Optimization Under Uncertainty Research at Sandia National Laboratories

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August 31, 2005

http://endo.sandia.gov/DAKOTA

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for the United States Department of Energy under contract DE-AC04-94AL85000.

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Introduction

Uncertainties/variabilities must be properly modeled in order to quantify risk and design systems that are robust and reliable

We use a UQ-based approach to optimization under uncertainty

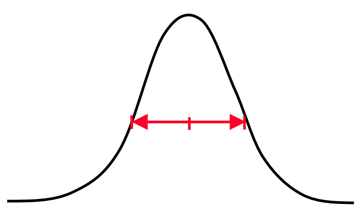
- **Concern: do safety factors, multiple operating conditions, or local sensitivity metrics accurately convey the full nature of the uncertainty?**

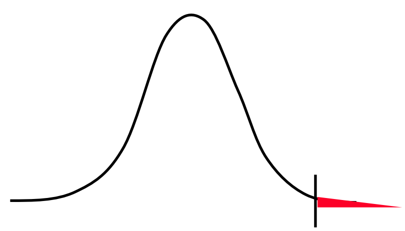
Uncertainty comes in different flavors:

- **Aleatory/irreducible: inherent uncertainty/variability with sufficient data → probabilistic models**
- **Epistemic/reducible: uncertainty from lack of knowledge → nonprobabilistic models** **Harder problem**

Optimization under uncertainty (OUU) methods encompass both:

- **design for robustness (moment statistics: mean, variance)**
- **design for reliability (tail statistics: probability of failure)** **Harder problem**





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Introduction (cont.)

Focus is simulation-based engineering applications

- response mappings are nonlinear and implicit
- distinct from chance-constrained stochastic programming (often linear/explicit)

Standard NLP:

$$\begin{array}{ll} \text{Minimize} & f(d) \\ \text{Subject to} & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \end{array}$$

Augment with statistics s_u (e.g., μ, σ, $z/\beta/p$) using a linear mapping:

$$\begin{array}{ll} \text{Minimize} & f(d) + W s_u(d) \\ \text{Subject to} & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & a_l \le A_i s_u(d) \le a_u \\ & A_e s_u(d) = a_t \\ & d_l \le d \le d_u \end{array}$$

Outline

Introduction

Foundations

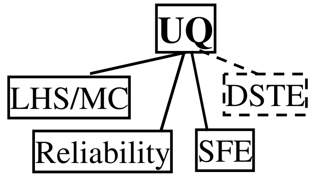
- **Uncertainty Quantification**
  - **Sampling methods**
  - **Reliability methods**
  - **Epistemic methods**
- **Surrogate-based optimization**
- **DAKOTA**

OUU Algorithms

- **Surrogate-based OUU methods: TR-SBOUU**
  - **Example: Robust capsule design for ICF**
- **Reliability-based Design Optimization (RBDO): bi-level, sequential, unilevel**
  - **Examples: computational benchmarks**
- **Intrusive OUU: SFE + SAND, Unilevel RBDO + SAND**

Concluding Remarks

Uncertainty Quantification



Active UQ development (new, developing, planned).

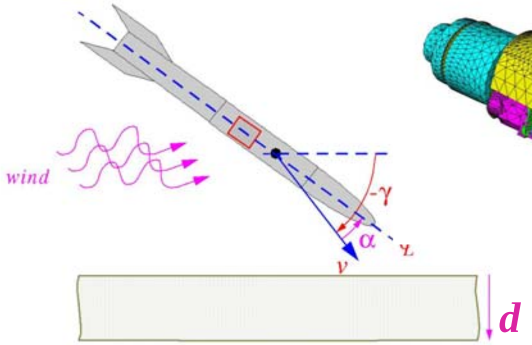
– **Sampling:** LHS/MC, QMC/CVT, Bootstrap/Importance/Jackknife.
Gunzburger collaboration.

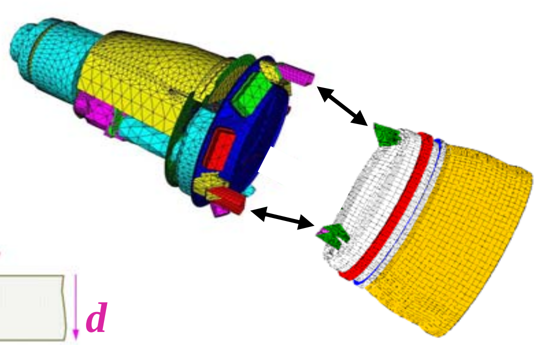
– **Reliability:** MVFOSM, x/u AMV, x/u AMV+, FORM (RIA/PMA mappings), MVSOSM, x/u AMV^2, x/u AMV^2+, TANA, SORM (RIA/PMA)
Renaud/Mahadevan collaborations.

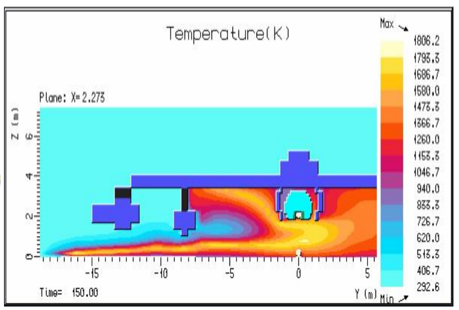
– **SFE:** Polynomial chaos expansions (quadrature/cubiture extensions).
Ghanem/Walters collaborations.

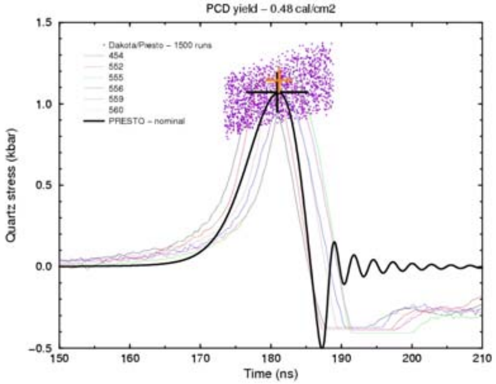
– **Metrics:** Importance factors, partial correlations, main effects, and variance decomposition.

– **Epistemic:** 2nd-order probability, Dempster-Schafer, Bayesian.









Uncertainty applications: penetration, joint mechanics, abnormal environments, shock physics, …

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Sampling Capabilities

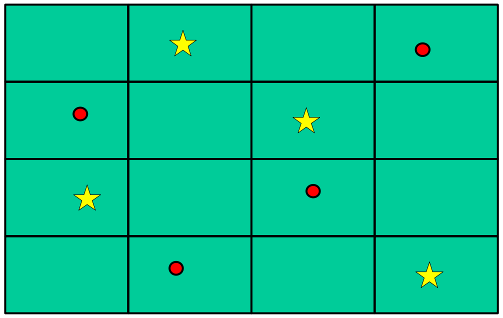
Motivations:

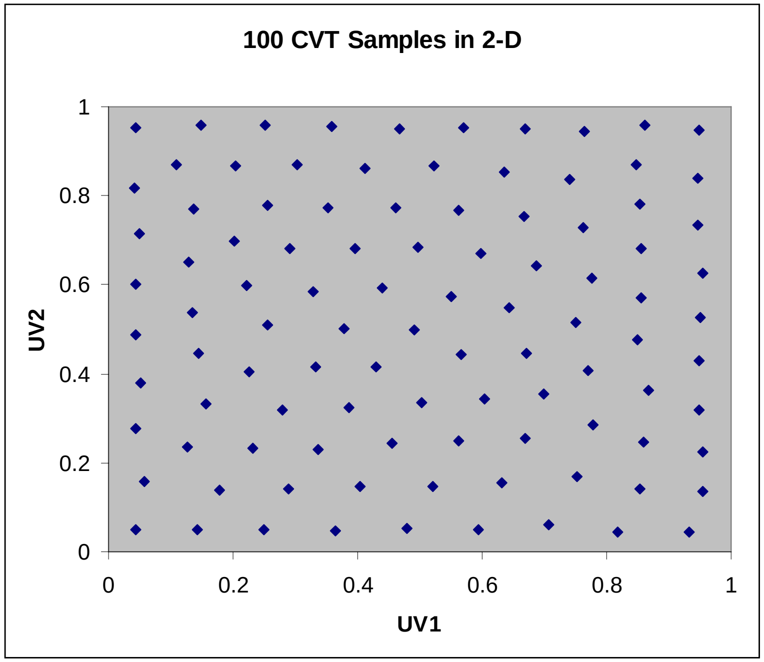
- Surrogates: Data fit, spanning ROM
- UQ

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**

UQ with Reliability Methods

Mean Value Method

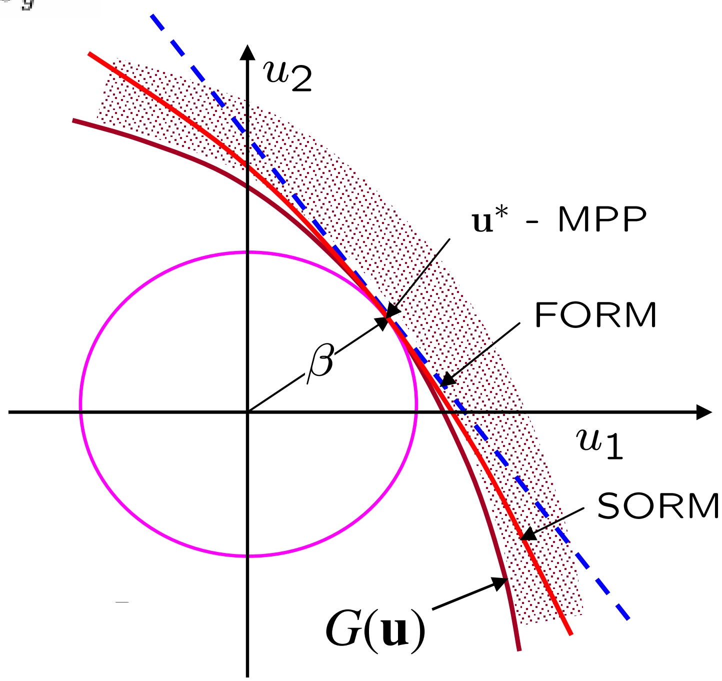
$$\mu_g = g(\mu_{\mathbf{x}})$$
$$\sigma_g = \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})$$

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

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

Frequently used by SNL analysts

MPP search methods



Reliability Index Approach (RIA)

$$\begin{array}{ll} \text{minimize} & \mathbf{u}^T\mathbf{u} \\ \text{subject to} & G(\mathbf{u}) = z_{target} \end{array}$$

Find min dist to G level curve
Better for $z \rightarrow p/\beta$

Performance Measure Approach (PMA)

$$\begin{array}{ll} \text{minimize} & G(\mathbf{u}) \\ \text{subject to} & \mathbf{u}^T\mathbf{u} = \beta^2_{target} \end{array}$$

Find min G at β radius
Better for $p/\beta \rightarrow z$

Variations: MPP search alg., Linearizations, Integrations, Warm starting

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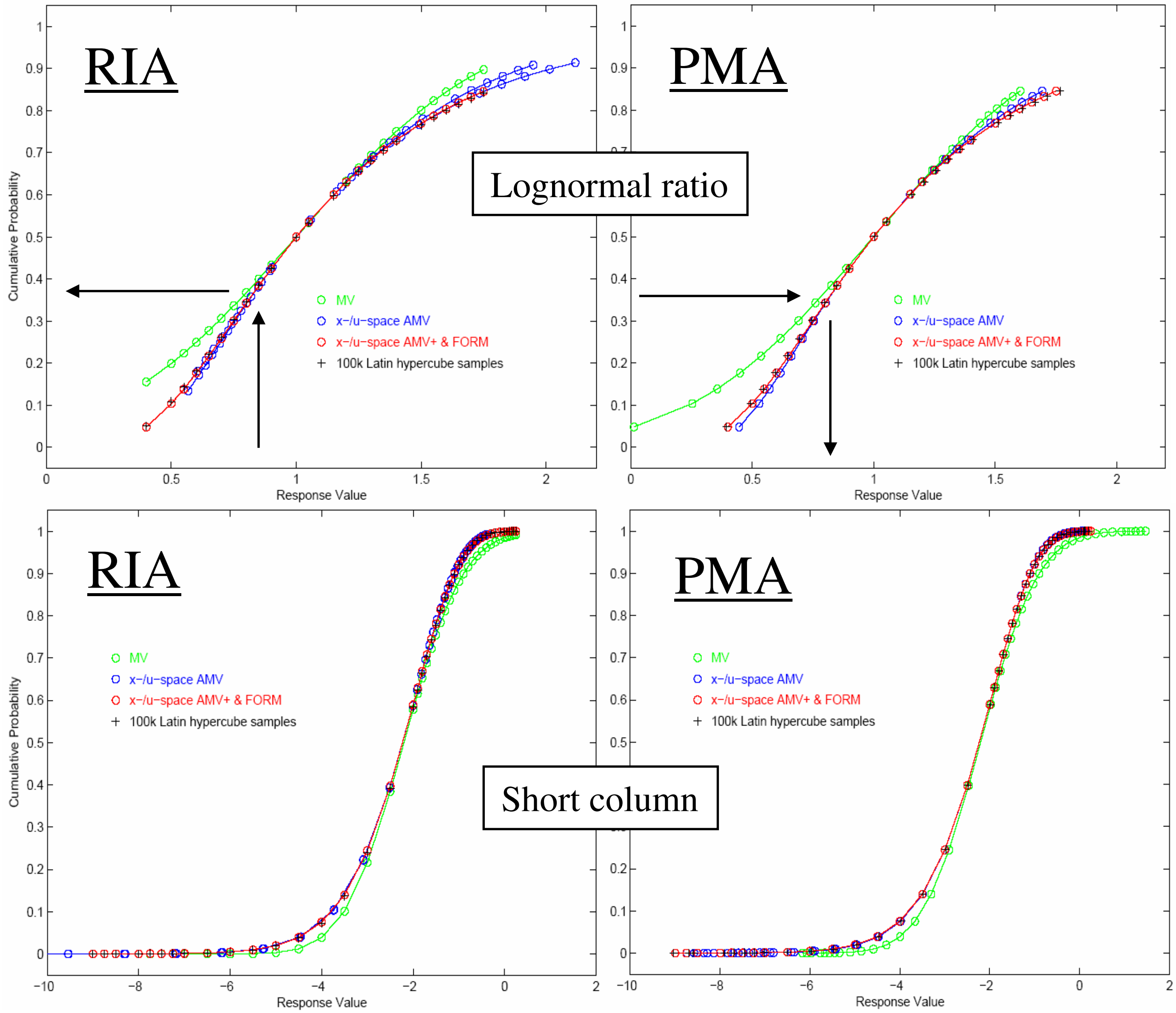
Uncertainty Quantification (cont.)
Reliability Index/Performance Measure



Cover range of accuracy vs. expense:

- **Relative to FORM:**
  - **MV ~100x faster but only accurate near means**
  - **AMV ~10x faster but MPP not converged**
  - **AMV+ ~3x faster with full accuracy**
- **Broad foundation for OUU via RBDO**

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Given success w/ 1st-order UQ/RBDO approximations → 2nd-order reliability methods for UQ/RBDO

2nd-order local limit state approximations

- **e.g., x-space AMV²+:**

$$g(\mathbf{x}) \cong g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T(\mathbf{x}-\mathbf{x}^*) + \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^T \nabla_x^2 g(\mathbf{x}^*)(\mathbf{x}-\mathbf{x}^*)$$

- **Hessians may be full/FD/Quasi**

Multipoint limit state approximations

- **e.g., TPEA, TANA:**

$$g(\mathbf{x}) \cong g(\mathbf{x}_2) + \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathbf{x}_2)\frac{x_{i,2}^{1-p_i}}{p_i}(x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2}\epsilon(\mathbf{x})\sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2$$

$$p_i = 1 + \ln\left[\frac{\frac{\partial g}{\partial x_i}(\mathbf{x}_1)}{\frac{\partial g}{\partial x_i}(\mathbf{x}_2)}\right] \Big/ \ln\left[\frac{x_{i,1}}{x_{i,2}}\right]$$

$$\epsilon(\mathbf{x}) = \frac{H}{\sum_{i=1}^{n}(x_i^{p_i} - x_{i,1}^{p_i})^2 + \sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2}$$

$$H = 2\left[g(\mathbf{x}_1) - g(\mathbf{x}_2) - \sum_{i=1}^{n}\frac{\partial g}{\partial x_i}(\mathbf{x}_2)\frac{x_{i,2}^{1-p_i}}{p_i}(x_{i,1}^{p_i} - x_{i,2}^{p_i})\right]$$

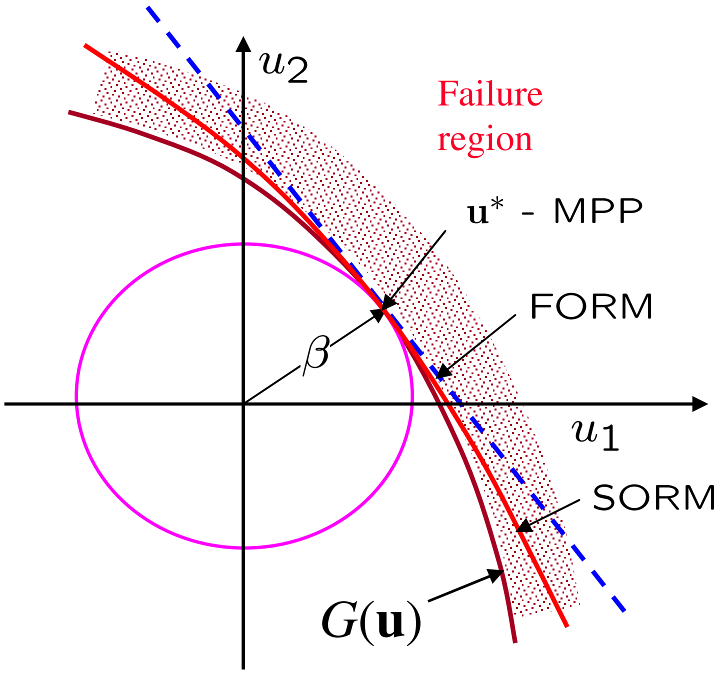
2nd-order integrations

(accounts for curvature in limit state):

$$p = \Phi(-\beta)\prod_{i=1}^{n-1}\frac{1}{\sqrt{1+\beta\kappa_i}}$$

curvature correction

Also, AIS, …



More accurate probability estimates

More rapid convergence

Best performer to date:

- **AMV²+ with SR1 Hessian updates**

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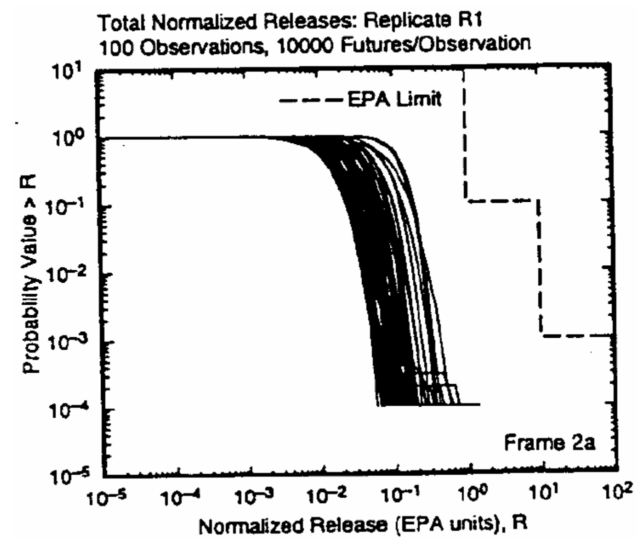
Epistemic UQ

Second-order probability

- Two levels: distributions/intervals on distribution parameters

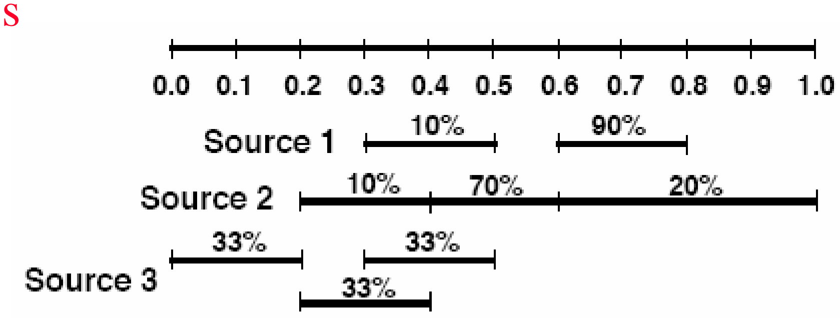
New
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).

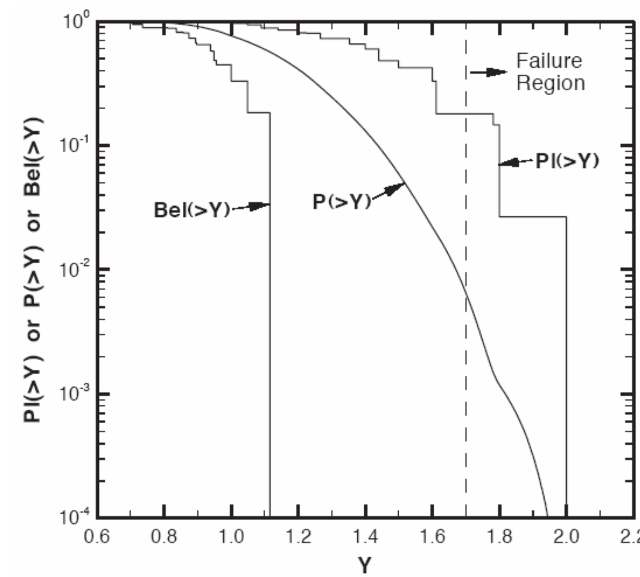


Dempster-Schafer theory of evidence

- Basic probability assignment (interval-based)

In progress
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals





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***

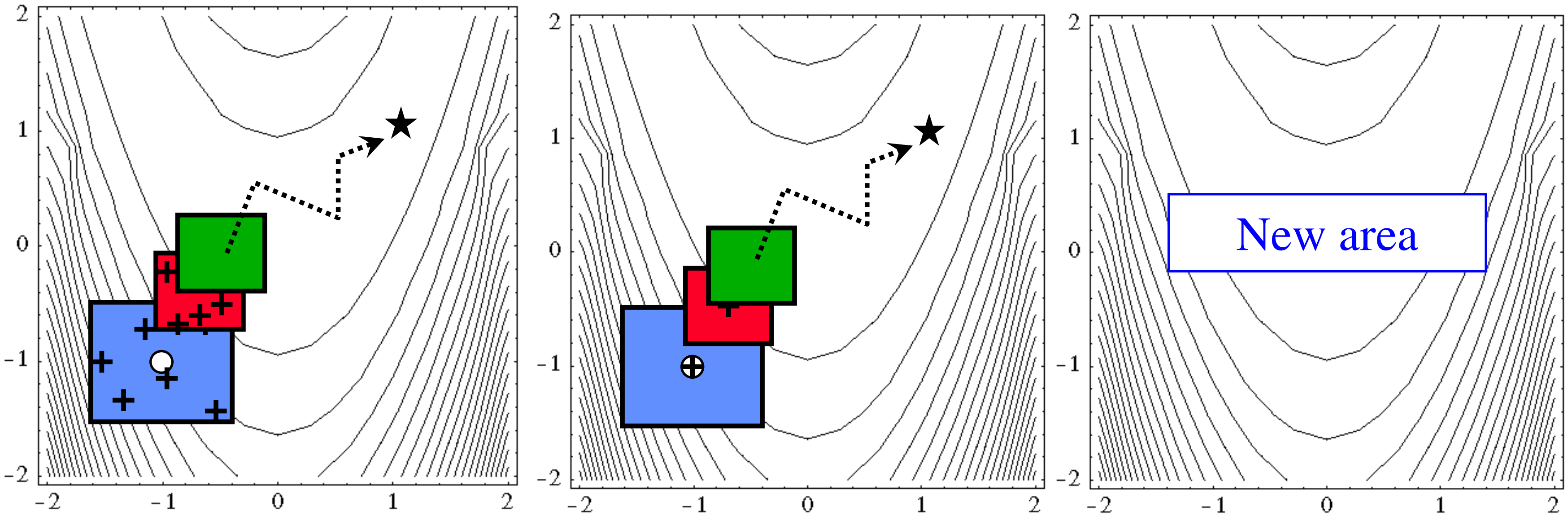
Surrogate models of interest:

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

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

Trust-Region Surrogate-Based Optimization

Data Fit* → *Multifidelity* → *ROM



Data fit surrogates:

- Global: polynomial regress., splines, neural net, kriging, radial basis fn
- Local: 1st/2nd-order Taylor
- Multipoint: 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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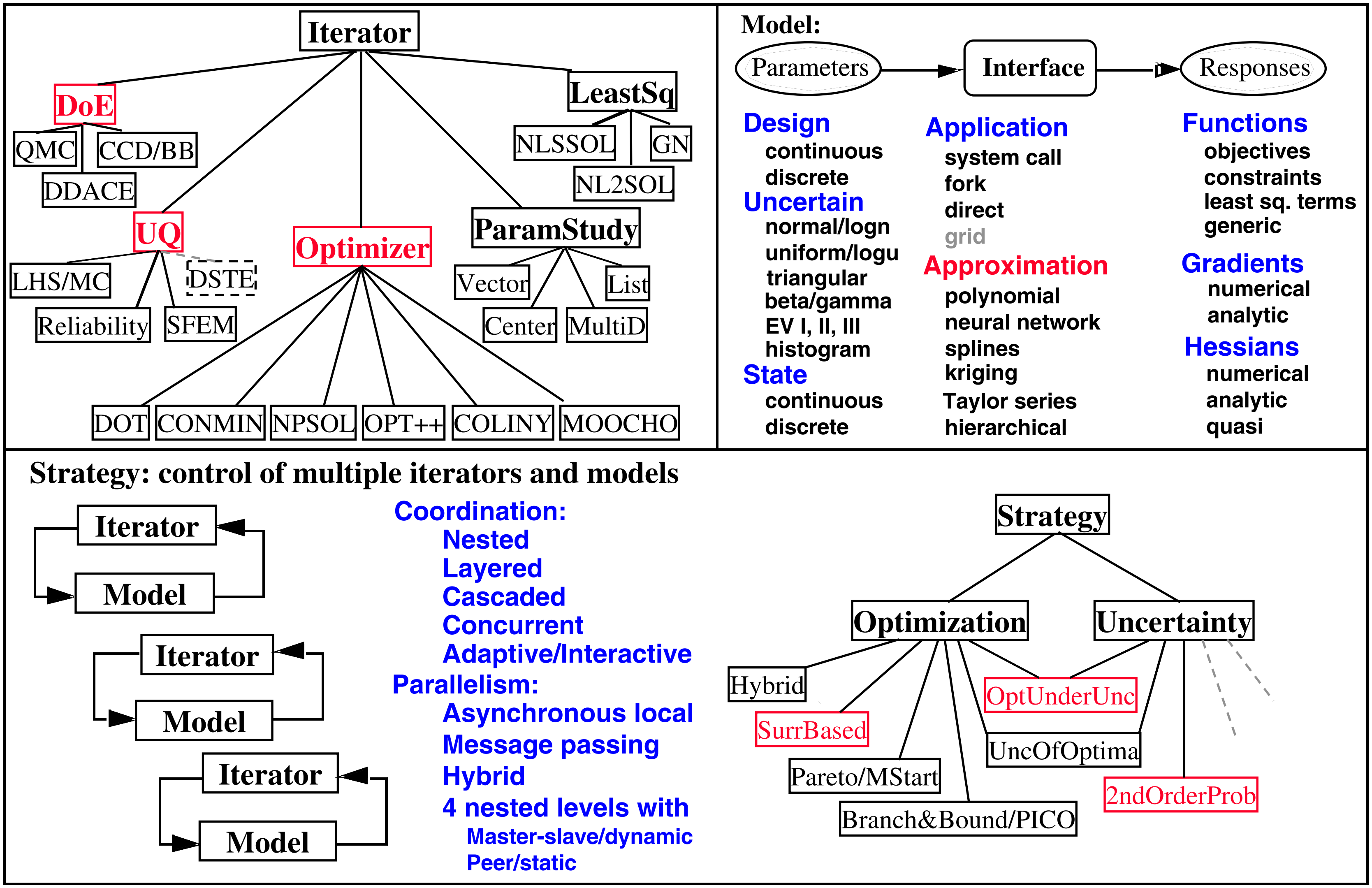
DAKOTA Framework



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Optimization Under Uncertainty

OUU techniques categorized based on UQ approach:

– **Sampling-based** (noise-tolerant opt.; design for robustness)

FY03
- TR-SBOUU: trust region surrogate-based
- Nongradient-based (Trosset)
- Robust design of experiments (Taguchi)

– **Reliability-based** (exploit structure; design for reliability)

FY04
- Bi-level RBDO (nested)

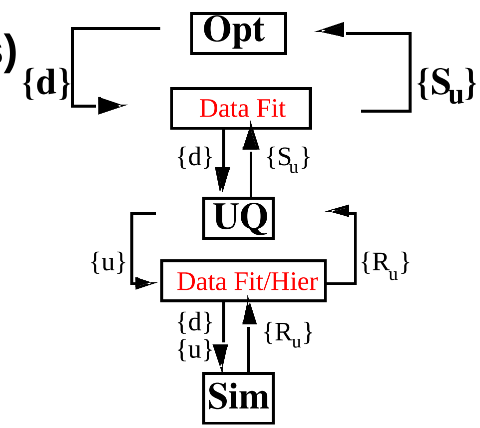
FY05
- Sequential RBDO (iterative)
- Unilevel RBDO (all at once)

– **Stochastic finite element-based** (multiphysics)

FY06
- Exploit PCE coeffs & random process structure
- Leverage SBO with deterministic ROMs

– **Epistemic uncertainty**
- Evidence theory-based (Agarwal)
- Bayesian inference: model calibration under uncertainty
- 2nd-order probability: 3-level SBOUU?

– **Intrusive OUU** (all at once approaches)
- SFE + SAND: intrusive PCE variant amenable to SAND
- Unilevel RBDO + SAND



Augment NLP with statistics $\mathbf{s_u}$ $(\mu, \sigma, p/\beta/z)$ *using a linear mapping:*

Minimize $f(d) + W s_u(d)$

Subject to

$$g_l \le g(d) \le g_u$$
$$h(d) = h_t$$
$$a_l \le A_i s_u(d) \le a_u$$
$$A_e s_u(d) = a_t$$
$$d_l \le d \le d_u$$

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SBOUU Formulations

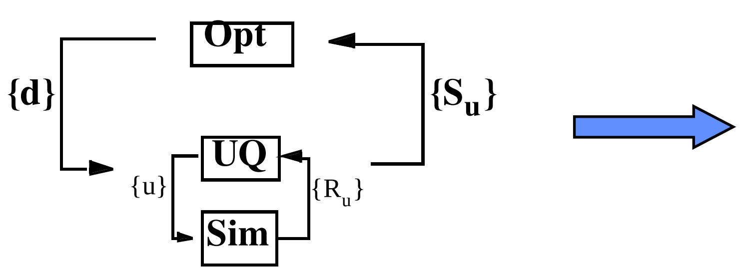
For surrogate-based OUU, the surrogate can appear

- at the **optimization level** (fit *S*(*d*))
- at the **UQ level** (fit *R*(*d*, *u*))
- at **both levels** (fit *S*(*d*) and *R*(*d*, *u*))

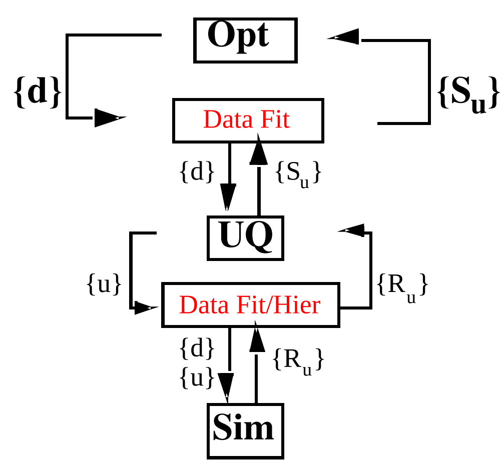
Surrogate can be

- local/global/multipoint data fit (either level)
- model hierarchy approximation (UQ level only)

Simple Nested OUU:



SBOUU with two surrogate levels:



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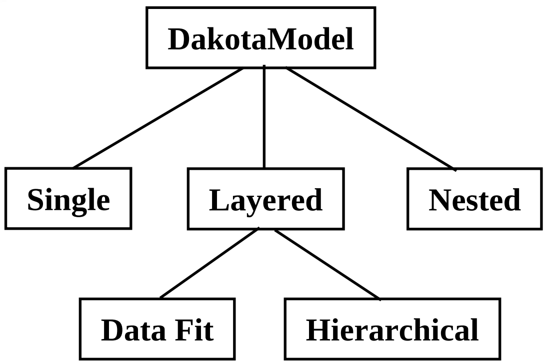
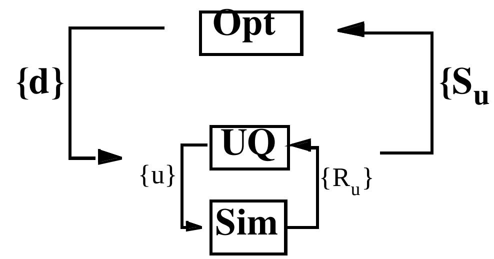
Optimization under Uncertainty with Surrogates



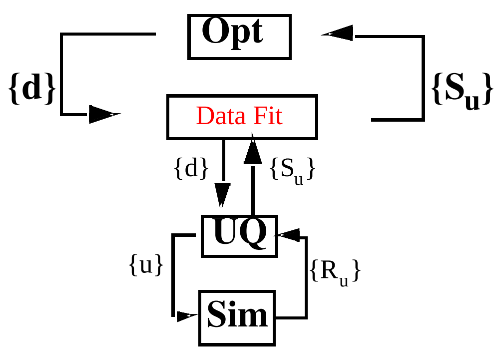
Nested model: internal iterators/models execute a complete iterative study as part of every evaluation.

Surrogate model: internal iterators/models used for periodic update and verification of data fit (global/local/multipoint) or hierarchical (variable fidelity) surrogates.

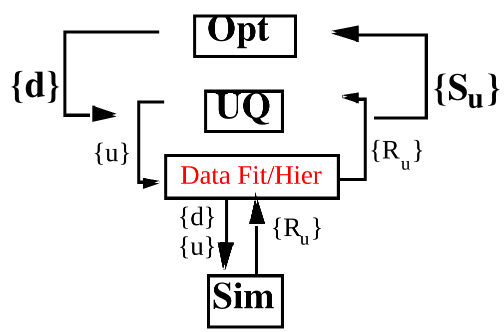
Nested/Surrogate models can recurse



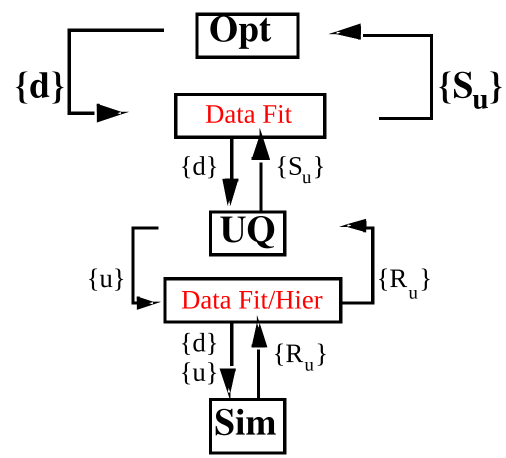
Formulation 1: Nested



Formulation 2: Surrogate containing Nested



Formulation 3: Nested containing Surrogate



Formulation 4: Surrogate containing Nested containing Surrogate

Formulations 2 & 4 amenable to trust-region approaches

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

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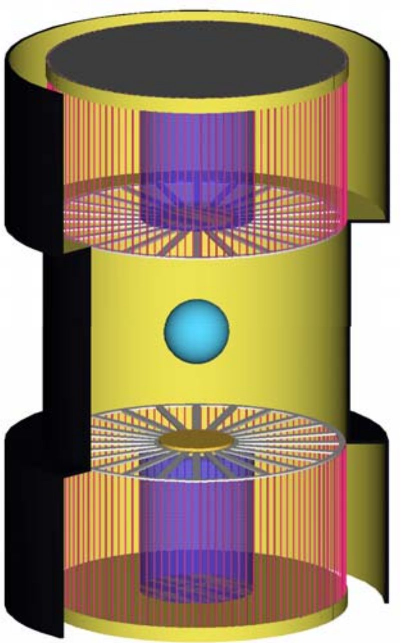
TR-SBOUU Results

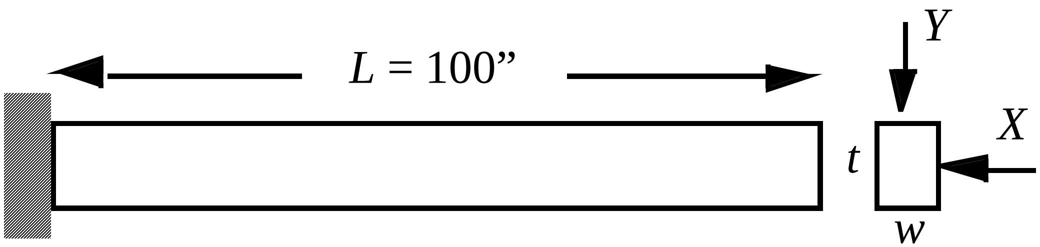
- **Direct nested OUU is expensive and requires seed reuse**
- **SBOUU expense much lower (up to 100x), but unreliable.**
- **TR-SBOUU maintains quality of results and reduces expense ~10x**
  - **Ex. 1: formulation 4 with TR 5-7x less expensive than direct nesting**
  - **Ex. 2: formulation 4 with TR 8-12x less expensive than direct nesting**
  - **ICF Ex.: formulations 2/4 with TR locate vicinity of a min in a single cycle**
- **Additional benefits:**
  - **Navigation of nonsmooth engineering problems**
  - **Less sensitive to seed reuse: variable patterns OK and often helpful, possibility of exploitation reduced**
  - **Less sensitive to starting point: data fit SBO provides some global ident.**



Minimize $f + p_{fail\_r1} + p_{fail\_r3}$

Subject to $g_i \leq 0$, for $i = 1,2,3$

$\mu_{r2} + 3\sigma_{r2} \leq 1.6e5$



Conference papers at 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."

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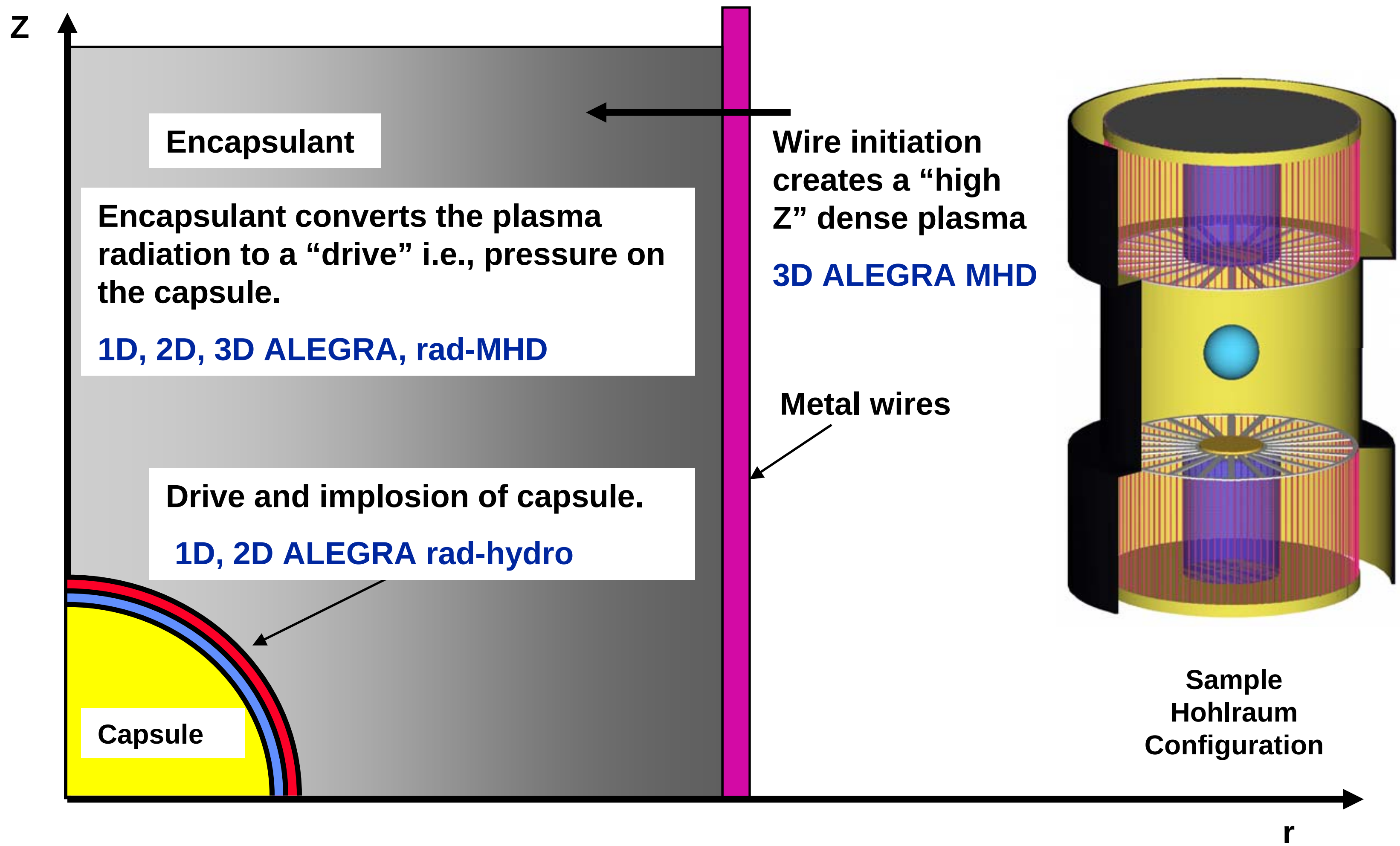
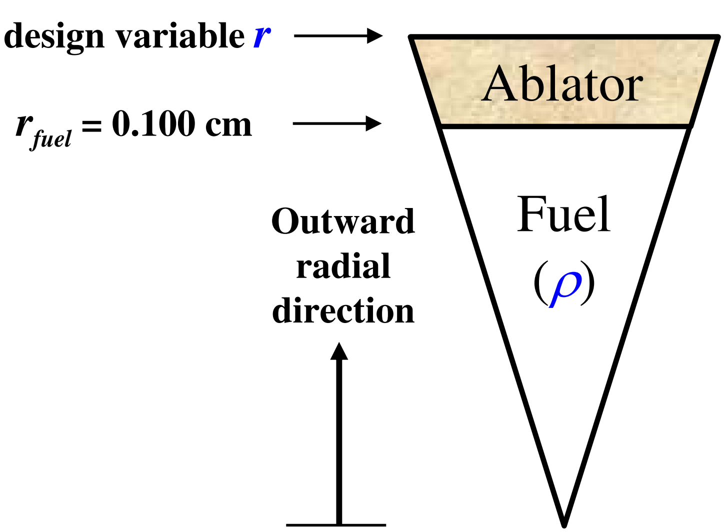
Robust Hohlraum Design for Inertial Confinement Fusion

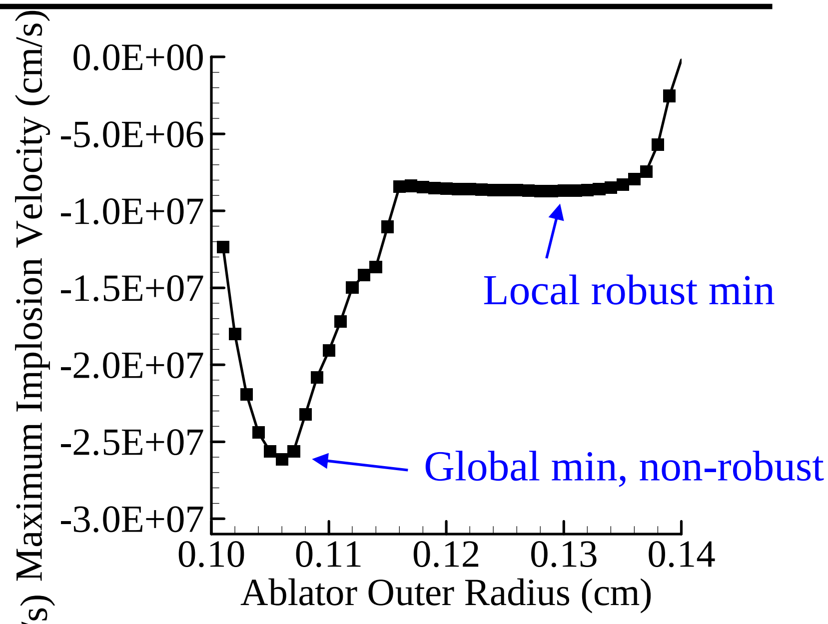


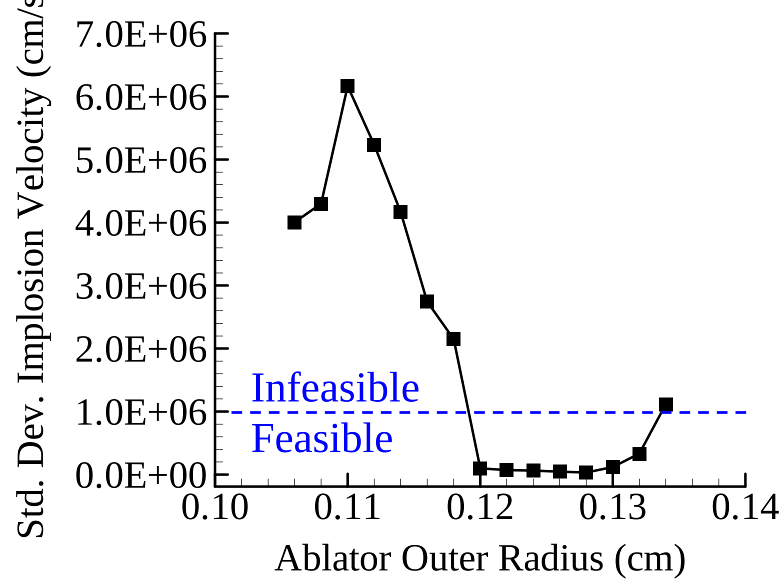
Uncertainties in: plasma, drive, and capsule characteristics

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







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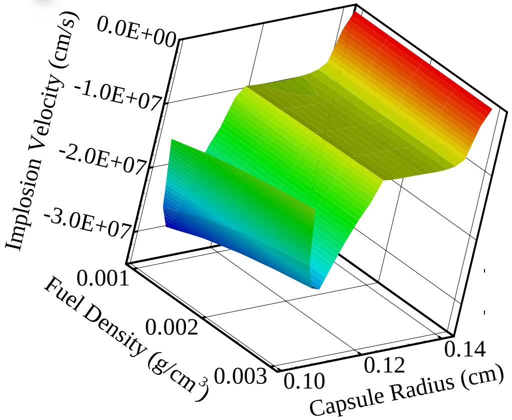
ICF Capsule Design
2D Optimization



Minimize $V(r, \rho)$

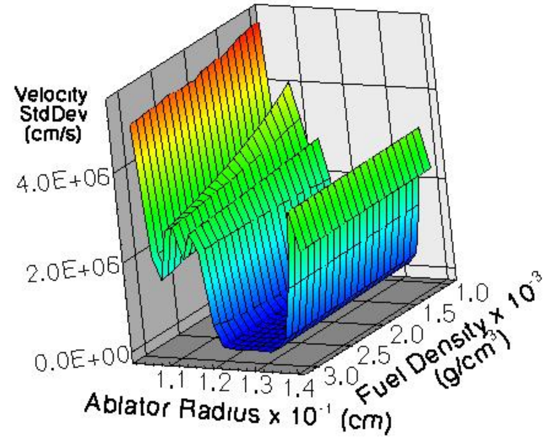
Subject to $\sigma_V(r, \rho) \leq$ **3.e+5 cm/s**

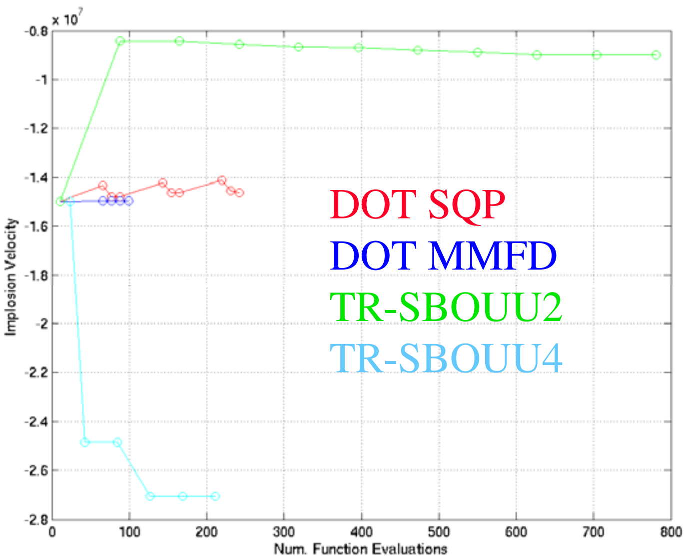
0.103 cm $\leq r \leq$ **0.14 cm**

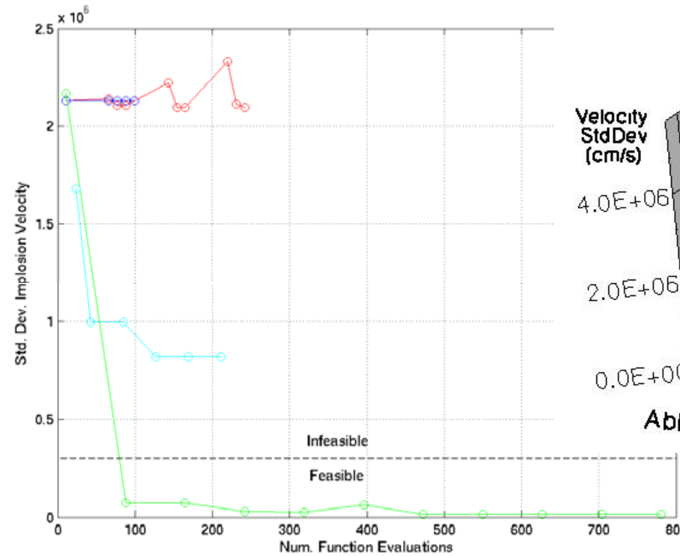
0.001 cm $\leq \rho \leq$ **0.003 g/cc**

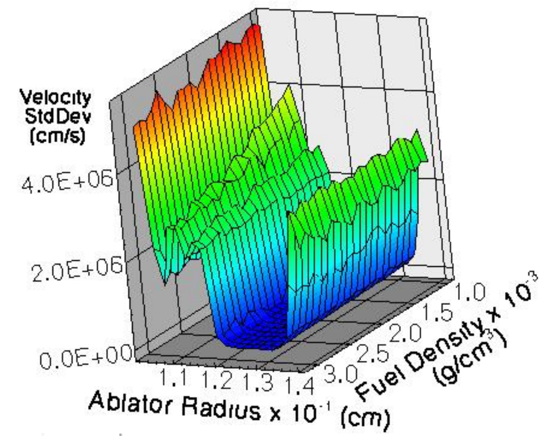
uniform: u_r **= [-2.5e-3, 2.5e-3]**

uniform: u_ρ **= [-2.5e-5, 2.5e-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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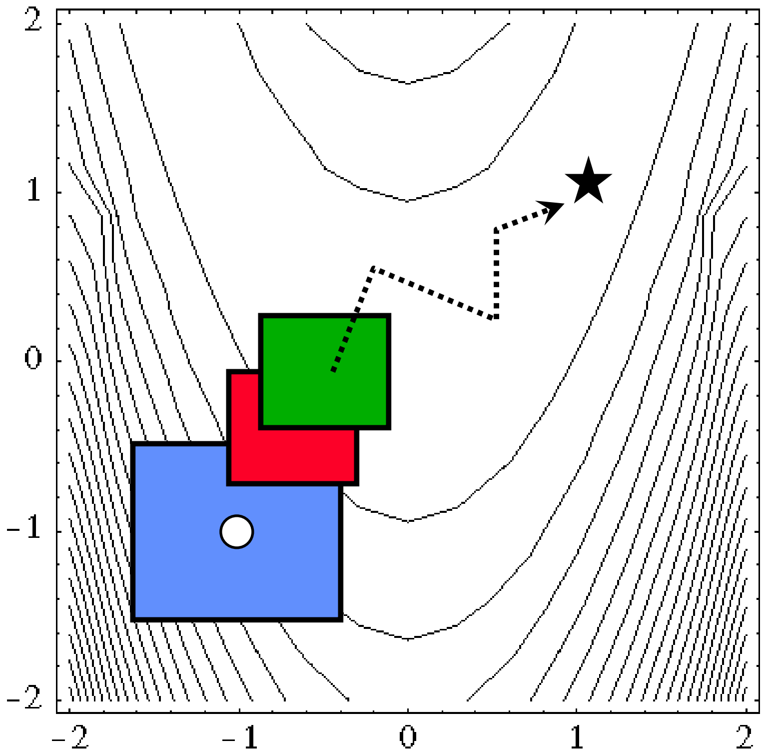
Trust Region Surrogate-Based Optimization under Uncertainty (TR-SBOUU)

Sequence of trust regions



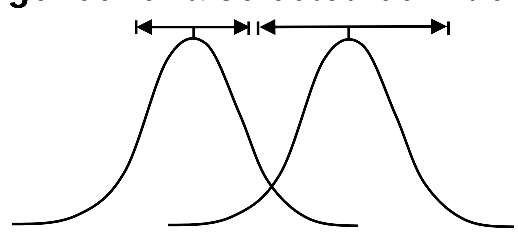
From SBO to SBOUU:

SBO is provably convergent with TR globalization

- **(at least) 1st order consistency with correction**
- **verification of approx. steps**

Extensions to SBOUU

- **1st order consistency, assuming a worthwhile stoch. gradient**
- **verification of stats. in relative sense. Three levels of verification rigor:**
  - **Least:** **nominal statistics.**
  - **Most:** **ordinal opt. (Chen/Romero) → nonoverlap confidence bounds on every step ("provable" convergence for a selected confidence level).**



  - **Affordable compromise:** **stochastic approximation (Igusa) → probability of erroneous TR steps is decreased in proportion to iteration count.**

RBDO Algorithms

Bi-level RBDO

- Constrain RIA $z \rightarrow p/\beta$ result
- Constrain PMA $p/\beta \rightarrow z$ 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
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Fully analytic Bi-level RBDO

- Analytic reliability sensitivities avoid numerical differencing at design level

$$\begin{aligned} \nabla_d z &= \nabla_d G \\ \nabla_d \beta_{cdf} &= \frac{1}{\| \nabla_u G \|_2} \nabla_d G \\ \nabla_d p_{cdf} &= -\phi(-\beta_{cdf}) \nabla_d \beta_{cdf} \end{aligned}$$

Sequential/Surrogate-based RBDO:

- Break nesting: iterate between opt & UQ until target is met. TR-SB linkage is non-heuristic.

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{d}_0) + \nabla_d f(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \\ \text{subject to} \quad & \beta(\mathbf{d}_0) + \nabla_d \beta(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \geq \bar{\beta} \\ & \| \mathbf{d} - \mathbf{d}_0 \|_\infty \leq \Delta^k \end{aligned}$$

1st order

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

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

KKT of MPP

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RBDO Results

Short Column

min *bh*

s.t. $\beta \geq 2.5$

$$g(\mathbf{x}) = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2}$$

Kuschel & Rackwitz, 1997

$P = N(500, 100)$ $\rho_{P,M} = 0.5$

$M = N(2000, 400)$ $b_{nom} = 5$

$Y = LogN(5, 0.5)$ $h_{nom} = 15$

Bi-level RBDO

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ MV	50	197.8	0.01913
RIA $z \to p$ x-space AMV	150	197.5	0.01962
RIA $z \to p$ u-space AMV	147	198.9	0.01721
RIA $z \to p$ x-space AMV+	370/354	217.1	0.0
RIA $z \to p$ u-space AMV+	400/371	217.1	0.0
RIA $z \to p$ FORM	1877/1781	217.1	0.0
RIA $z \to \beta$ MV	16	197.7	0.5475
RIA $z \to \beta$ x-space AMV	48	197.4	0.5559
RIA $z \to \beta$ u-space AMV	48	198.2	0.5326
RIA $z \to \beta$ x-space AMV+	195/185	216.7	0.0
RIA $z \to \beta$ u-space AMV+	211/193	216.7	0.0
RIA $z \to \beta$ FORM	916/1088	216.7	0.0
PMA $p, \beta \to z$ MV	35	197.7	0.1547
PMA $p, \beta \to z$ x-space AMV	124	214.8	0.01367
PMA $p, \beta \to z$ u-space AMV	124	215.6	0.008390
PMA $p, \beta \to z$ x-space AMV+	268/212	216.8	0.0
PMA $p, \beta \to z$ u-space AMV+	328/214	216.8	0.0
PMA $p, \beta \to z$ FORM	1567/707	216.8	0.0

Analytic bi-level RBDO

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ x-space AMV+	161/149	217.1	0.0
RIA $z \to p$ u-space AMV+	171/160	217.1	0.0
RIA $z \to p$ FORM	865/911	217.1	0.0
RIA $z \to \beta$ x-space AMV+	76/72	216.7	0.0
RIA $z \to \beta$ u-space AMV+	82/76	216.7	0.0
RIA $z \to \beta$ FORM	538/612	216.7	0.0
PMA $p, \beta \to z$ x-space AMV+	105/100	216.8	0.0
PMA $p, \beta \to z$ u-space AMV+	125/102	216.8	0.0
PMA $p, \beta \to z$ FORM	508/285	216.8	0.0

Surrogate-based RBDO

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ x-space AMV+	77/75	216.9	0.0
RIA $z \to p$ u-space AMV+	82/81	216.9	0.0
RIA $z \to p$ FORM	573/577	216.9	0.0
RIA $z \to \beta$ x-space AMV+	67/65	216.7	0.0
RIA $z \to \beta$ u-space AMV+	72/72	216.7	0.0
RIA $z \to \beta$ FORM	508/561	216.7	0.0
PMA $p, \beta \to z$ x-space AMV+	79/76	216.7	2.1e-4
PMA $p, \beta \to z$ u-space AMV+	87/79	216.7	2.1e-4
PMA $p, \beta \to z$ FORM	333/228	216.7	2.1e-4

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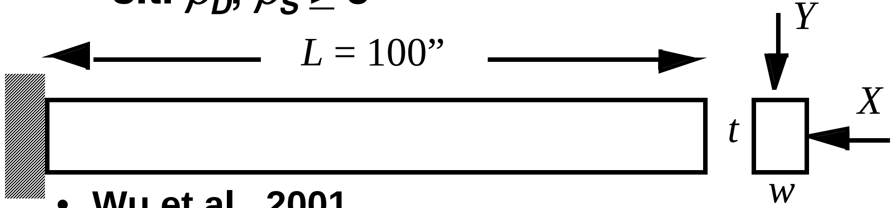
RBDO Results

Cantilever

min *wt*

s.t. β_D, $\beta_S \geq 3$



- **Wu et al., 2001**
- **2 design vars: *w*, *t***
- **4 uncorr. normal uncertain vars: *E*, *R*, *X*, *Y***

Limit state eqns (unnormalized):

$$stress = \frac{600}{wt^2}Y + \frac{600}{w^2 t}X \leq R$$

$$displacement = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \leq D_0$$

Bi-level RBDO

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ MV	95	11.37	0.0
RIA $z \to p$ x-/u-space AMV	285	11.37	0.0
RIA $z \to p$ x-/u-space AMV+	597/624	9.563	0.0
RIA $z \to p$ FORM	1522/1111	9.563	0.0
RIA $z \to \beta$ MV	44	9.392	0.2958
RIA $z \to \beta$ x-/u-space AMV	132	9.392	0.2958
RIA $z \to \beta$ x-/u-space AMV+	540/493	9.520	0.0
RIA $z \to \beta$ FORM	1082/865	9.520	0.0
PMA $p, \beta \to z$ MV	53	9.393	0.03216
PMA $p, \beta \to z$ x-/u-space AMV	159	9.504	0.003602
PMA $p, \beta \to z$ x-/u-space AMV+	547/428	9.521	0.0
PMA $p, \beta \to z$ FORM	3631/1148	9.521	0.0

Analytic bi-level RBDO

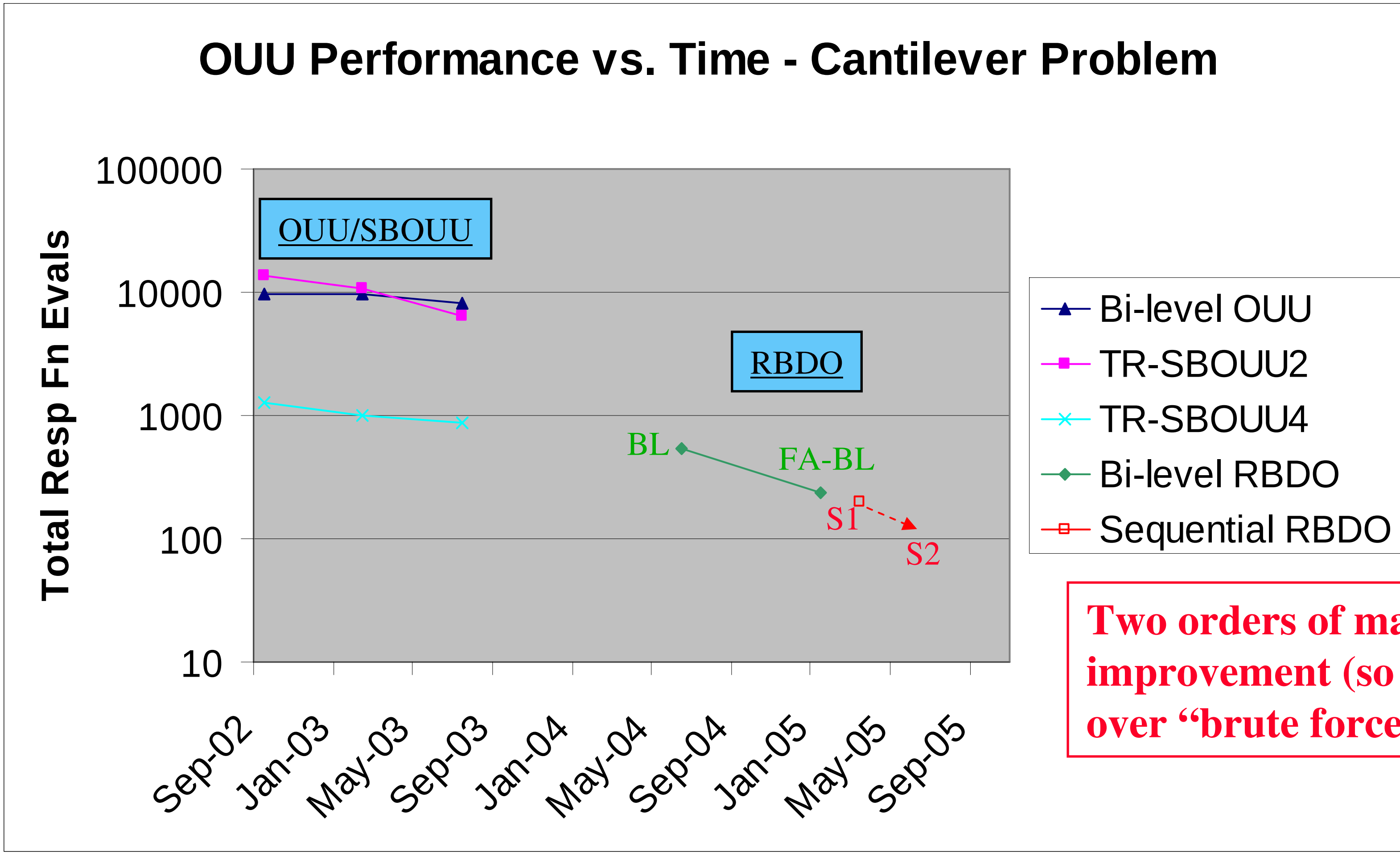
RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ x-/u-space AMV+	279/319	9.529	1.1e-5
RIA $z \to p$ FORM	623/531	9.563	0.0
RIA $z \to \beta$ x-/u-space AMV+	207/208	9.520	0.0
RIA $z \to \beta$ FORM	367/324	9.520	0.0
PMA $p, \beta \to z$ x-/u-space AMV+	247/232	9.521	0.0
PMA $p, \beta \to z$ FORM	1408/843	9.521	0.0

Surrogate-based RBDO

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \to p$ x-/u-space AMV+	197/186	9.520	1.0e-9
RIA $z \to p$ FORM	342/457	9.520	1.0e-9
RIA $z \to \beta$ x-/u-space AMV+	189/203	9.520	9.5e-5
RIA $z \to \beta$ FORM	372/442	9.520	9.5e-5
PMA $p, \beta \to z$ x-/u-space AMV+	181/181	9.520	2.7e-9
PMA $p, \beta \to z$ FORM	759/487	9.520	2.7e-9

OUU Progress To Date

- **2003:** **Surrogate-based OUU with sampling methods**
- **2004:** **Bi-level RBDO with numerical reliability gradients**
- **2005:** **Fully analytic bi-level RBDO**
  Sequential/surrogate-based RBDO (1st-order)



Two orders of magnitude improvement (so far) over "brute force" OUU

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Intrusive OUU:
DAKOTA/MOOCHO w/ SIERRA/NEVADA

Next-generation multi-physics simulation architectures:

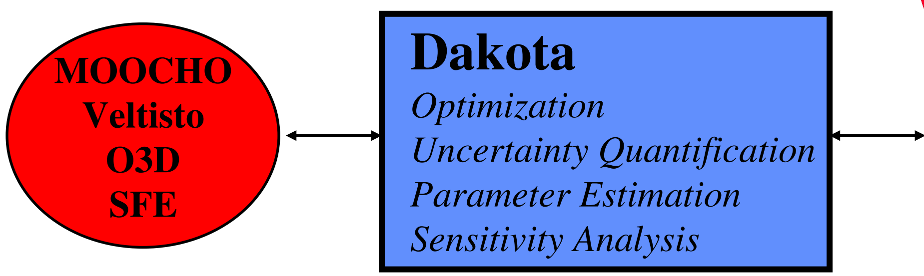
- **SIERRA: mechanics framework (“S. DAKOTA”)**
- **NEVADA: physics framework (“N. DAKOTA”)**

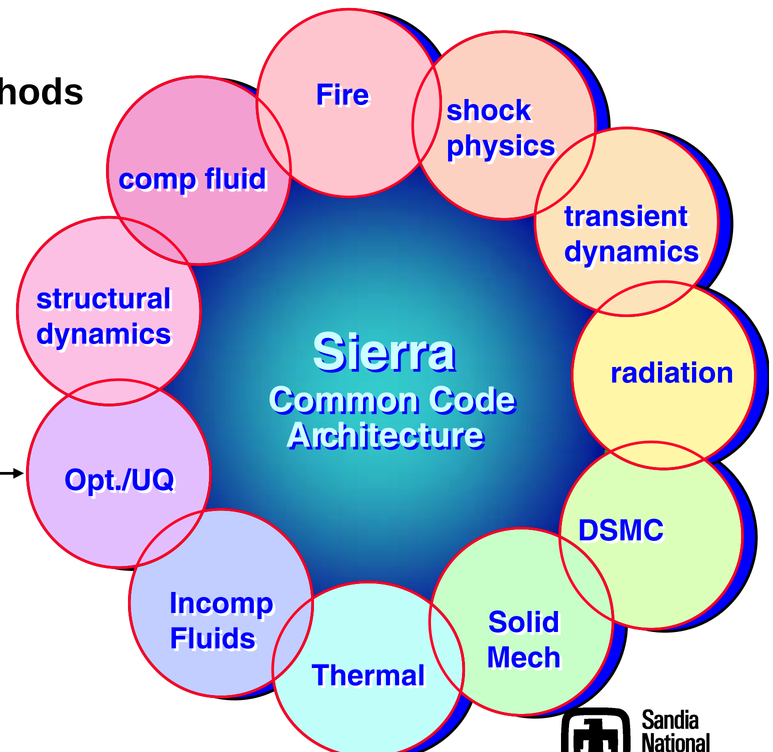
Architecture extensions underway for:

- **Opt.: SAND optimization (MOOCHO)**
- **UQ: (intrusive) stochastic finite elements**
- **Other: Stability analysis (LOCA), Nonlinear equations (NOX), Fully-coupled MDA**

Impact:

- **Performance enhancements for existing nested methods**
  - **Model I/O in core in parallel**
  - **SPMD execution on compute nodes of ASCI MPPs**
- **Next-generation, tightly-coupled opt. & UQ**
  - **Direct/adjoint sensitivities & AD**





Intrusive OUU:

- **SFE + SAND**
- **Unilevel RBDO + SAND**

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Conclusions

OUU Aspects:

- **UQ-based**
- **Aleatory and Epistemic uncertainties**
- **Design for Robustness and Reliability**
- **Nonlinear, implicit, large-scale, expensive simulations**

OUU Algorithms:

- **SBOUU**
  - **Good:** **trustworthy UQ, TR-SBOUU ~10x better than brute force w/ additional benefits (nonsmooth navigation/limited global ID/seed insensitivity)**
  - **Bad:** **low probability events/reliability constraints difficult to resolve efficiently**
  - **Ugly:** **multiple surrogates lead to complex input specifications**
- **RBDO**
  - **Good:** **efficient for well-behaved problems, handles low prob. events, industry workhorse**
  - **Bad:** **UQ not trustworthy for nonsmooth/highly nonlinear problems or multiple failure pts.**
  - **Ugly:** **high-consequence apps? (some communities possibly over-subscribed to this approach)**
- **Intrusive OUU**
  - **Good:** **next level of performance**
  - **Bad:** **requires simulation code intrusion (few sites w/ in-house sim code development)**
  - **Ugly:** **level of effort is extensive for general support of production-scale apps.**

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