2004 Department Review

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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

Project leadership & programmatics

- DAKOTA PI
- Internal Impact
- External Partnerships

Algorithm Research

- **Surrogate-Based Optimization**
- **Uncertainty Quantification**
- **Optimization Under Uncertainty**
- **Publications**

Architecture development

- **DAKOTA/SIERRA integration**
- **DAKOTA interim and major releases**

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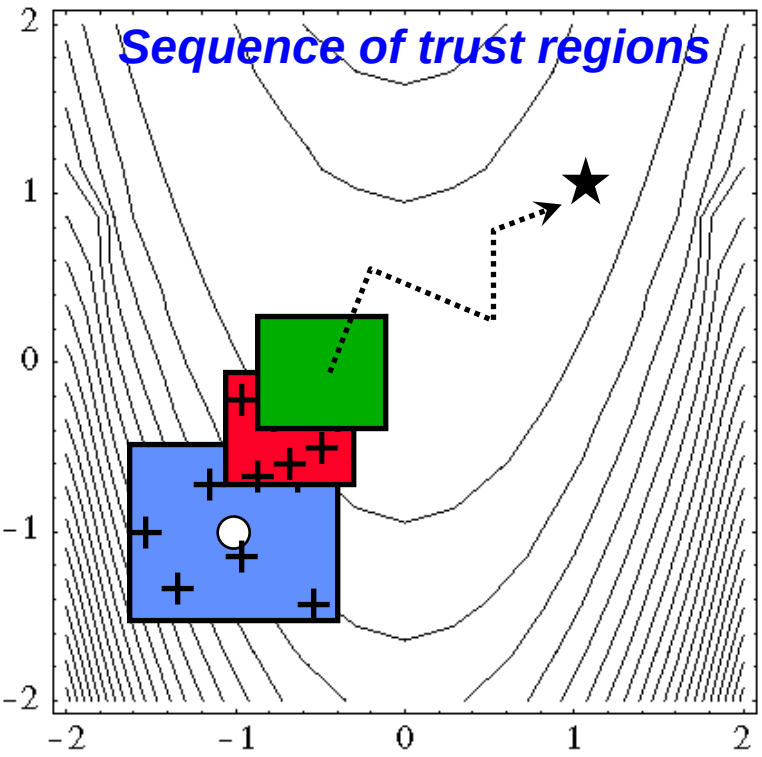
Trust Region Surrogate-Based Optimization (SBO)



Data fit case

- Global: Poly, NN, MARS, Kriging
- Local: 1st/2nd-order Taylor

Model hierarchy case

- truth eval only at center (scales better with des vars)
- correction quality is crucial

Correction approaches

Additive: $f(x)_{HF} = f(x)_{LF} + \alpha(x)$

Multiplicative: $f(x)_{HF} = f(x)_{LF}\ \beta(x)$

$\alpha(x)$, $\beta(x)$ may support local, multipt, or global correction

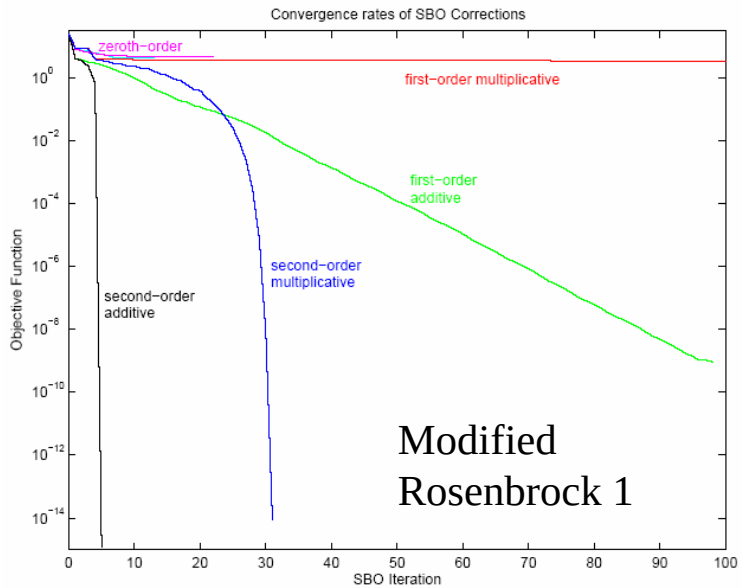
0th-order local: α, β = scalars; match HF value @1 pt

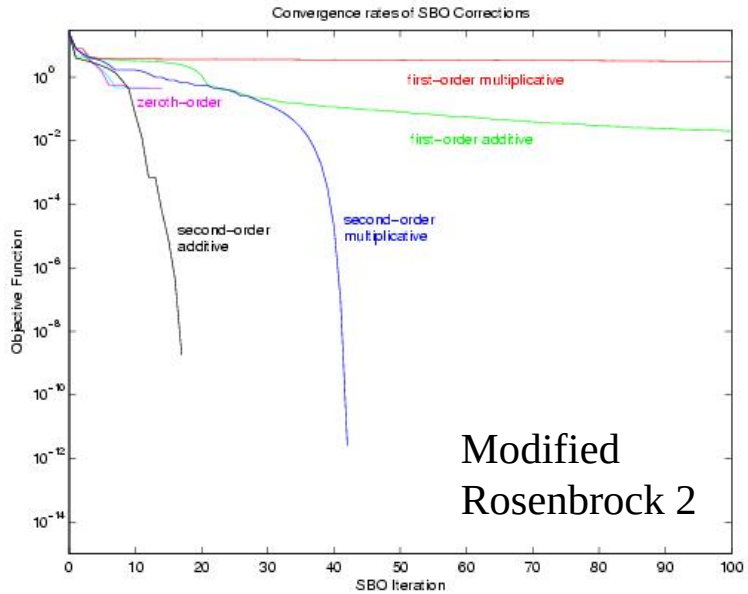
1st-order local: α, β = linear fns; match HF val/grad @1 pt

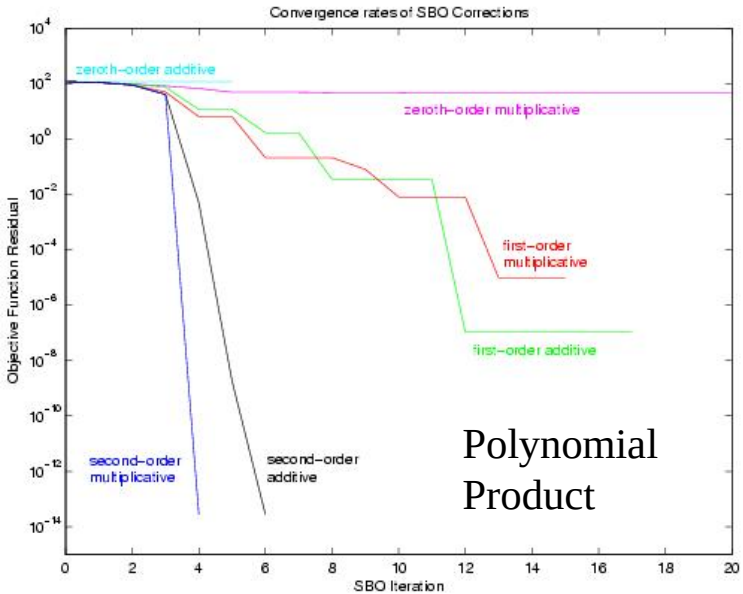
2nd-order local: α, β = quad fns; match HF val/grad/Hess @1 pt

- 0th order approaches are better than nothing, but are generally insufficient
- 1st-order approaches are sufficient to prove convergence, but rates can be unacceptably slow (current SOA)
- *New 2nd-order corrections significantly improve convergence rates* (quadratic/superlinear for full-/quasi-2nd-order)

Multi-fidelity Surrogate Corrections







Ongoing multi-fidelity work:

- **Quasi-2nd-order: BFGS, SR1**
- **Multipoint:** $f(x)_{HF} = \gamma f(x)_{\alpha} + (1-\gamma) f(x)_{\beta}$
- **CFD applications with DGM (Scott Collis)**

Additional SBO research topics:

- **Constraint management (CSRI w/ V. Perez):**
  - **Constraint relaxation (homotopy, FCD)**
  - **Penalty-free SBO TR logic (filter methods)**
- **Surrogate-based OUU**
- **Longer term: multigrid, multiscale**

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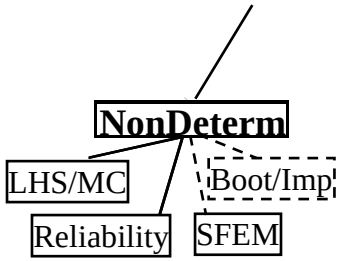
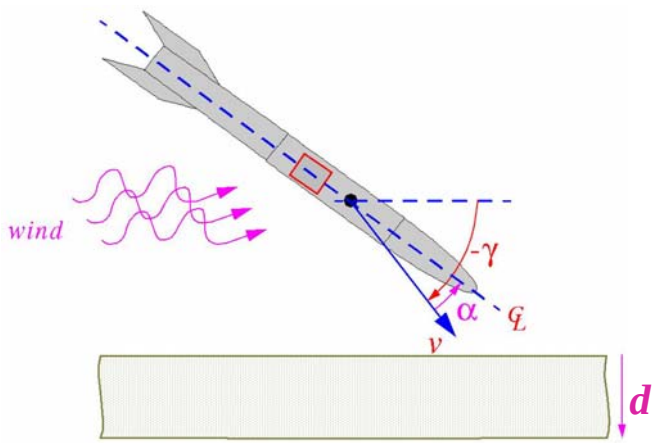
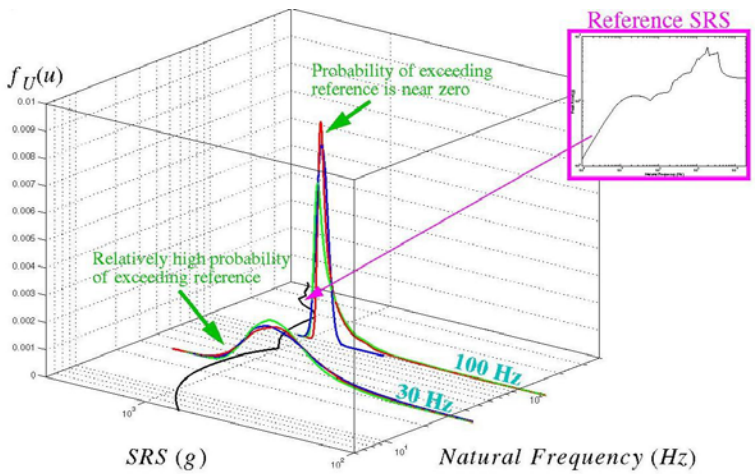
Uncertainty Quantification

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



- **Sampling:** LHS, MC (Hammersley/QMC, Bootstrap/AIS/Jackknife) Diwekar and Gunzburger collaborations.
- ★ **Reliability:** MV/AMV/AMV+/FORM (RIA z → p/β and PMA p/β → z mappings for μ_x/μ_u/x*/u*/no linearization with FORM/SORM/AIS integrations). Renaud collaboration.
- **SFE:** Polynomial chaos expansions (quadrature/cubiture extensions). Ghanem collaboration.
- **Metrics:** Importance factors, partial correlations, and variance decomposition.
- **Epistemic:** Bayesian, 2nd-order probability, Dempster-Schafer





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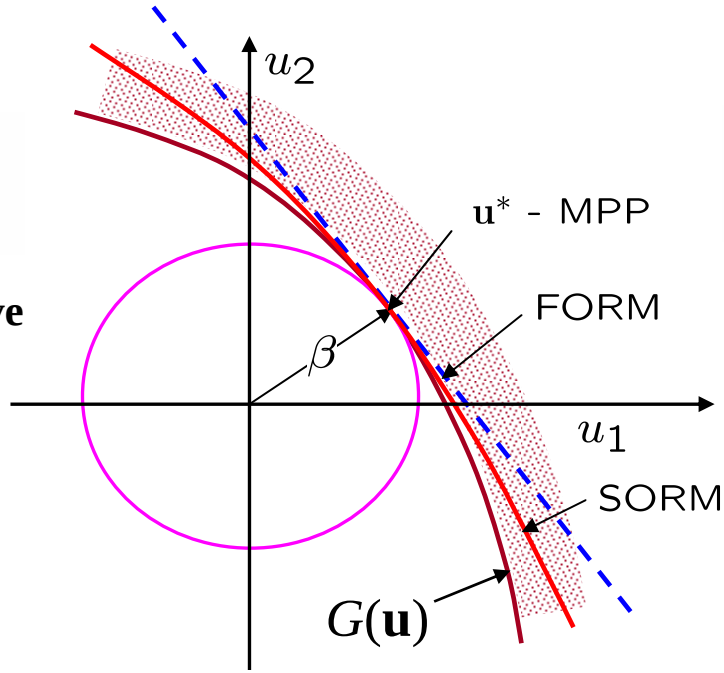
Uncertainty Quantification (cont.)
Reliability Index/Performance Measure

RIA

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

Find min dist to *G* level curve
Better for *z* → *p/β*



PMA

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

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

AMV: $g(\mathbf{x}) = g(\mu_\mathbf{x}) + \nabla_x g(\mu_\mathbf{x})^T(\mathbf{x} - \mu_\mathbf{x})$

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

AMV+: $g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*)$

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

FORM: no linearization (plus 1st-order integration)

From 4 → 11 reliability analysis methods

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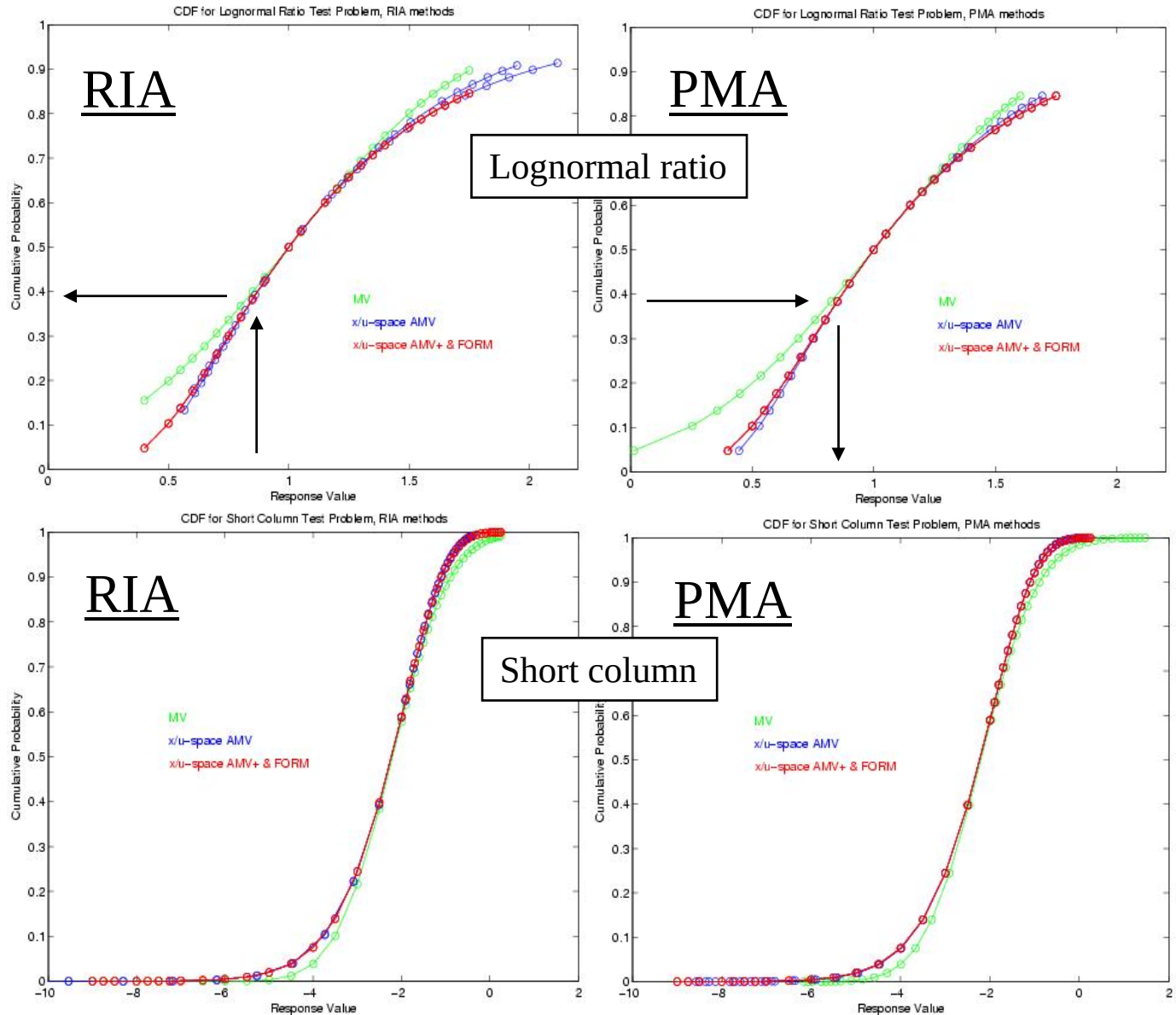
Uncertainty Quantification (cont.)
Reliability Index/Performance Measure



Novel aspects:

- **Full CDF/CCDF**
- **PMA linearizations**
- **Warm starting by projection (avoids premature convergence)**
- **SQP vs. NIP**

Performance:

- **Relative to FORM:**
  - **MV 100-200x faster but only accurate near means**
  - **AMV 20-40x faster but MPP not converged**
  - **AMV+ 2-3x faster with full accuracy**
- **Warm starts: 7x reduction best case, 30% typical**

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OUU Formulations

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 can be categorized based on UQ approach:

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

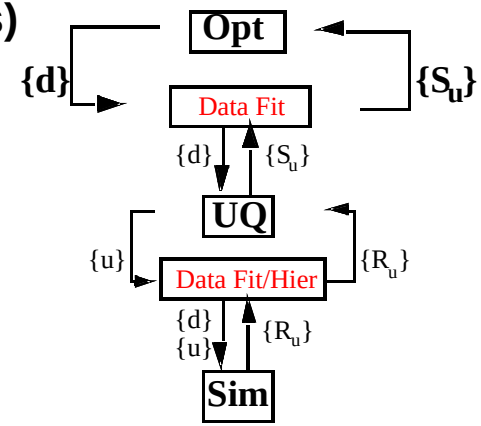
Refined this year

  - TR-SBOUU: trust region surrogate-based (5-12x)
  - Nongradient-based (Trosset)

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

New this year

  - Nested RBDO (nested)
  - Sequential RBDO (iterative)
  - Unilevel RBDO (all at once)



- **Stochastic finite element-based** (multiphysics)
  - novel formulations exploiting 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

Reliability-Based Design Optimization Bi-level (Nested) & Unilevel

- First approach: nest MPP search within outer opt. and use warm starts
- Since p/β and z must *both* be specified, RBDO can employ either an RIA or PMA formulation for the UQ portion:
  - RIA maps $z \rightarrow p/\beta$ for particular d, optimizer constrains $p(d)$ or $\beta(d)$
  - PMA maps $p/\beta \rightarrow z$ for particular d, optimizer constrains $z(d)$

RBDO results, short column test problem.

RBDO Approach	Function Evals (Cold/Warm Start)	Objective Function	Constraint Violation
RIA $z \rightarrow p$ AMV+	420/382	217.1	0.0
RIA $z \rightarrow p$ FORM	2108/1901	217.1	0.0
RIA $z \rightarrow \beta$ AMV+	218/194	216.7	0.0
RIA $z \rightarrow \beta$ FORM	938/1104	216.7	0.0
PMA $p \rightarrow z$ AMV+	308/226	216.8	0.0
PMA $p \rightarrow z$ FORM	1688/729	216.8	0.0
PMA $\beta \rightarrow z$ AMV+	308/226	216.8	0.0
PMA $\beta \rightarrow z$ FORM	1523/745	216.8	0.0

- Provides important capability for prescribed reliability (e.g., DFSS)
- Nested/warm-started RBDO expense already on par with TR-SBOUU (~200 fev)
- β preferred to p in RIA RBDO (more linear/well-scaled)
- AMV+ preferred to FORM

- Next approaches: reduce nested expense with ***sequential/unilevel*** approaches.
  - Sequential iterates between opt and UQ until desired reliability is met
  - Unilevel applies the KKT conditions of the MPP search as equality constraints in the outer optimization (SAND-like: SRND?)
    - outer optimization increases in scale, require 2nd-order information for derivatives of first-order KKT constraints
    - Victor & I exploring rSQP approach for reducing scale of AAO RBDO

2004 Publications

Journal (4 first author: 1 in press, 3 in prep):

MLP
- Eldred, M.S., Giunta, A.A., and van Bloemen Waanders, B.G., "Multilevel Parallel Optimization Using Massively Parallel Structural Dynamics," *Structural and Multidisciplinary Optimization*, Springer-Verlag, Vol. 27, Nos. 1-2, May 2004, pp. 97-109.
- 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. **[99% complete]**

OUU
- 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. **[95% complete]**

SBO
- 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. **[75% complete]**

Conference (11: 3 first author/presenter, 8 coauthor):

SBO
- Eldred, M.S., Giunta, A.A., and Collis, S.S., "Second-Order Corrections for Surrogate-Based Optimization with Model Hierarchies," to appear in *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," to appear in *Proceedings of the 10th MA&O*, Albany, NY, Aug. 30 - Sept. 1, 2004.
- Giunta, A.A., Eldred, M.S., Wojtkiewicz, S.F., Jr., Trucano, T.G., and Castro, J.P., "Surrogate-Based Optimization Methods for Engineering Design," abstract in *Proc. of the Fifth Biennial Tri-Lab. Conference*, Santa Fe, NM, October 21-23, 2003.
- Giunta, A.A. and Eldred, M.S., "Engineering Design Optimization Algorithms: Theory and Practice," abstract in *Proceedings of the 7th USNCCM*, Albuquerque, NM, July 28-30, 2003.

UQ
- Eldred, M.S., Agarwal, H., Perez, V.M., Wojtkiewicz, S.F., Jr., and Renaud, J.E., "Investigation of Reliability Method Formulations in DAKOTA/UQ," to appear in *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," to appear in *Proceedings of the 9th PMC*, Albuquerque, NM, July 26-28, 2004.

OUU
- Giunta, A.A., Eldred, M.S., Hough, P.D., Perez, V.M., Trucano, T.G., Ghanem, R., Igusa, T., Maute, K., Royset, J.O., Shoemaker, C.A., and Trosset, M., "Perspectives on Optimization Under Uncertainty: Algorithms and Applications" to appear in *Proceedings of the 10th MA&O*, Albany, NY, Aug. 30 - Sept. 1, 2004.
- Perez, V.M., Eldred, M.S., and Renaud, J.E., "An rSQP Approach for a Single-Level Reliability Optimization," to appear in *Proceedings of the 9th PMC*, Albuquerque, NM, July 26-28, 2004.
- Giunta, A.A. and Eldred, M.S., "Robust Design Optimization Using Surrogate Models," abstract submitted for the *Robust Optimization-Directed Design (RODD) Conference*, Shalimar, FL, April 19-21, 2004.
- Giunta, A. A., and Eldred, M. S., "Surrogate-Based Optimization Under Uncertainty: Formulations and Applications" abstract in the *Proceedings of the 18th International Symposium on Mathematical Programming*, Copenhagen, Denmark, Aug. 2003.
- Eldred, M.S., Giunta, A.A., Wojtkiewicz, S.F., Jr., and Trucano, T.G., "Formulations for Surrogate-Based Optimization Under Uncertainty," abstract in *Proceedings of the 7th USNCCM*, Albuquerque, NM, July 28-30, 2003.

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Algorithm Research

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Architecture development

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Enhancements enabling next level of deployment

Feedback:

- **Power users (enjoy flexible do-anything simulation interfaces)**
- **New users (desire simplified, user-friendly tools)**

Three inter-related initiatives to simplify new application development:

- **DAKOTA integration within SIERRA/NEVADA**
  - **Custom interface dev. not required, pre-/post- in core in parallel, SPMD executions**
  - **Special facilities for work-horse SNL ASC codes**
- **JAGUAR GUI development (based on SwRI/LANL GUI, outsourced to Strikewire)**
  - **Symbolic problem specification and graphical interface definition**
  - **Emphasis is general applications (although SIERRA/NEVADA will also be supported)**
- **New DAKOTA-optimized interfacing utilities (DPrePro/DPostPro)**
  - **Simplify input parameterizations and output data capture**
  - **To be used by JAGUAR-generated simulation interfaces behind scenes**

DAKOTA/SIERRA Integration

I completed an initial DAKOTA interface within SIERRA in Q4FY02

- interface at SIERRA Procedure level
- no Framework intrusion, but had a number of limitations

This year, C. Edwards and I designed a new interface as part of the recent SIERRA mechanics refactoring, and I have recently completed a derived DAKOTA Domain

- interface at SIERRA Domain level allows for top level control (MPI Comms, I/O registrations)
- SIERRA code teams can activate DAKOTA within their apps with a single line in main

User Impact:

- Opt./UQ studies managed within the same simulation executables and input files
- Multilevel-parallel SPMD runs on a single compute node partition of an ASC MPP

SIERRA development activities are leveraged:

- top level: DAKOTA interface (Mike + Carter)
- mid level: Mechanics instances for metric recovery (David + Alfred)
- low level: FEI extension with TSFCore (Ross + Alan)

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

Initial cut: nested procedures

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

New: derived domain

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

Future: full SAND/NAND

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DAKOTA Version 3.1.2 Interim Release
DAKOTA Version 3.2 Major Release

3.2 Release scheduled for May 2004:

- **New strategies:**
  - **Enhanced TR-SBOUU, first RBDO**
  - **SBO enhancements: 2nd-order corrections, constraint management**
- **New iterative methods:**
  - **New COLINY optimizers**
  - **New JEGA optimizers**
  - **New DAKOTA/UQ: reliability methods, sampling correlations and full *p*/*β*/*z* mappings**
  - **New NL2SOL least squares solver**
- **Coordination with SGOPT/COLINY, PICO, UTILIB, OPT++, DDACE, APPS teams**
- **Updating Users, Reference, & Developers Manuals**
- **Training sessions TBA**

External VOTD activated early April for beta testing

Metrics:

- **~300 software commits, ~1/3 of time**
- **Greater than *1600 external download registrations* since 12/01**
- **ASC SQE assessment: improvement from 64.8 (FY02) to 102.3 (FY03)**

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Service/Publications/Awards

Service:

- **Editorial Board:** ***Structure and Infrastructure Engineering***
- **Sandia Service:** **ASC Algorithms & ET PI team**
- **External Service:** **ASCE PMC conference committee; AIAA SDM and MDO conference abstract review teams (reviewed 9 abstracts)**
- **CSRI interactions:** **faculty (Renaud, Gunzburger, Dennis, Igusa, Ghanem) and students (Perez, Agarwal, Eddy, Ricco)**
- **Internal consulting:** **13 optimization/UQ applications**

Publications/Talks:

- **4 journal papers**
- **11 conference papers/abstracts (3 presentations)**
- **3 SAND report updates**
- **9 other optimization talks (program briefings, etc.)**
- **Led 3 v3.1 training sessions, v3.2 sessions TBA**
- **Invited contributor to new AIAA MDO White Paper (DOE optimization R/D/A)**

Awards:

- **SAFE (1):** ***Leadership of ASC Optimization***
- **ERA nominations (2):** ***individual leadership*** **and** ***ASC SQE team***

Closing Remarks

Observations on P/R/D/A balance

- 2004 good year for algorithms: ~ 50% R↑, 35% D↓, 10% P↓, 5% A↓
- CSRI has been a big driver for R
- Balancing research focus with production focus

Research focus (current → future)

- SBO: multifidelity → multigrid, multiscale
- UQ: reliability methods → epistemic methods
- OUU: nested RBDO → unilevel RBDO, SFE-based OUU, intrusive OUU
- Publications have received renewed emphasis
- New collaborations: Renaud/Perez/Agarwal, Alexandrov/Lewis, Maute, Gunzburger