2005 Department Review

Michael S. Eldred

Dept. 9211: Optimization & Uncertainty Estimation

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

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Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

MESA | DART | HPC | SIERRA | Xyce | Entero | PRIDE

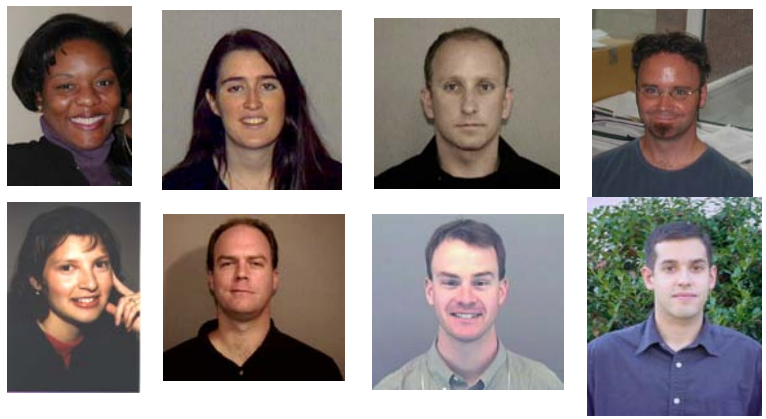
Research:
Optimization
Uncertainty quantification
Opt under uncertainty

Development:
Framework architect
DAKOTA releases

Deployment:
Use/access initiatives
External/internal impact

Project Leadership

- **Leadership of DAKOTA team**
  - **Vision, strategic planning, and technical leadership**
  - **Mentoring of new staff and LTEs**
  - **Supervision of contractors**
- **Responsible for multiple projects and their deliverables**
  - **PI for ASC Algorithms, LM Shared Vision**
  - **Team member for ASC V&V (DAKOTA/UQ, D-S TofE), GY, CSRF OUU**
  - **Met 3 FY05 L3 milestones thus far: Algs Q2, V&V Q3/Q4**



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New Directions

New outreach/connectivity:

Deployment

- *DART:* APC, ASETS, WISDM, SIMBA → Tiger team for ensemble computing
- *SIERRA:* new reqmts for instrumentation subsystem and XML schema plug-ins
- *Xyce/ICC:* HPEMS interface and deployment
- *MESA-TOP/MESA-CA:* Gianoulakis, Wittwer, Fulcher, Thomas → thermal/RF/SiReS
- *ICC/NWCC/Red Storm:* mpiexec (Evensky, Wycoff), multilevel parallel reqmts (Kelly, Tomkins)

Research

- *Entero:* integration of space mapping research w/ POD and correction research
- *PRIDE:* connection of SBO to Bayesian updating of surrogate models
- *Verification:* connection to planned toolbox (MMS, Richardson Extrap.)

New research directions:

- *ROMs:* 9211/9214/9233 proposal (LDRD → CSRF)
- *MEMS:* 9211/9124 proposal (CSRF)

New coordination activities:

- Weekly DAKOTA team luncheons
- Quarterly ASC Optimization coordination meetings

Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

Impact: shared vision, enhanced connectivity, critical mass

Research:
Optimization
Uncertainty quantification
Opt under uncertainty

Development:
Framework architect
DAKOTA releases

SBO | RBDO | AMV+^{2} | Epistemic | CSRI

Deployment:
Use/access initiatives
External/internal impact

Trust Region Methods for Approximation Management

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

Workhorse techniques

→ Methods used extensively by SNL, GY, LM Aero

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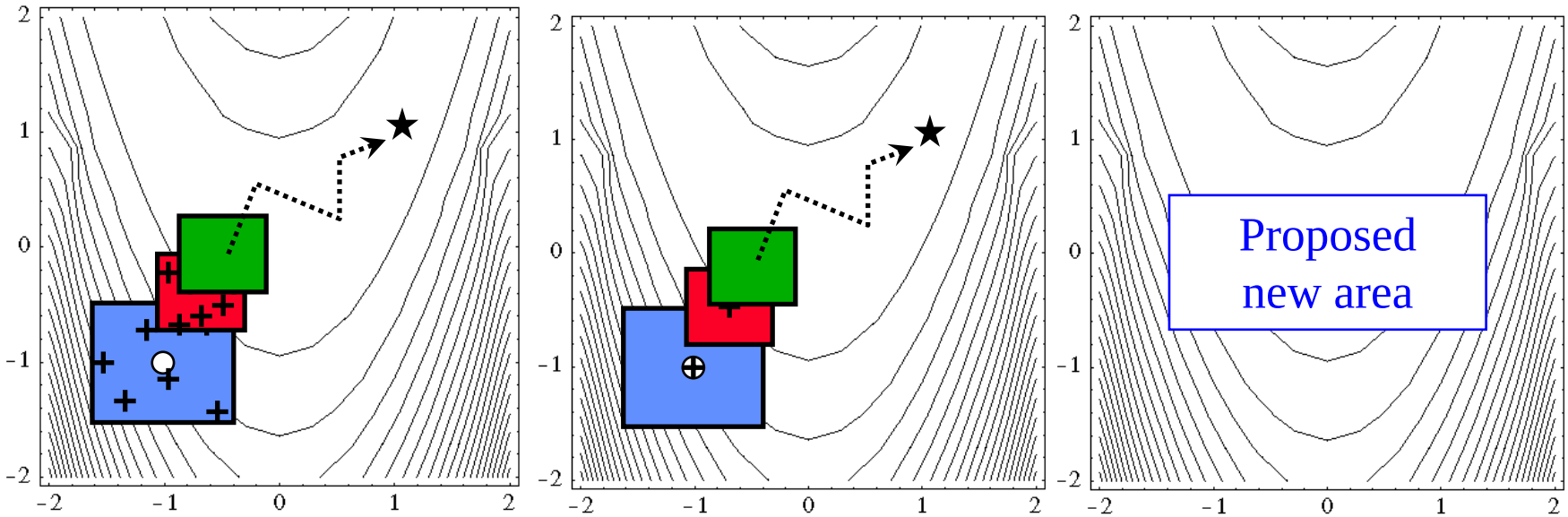
Trust-Region Surrogate-Based Optimization

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
- 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 and multifidelity cases

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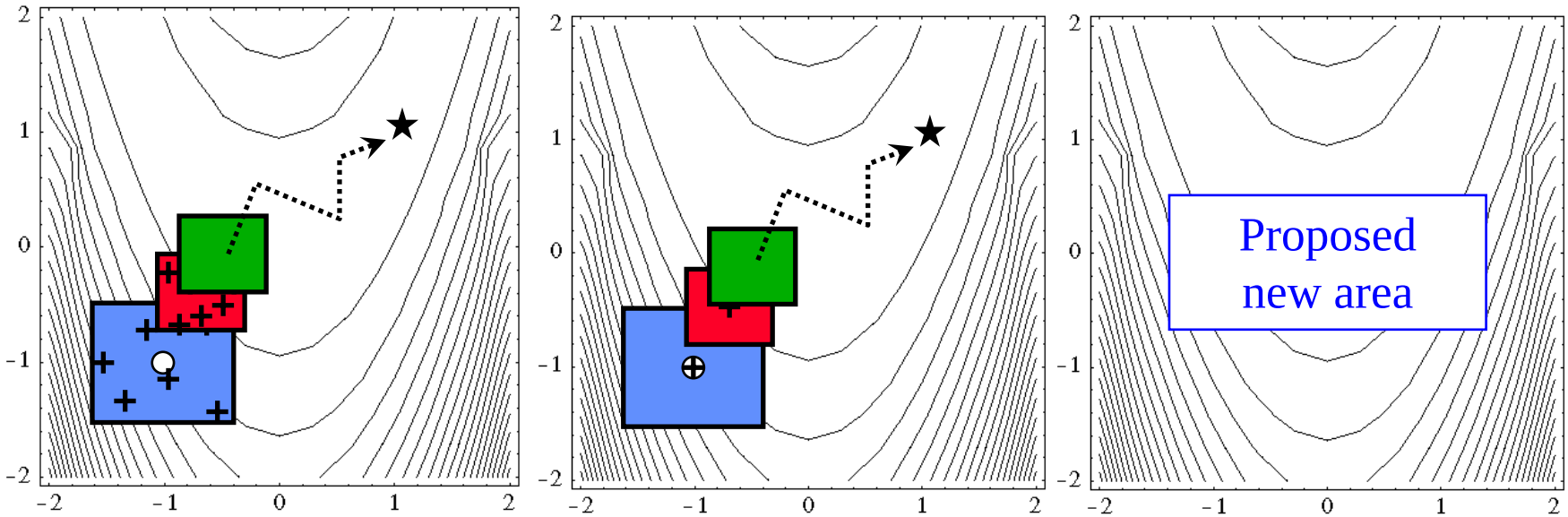
Trust-Region Surrogate-Based Optimization

Data Fit → ***Multifidelity*** → ***ROM***



Research areas (new, developing, planned):

Nonlinear constraint management (2004 CSRI: ND)

Homotopy/composite step → efficiency through balance of feasibility/optimality

Filter methods → robustness through penalty-free iterate selection & TR logic

Global fits w/ local consistency (e.g., constrained LLS)

Response Corrections
Variable mappings
(2005 CSRI: MIT)

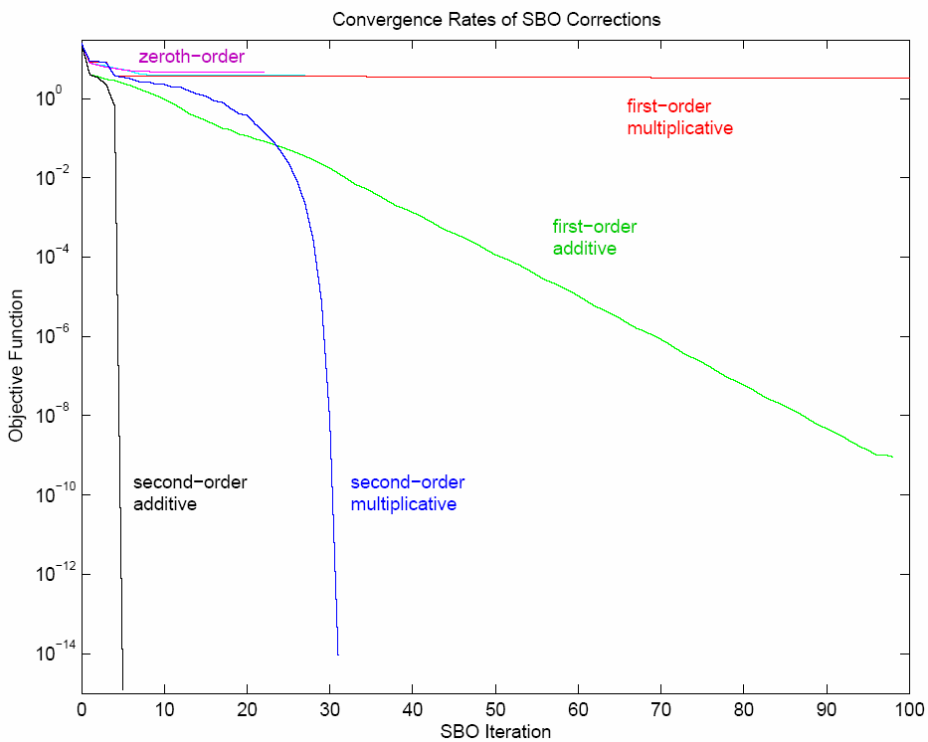
Extended/spanning ROMS
(2005 CSRI: CU Boulder)

2nd-order Corrections in Multifidelity SBO
FD- and Quasi-2nd-order, Multipoint

PY04

Additive: $\hat{f}_{hi_\alpha}(\mathbf{x}) = f_{lo}(\mathbf{x}) + \alpha(\mathbf{x})$

Multiplicative: $\hat{f}_{hi_\beta}(\mathbf{x}) = f_{lo}(\mathbf{x})\beta(\mathbf{x})$



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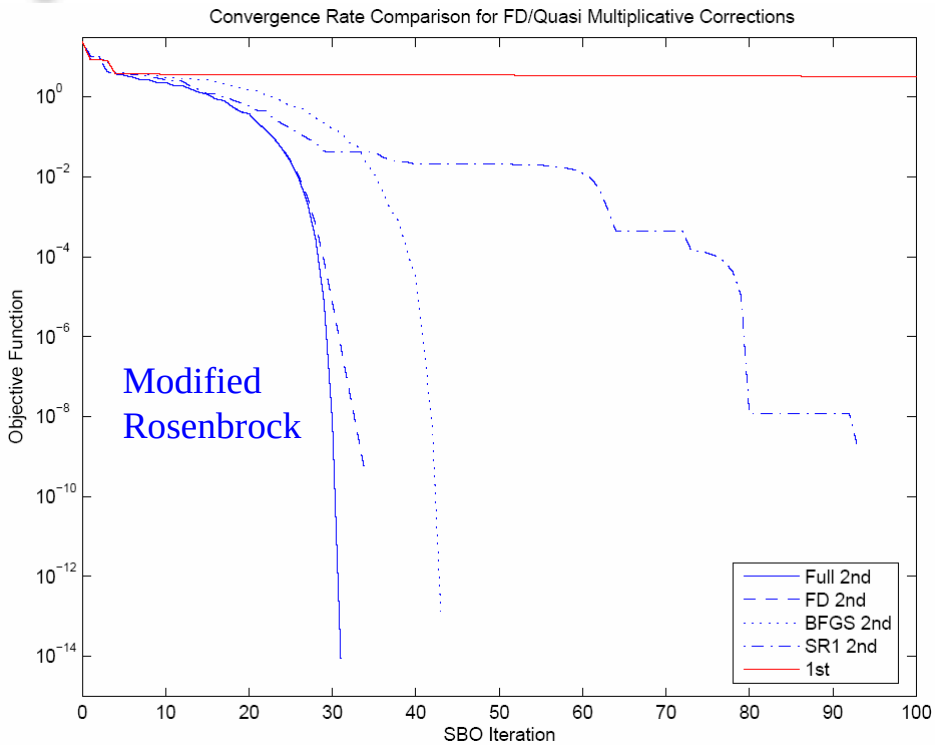
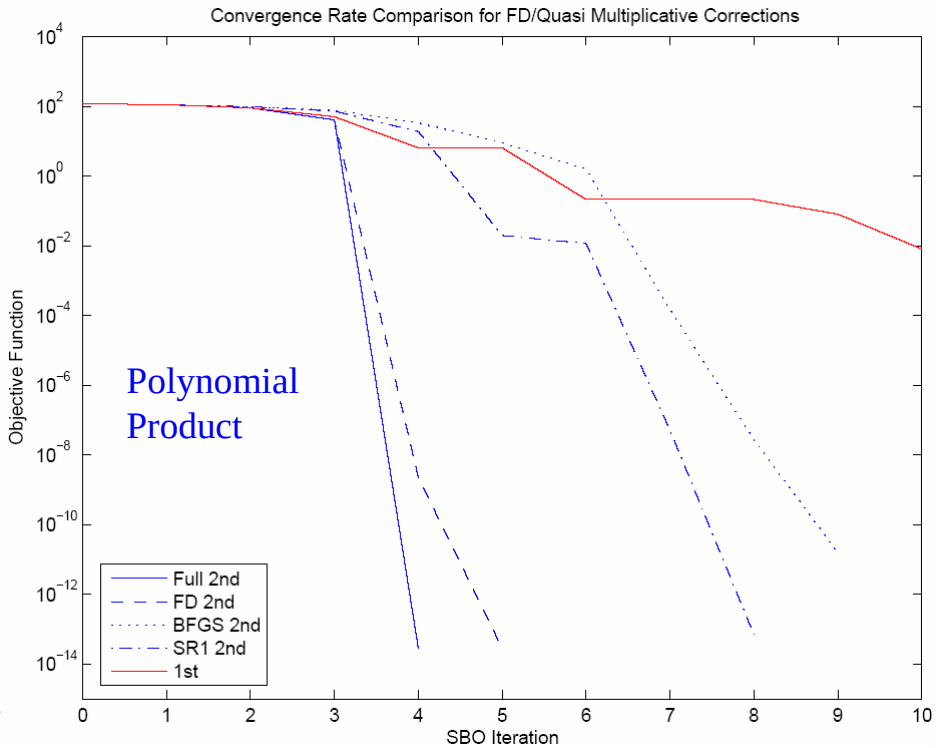
2nd-order Corrections in Multifidelity SBO
FD- and Quasi-2nd-order, Multipoint





Finite diff. Hessians **(1st & 2nd-order diffs) are expensive, but mirror full 2nd-order**

Quasi-Newton Hessians **(BFGS, SR1) require no addtl evals and are effective:**

- **Consistently outperform 1st-order corrections**
- **Lag relative to full/FD 2nd-order as curvature is accumulated**

Multipoint corrections **address global accuracy & adaptively select among add/mult**

$$\hat{f_{hi_\gamma}}(\mathbf{x}) = \gamma \hat{f_{hi_\alpha}}(\mathbf{x}) + (1-\gamma)\hat{f_{hi_\beta}}(\mathbf{x})$$

Ongoing: **SAGE CFD applications with Scott Collis**

Optimization Under Uncertainty

Many opt. problems must be solved in the presence of uncertainty

- inherent: aleatory/irreducible (probabilistic models)
- lack of knowledge: epistemic/reducible (nonprobabilistic models)

OUU techniques categorized based on UQ approach:

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

FY03

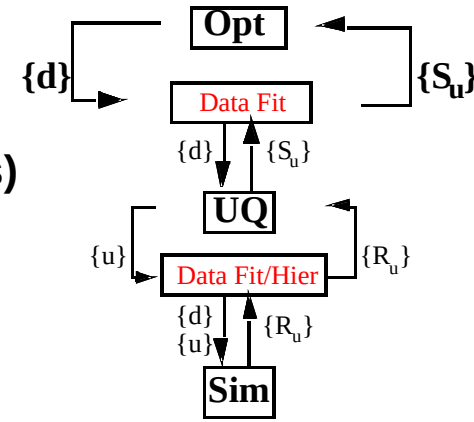
  - TR-SBOUU: trust region surrogate-based
  - Nongradient-based (Trosset)

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

FY04
FY05

  - Bi-level RBDO (nested)
  - Sequential RBDO (iterative)
  - Unilevel RBDO (all at once)

- **Stochastic finite element-based** (multiphysics)
  - exploit PCE coeffs & random process structure
- **Epistemic uncertainty**
  - Evidence theory-based
  - Bayesian inference: model calibration under uncertainty
  - 2nd-order probability: 3-level SBOUU
- **Intrusive OUU**
  - SFE + SAND: intrusive PCE variant amenable to SAND
  - Unilevel RBDO + SAND



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

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

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RBDO Algorithms

Bi-level RBDO

- **Constrain RIA *z* → *p*/β result**
- **Constrain PMA *p*/β → *z* result**

$$\text{RIA RBDO}\begin{cases}\text{minimize} & f\\ \text{subject to} & \beta \geq \bar{\beta}\\ \text{or} & p \leq \bar{p}\end{cases}$$

$$\text{PMA RBDO}\begin{cases}\text{minimize} & f\\ \text{subject to} & z \geq \bar{z}\end{cases}$$

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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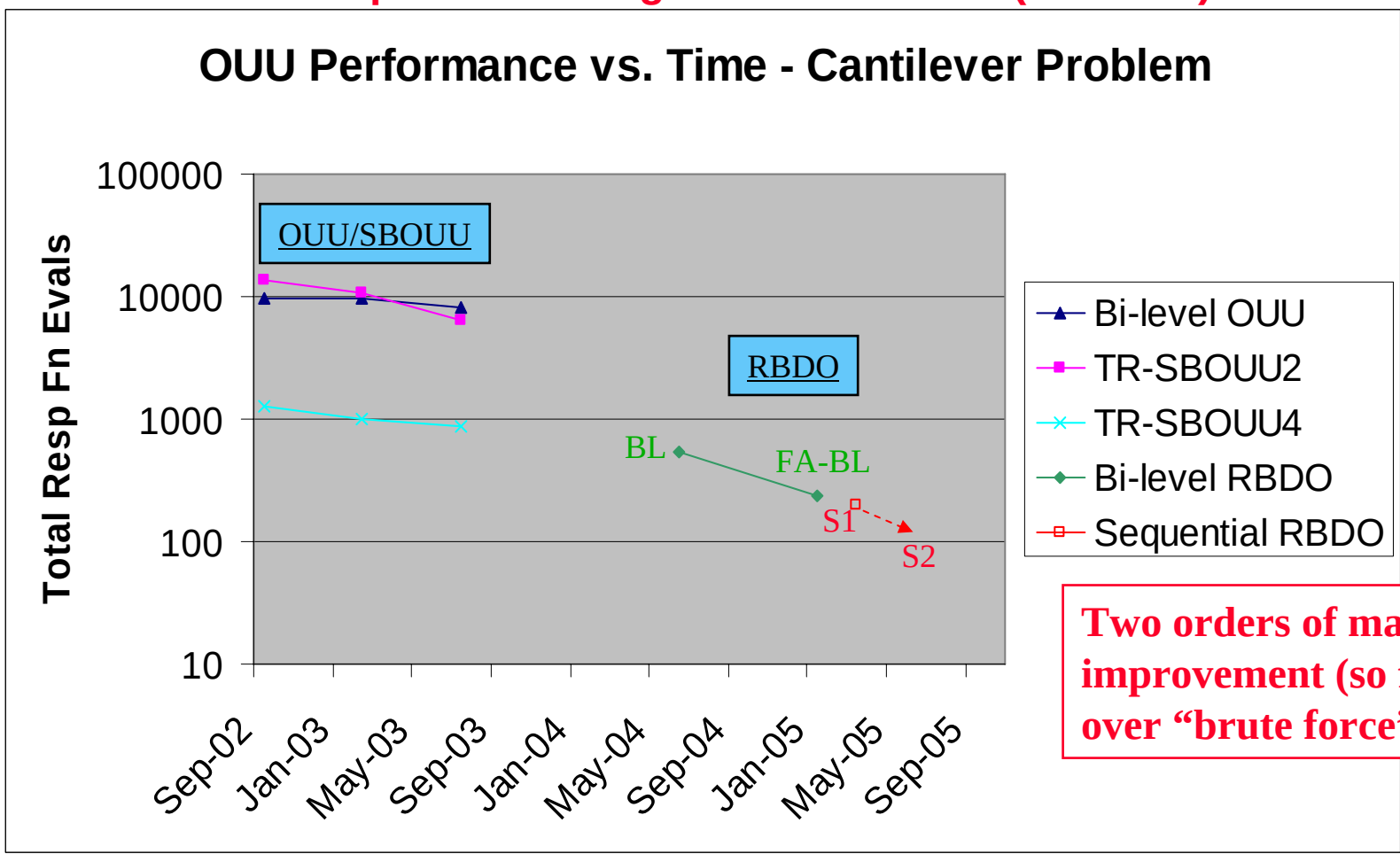
OUU Progress

- **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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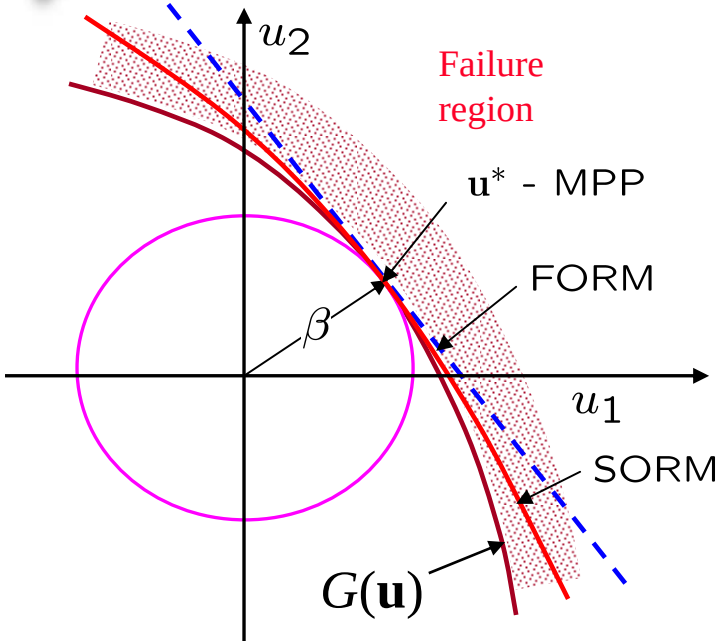
Given success w/ 1st-order UQ/RBDO approximations

→ 2nd-order reliability methods for UQ/RBDO



2nd-order limit state approximations

- **e.g., x-space AMV+²:**

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

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

2nd-order integration

(accounts for curvature in limit state):

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

curvature correction

2nd-order sequential RBDO

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{d}_0) + \nabla_d f(\mathbf{d}_0)^T(\mathbf{d}-\mathbf{d}_0) + \tfrac{1}{2}(\mathbf{d}-\mathbf{d}_0)^T\nabla_d^2 f(\mathbf{d}_0)(\mathbf{d}-\mathbf{d}_0) \\ \text{subject to} \quad & \beta(\mathbf{d}_0) + \nabla_d \beta(\mathbf{d}_0)^T(\mathbf{d}-\mathbf{d}_0) + \tfrac{1}{2}(\mathbf{d}-\mathbf{d}_0)^T\nabla_d^2\beta(\mathbf{d}_0)(\mathbf{d}-\mathbf{d}_0) \geq \bar{\beta} \\ & \| \mathbf{d}-\mathbf{d}_0 \|_\infty \leq \Delta^k \end{aligned}$$

2nd order

Leverages 2nd-order optimization
Invited journal paper in preparation

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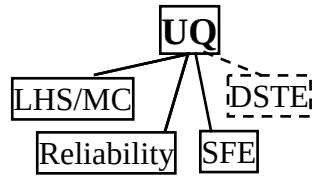
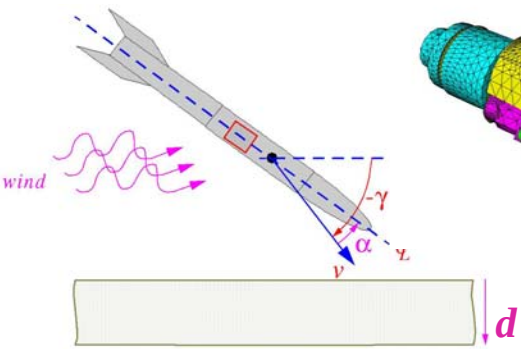
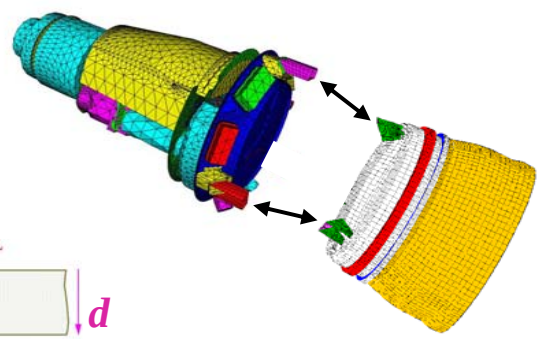
Uncertainty Quantification
(jointly funded by ASC Algs/ASC V&V)

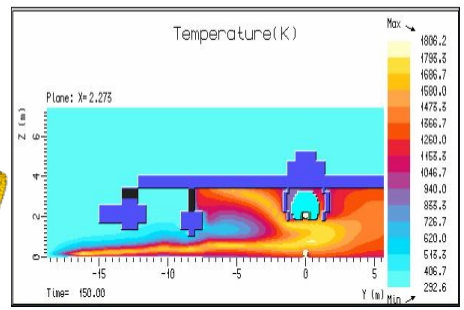


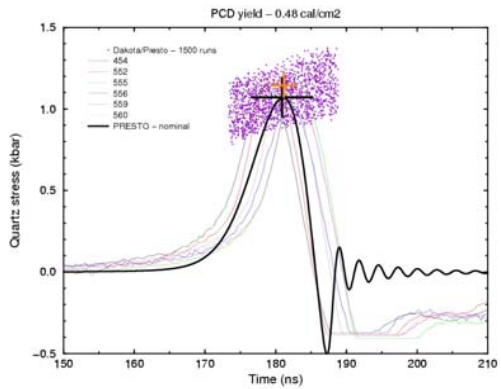
Active DAKOTA/UQ development (new, developing, planned).

- **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}, SORM (RIA/PMA mappings) Renaud collaboration.
- **SFE:** Polynomial chaos expansions (quadrature/cubiture extensions). Ghanem collaboration.
- **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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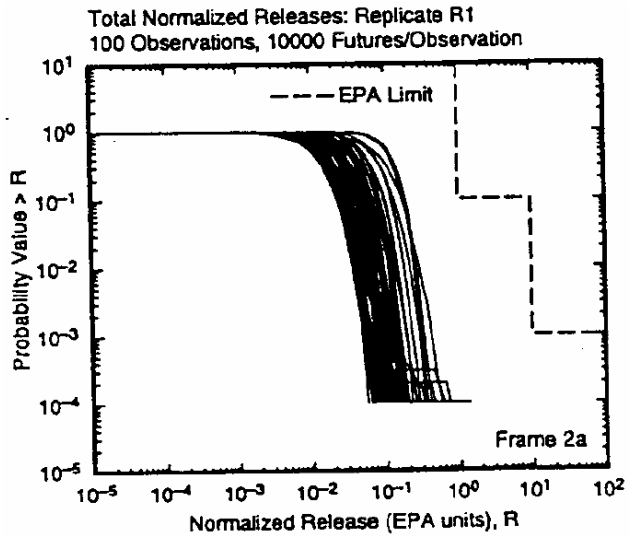
Epistemic UQ

Second-order probability

New

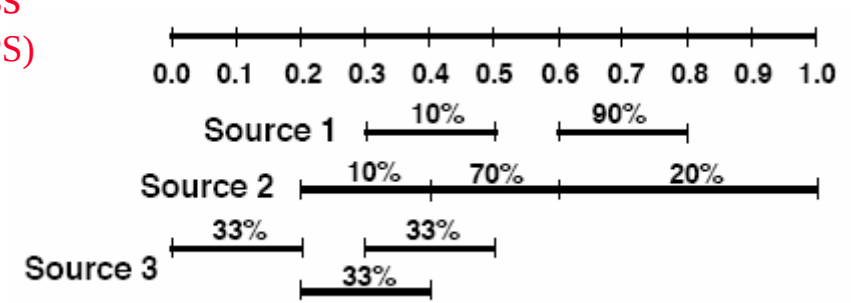
- Two levels: distributions/intervals on distribution parameters (leveraged w/ RBDO)
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP) for enabling SNL certification & QMU

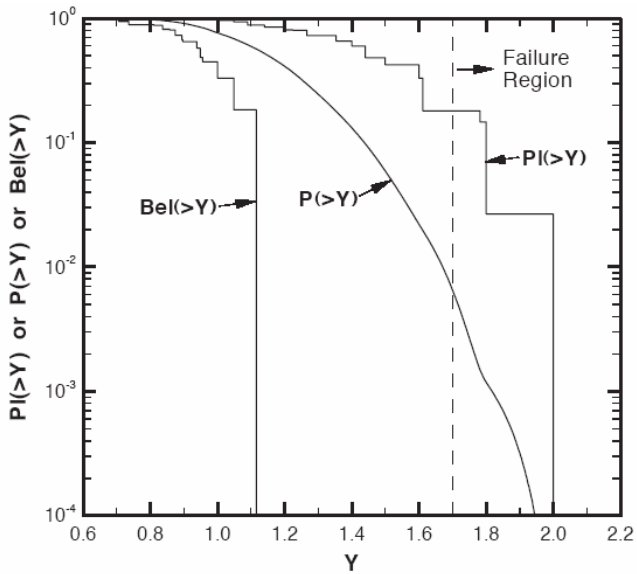


Dempster-Schafer theory of evidence

In progress (led by LPS)

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





Collaborative Research (CSRI)

2004 CSRI research

SBO:

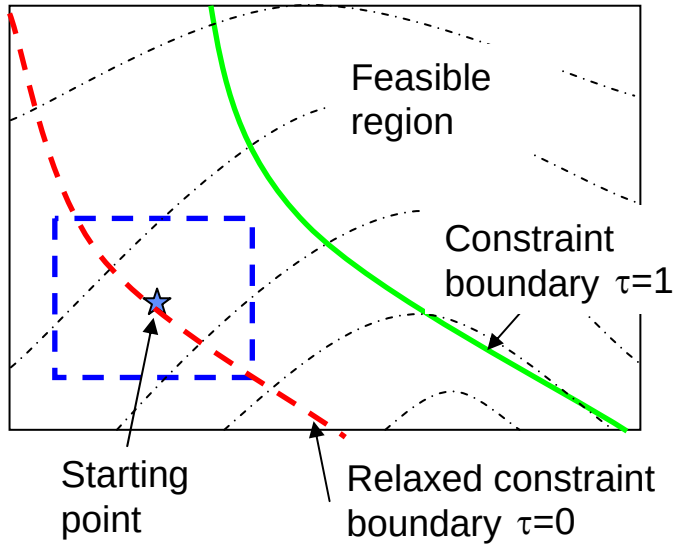
- **Constraint management (Perez):**
  - **Constraint relaxation (homotopy, composite step)**
  - **Penalty-free SBO TR logic (filter methods)**

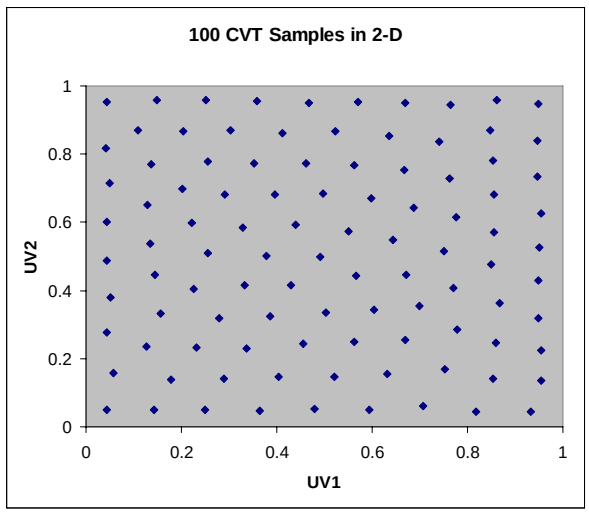
OUU:

- **rSQP for unilevel RBDO (Perez)**

UQ:

- **FSU QMC/CVT (Gunzburger, Burkardt w/ LPS)**





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\begin{aligned}
\min_{\mathbf{d}_{aug}=(\mathbf{d},\mathbf{u}_1,..,\mathbf{u}_{N_{hard}})} &: f(\mathbf{d},\mathbf{p},\mathbf{y}(\mathbf{d},\mathbf{p})) \\
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&\beta_{allowed} - \beta_i \geq 0 \\
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&\beta_i = ||\mathbf{u}_i|| \\
&\mathbf{d}^l \leq \mathbf{d} \leq \mathbf{d}^u
\end{aligned}
$$

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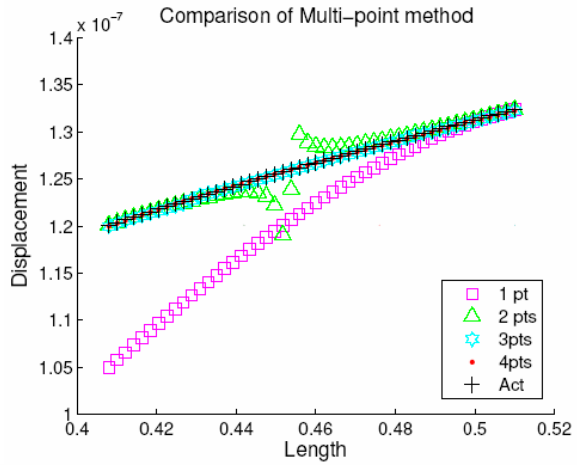
2005 CSRI research

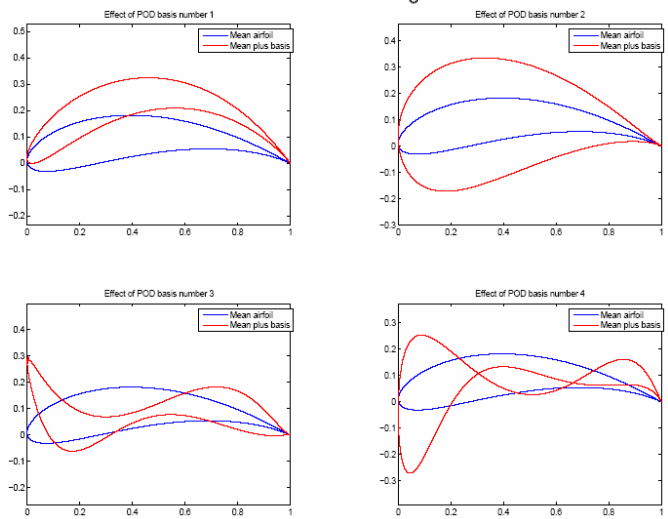
SBO/ROM:

- **Extended/spanning ROMs (Maute, Weickum)**
- **POD space mapping (Willcox, Robinson)**

UQ/RBDO:

- **V&V (Mahadevan, McFarland w/ AAG)**
- **Reliability/RBDO (Mahadevan, Bichon w/ LPS)**





$$\mu' = x^* - \sigma' \cdot \Phi^{-1}[F(x^*)]$$

$$\sigma' = \frac{\varphi\{\Phi^{-1}[F(x^*)]\}}{f(x^*)}$$

2004-2005 PY Publications

Journal (5 first author: 1 in press, 4 in prep, 2 invited):

- Eldred, M.S., Agarwal, H., Perez, V.M., Wojtkiewicz, S.F., Jr., and Renaud, J.E., "Investigation of Reliability Method Formulations in DAKOTA/UQ," (invited, to appear) *Structure & Infrastructure Engineering*, Taylor & Francis Group.
- Eldred, M.S. and Wojtkiewicz, S.F., Jr., "Investigation of Second-Order Reliability Method Formulations in DAKOTA/UQ," (invited, in preparation) *Structure & Infrastructure Engineering: Maintenance, Management, Life-Cycle Design & Performance*, T&F Group.
- Eldred, M.S. and Hart, W.E., "Multilevel Parallelism for Optimization on MP Computers: Theory and Experiment," (in preparation) *Structural and Multidisciplinary Optimization*, Springer-Verlag.
- Eldred, M.S., Giunta, A.A., Wojtkiewicz, S.F., Jr., and Trucano, T.G., "Formulations for Surrogate-Based Optimization Under Uncertainty," (in preparation) *Optimization and Engineering*, Kluwer Academic Publishers.
- Eldred, M.S., Giunta, A.A., and Collis, S.S., "Second-Order Corrections for Surrogate-Based Optimization with Model Hierarchies," (in preparation) *Optimization and Engineering*, Kluwer Acad. Publ.

Conference (8: 2 first author, 6 coauthor, 4 presented):

- Eldred, M.S., Giunta, A.A., and Collis, S.S., "Second-Order Corrections for Surrogate-Based Optimization with Model Hierarchies," *Proceedings of the 10th MA&O*, Albany, NY, Aug. 30 - Sept. 1, 2004.
- Giunta, A.A., Eldred, M.S., Swiler, L.P., Trucano, T.G., and Wojtkiewicz, S.F., Jr., "Perspectives on Optimization Under Uncertainty: Algorithms and Applications" *Proceedings of the 10th MA&O*, Albany, NY, Aug. 30 - Sept. 1, 2004.
- Perez, V.M., Eldred, M.S., and Renaud, J.E., "Solving the Infeasible Trust-region Problem Using Approximations," *Proceedings of the 10th MA&O*, Albany, NY, Aug. 30 - Sept. 1, 2004.
- Eldred, M.S., Agarwal, H., Perez, V.M., Wojtkiewicz, S.F., Jr., and Renaud, J.E., "Investigation of Reliability Method Formulations in DAKOTA/UQ," *Proceedings of the 9th PMC*, Albuquerque, NM, July 26-28, 2004.
- Giunta, A.A., Eldred, M.S., and Castro, J.P., "Uncertainty Quantification Using Response Surface Approximations," *Proceedings of the 9th PMC*, Albuquerque, NM, July 26-28, 2004.
- Perez, V.M., Eldred, M.S., and Renaud, J.E., "An rSQP Approach for a Single-Level Reliability Optimization," *Proceedings of the 9th PMC*, Albuquerque, NM, July 26-28, 2004.
- Collis, S.S., Eldred, M.S., and Chen, G., "Multi-Fidelity and Multi-Scale Optimization within a Discontinuous Galerkin Framework," abstract in *Proc. of SIAM Conference on Optimization*, Stockholm, Sweden, May 15-19, 2005.
- Giunta, A.A., Castro, J.P., Hough, P.D.,Gray, G.A., Eldred, M.S., "Multifidelity Modeling Approaches in Simulation-Based Optimization," abstract in *Proc. of SIAM Conference on Optimization*, Stockholm, Sweden, May 15-19, 2005.

SAND report (3 DAKOTA manual updates):

- Eldred, M.S., Giunta, A.A., Swiler, L.P., Wojtkiewicz, S.F., Jr., Hart, W.E., Watson, J.P., Gay, D.M., and Brown, S.L., "DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis."
  - Version 4.0 Users Manual. Sandia Tech Report SAND2001-3796, April 2002. Updated 2005 (in preparation).
  - Version 3.3 Reference Manual. Sandia Technical Report SAND2001-3515, April 2002. Updated Dec. 2004.
  - Version 3.3 Developers Manual. Sandia Technical Report SAND2001-3514, April 2002. Updated Dec. 2004.

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Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

Research:
Optimization
Uncertainty quantification
Opt under uncertainty

Development:
Framework architect
DAKOTA releases

Impact: algorithmic performance (OUU/SBO), (invited) publications, new university collaborations

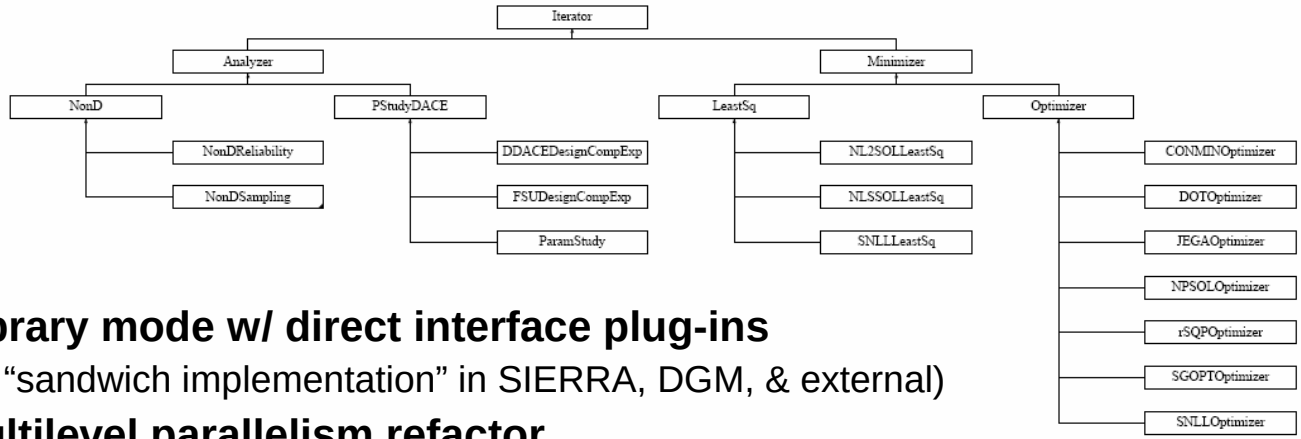
3.2 | 3.3 | 4.0 | SQE

Deployment:
Use/access initiatives
External/internal impact

Enabling Framework Development

Enable team development by providing OO infrastructure:

- **Iterator hierarchy → Minimizer & Analyzer branches**
  (collocates UQ, DACE, and PStudy for enhanced code sharing/reuse)



- **Library mode w/ direct interface plug-ins**
  (→ "sandwich implementation" in SIERRA, DGM, & external)
- **Multilevel parallelism refactor**
  (more modular/extensible, allows multiple parallelism configurations to coexist → MF SBO)
- **Enhanced model recursion → "model" as 6th keyword block**
  (generalizes local/hierarchical approxs. for arbitrary recursion)
- **Generalized data insertion and extraction**
  (enables RBDO/2nd-order probability and iterator final result sensitivities)
- **Native Hessian estimation/approximation routines**
  (enables 2nd-order surrogate corrections, 2nd-order UQ/RBDO)
- **SQE: process docs, requirements, test harness, TPL management**
- **Misc: dependency management, fine-grain eval reporting, parser**

DAKOTA/JAGUAR Releases

DAKOTA 3.2 Release – July 21, 2004

DAKOTA 3.3 Release – Dec 23, 2004

- **Coordination: deliverables, timelines, library releases, SQE**
- **New iterative methods:**
  - **Optimization: OPT++, COLINY/APPS/DIRECT, JEGA**
  - **UQ: FSU DACE, reliability, metrics (correlations, VBD)**
  - **Nonlinear least squares: NL2SOL, GNewton NIP**
- **New strategies:**
  - **Opt: Multifidelity SBO with 2nd-order corrections**
  - **UQ: 2nd-order probability**
  - **OUU: SBOUU, RBDO (bi-level, fully analytic bi-level, sequential/surrogate-based), calibration under uncertainty**

4.0 Release scheduled for late 2005/early 2006

Metrics:

- **SQE assessment: 75% FY02 → 110% FY03; FY05 NNSA audit completed**
- **Approximately *2400 external, unique download registrations* since 12/01**

JAGUAR 1.0-Alpha Release – Jan 28, 2005

- **Copyright in process → LM, GY, LANL**

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Impact: flexible & extensible architecture, effective delivery vehicle for algorithms

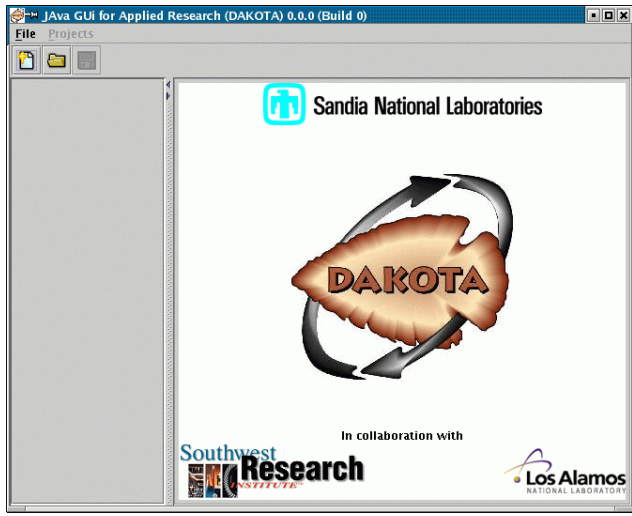
Deployment:
Use/access initiatives
External/internal impact

SIERRA	JAGUAR	DPrePro/DPostPro	Milestones	Impact

DAKOTA Deployment : Streamlining Set-Up and Interfacing

Three inter-related initiatives

- **JAGUAR (based on SwRI/LANL GUI, outsourced to Strikewire)**
  - **Symbolic problem spec. and graphical interface definition**
  - **Emphasis is general applics. (SIERRA/NEVADA also supported)**
  - **This year: 1.0 alpha release of functional GUI**
- **DAKOTA-optimized interfacing utilities (DPrePro/DPostPro)**
  - **Simplify input parameterizations and output data capture**
  - **This year: DPrePro enhancements, DSTK → DPostPro**
- **Intrusive DAKOTA integration within SIERRA/NEVADA**
  - **Special facilities for work-horse SNL ASC codes**
  - **Custom interface dev. not required; pre-/post- in core in parallel**
  - **SIERRA code teams can activate DAKOTA within their apps *with a single line in main***
  - **Opt./UQ studies managed within *same simulation executables and input files***
  - **Multilevel-parallel SPMD runs on a *single compute node partition***
  - **This year: prototype → Fmwk requirements → production**




```
begin sierra dakota (domain)
   begin calore procedure
      …
   end
end
```

Derived domain
→ sandwich implementation
→ library mode w/ interface plug-in

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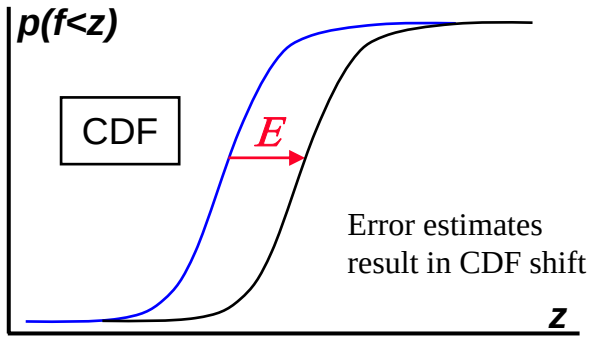
FY06 L1 & L2 Milestones

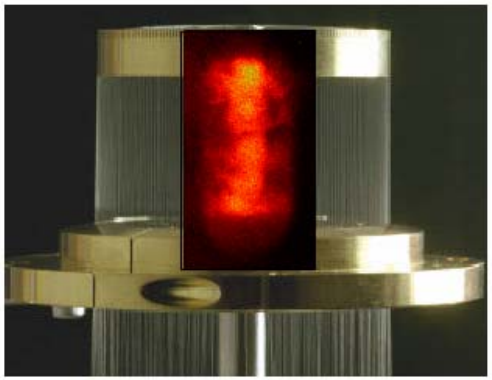
- **Level 2: UQ + EE**
  - **Error-corrected reliability analysis (and RBDO) of MEMS**
  - **Account for error or adapt mesh to control it**
  - **Showcase DAKOTA/SIERRA interface**



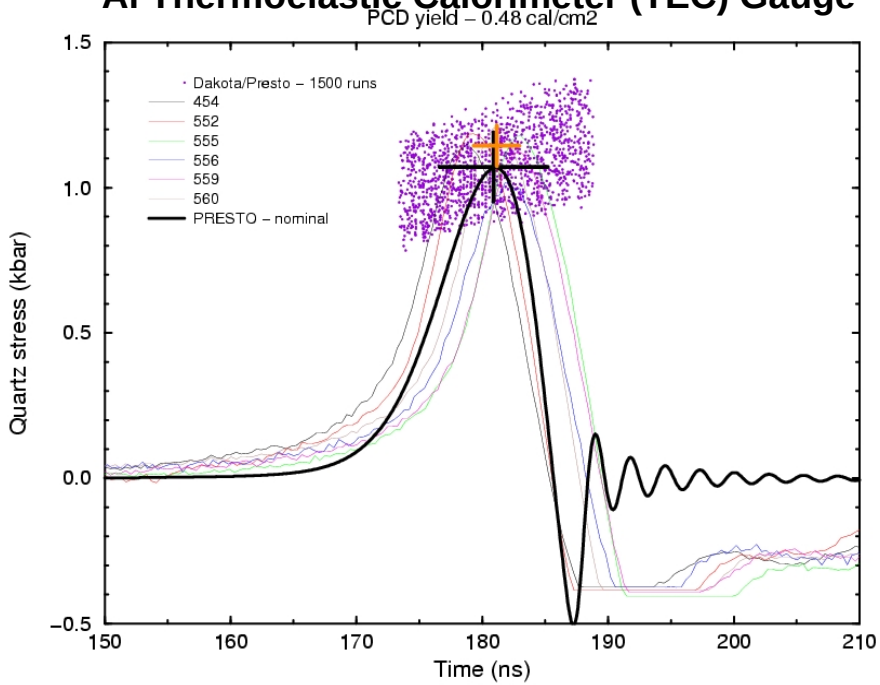
- **Level 1: Validation**
  - ***System level UQ and sensitivity analyses using DAKOTA to estimate design margins acknowledging uncertainties throughout the modeling process***
  - ***Evidence that DAKOTA is managed to institutional software requirements (selected for recently completed FY05 SQE review)***
  - ***Evidence of code verification (SQE)***
  - ***Demonstrated capability to perform ensemble computing w/ parallel codes and various platforms (multilevel parallelism)***

Recent successes - Internal

Wire array and Z pinch



Al Thermoelastic Calorimeter (TEC) Gauge



- **Joel Lash 2004**
  - **DAKOTA + Presto: UQ for V&V**
- **Ray Lemke 2005 (recent 1600 news note, related Lab News story)**
  - **DAKOTA + ALEGRA for isentropic compression experiment (ICE) on Z**
  - **Reverse engineer magnetic pressure drive history (cannot be precisely measured at this time on Z) that matches measured flyer velocity**
  - **Waveform was then optimized to eliminate undesirable features observed in a previous similar shot**
  - **Verified that part of aluminum flyer remains intact at the target (despite ~5 Mbar pressure) → reqmt for obtaining useful EOS data**

Recent successes - External

- **JSF → ERA winner**

Lockheed Martin Aeronautics conducted a trade study for the F-35 Joint Strike Fighter (JSF) aircraft to design the external fuel tank for improved performance, store separation, and flutter. CFD was used in conjunction with Sandia National Laboratories' Dakota optimization code to determine the optimal shape of the tank that minimizes drag for maximum range and minimizes yawing moment for separation of adjacent stores. Data obtained at several wind tunnel facilities verified the predicted performance of the new aeroshaped, compartmented tank for separation and flutter, as well as acceptable characteristics for loads, stability, and control.

Service/Publications/Awards

Service:

- 9200 Service: ASC Algorithms PI team, Ext Panel Review
- External Service:
  - Editorial Board: *Structure and Infrastructure Engineering*
  - CU Boulder thesis committee, 3 reviews, 2 session chair

Publications/Talks:

- 1 journal paper in press, 4 in prep, 2 invited
- 8 conference papers/abstracts (4 presented)
- 3 SAND report updates
- 8 other optimization talks (panel/program reviews, etc.)

Awards:

- Associate Fellow AIAA
- *SAFE:* DAKOTA Release
- *ERA:* Sandia/LM JSF Team

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Closing Remarks

Observations on balance

- Another good year for algorithms
  (enablers: CSRI, telecommuting)
- A renewed emphasis on program leadership
- Development → enabling architecture
- Deployment → new Product Manager (Tony)
  & contracts (Strikewire)

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R&D (current → future)

- SBO: data fit → multifidelity → ROMs, multigrid, multiscale
- UQ: reliability methods → epistemic methods
- OUU: SBOUU → RBDO (bi-level → sequential → unilevel) → SFE/stochastic ROMs
- New 2005 CSRI collaborations: Maute, Willcox, Mahadevan

Deployment/Impact

- Internal – L1/L2/L3 milestones & production computing
- External – Tri-lab, LM, GY, Caterpillar, IHAT, NEVOT, open source
- Initiatives to streamline interfaces and problem setup → 4.0 release next