Model (simulation)

- **Black box:** any code: mechanics, circuits, high energy physics, biology, chemistry
- **Semi-intrusive:** Matlab, ModelCenter, Python SIERRA multi-physics, SALINAS, Xyce

Sandia National Laboratories

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)

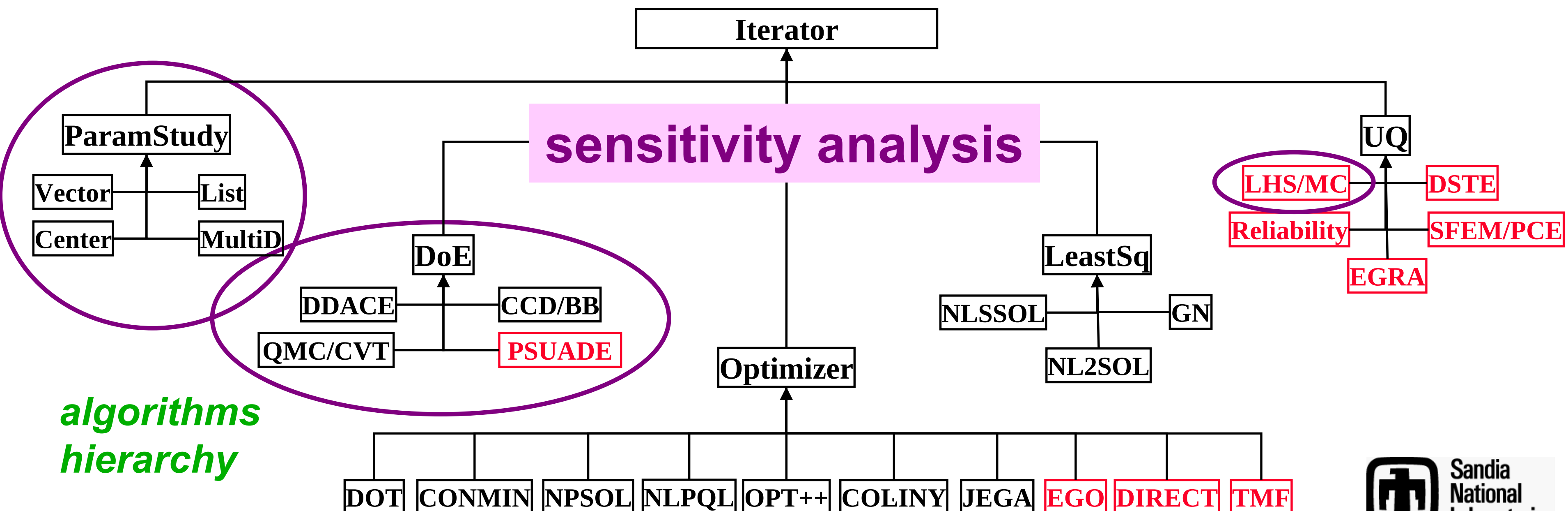


algorithms hierarchy

Sandia National Laboratories

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

Sandia National Laboratories

Flexibility with Models

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**

integrate parameters into application inputs

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**

extract relevant metrics

responses

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

Flexible interface to user application (computational model/simulation)

- **May be cheap (analytic function, linear analysis); typically costly (finite element mesh with millions of DOF, transient analysis of integrated circuit with millions of transistors)**

- **May run tightly-coupled, locally as separate process, in parallel on a cluster, remotely on a distributed resource**

Optimization Methods

Gradient-based methods

(DAKOTA will compute finite difference gradients and FD/quasi-Hessians if necessary)

- *DOT (various constrained)*
- CONMIN (FRCG, MFD)
- *NPSOL (SQP)*
- *NLPQL (SQP)*
- OPT++ (CG, Newton)

Calibration (least-squares)

- NL2SOL (GN + QH)
- *NLSSOL (SQP)*
- OPT++ (Gauss-Newton)

Derivative-free methods

- COLINY (PS, APPS, Solis-Wets, COBYLA2, EAs, DIRECT)
- JEGA (single/multi-obj GAs)
- EGO (efficient global opt via Gaussian Process models)
- DIRECT (Gablonsky)
- OPT++ (parallel direct search)

- *TMF (templated meta-heuristics framework)*

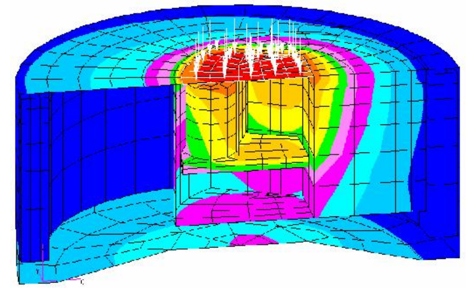
Uncertainty Quantification

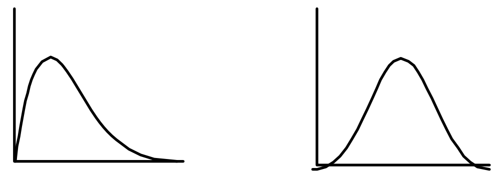
- **A single optimal design or nominal performance prediction is often insufficient for decision making**

- ***Need to make risk-informed decisions, based on an assessment of uncertainty***

Uncertainty Quantification Example

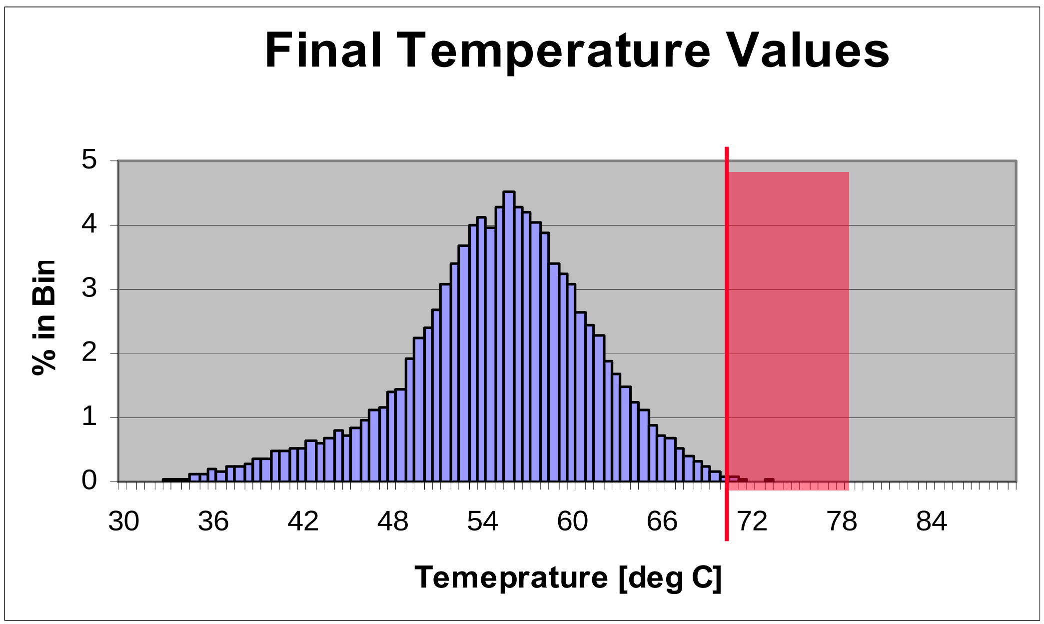
- Device subject to heating (experiment or computational simulation)
- Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by $u_1, \ldots, u_N$
- Response temperature $T(u_1, \ldots, u_N)$ calculated by heat transfer code





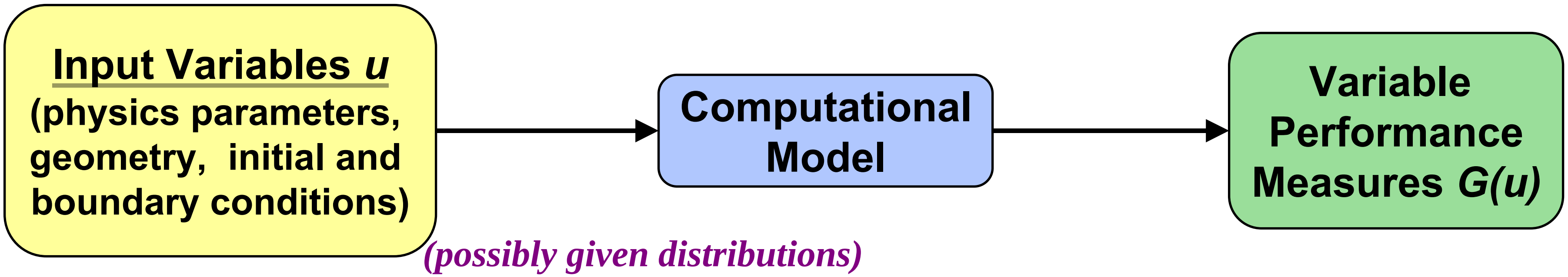
Given distributions of $u_1,\ldots,u_N$, UQ methods calculate statistical info on outputs:

- Probability distribution of temperatures
- Correlations (trends) and sensitivity of temperature
- Mean(T), StdDev(T), Probability($T \geq T_{critical}$)



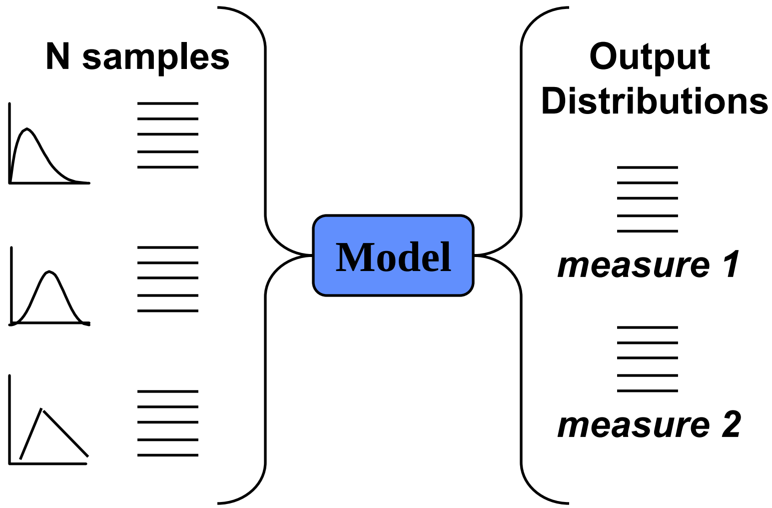
Uncertainty Quantification (UQ)

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*



Typical method: Monte Carlo Sampling

Sandia National Laboratories

UQ Algorithms

Goal: bridge robustness/efficiency gap

	Production	New	Under dev.	Planned
Sampling	LHS/MC, QMC/CVT	IS/AIS/MMAIS, Incremental LHS		Bootstrap, Jackknife
Reliability	1st/2nd-order local: MVFOSM/SOSM, x/u AMV/AMV^2/ AMV+/AMV^2+, x/u TANA, FORM/SORM	Global: EGRA		
Polynomial Chaos		Wiener-Askey gPC: sampling, quadrature, pt collocation	Cubature	Adaptivity, Wiener-Haar
Other probabilistic				Dimension reduction
Epistemic	Second-order probability	Dempster-Shafer evidence theory		Bayesian, Imprecise probability
Metrics	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression	

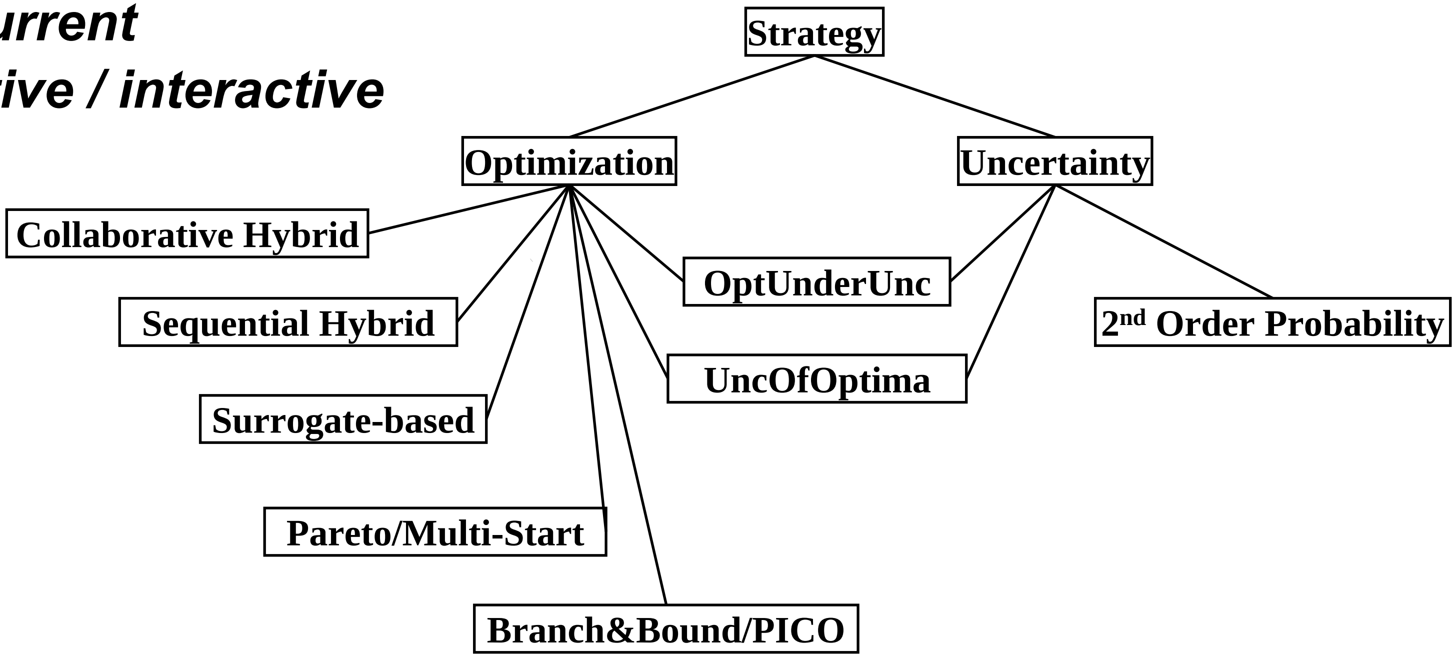
Outline

- The DAKOTA framework and design concepts
- Tour of methods
- Strategies combining methods
  - Surrogate-based optimization
  - Optimization for uncertainty quantification
  - Reliability-based design (OPT+UQ)
- Ongoing research

Strategies Enable Algorithm Combination

DAKOTA <u>strategies</u> enable flexible combination of multiple models and algorithms.

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



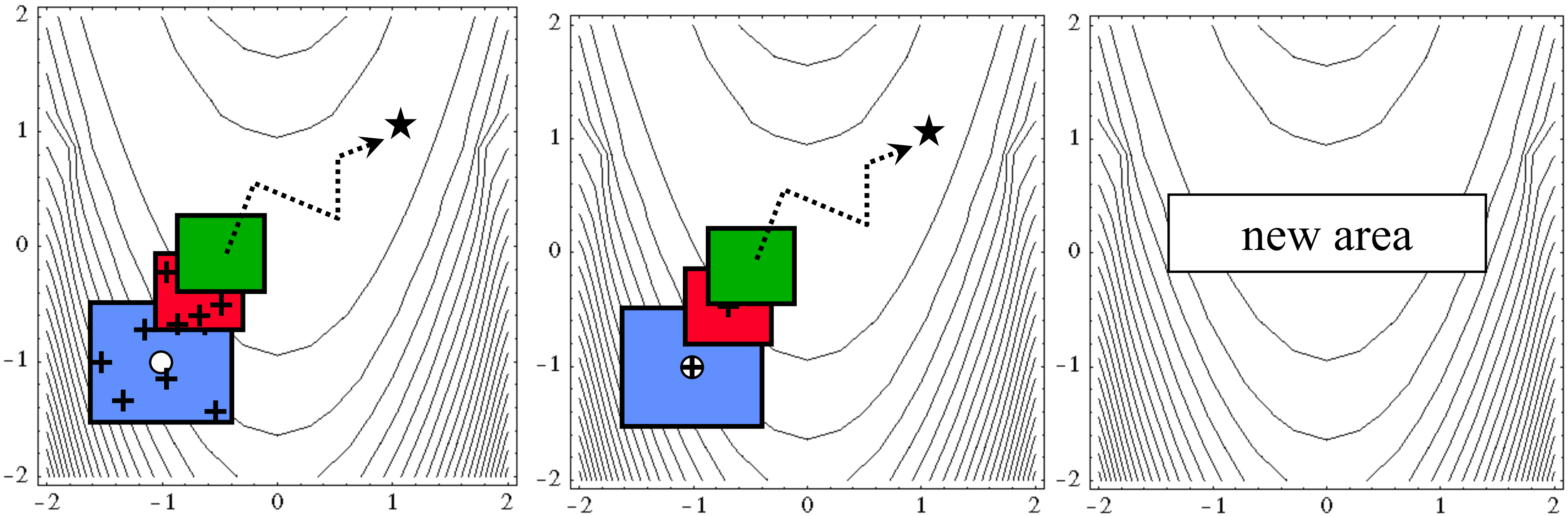
Sample Algorithm Combinations

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
- **Optimization under uncertainty:** robust or reliability-based design, design with probabilistic constraints

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.)

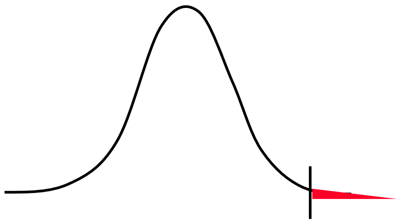
ROMs in SBO

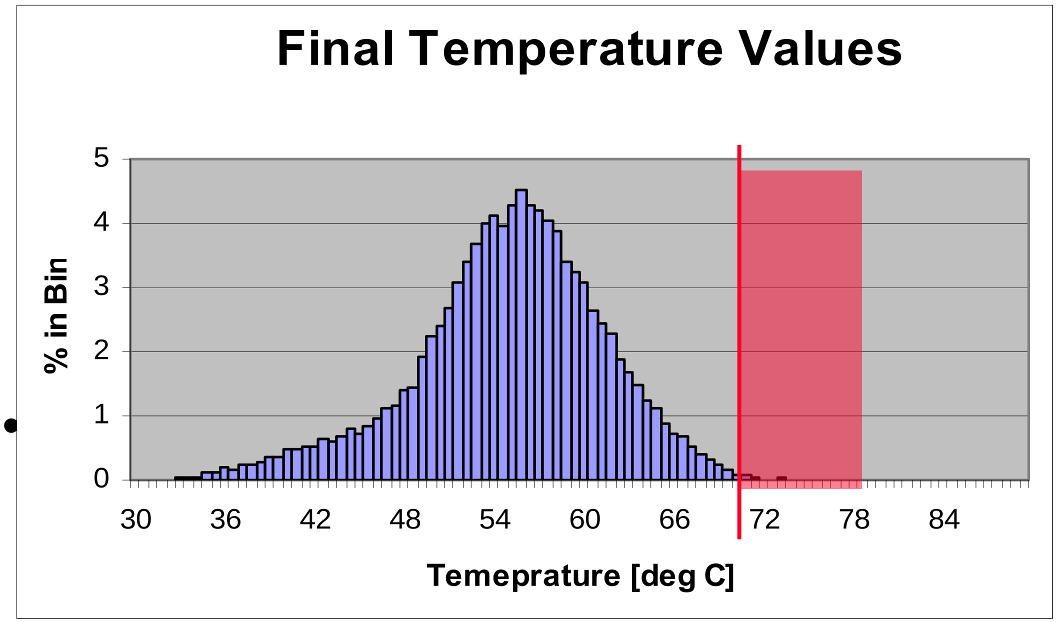
- Key issue: capture parameter changes
  - E- ROM, S-ROM, tensor SVD
- Some simulation intrusion to re-project
- TR progressions resemble local, multipoint, or global

Sandia National Laboratories

Calculating Probability of Failure

- *Given uncertainty in materials, geometry, and environment, determine likelihood of failure Probability($T \geq T_{critical}$)*





- **Could perform 10,000 Monte Carlo samples and count how many exceed the threshold…**

- **Or directly determine input variables which give rise to failure behaviors by solving an optimization problem.**

Sandia National Laboratories

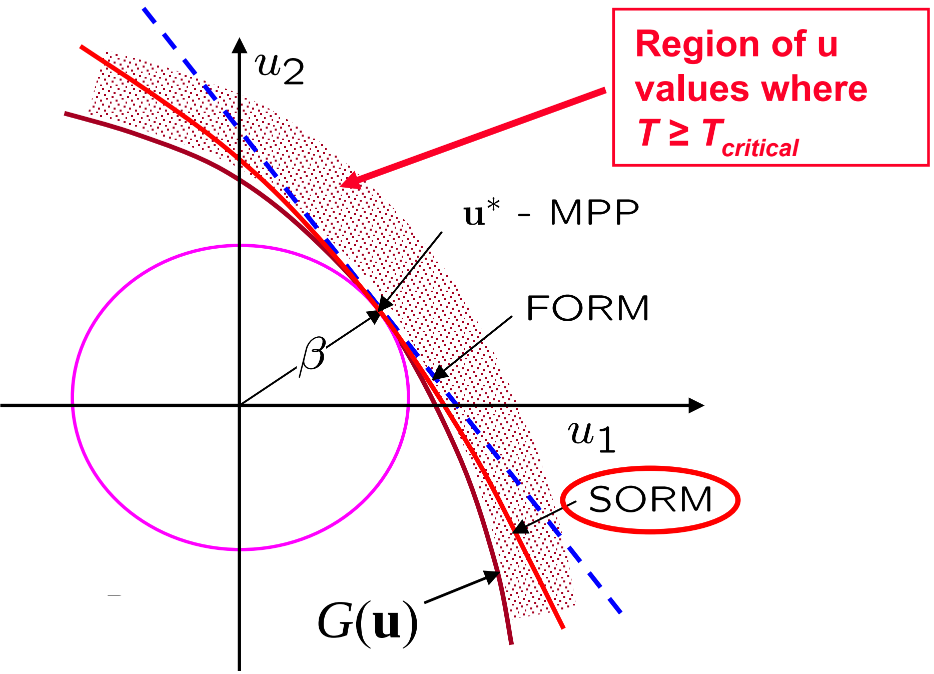
Analytic Reliability: MPP Search

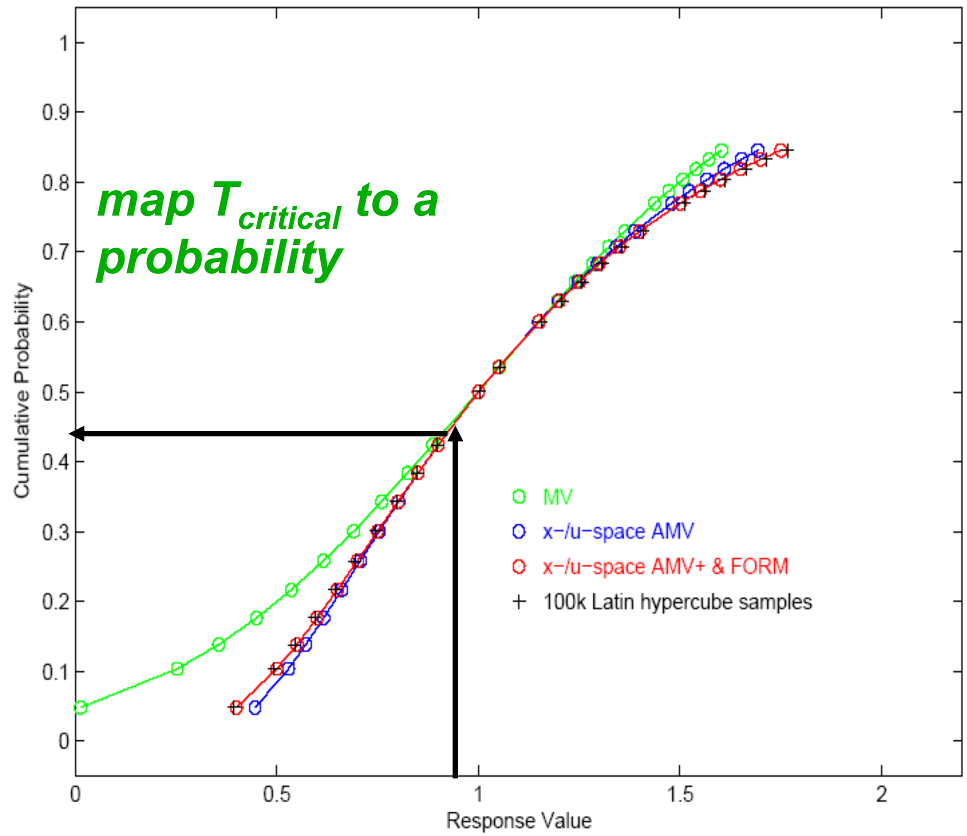
Perform optimization **in uncertain variable space to determine Most Probable Point (of response or failure occurring) for *G(u)* = *T(u)*.**

Reliability Index Approach (RIA)

$$\text{minimize} \quad \mathbf{u}^T \mathbf{u}$$

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





Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

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

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

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

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

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

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

1st-order: $\begin{cases} p(g \leq z) &= \Phi(-\beta_{cdf}) \\ p(g > z) &= \Phi(-\beta_{ccdf}) \end{cases}$

2nd-order: $\left\{ p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta \kappa_i}} \right.$

curvature correction

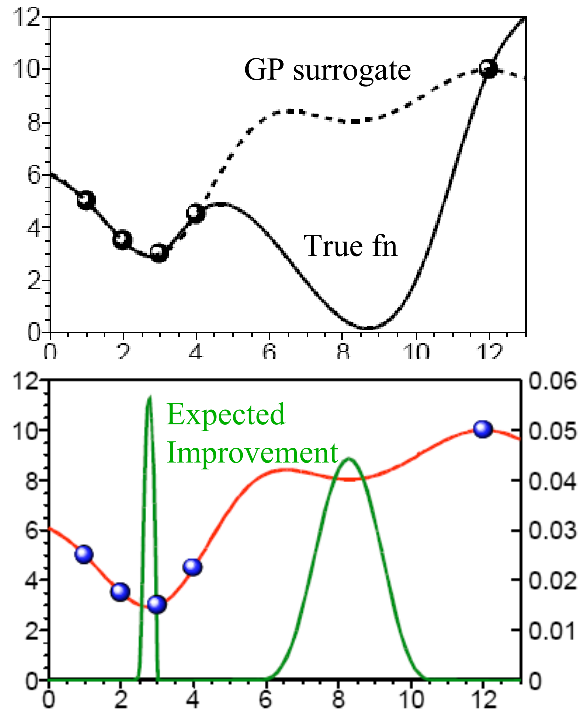
- **MPP search algorithm:** Sequential Quadratic Prog. (SQP) vs. Nonlinear Interior Point (NIP)
- **Warm starting (for linearizations, initial iterate for MPP searches):** speeds convergence when increments made in: approximation, statistics requested, design variables

Sandia National Laboratories

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-modal limit states in MPP searches.**



From Jones, Schonlau, Welch, 1998

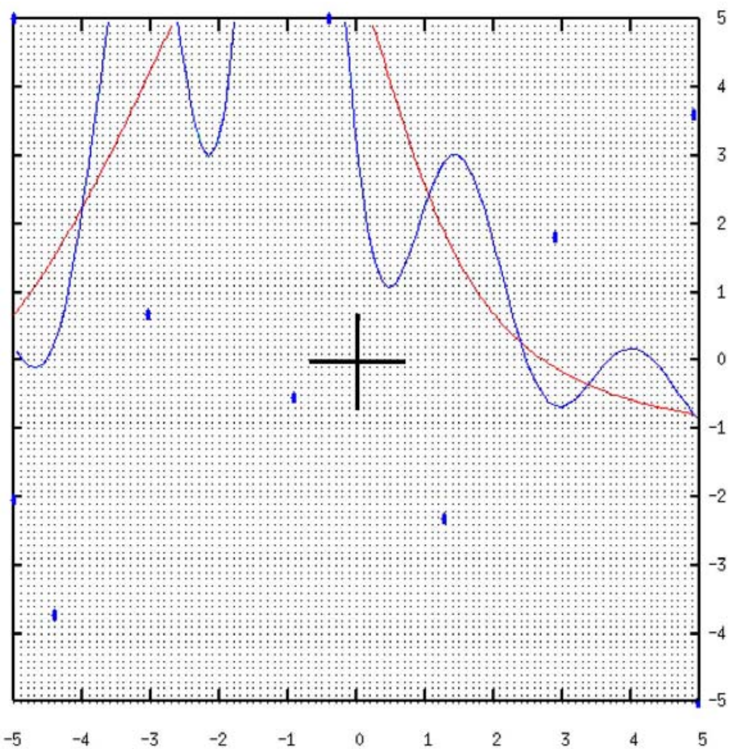
Efficient Global Reliability Analysis

- **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.

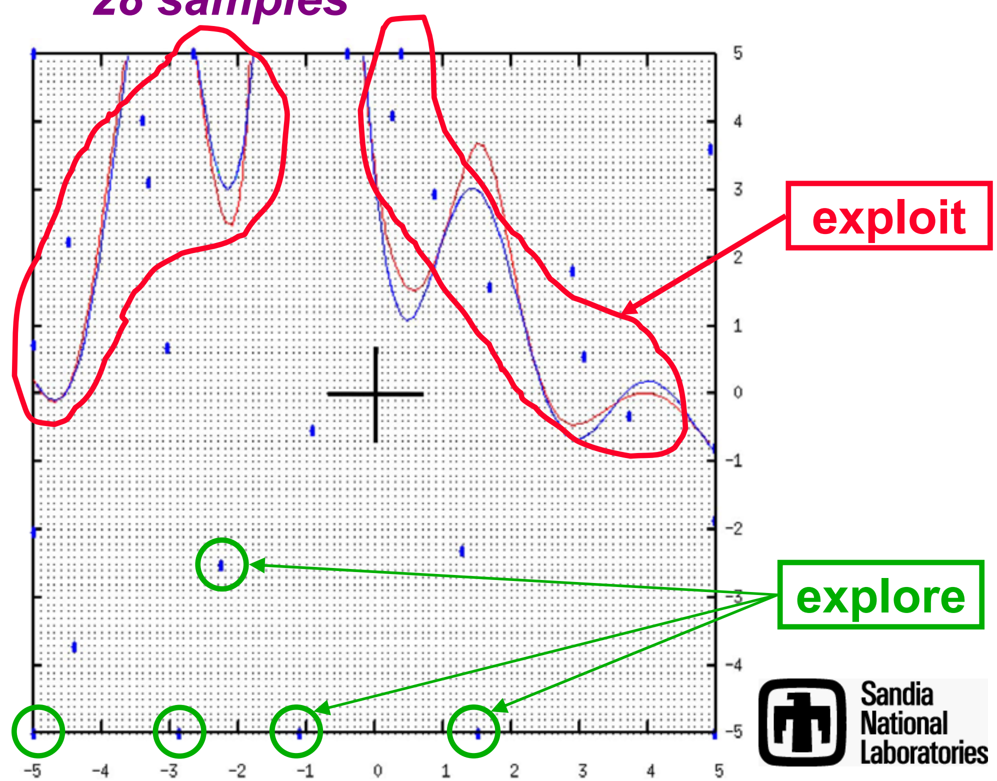
- Created to address nonlinear and/or multi-modal limit states in MPP searches.

Gaussian process model of reliability limit state with

10 samples



28 samples

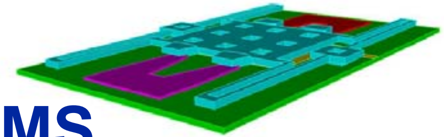


Sandia National Laboratories

DAKOTA/EGRA: Superior Performer

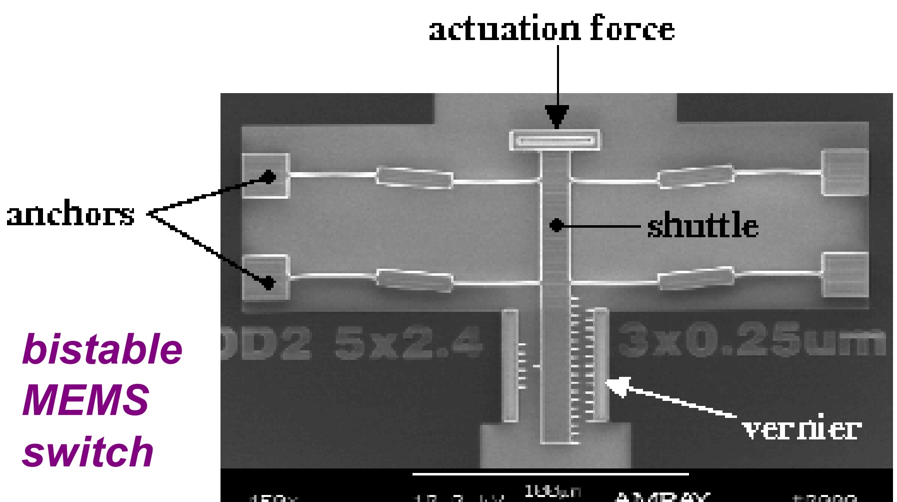
Reliability Method	Function Evaluations	First-Order p_f (% Error)	Second-Order p_f (% Error)	Sampling p_f (% Error, Avg. Error)
No Approximation	66	0.11798 (276.3%)	0.02516 (-19.7%)	—
x-space AMV^2+	26	0.11798 (276.3%)	0.02516 (-19.7%)	—
u-space AMV^2+	26	0.11798 (276.3%)	0.02516 (-19.7%)	—
x-space TANA	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**



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)



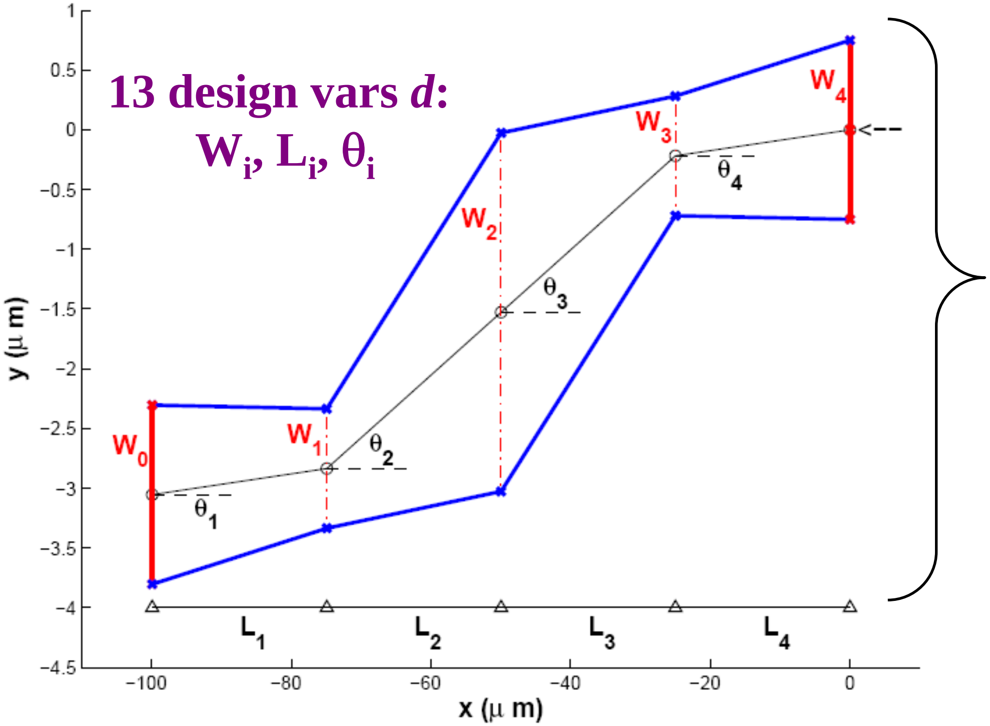
bistable MEMS switch

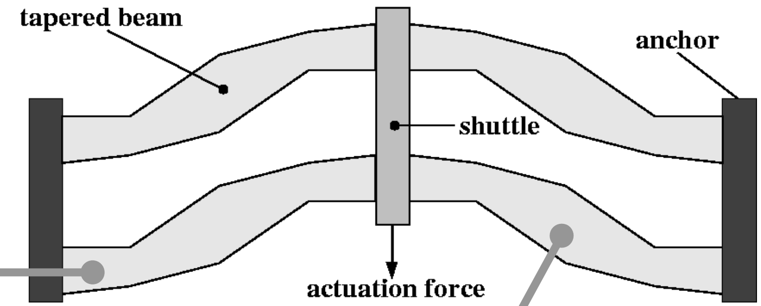
uncertainties to be considered (edge bias and residual stress)

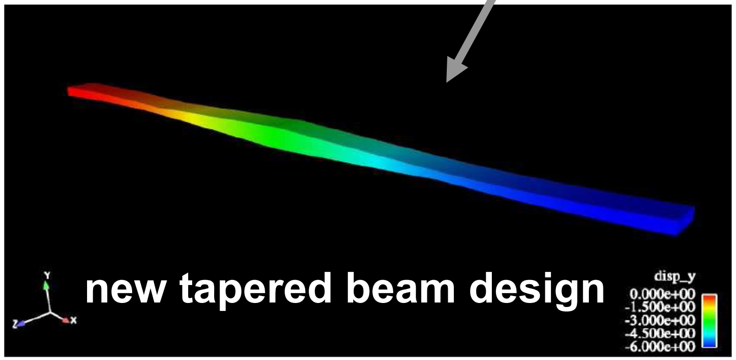
variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

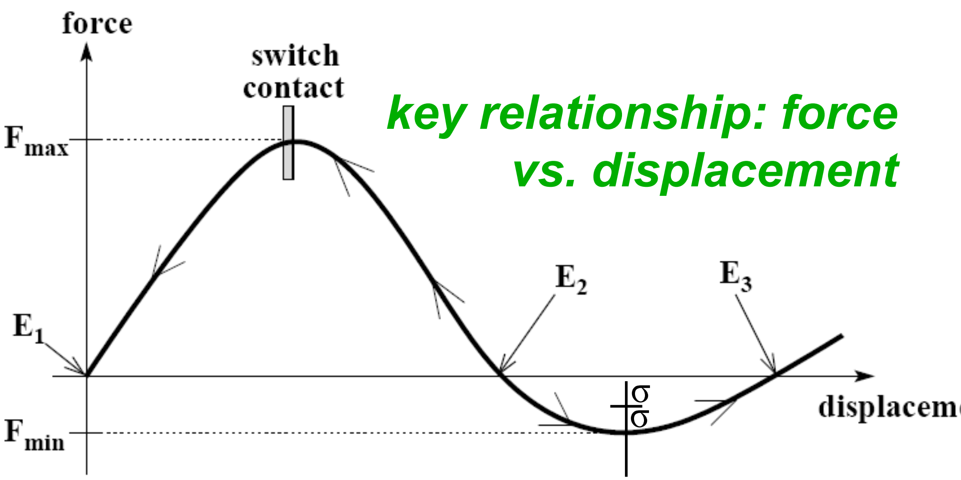
Sandia National Laboratories

Tapered Beam Bistable Switch: Performance Metrics









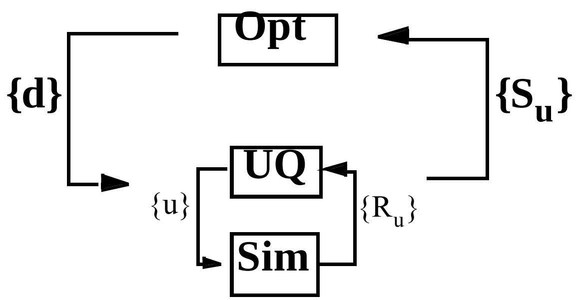
key relationship: force vs. displacement

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:



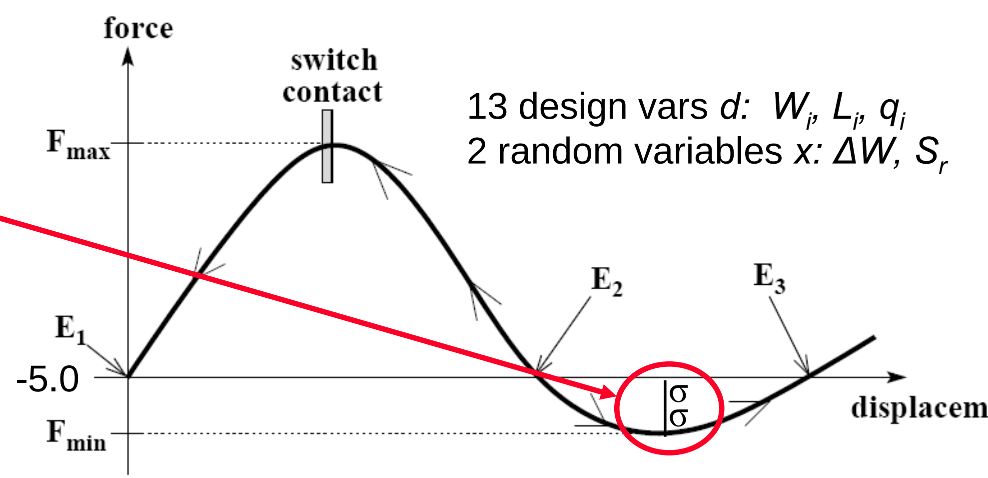
(nested paradigm)

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

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

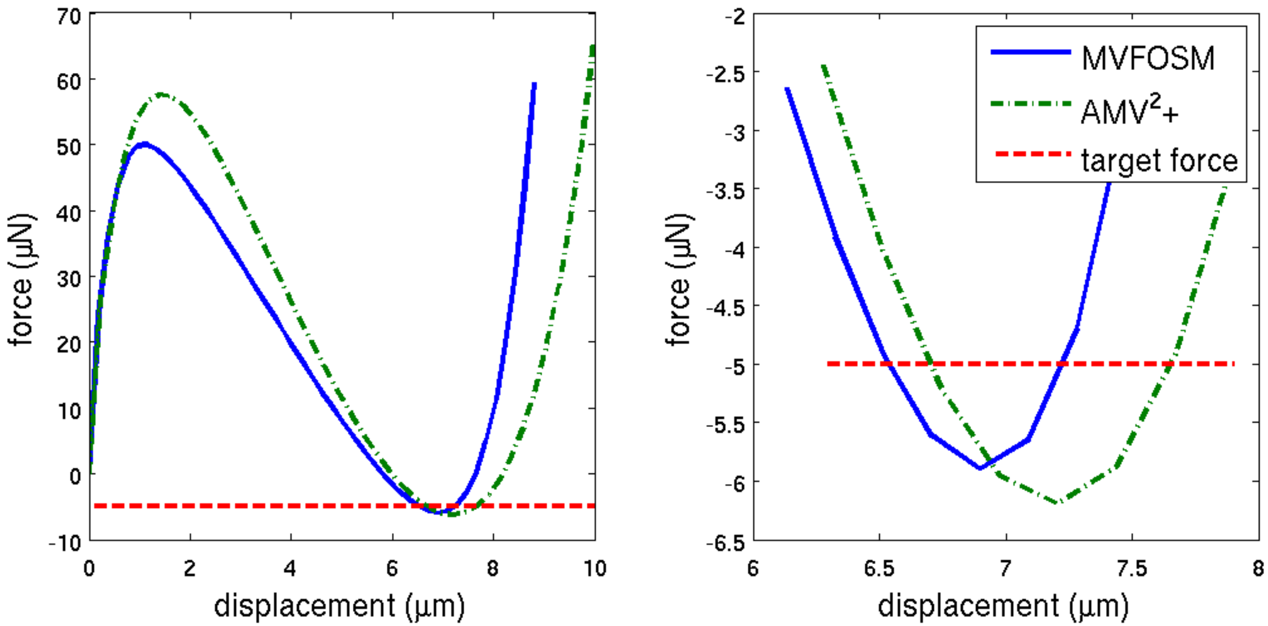
simultaneously reliable and robust designs

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



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	-

Sandia National Laboratories

Research Directions

DAKOTA's power comes partially from numerous iterative methods and flexible interfaces, but largely from its flexibility in combining methods for uncertainty-aware analysis of expensive simulations

Work in progress…

- **Polynomial Chaos and Stochastic Collocation (and their use in design optimization: tailor opt to UQ method)**
- **Model calibration under uncertainty,**
- **Better epistemic methods, including for OUU**
- **General weighted nonlinear least squares for calibration problems**
- **Advanced surrogate models and ROMs**
- **Improved user interface and XML problem specifications**

Thank you for your attention!

briadam@sandia.gov
http://www.sandia.gov/~briadam

Sandia National Laboratories