Uncertainty Quantification for Credible Simulation and Risk Analysis:
methods, software tools, and research needs

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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

- **Motivation for sensitivity analysis (SA) and uncertainty quantification (UQ), including application to code V&V**
- **Using computational models for design, margin evaluation, reliability analysis, prediction, etc.**
- **The DAKOTA toolkit and UQ methods implemented, focusing on sampling, epistemic, and reliability methods**
- **Sample application of reliability analysis to MEMS**
- **Our view on relevant future research directions and challenges**

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Why Uncertainty Quantification (UQ)?

Need to design systems given <u>uncertain/variable</u> material properties, manufacturing processes, operating conditions, models (including science, equations, numerics, and code), measurements…

Uncertainty must be properly modeled to <u>quantify risk</u> and design <u>robust and reliable</u> systems.

<u>Aleatory / irreducible</u> inherent variability with sufficient data (probabilistic models)	vs.	**<u>Epistemic / reducible</u>** uncertainty from lack of knowledge (non-probabilistic models)

Crucial: recognize difference between design/test conditions vs. operation (e.g., component tests vs. full system operation, calibration in one regime to operate in another): based on uncertainty, in what regime do we trust the results?

Example of UQ aware design: UQ-based approach to optimization under uncertainty (OUU) – helpful when safety factors, multiple operating conditions, local sensitivities insufficient.

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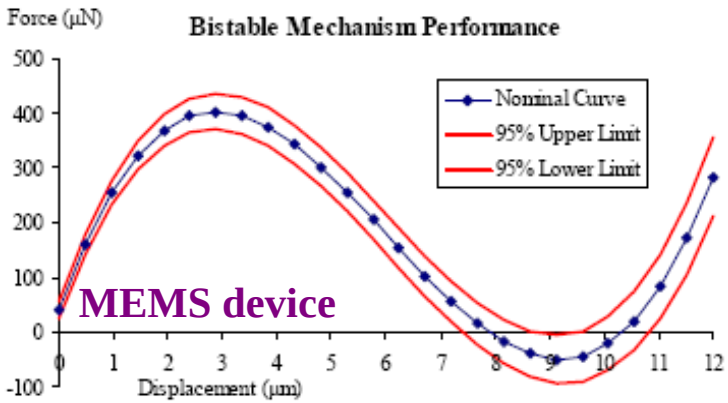
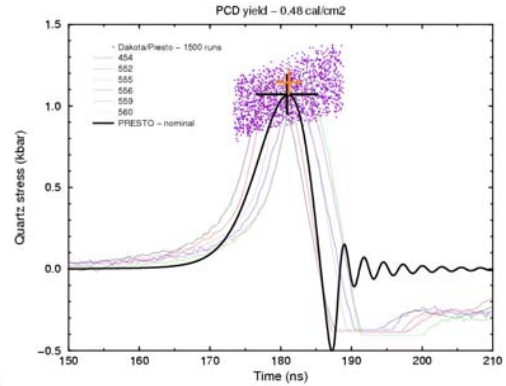
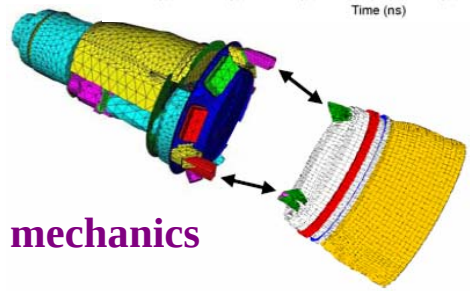
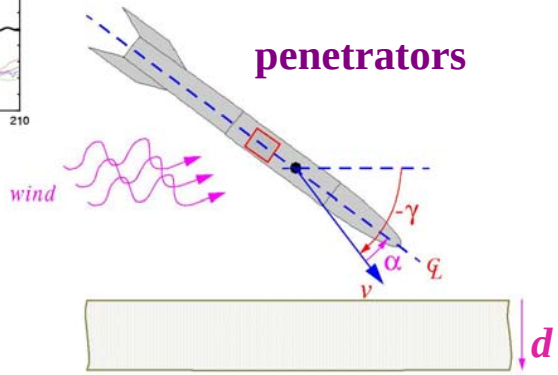
Sample SNL UQ Applications









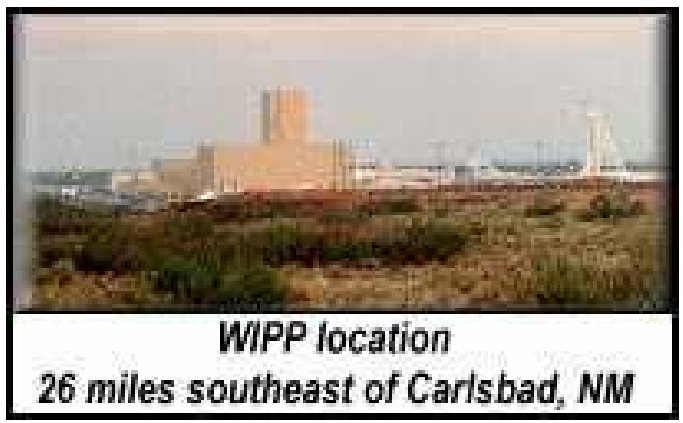
Nuclear power-related projects

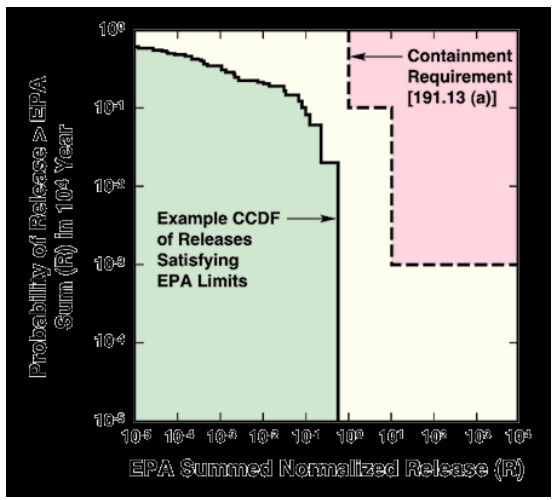
- Yucca Mountain analysis, including multi-fidelity reactions, geochemistry, hydrology, geology, flow UQ (1M year scale)
- Waste Isolation Pilot Plant (Carlsbad, NM) long-term safety
- Nuclear reactor safety (Rod Schmidt)

* Expertise in fault trees, including aggregating probabilities, performing sensitivity analysis, and impact of terrorist attacks

Waste Isolation Pilot Plant (WIPP)

- Sandia responsible for ongoing evaluation and recertification (http://www.sandia.gov/E&E/risk/wast2.html)
- Consequence and uncertainty analysis, including:
  - probabilistic characterization of likelihood of different futures occurring at WIPP site over 10,000 year period
  - estimating radionuclide releases to accessible environment in each scenario
  - probabilistic characterization of uncertainty in models/parameters on which regulation and performance assessment are based





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UQ and Verification & Validation

- Analysis based on (possibly coupled) computer models of complex systems with many uncertain calibration and input parameters, numerical approximations, possible error cancellation
  - Discrete event and logistics simulators (e.g., to model waste handling or supply chain) expensive to solve
  - Large-scale physics or chemistry-based models (e.g., to model reactions, long-term degradation) often finite element, nonlinear, expensive to solve
- Need to change the engineering simulation culture from "high fidelity, deterministic physics" to "best estimate plus uncertainty"
- Codes implementing complex simulations need fidelity in
  - correctly representing phenomena; and
  - accurately solving for that representation with computers

model to experiment comparison uncertain → inference from comparison uncertain → decisions must include credibility statements that account for uncertainty

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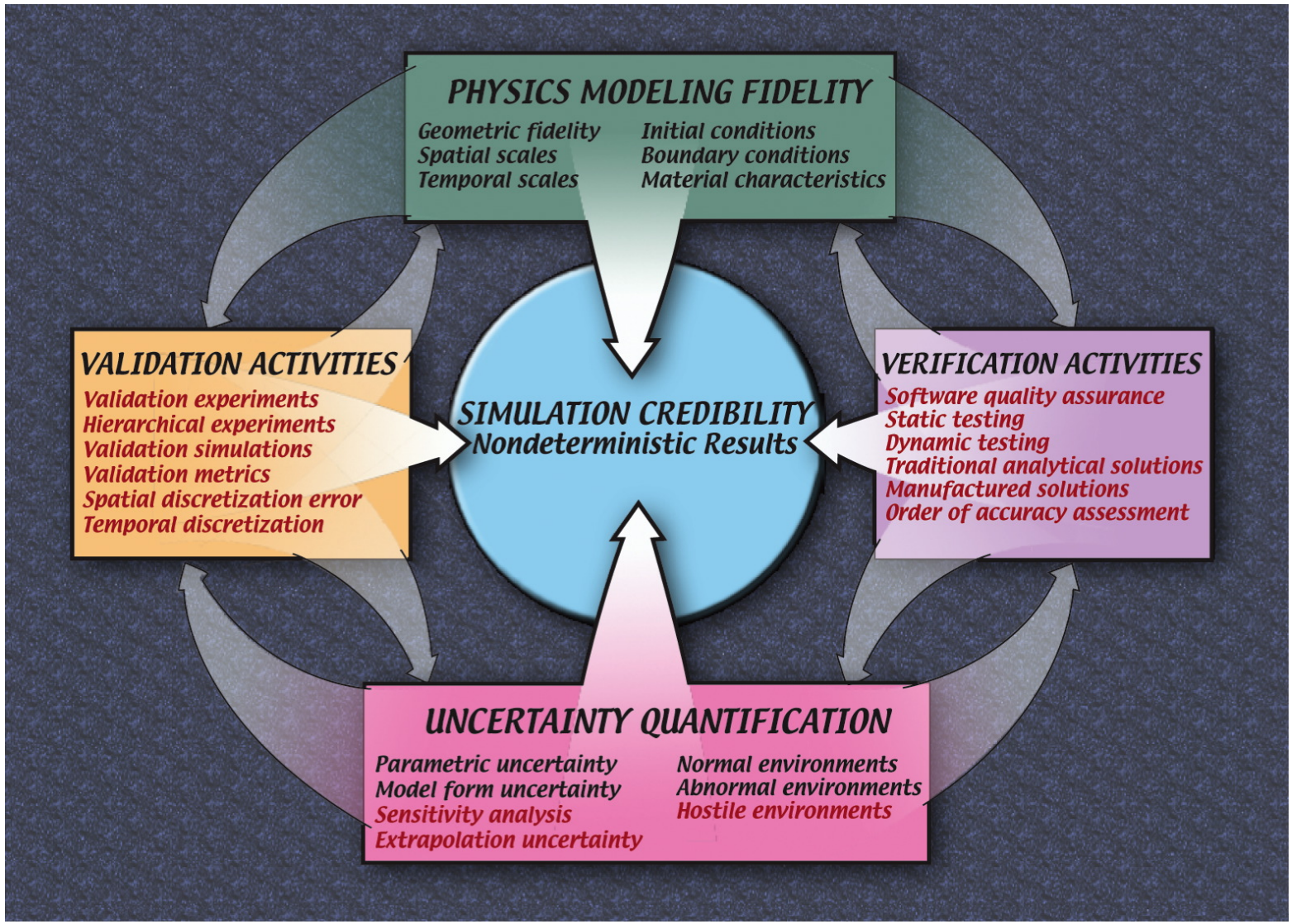
Components of Credible Simulation



graphic courtesy Bill Oberkampf

SNL/ASC targeting all four areas

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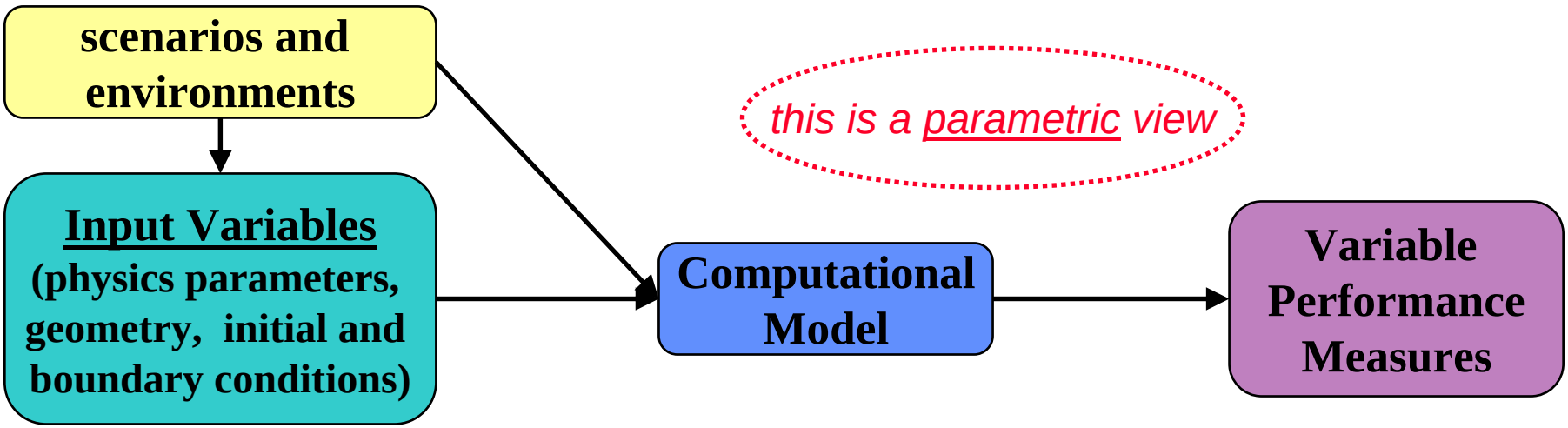
Model-based Uncertainty Quantification

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



(possibly given distributions)

GOALS:

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

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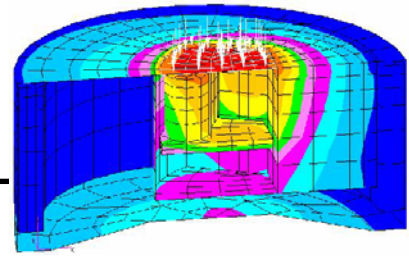
DAKOTA Overview



iterative analysis…

DAKOTA
optimization, uncertainty quant, parameter est., sensitivity analysis

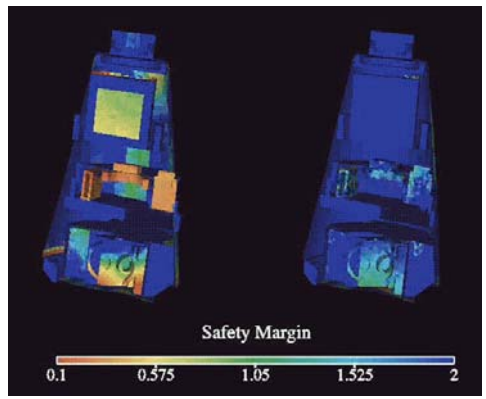
parameters
(design, UC, state)

response metrics

Computational Model
- Black box: Sandia or commercial simulation codes
- Semi-intrusive: SIERRA multi-physics, SALINAS, Xyce, Matlab, ModelCenter

Goal: answer fundamental engineering questions
- What is the best design? How safe is it?
- How much confidence do I have in my answer?

Challenges
- **Software:** reuse tools and common interfaces
- **Algorithm R&D:** nonsmooth/discontinuous/multimodal, mixed variables, unreliable gradients, costly sim. failures
- **Scalable parallelism:** ASCI-scale apps & architectures



Nominal Optimized

Impact: Tool for DOE labs and external partners, broad application deployment, free via GNU GPL (~3000 download registrations)

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DAKOTA UQ Methods

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

- **Sampling:** LHS/MC, QMC/CVT, Bootstrap/Importance/Jackknife
  Gunzburger collaboration
  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)
  Renaud/Mahadevan collaborations
- **SFE:** Polynomial chaos expansions (quadrature/cubiture extensions).
  Ghanem (Walters) collaborations
- **Metrics:** Importance factors, partial correlations, main effects, and variance-based decomposition.
- **Epistemic:** 2nd-order probability: combines epistemic and aleatory; Dempster-Schafer: basic probability assignment (intervals); Bayesian

With DAKOTA, these methods can be readily combined with surrogates (creating/sampling), optimization, and more

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Sampling Capabilities

Parameter Studies

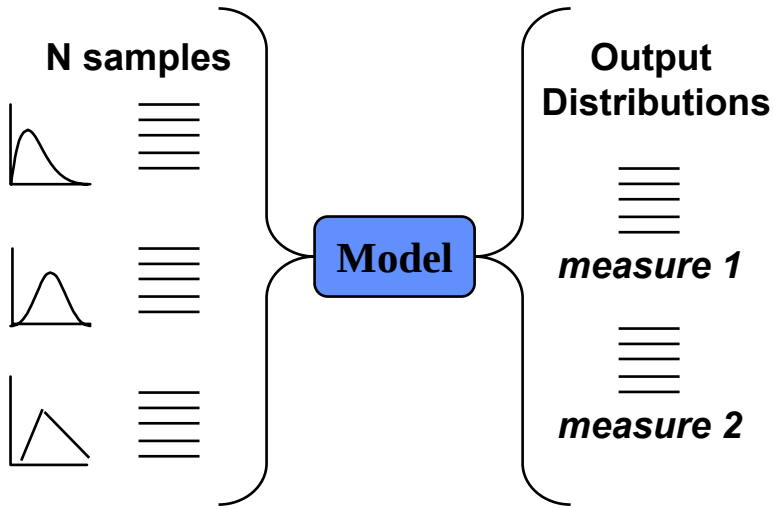
- perturb each variable
- “one-off” or one at a time
- simple but inefficient

Design of Computer Experiments (DACE) and Design of Experiments (DOE)

- LHS, Box-Behnken, Central Composite
- factorial and fractional designs
- orthogonal arrays, OA-LHS

Sampling Methods – typical for forward UQ propagation

- Standard Monte Carlo
- Pseudo-Monte Carlo: Latin Hypercube Sampling (samples from equi-probability bins for all 1-D projections)
- Quasi-Monte Carlo (low discrepancy): Hammersley, Halton
- Centroidal Voroni Tesselation (CVT): approx. uniform samples over arbitrarily shaped parameter spaces



- ***Support distributions:*** *normal, lognormal, uniform, loguniform, triangular, gamma, gumbel, frechet, weibull, histogram, interval* ← including correlations

- ***Also useful for constructing data fit or spanning ROM surrogates.***

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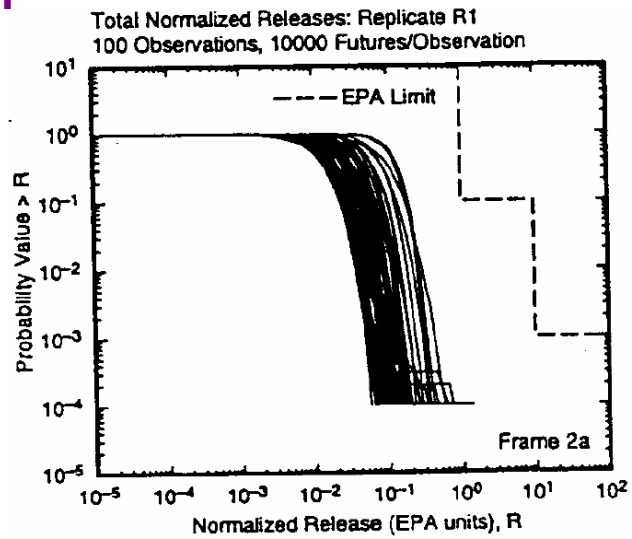
Epistemic UQ

Insufficient knowledge to specify prob. distribution (subjective, reducible uncertainty)

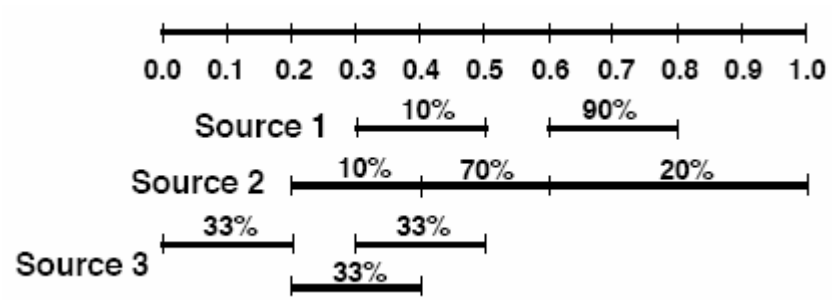
New **Second-order probability**

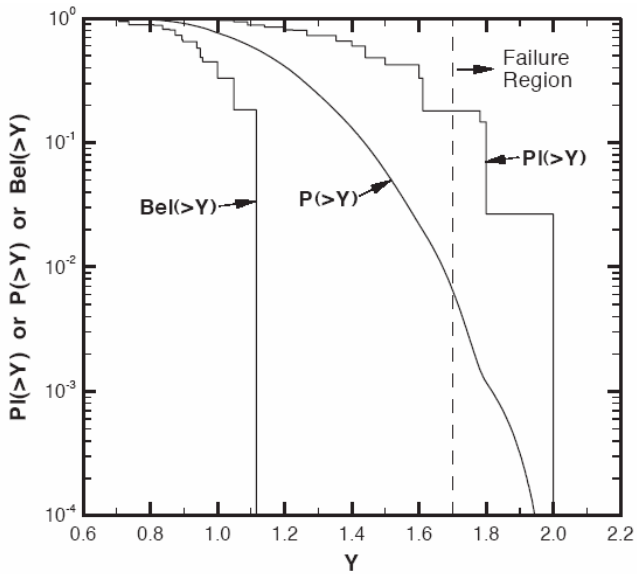
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).



New **Dempster-Shafer theory of evidence**

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





Analytic Reliability Methods for UQ

- **Define limit state function *g(x)* for response metric (model output) 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.**

<u>Mean Value (first order, second moment – MVFOSM)</u>

determine mean and variance of limit state:

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

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

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

simple approximation, but widely used by analysts

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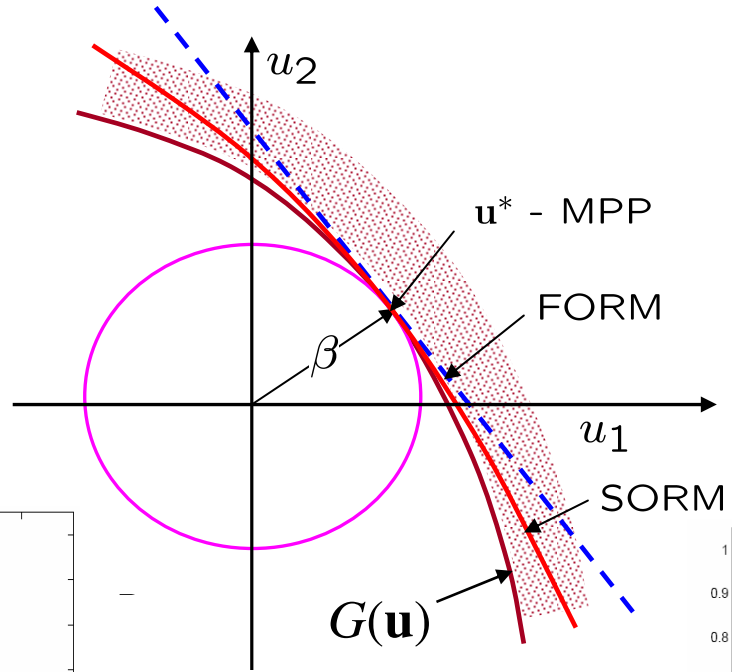
Analytic Reliability: MPP Search

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)

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

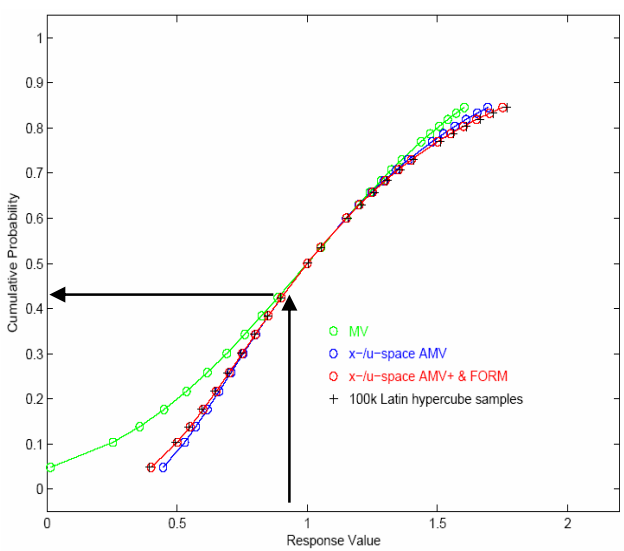
Find min dist to *G* level curve
Used for fwd map *z* → *p/β*



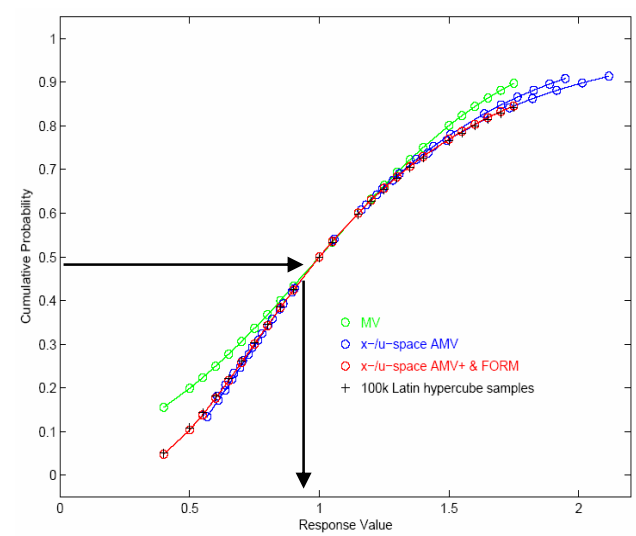
Performance Measure Approach (PMA)

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

Find min *G* at *β* radius
Better for inv map *p/β* → *z*



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



Uncertainty-Aware Design

Rather than designing and then post-processing to evaluate uncertainty…

Standard NLP

$$\begin{aligned} \text{minimize} \quad & f(d) \\ \text{subject to} \quad & g_l \leq g(d) \leq g_u \\ & h(d) = h_t \\ & d_l \leq d \leq d_u \end{aligned}$$

…actively design while accounting for uncertainty/reliability metrics

Augment with general response statistics $\boldsymbol{s_u}$ *(e.g.* μ, σ, *or reliability* $\mathbf{z}/\beta/\mathbf{p}$*) with linear map*

$$\begin{aligned} \text{minimize} \quad & f(d) + W s_u(d) \\ \text{subject to} \quad & g_l \leq g(d) \leq g_u \\ & h(d) = h_t \\ & d_l \leq d \leq d_u \\ & a_l \leq A_i \, s_u(d) \leq a_u \\ & A_e \, s_u(d) = a_t \end{aligned}$$

Focus on large-scale simulation-based engineering applications:

- **mostly PDE-based, often transient, some agent-based/discrete event models**
- **response mappings (fns. and constraints) are nonlinear and implicit**

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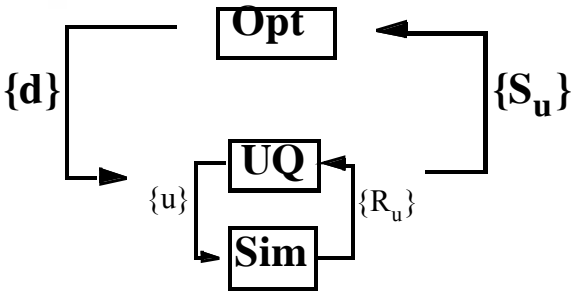
Optimization Under Uncertainty



nested paradigm

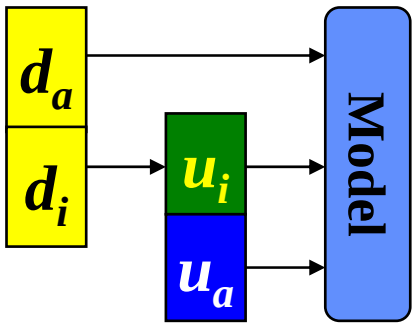
optimize, accounting for uncertainty metrics

(use any of surveyed UQ methods)

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

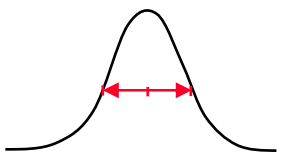
Input design parameterization

- **Uncertain variables augment design variables in simulation**
- **Inserted design variables: an optimization design variable may be a parameter of an uncertain distribution, e.g., design the mean of a normal.**

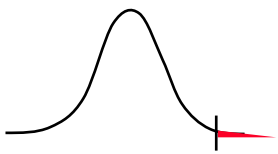


Response metrics to design for…

…robustness:
min/constrain μ, σ², moments or G(β) range



…reliability:
max/constrain *p*/β (minimize tail stats, failure)



…combined/other:
pareto tradeoff, LSQ: model calibration under uncertainty

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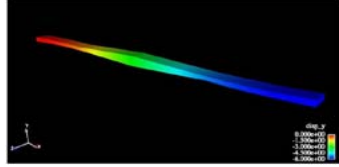
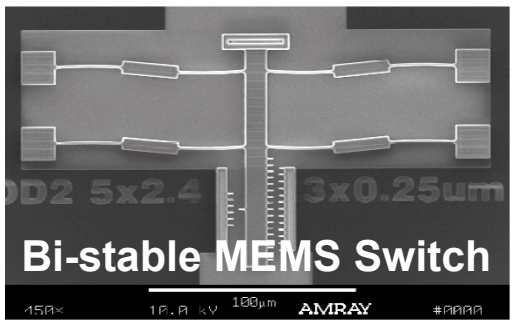
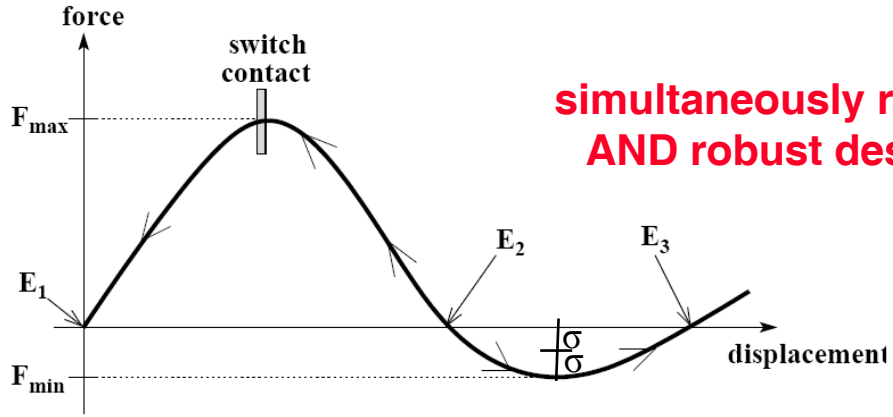
Engineering Application Deployment:

Shape Optimization of Compliant MEMS

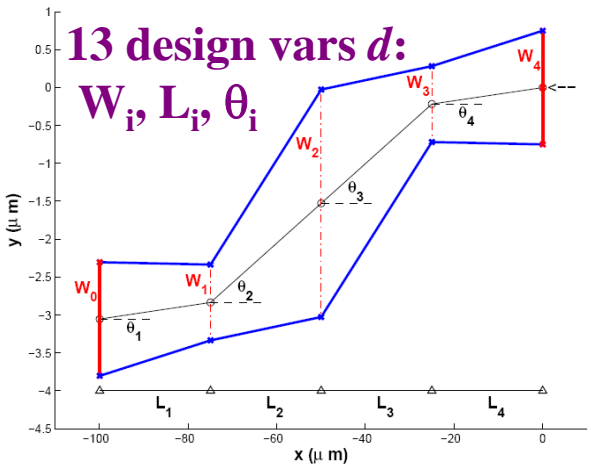


- **Micro-electromechanical system (MEMS) designs are subject to substantial variabilities and lack historical knowledge base**
- **Sources of parametric uncertainty (μ):** Material properties, manufactured geometries, residual stresses
- **Goal: shape optimization of nonlinear FEM** to achieve prescribed reliability and minimize sensitivity to uncertainties (robustness)





simultaneously reliable AND robust designs



$$
\begin{array}{llcll}
\max & & & F_{min}(\mathbf{d}, \mu) & \\
\text{s.t.} & 2 & \leq & \beta(\mathbf{d}) & \\
 & 50 & \leq & F_{max}(\mathbf{d}, \mu) & \leq 150 \\
 & & & E_2(\mathbf{d}, \mu) & \leq 8 \\
 & & & S_{max}(\mathbf{d}, \mu) & \leq 1200
\end{array}
$$

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General Comments on UQ Needs

- Even with good tools, it is difficult to enumerate and quantify input uncertainties, propagate them through models of complex systems, and analyze the results
- How to properly integrate UQ and V&V into a risk-informed decision making process is not always (often) clear
- Naively applied sampling methods can be too costly for complex computer models – need more efficient sampling methods (surrogates may help) and efficient alternatives
- Need better failure and tail probability analysis (e.g., via analytic reliability methods) and epistemic UQ (esp. for numerics)
- Education: crucial to connect scientists, analysts with breadth of available tools for SA, UQ, V&V; help select job-appropriate tools
- Impact: demonstrate importance of these techniques – they are not a burden, rather crucial components of risk analysis

5 Year Outlook on UQ Method Needs

- Quantify predictive/extrapolative confidence: requires response surface methods which handle uncertainty
- Sampling stochastic processes (random fields): in space and/or time, possibly non-stationary and non-Gaussian, not just random variables.
- Intrinsic / Analytic UQ capability: expand role of expansion methods such as Polynomial Chaos; solving DEs with random coefficients; issues include set of points on which to construct basis for different distribution types, type of integration method, etc.
- Efficient methods for higher order moments and tail statistics: success of surrogates depends on quantification of surrogate accuracy
- Adaptive Experimental Design
  - Importance Sampling, Adaptive OAs
- Efficient sensitivity analysis, better sensitivity metrics
- Epistemic UQ (fuzzy sets, imprecise prob., possibility, info gap, Bayesian)
  - Capability to combine aleatory and epistemic uncertainty in one analysis
- UQ treatment in multi-fidelity and/or hierarchical models: Need efficiency, but more important is handling uncertainty at different time or length scales across simulations
- 2nd order probability and evidence theory

Conclusions

- Modeling fidelity, sensitivity analysis, uncertainty quantification, verification, and validation are crucial to have faith in simulation-based analysis and quantify risk.
- Uncertainty-aware design optimization is helpful in engineering applications where robust and/or reliable designs are essential.
- SNL's DAKOTA toolkit includes algorithms for uncertainty quantification and optimization of computational models.
- DAKOTA strategies enable combination of algorithms, use of surrogates and warm-starting, and leveraging massive parallelism.
- Further UQ and OPT capabilities are in development in collaboration with the academic community as is deployment to additional applications.

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http://endo.sandia.gov/DAKOTA

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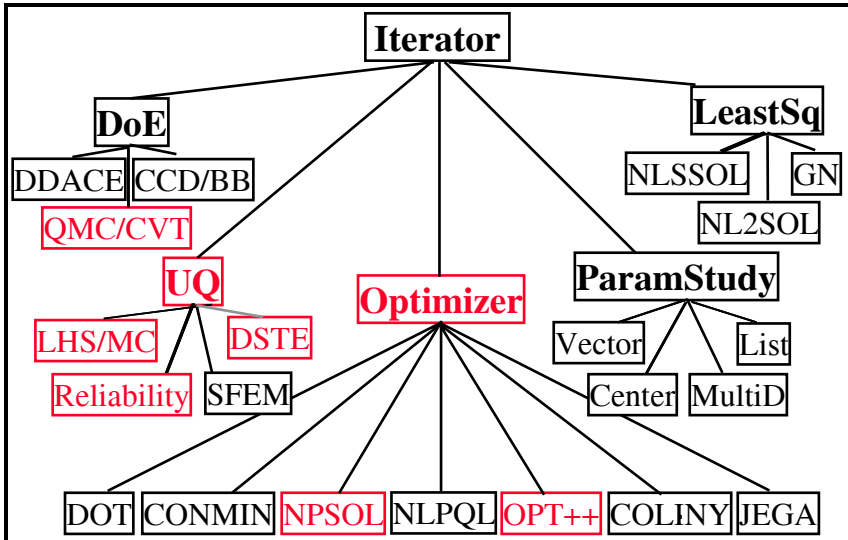
Extra Slides

DAKOTA Framework



Model:

Design
- continuous
- discrete

Uncertain
- normal/logn
- uniform/logu
- triangular
- beta/gamma
- EV I, II, III
- histogram
- interval

State
- continuous
- discrete

Application
- system
- fork
- direct
- grid

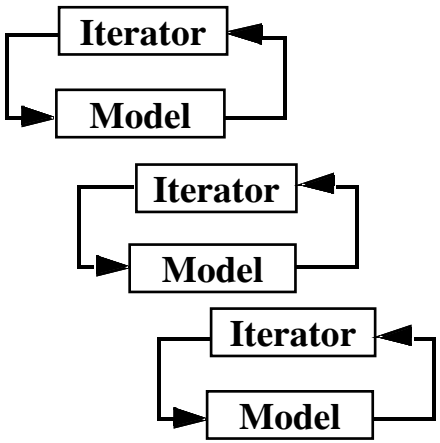
Approximation
- global
  - polynomial 1/2/3, NN, kriging, MARS, RBF
- multipoint – TANA3
- local – Taylor series
- hierarchical

Functions
- objectives
- constraints
- least sq. terms
- generic

Gradients
- numerical
- analytic

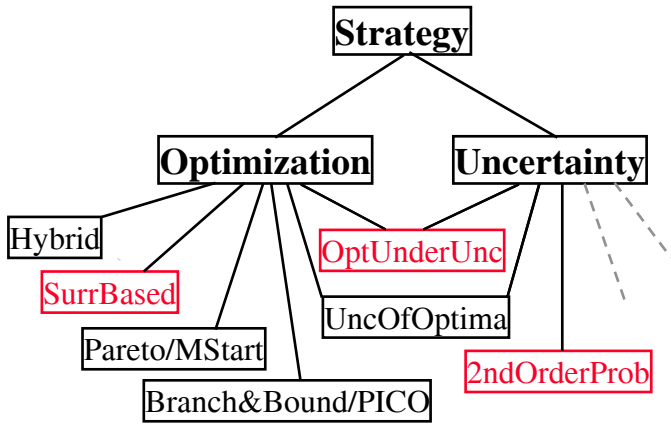
Hessians
- numerical
- analytic
- quasi

Strategy: control of multiple iterators and models



Coordination:
- Nested
- Layered
- Cascaded
- Concurrent
- Adaptive/Interactive

Parallelism:
- Asynchronous local
- Message passing
- Hybrid
- 4 nested levels with
  - Master-slave/dynamic
  - Peer/static



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Sampling Capabilities

Motivations:

- **Surrogates: Data fit, spanning ROM**
- **UQ**

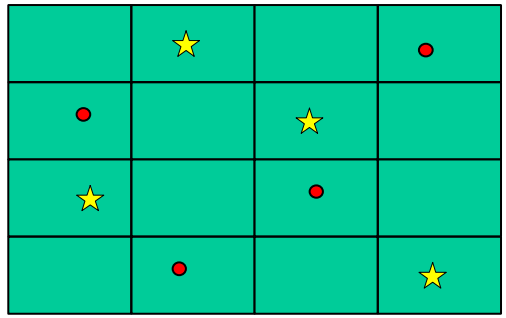
Types:

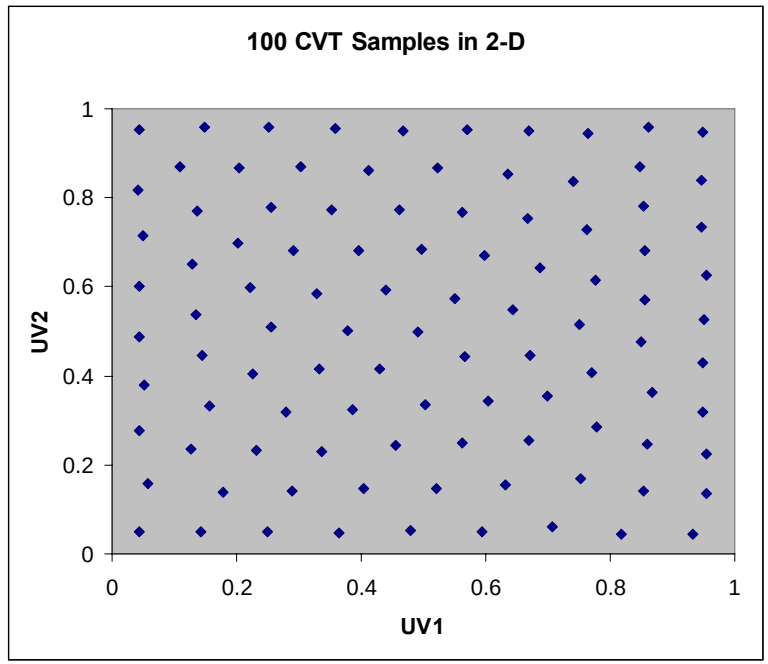
- Pseudo Monte Carlo: **Latin Hypercube Sampling (LHS) is a stratified, structured sampling method that picks random samples from equal probability bins for all 1-D projections.**
- Quasi Monte Carlo**: deterministic sequences constructed to uniformly cover a unit hypercube with low discrepancy.**
  E.g., Halton, Hammersley, Sobol
- Centroidal Voronoi Tesselation (CVT): **generates nearly uniform spacing over arbitrarily shaped parameter spaces; originally developed for "meshless" mechanics methods.**

New

Associated Tools:

- **Volumetric quality, Latinization**
- **Correlations, variance-based decomposition**





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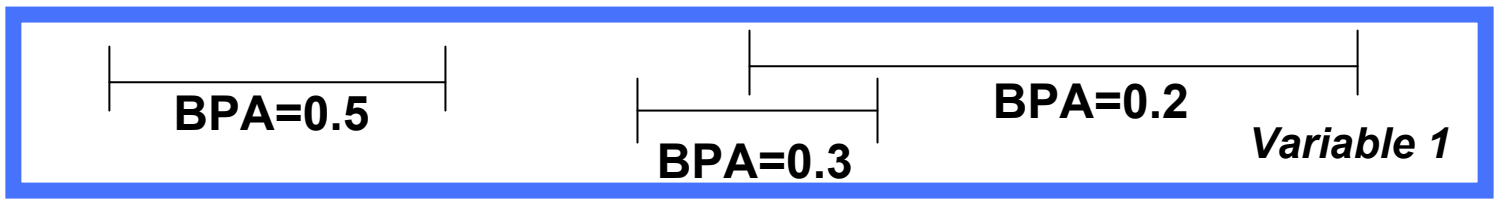
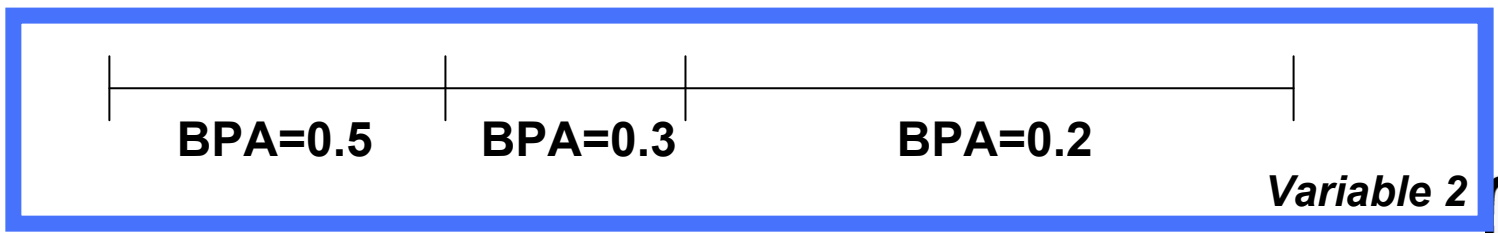
Epistemic Uncertainty Quantification

- Epistemic uncertainty refers to the situation where one does not know enough to specify a probability distribution on a variable
- Sometimes it is referred to as subjective, reducible, or lack of knowledge uncertainty
- The implication is that if you had more time and resources to gather more information, you could reduce the uncertainty
- Initial implementation in DAKOTA uses Dempster-Shafer belief structures. For each uncertain input variable, one specifies "basic probability assignment" for each potential interval where this variable may exist.
- Intervals may be contiguous, overlapping, or have "gaps"





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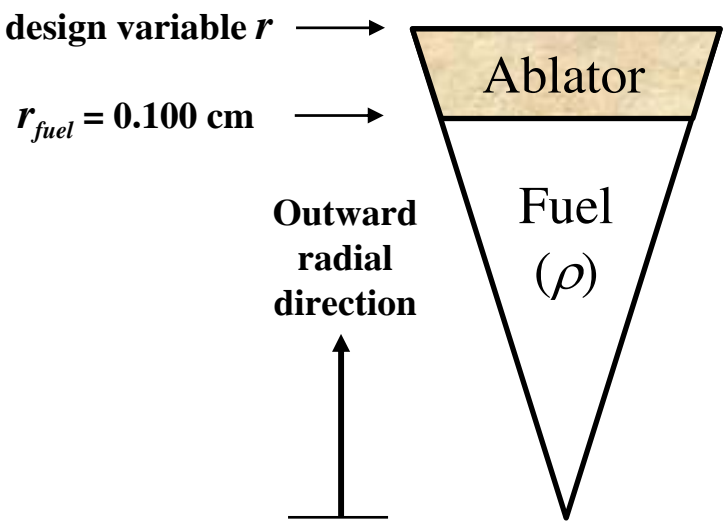
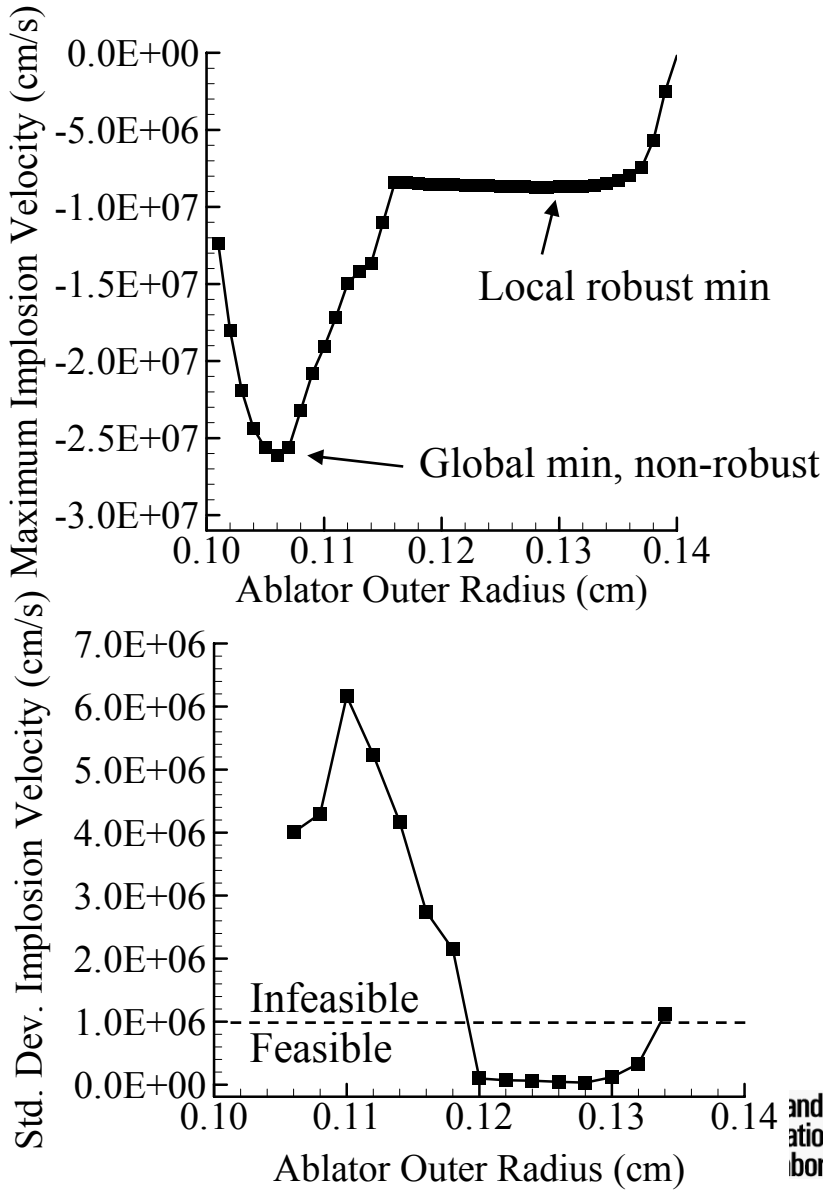
Outputs from DAKOTA/UQ

- Response metrics evaluated at samples
- Input/output correlations
- Variance-based decomposition (VBD) global sensitivity analysis indices
- Quality metrics (e.g., point distribution norm)
- Sample to generate and evaluate surrogates
- Bases for Polynomial Chaos Expansions
- Probability/reliability metrics
- Epistemic complementary cumulative belief and plausibility functions (CCBF and CCPF)

ICF Capsule Design – 1D Param Study

Design goal: maximize the implosion velocity w.r.t. ablator radius *r* and fuel density ρ, but remain robust w.r.t. manufacturing variability





Optimization with Surrogate Models

Purpose:

- **Reduce the number of expensive, high-fidelity simulations by using a succession of approximate (surrogate) models**
- **Approximations generally have a limited range of validity**
- **Trust regions adaptively manage this range based on efficacy during opt**
- **With trust region globalization and local 1st-order consistency, SBO algorithms are *provably-convergent***

Surrogate models of interest:

- ***Data fits***
- ***Multifidelity*** **(special case:** ***multigrid*** **optimization)**
- ***Reduced-order models***

Future connections to ***multi-scale*** **for managing approximated scales**

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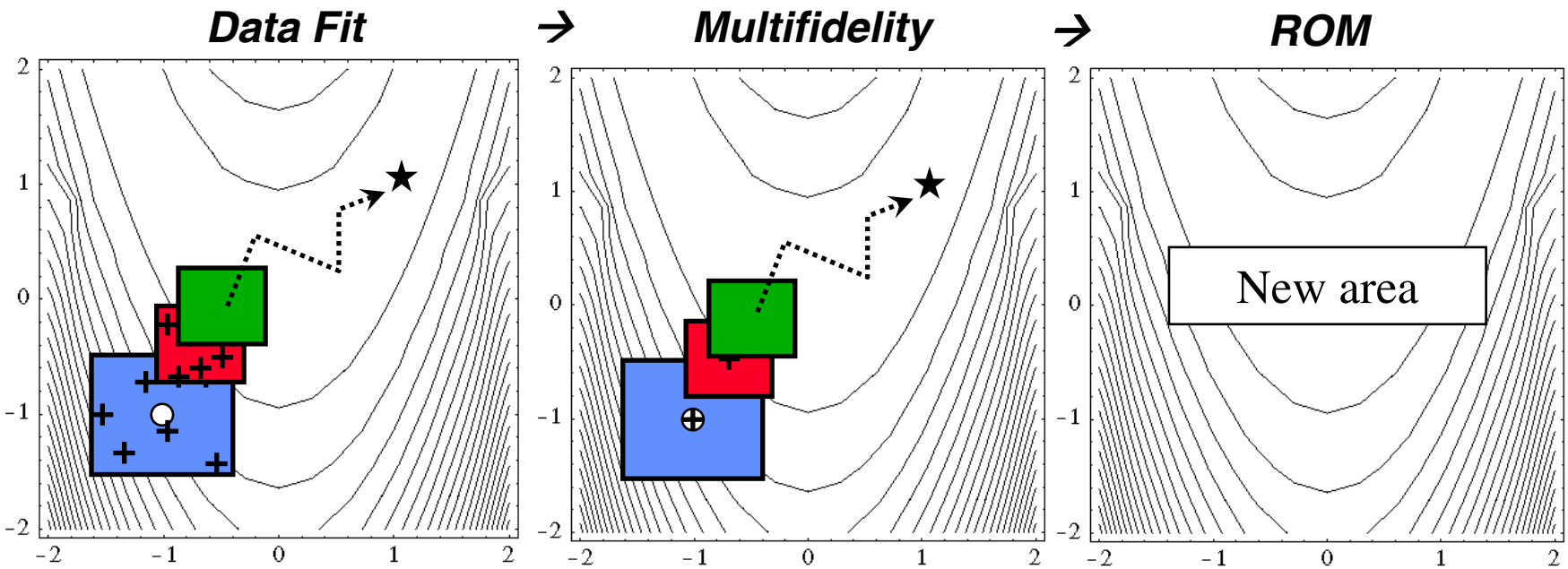
Trust-Region Surrogate-Based Optimization



Data fit surrogates:

- Global: polynomial regress., splines, neural net, kriging, 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
- Design vector maps may be reqd.
- Correction quality is *crucial*

ROM surrogates:

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

ROMs in SBO

- Key issue: capture parameter changes
  - Extended ROM, Spanning ROM
- Shares features of data fit

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New representations of uncertainty

- Fuzzy sets (Zadeh)
- Imprecise Probability (Walley)
- Dempster-Shafer Theory of Evidence (Klir, Oberkampf, Ferson)
- Possibility theory (Joslyn)
- Probability bounds analysis (p-boxes)
- Info-gap analysis (Ben-Haim)
- Bayesian approaches: Bayesian belief networks, Bayesian updating, Robust Bayes, etc.
- Scenario evaluation

Bi-Stable Switch: Results (DOT/MMFD)

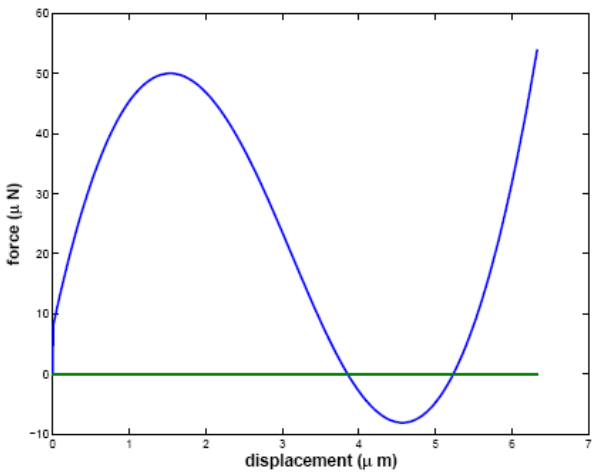
lower bound	RBDO metric	upper bound	MVFOSM initial	MVFOSM optimal	AMV+/FORM initial	AMV+/FORM optimal
	F_{min} (μN)		-23.03	-8.08	-23.03	-9.37
2	β		5.66	2.00	4.02	2.00
50	F_{max} (μN)	150	67.35	50.0	67.35	50.0
	E_2 (μm)	8	4.06	3.85	4.06	3.76
	S_{max} (MPa)	1200	396	313	396	323
	Verified β		4.02	1.75		

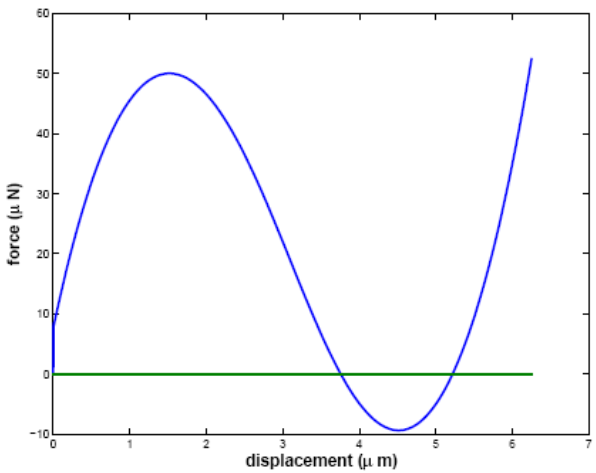
Reliability: target achieved for AMV+/FORM; target approximated for MV

Robustness: variability in F_{min} reduced from 5.7 to 4.6 μN per input σ [$\mu_{F_{min}}/\beta$]

Ongoing: quantity of interest error estimates → error-corrected UQ/RBDO

MVFOSM-based RBDO





AMV+/FORM-based RBDO

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