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Derivative-free Optimization Methods in DAKOTA, with Applications

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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`

- **Survey DAKOTA framework and its key capabilities**
- **Current and developing capabilities for local and global derivative-free optimization**
- **Demonstrate powerful combination of algorithms**

Thanks to Barron Bichon, Mike Eldred, and Jean-Paul Watson for slide content.

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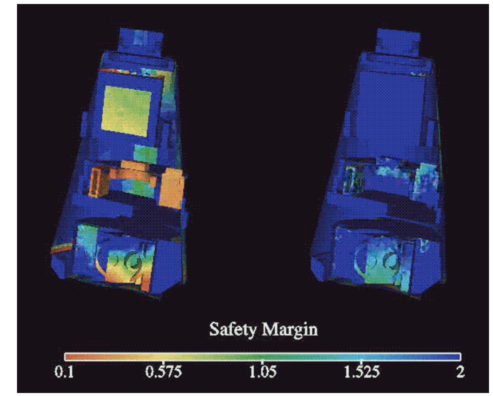
DAKOTA Motivation

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

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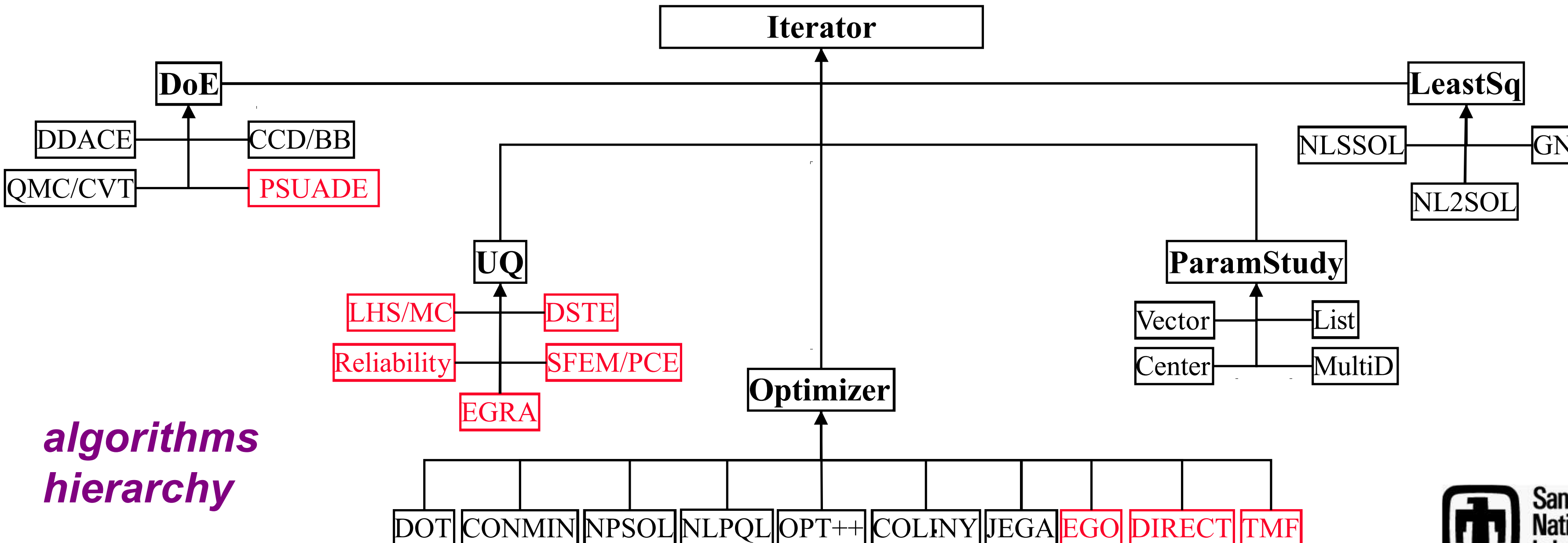
DAKOTA C++/OO Framework Goals

- **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
- **Impact:** tool for DOE labs and external partners; broad application deployment; free via GNU GPL (>3000 download registrations)



algorithms hierarchy

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

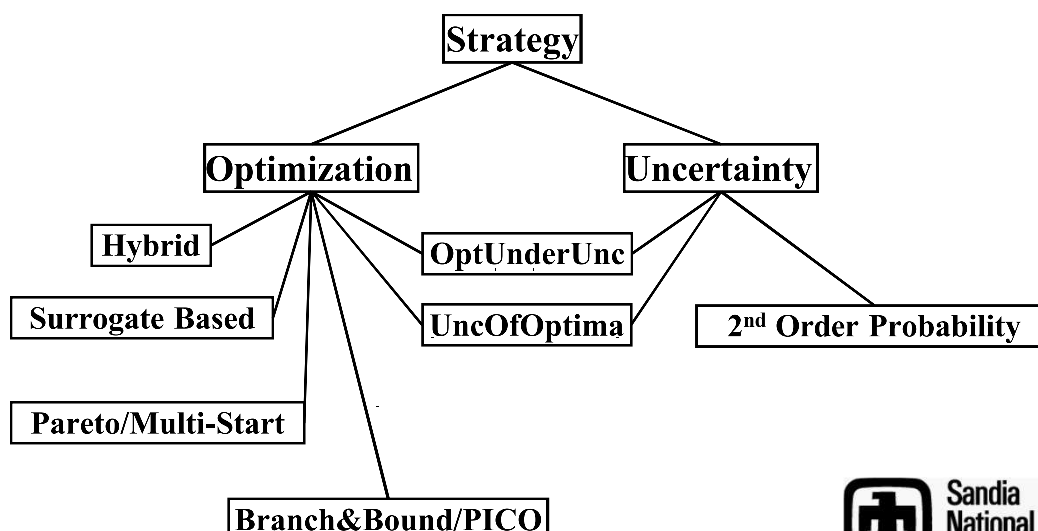
→

responses

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

DAKOTA strategies enable flexible combination of multiple models and algorithms. These can be:

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



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Current Derivative-free Methods

- **COLINY (interfaced through ACRO; W.E. Hart, et al.)**
  - **Asynchronous Parallel Pattern Search (APPSPACK; T.G. Kolda, et al.)**
  - **Pattern Search** *(enhanced with basis and move selection options)*
  - **Solis-Wets** *(greedy local search heuristic w/ MV Gaussian distribution)*
  - **COBYLA2** *(Nelder-Mead w/ linear & non-linear constraint support)*
  - **Evolutionary Algorithms** *(several variants)*
  - **Division of Rectangles (DIRECT)**
- **OPT++ Parallel Direct Search (PDS; J.C. Meza, et al.)**
- **John Eddy's Genetic Algorithms (JEGA)**
  - **Single-objective (SOGA)**
  - **Multi-objective Pareto (MOGA)**
- **DIRECT (as implemented by J.M. Gablonsky, et al.)**

Excepting OPT++, these all support general nonlinear constraints, either natively or through framework-supplied penalty functions.

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Developing Derivative-free Methods

- **Templatized Metaheuristics Framework (TMF; J-P. Watson): Includes text-based parameter initialization, solution-attribute caching, analysis observers / functors, eventually algorithm engineering. Algorithms include:**
  - **Metropolis sampling**
  - **Simulated annealing**
  - **Iterated local search**
  - **Basin hopping**
  - **Variable-neighborhood search**
  - **Elite pool maintenance schemes**
  - ***(eventually)* Evolutionary computing, constructive heuristics**

- **Efficient Global Optimization (EGO; B.J. Bichon): Uses a Gaussian Process model with expected improvement function to manage exploit vs. explore samples in search of optimum *(due to Jones, et al., 1998).***

- **Direct interface to APPSPACK / NAPPSPACK (Kolda & Griffin): APPS now supports nonlinear constraints through l_1, l_2, l_∞ penalty fns and solving a sequence of linearly constrained subproblems.**

Sample Algorithm Combinations

- **Global/local optimization:** **perform (1) sampling, parameter study, or global opt; then (2) local (gradient or non-gradient) opt at each promising point.**

- **Surrogate globalization** **of derivative-free local methods such as pattern search** ***(however not close-coupled as Taddy, et al.).***

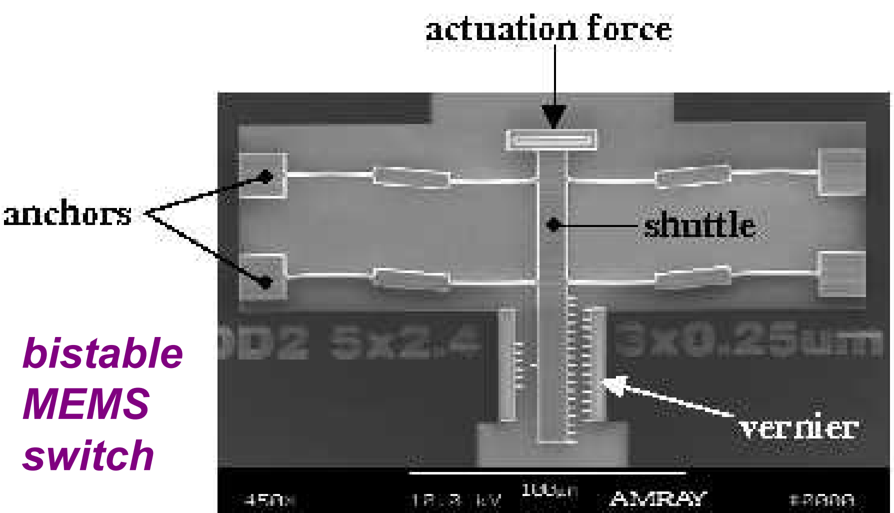
detailed examples coming up

- **Optimization under uncertainty for MEMS**

- **EGRA:** **Efficient Global Reliability Analysis**

Shape Optimization of Compliant MEMS

- **Micro-electromechanical system (MEMS)** made from silicon, polymers, and metals; used as micro-scale sensors, actuators, switches, and machines
- **MEMS designs are subject to substantial variabilities** and lack historical knowledge base. Micromachining, photo lithography, etching processes yield uncertainty:
  - Material properties, manufactured geometries, residual and yield stresses
  - Material elasticity and geometry key for bistability
  - Data can be obtained to inform probabilistic approaches
- 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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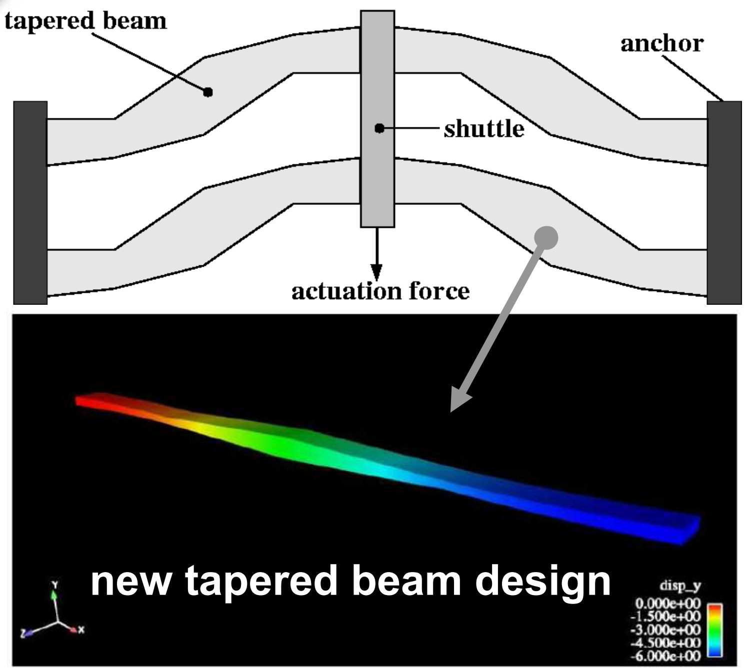
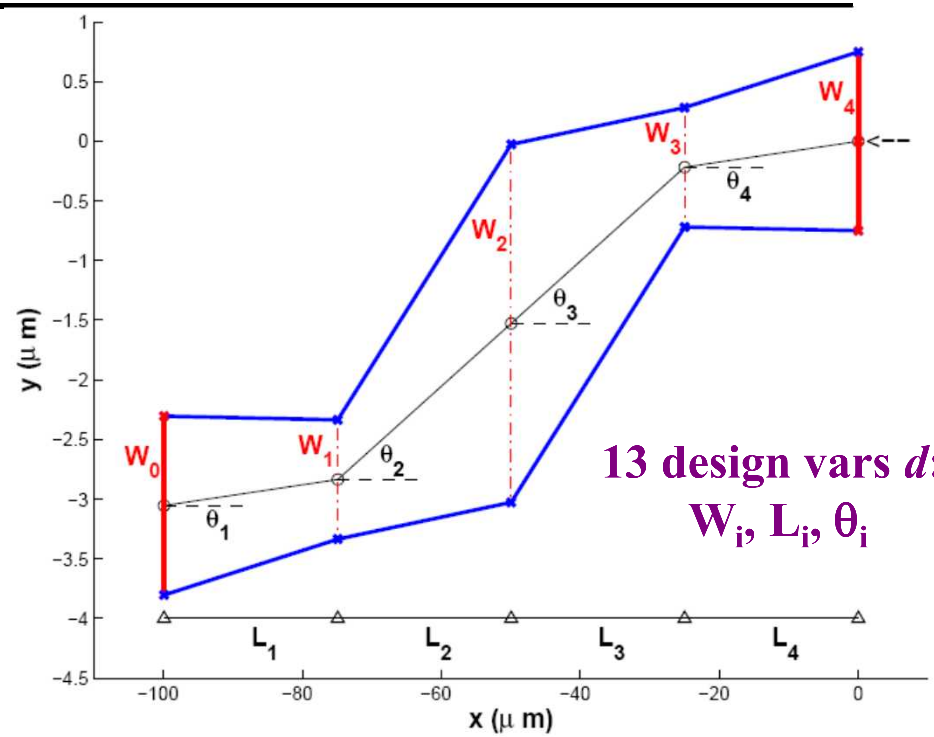
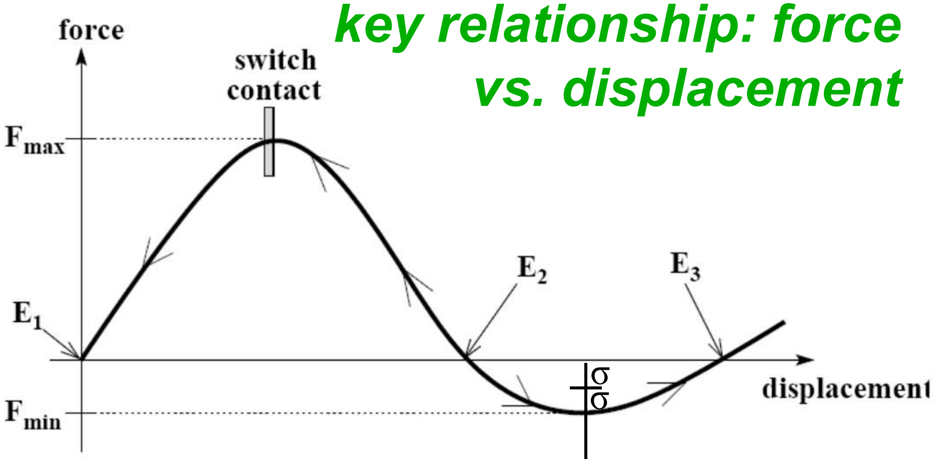
Tapered Beam Bistable Switch: Performance Metrics





13 design vars d: W_i, L_i, θ_i

key relationship: force vs. displacement

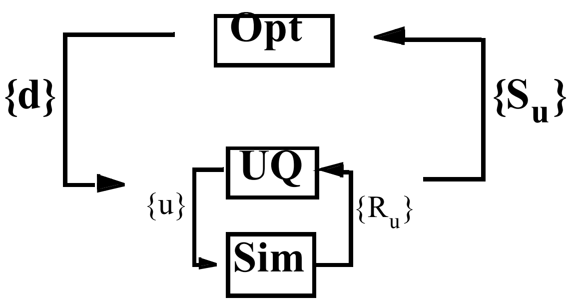


Typical design specifications:

- 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:



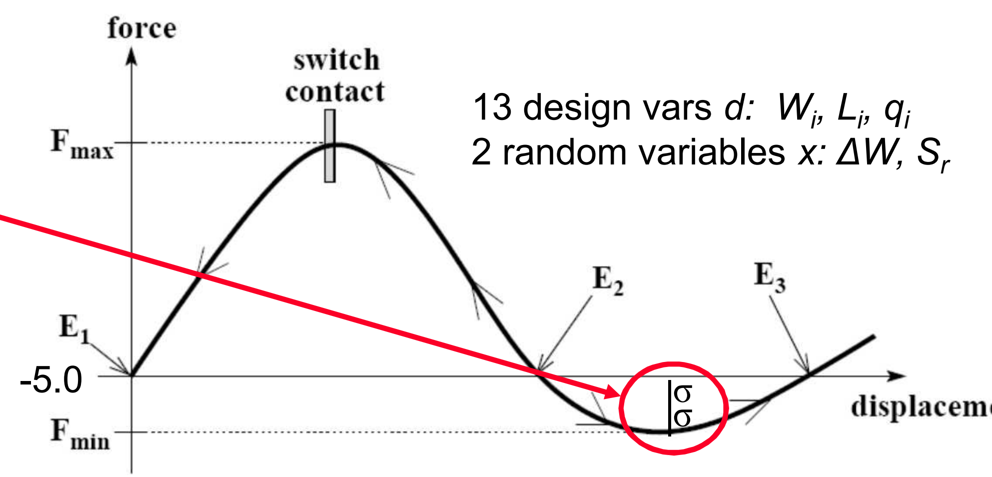
(nested paradigm)

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

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

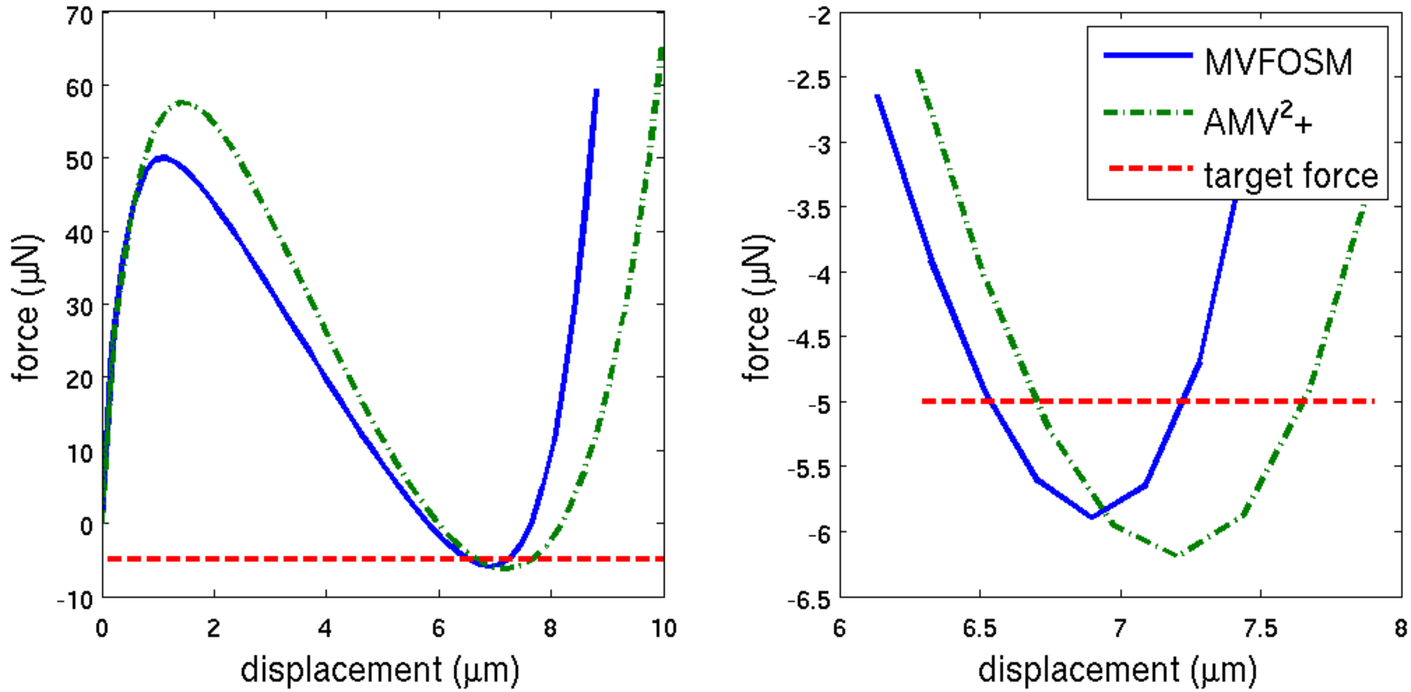
simultaneously reliable and robust designs

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



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

RBDO Finds Optimal & Robust Design



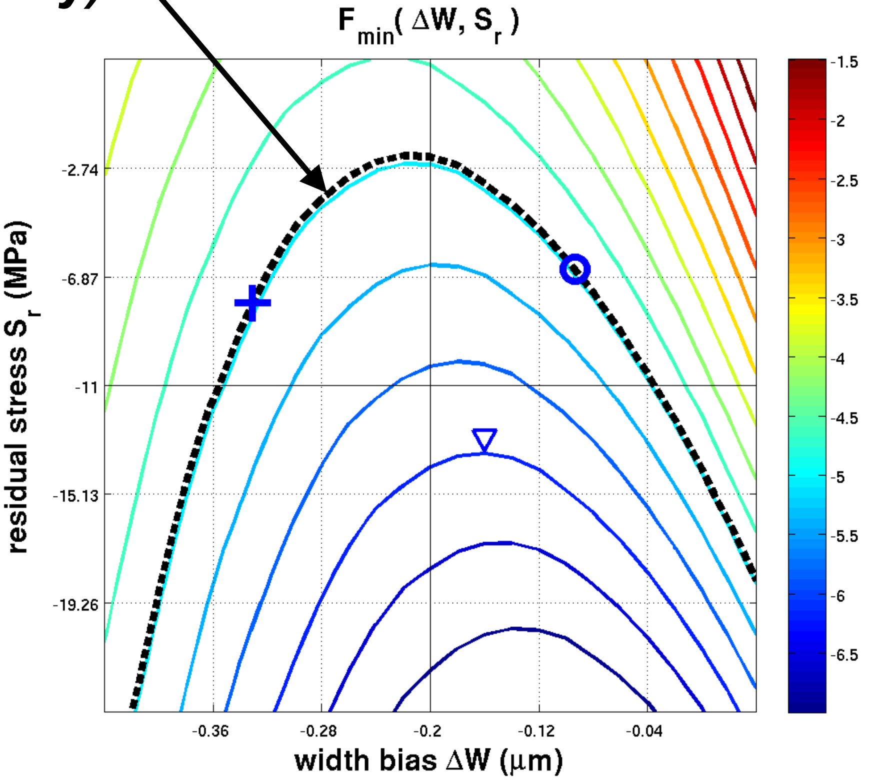
Close-coupled results: optimal and reliable/robust design:

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	-

UQ Challenge: Nonlinear/Multimodal Limit States

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

- **AMV^2+ and FORM converge to different MPPs (+ and O respectively)**
- **Challenge: limit states with multiple legitimate candidates for most probable point of failure**
- **Challenge: local first order probability integrations may not be accurate enough for nonlinear limit state**



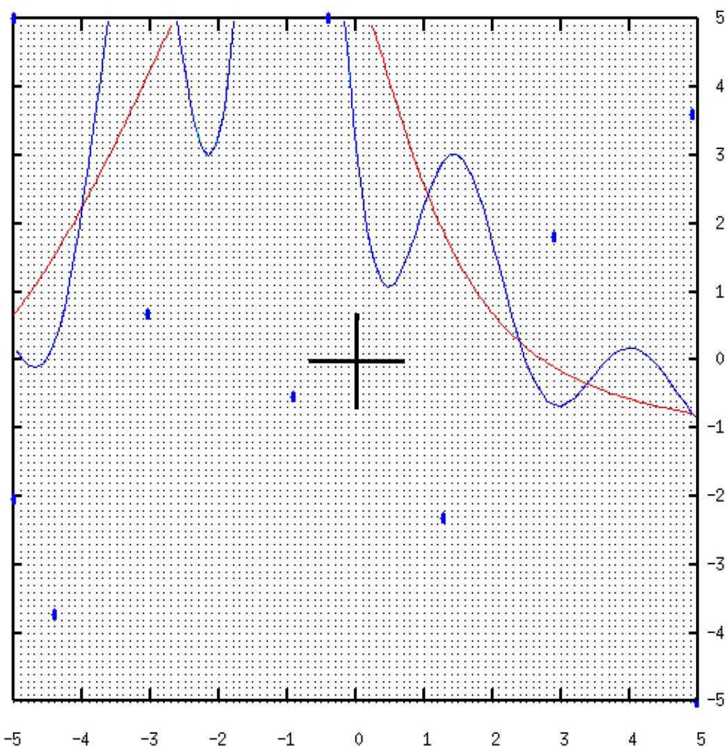
Efficient Global Reliability Analysis

- **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.**

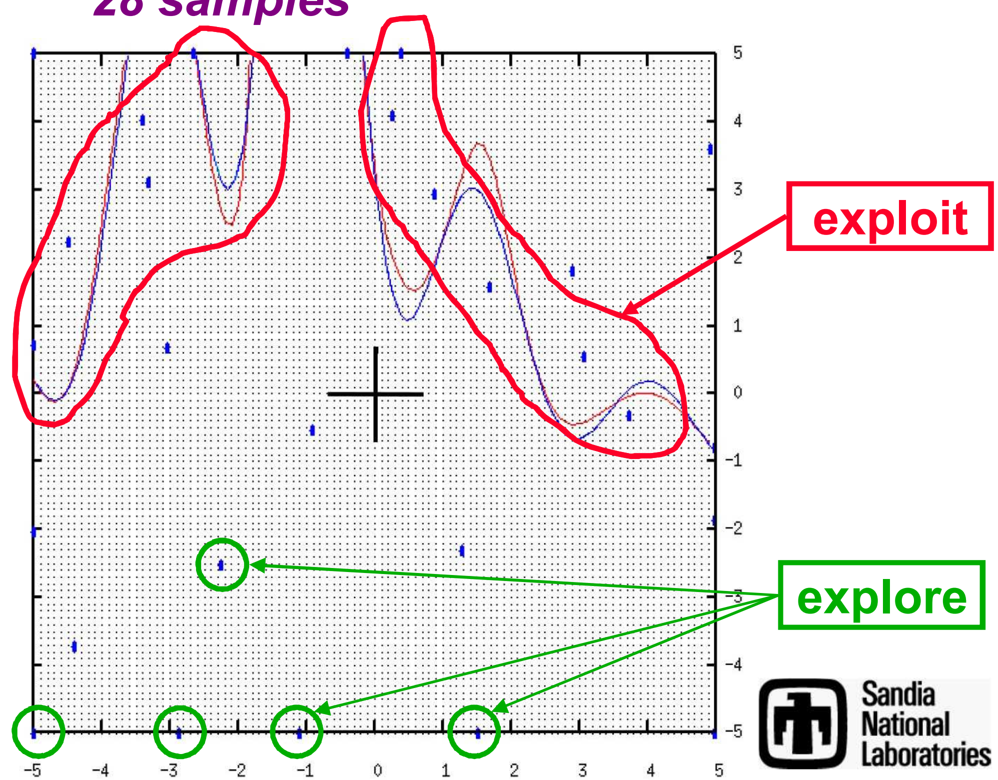
- **Created to address nonlinear and/or multi-model limit states in MPP searches.**

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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Conclusions

- The DAKOTA toolkit includes algorithms for massively parallel uncertainty quantification and optimization with large-scale computational models.
- The framework is publicly distributed with a growing number of derivative-free optimization algorithms.
- 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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http://www.cs.sandia.gov/DAKOTA