2006 Department Review

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Dept. 1411: Optimization & Uncertainty Estimation

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
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Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

ASC Algs | ASC V&V | MICS | CSRF | CSRI | LM SV | Goodyear

Research:
Opt, UQ, OUU Algorithms
CSRI Collaborations
Publications

Development:
Framework architect
DAKOTA 4.0 release

Deployment:
Use/access initiatives
External/internal impact
MESA: ASC L2, RF

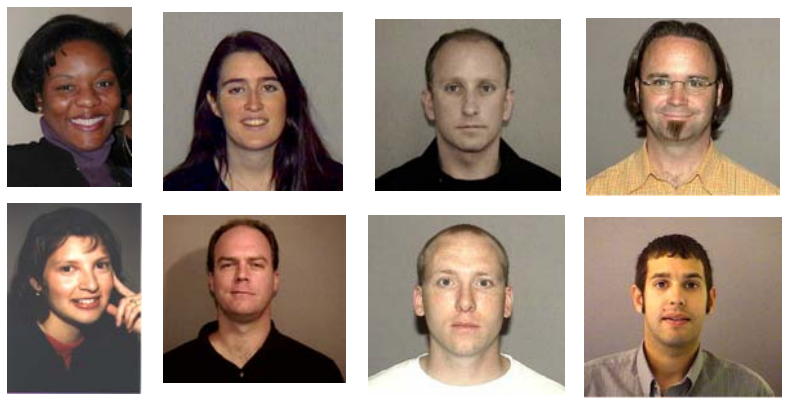
Sandia Project Leadership

ASC Algorithms/MICS, ASC V&V, CSRF, CSRI, LM Shared Vision, Goodyear

- PI for much of above, plus helping define direction for other efforts
- ASC leadership is largest commitment, but investing time in many ***new opportunities*** (ROM, MESA, SciDAC2, climate UQ/MCUU, V&V COE, Next gen UQ LDRD, DART, DDRIV, …)

Leadership of DAKOTA team from 1411/1415/1533/6642/8962

- Vision, strategic planning, and technical leadership
- Mentoring of new staff (Adams, Dunlavy, Eddy) and students (Bichon, Robinson, Weickum)
- Supervision of contractors (Bartz (Strikewire))



New research directions

- ***ROM:*** joint 1411/1414/1433 CSRF project
- ***MEMS:*** ASC L2 milestone (bistable), production MESA-TOP support (RF)

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Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

Impact: expanding mission space, high performing team

Research:
Opt, UQ, OUU Algorithms
CSRI
Publications

Development:
Framework architect
DAKOTA 4.0 release

SBO | UQ | RBDO | ROM | CSRI

Deployment:
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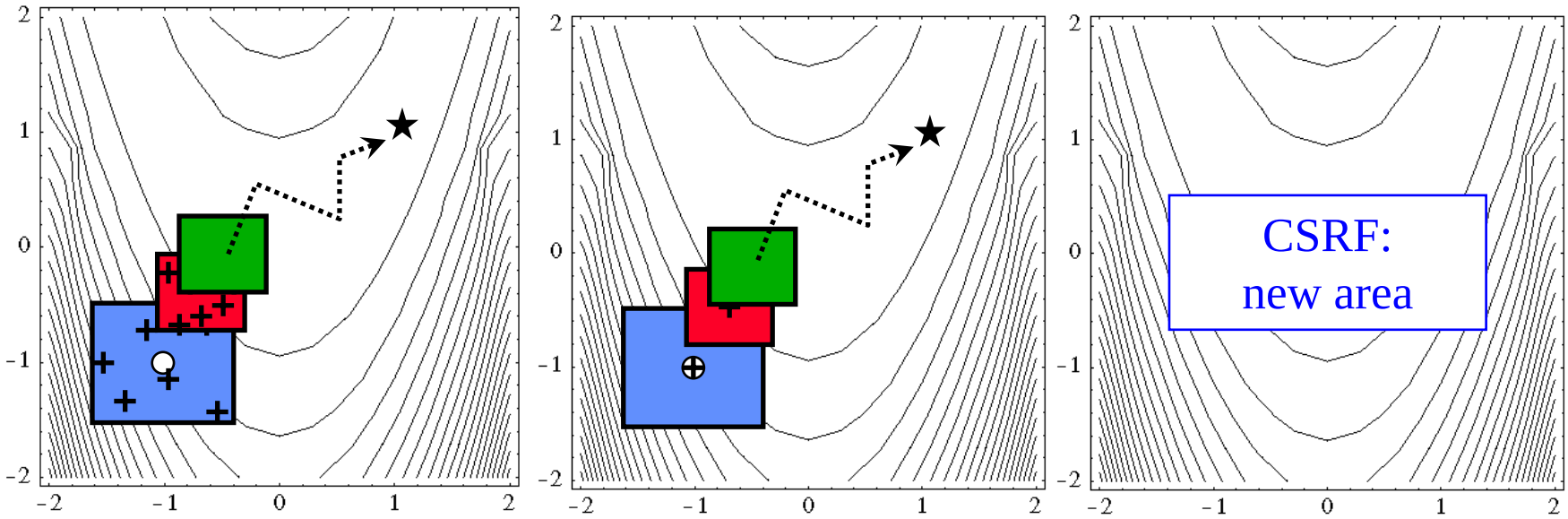
MESA: ASC L2, RF

Trust-Region Surrogate-Based Optimization

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



Research areas (last year, new DAKOTA, new CSRI):

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)

SBO 2006: Core Algorithm Refactor

- **Merit fns:** penalty, adaptive penalty, Lagrangian, augmented Lagrangian

$$\Phi(\mathbf{x}, \lambda_\psi, \lambda_h, r_p) = f(\mathbf{x}) + \lambda_\psi^T \psi(\mathbf{x}) + r_p \psi(\mathbf{x})^T \psi(\mathbf{x}) + \lambda_h^T \mathbf{h}(\mathbf{x}) + r_p \mathbf{h}(\mathbf{x})^T \mathbf{h}(\mathbf{x})$$

$$\psi_i = \max\left\{ g_i, -\frac{\lambda_{\psi_i}}{2r_p} \right\}$$

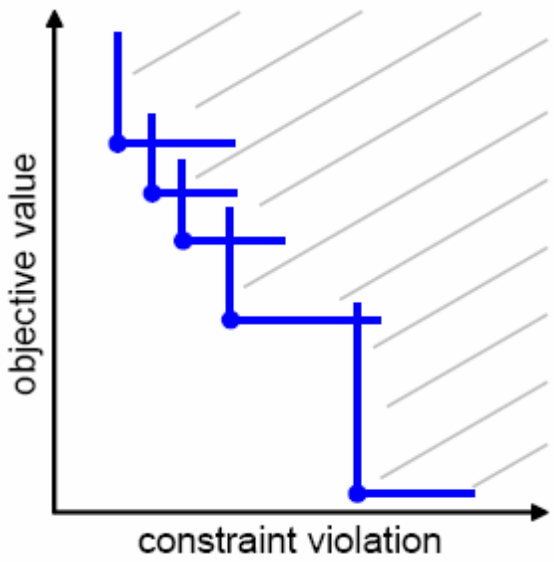
- **Iterate acceptance:** trust region ratio, filter method

$$\rho^k = \frac{\Phi(\mathbf{x}_c^k) - \Phi(\mathbf{x}_*^k)}{\hat{\Phi}(\mathbf{x}_c^k) - \hat{\Phi}(\mathbf{x}_*^k)}$$

- **Hard conv. assessment:** bound constr-LLS Lagrange multiplier estimation

$$\nabla_x \Phi(\mathbf{x}, \lambda_g, \lambda_h) = \nabla_x f(\mathbf{x}) + \lambda_g^T \nabla_x \mathbf{g}^+(\mathbf{x}) + \lambda_h^T \nabla_x \mathbf{h}(\mathbf{x})$$

$$\mathbf{A}\lambda = -\nabla_x f$$



- **Constraint relaxation:** homotopy (with Danny Dunlavy)

$$\begin{array}{ll} \text{minimize} & \hat{f}^k(\mathbf{x}) \\ \text{subject to} & \mathbf{g}_l \le \hat{\mathbf{g}}^k(\mathbf{x}) \le \mathbf{g}_u \\ & \hat{\mathbf{h}}^k(\mathbf{x}) = \mathbf{h}_t \\ & \| \mathbf{x} - \mathbf{x}_c^k \|_\infty \le \Delta^k \end{array}$$

$$\Rightarrow \quad \begin{aligned} \tilde{\mathbf{g}}^k(\mathbf{x}, \tau) &= \hat{\mathbf{g}}^k(\mathbf{x}) + (1-\tau)\mathbf{b}_g \\ \tilde{\mathbf{h}}^k(\mathbf{x}, \tau) &= \hat{\mathbf{h}}^k(\mathbf{x}) + (1-\tau)\mathbf{b}_h \end{aligned} \quad \Rightarrow$$

$$\begin{array}{ll} \text{minimize} & \hat{f}^k(\mathbf{x}) \\ \text{subject to} & \mathbf{g}_l \le \tilde{\mathbf{g}}^k(\mathbf{x}, \tau^k) \le \mathbf{g}_u \\ & \tilde{\mathbf{h}}^k(\mathbf{x}, \tau^k) = \mathbf{h}_t \\ & \| \mathbf{x} - \mathbf{x}_c^k \|_\infty \le \Delta^k \end{array}$$

Impact: 1st filter SBO, improved perf, balance of optimality and feasibility, degeneracies eliminated

Eldred, M.S. and Dunlavy, D.M., "Formulations for Surrogate-based Optimization with Data Fit, Multifidelity, and Reduced-Order Models," to appear in *Proceedings of 11th AIAA MA&O Conference*, Sept. 2006.

Reduced-Order Modeling (ROM)

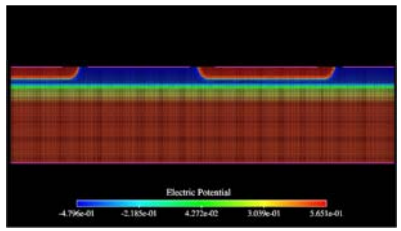
ROM (e.g., modal analysis, POD) captures critical aspects of HF simulations by using a reduced basis for projections of the system response

$$M\ddot{u} + C\dot{u} + Ku = f \qquad u(t) = \sum_{j=1}^{k} \eta_j(t)\phi_{(j)} = \Phi\eta(t)$$

$$\Phi^T M\Phi\ddot{\eta}(t) + \Phi^T C\Phi\dot{\eta}(t) + \Phi^T K\Phi\eta(t) = \Phi^T f(t)$$

$$M_R\ddot{\eta} + C_R\dot{\eta} + K_R\eta = f_R$$

Example:



Charon semiconductor: O(10^6) unknowns

→ ROM →

O(10^1) unknowns using reduced basis

Xyce™ Parallel Electronic Simulator

Detailed system integration studies

New CSRF effort targets 3 inter-related research areas:

- ***SBO with ROMs:*** **effective use of parametric ROMs in opt./UQ/OUU**
- ***Goal-oriented ROMs:*** **calculation of bases tailored to specific simulation metrics**
- ***Nonlinear multi-parameter ROMs:*** **increased accuracy/stability/efficiency for nonlinear sys.**

CSRI: parametric ROMs (w/ Maute, Weickum)

Most ROM-based opt. to date: restricted, design changes = ROM inputs (e.g., Dirichlet BC control).

General case: design changes influence system matrices → updates to basis and projected model

→ Extended ROM (E-ROM), Spanning ROM (S-ROM)

Results to date: Multipoint E-ROM using design history

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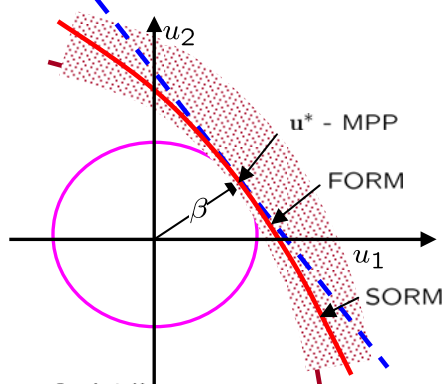
Reliability Analysis & RBDO:
Second-Order Methods



2nd-order local limit state approximations

- MVSOSM, x-/u-AMV^2, x-/u-AMV^2+
- Hessians may be full, FD, or Quasi (BFGS or SR1)

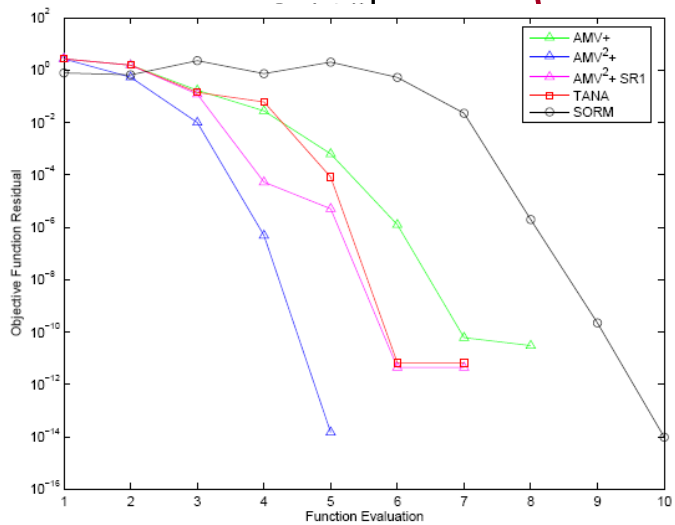
Multipoint limit state approximations

- TANA-3 (Xu and Grandhi)
- Extensions for scaling, safeguarding

2nd-order integrations

- Breitung, Hohenbichler-Rackwitz, Hong
- Extensions to support full/FD/Quasi Hessians

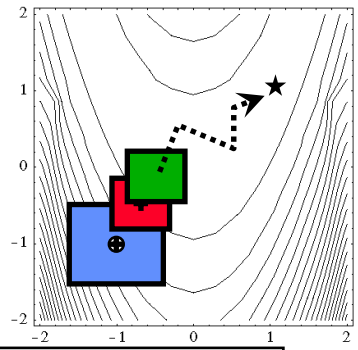
New distributions and full design SA support



Sequential RBDO:

- Trust-region surrogate-based linkage is ***first rigorous approach***

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



Impact:

Novel UQ algorithms: AMV^2/AMV^2+, 2nd-order PMA, QN 2nd-order integrations

Novel RBDO algorithms: 2nd-order sensitivities, 2nd-order TR-SB for sequential RBDO

More rapid convergence, more robust performance, more accurate probability integrations

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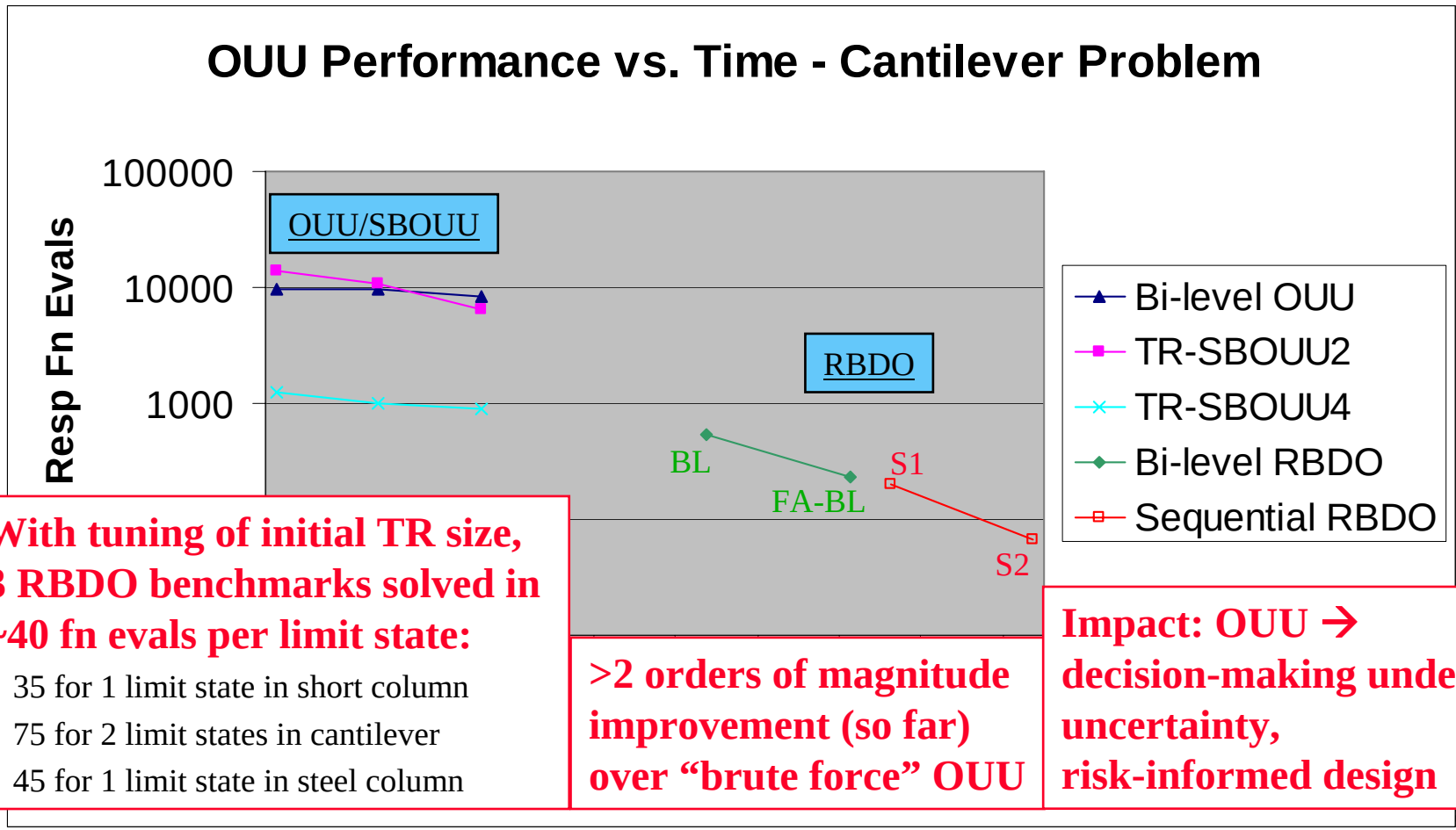
OUU Progress To Date

- **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, 2nd-order)



With tuning of initial TR size, 3 RBDO benchmarks solved in ~40 fn evals per limit state:

- 35 for 1 limit state in short column
- 75 for 2 limit states in cantilever
- 45 for 1 limit state in steel column

>2 orders of magnitude improvement (so far) over "brute force" OUU

Impact: OUU → decision-making under uncertainty, risk-informed design

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RBDO Closure

4 invited university talks/lectures on OUU research:

- **Spring seminars: USC, Arizona**
- **Spring class lecture: MIT**
- **Fall seminar: Johns Hopkins**

Invited book chapter (in preparation)

Eldred, M.S., Bichon, B.J., Adams, B.M., and Mahadevan, S., "Overview of Reliability Analysis and Design Capabilities in DAKOTA with Application to Shape Optimization of MEMS," in *Structural Design Optimization Considering Uncertainties*, edited by Y. Tsompanakis and N. Lagaros, Springer.

Several remaining research issues are targeted in Bichon thesis

- **Target issues with realistic engineering apps**
  - **nonsmooth limit states**
  - **multiple failure modes**

Deployment to MESA: bi-stable (ASC L2 milestone), RF

On to OUU with PCE, epistemic methods…

Collaborative Research (CSRI)

2005 CSRI summer research

SBO/ROM:

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

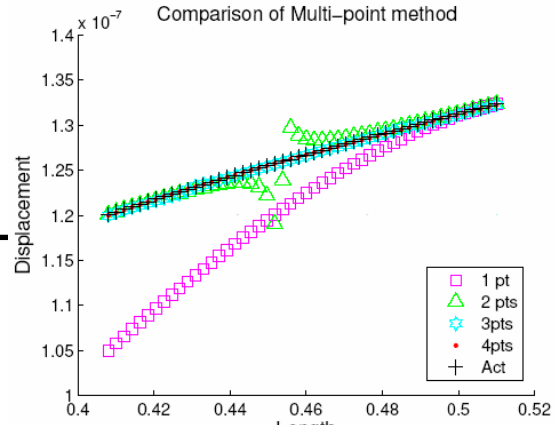
UQ/RBDO:

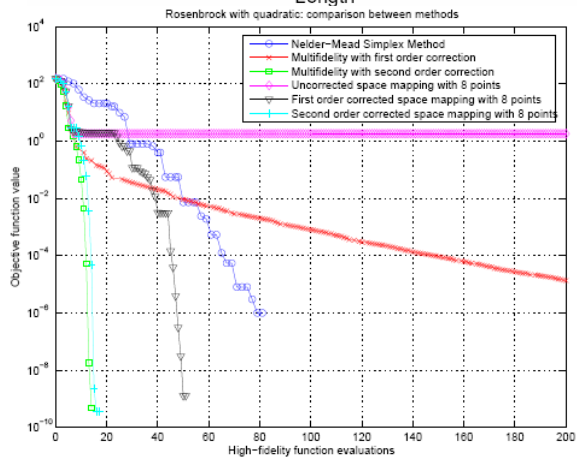
- **Reliability/RBDO (Mahadevan, Bichon)**

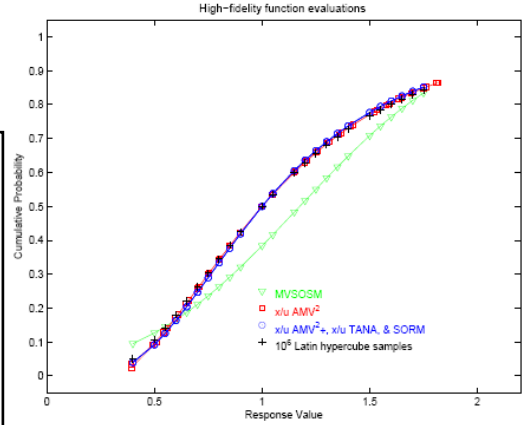
2006 CSRI research

Continuing each of these 2005 activities (5 joint conf papers → joint journal)

Barron Bichon extended 2006 stay (May-Dec.) to focus on MEMS RBDO







Impact:

Novel multifidelity: First-ever multifidelity SBO with variable dimensionality

- Corrected space mapping
- POD mapping
- Hybrid POD/space mapping

Novel ROM: parametric ROM for general opt/UQ/OUU

- Single-point E-ROM
- Multipoint/global E-ROM
- global S-ROM

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2005-2006 PY Publications

Journal (3 invited: 2 in press, 1 in review):

- Eldred, M.S. and Bichon, B.J., "Second-Order Reliability Method Formulations in DAKOTA/UQ," (invited, in review) *Structure & Infrastructure Engineering (SIE)*, Taylor & Francis Group.
- Giunta, A.A., McFarland, J. M., Swiler, L.P., and Eldred, M.S., "The promise and peril of uncertainty quantification using response surface approximations," (invited, in press) *SIE*, special issue on UQ and Design under Uncertainty of Aerospace Systems, Taylor & Francis Group.
- 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, in press) *SIE*, Taylor & Francis Group.

Conference/Workshop (9: 4 first author, 5 presented):

- Adams, B.M., Eldred, M.S., Wittwer, J., and Massad, J., "Reliability-Based Design Optimization for Shape Design of Compliant Micro-Electro-Mechanical Systems," to appear as paper AIAA-2006-7000 in the *Proceedings of the 11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference (MA&O)*, Portsmouth, VA, Sept. 6-8, 2006.
- Eldred, M.S. and Dunlavy, D.M., "Formulations for Surrogate-Based Optimization with Data Fit, Multifidelity, and Reduced-Order Models," to appear as paper AIAA-2006-7117 in the *Proceedings of the 11th MA&O*, Portsmouth, VA, Sept. 6-8, 2006.
- Giunta, A.A., Swiler, L.P., Brown, S.L., Eldred, M.S., Richards, M.D., and Cyr, E.C. , "The Surfpack Software Library for Surrogate Modeling of Sparse Irregularly Spaced Multidimensional Data," to appear as paper AIAA-2006-7049 in the *Proceedings of the 11th MA&O*, Portsmouth, VA, Sept. 6-8, 2006.
- Robinson, T.D., Willcox, K.E., Eldred, M.S., and Haimes, R., "Multifidelity Optimization for Variable-Complexity Design," to appear as paper AIAA-2006-7114 in the *Proceedings of the 11th MA&O*, Portsmouth, VA, Sept. 6-8, 2006.
- Eldred, M.S. and Bichon, B.J., "Second-Order Reliability Formulations in DAKOTA/UQ," paper AIAA-2006-1828 in *Proceedings of the 47th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference (SDM),* Newport, Rhode Island, May 1 - 4, 2006.
- Robinson, T.D., Eldred, M.S., Willcox, K.E., and Haimes, R., "Strategies for Multifidelity Optimization with Variable Dimensional Hierarchical Models," paper AIAA-2006-1819 in *Proceedings of the 47th SDM*, Newport, Rhode Island, May 1 - 4, 2006.
- Weickum, G., Eldred, M.S., and Maute, K., "Multi-point Extended Reduced Order Modeling For Design Optimization and Uncertainty Analysis," paper AIAA-2006-2145 in *Proceedings of the 47th SDM*, Newport, Rhode Island, May 1 - 4, 2006.
- Eldred, M.S., Bichon, B.J., and Adams, B.M., "Overview of Reliability Analysis and Design Capabilities in DAKOTA," *Proceedings of the NSF Workshop on Reliable Engineering Computing (REC 2006),* Savannah, GA, February 22-24, 2006.
- Eldred, M.S., "Optimization Under Uncertainty Research at Sandia National Laboratories," abstract in *Proceedings of Large-Scale Robust Optimization Workshop*, Santa Fe, NM, Aug. 2005.

SAND report (3 DAKOTA manual updates):

- Eldred, M.S., Giunta, A.A., Brown, S.L., Adams, B.M., Dunlavy, D.M., Eddy, J.P., Gay, D.M., Griffin, J.D., Hart, W.E., Hough, P.D., Kolda, T.G., Martinez-Canales, M.L., Swiler, L.P., Watson, J.-P., Williams, P.J., "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 SAND2006-xxxx, May 2006 (in preparation).
  - •Version 4.0 Reference Manual. Sandia Technical Report SAND2006-xxxx, May 2006.
  - •Version 4.0 Developers Manual. Sandia Technical Report SAND2006-xxxx, May 2006.

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Highlights this performance year

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

Research:
Opt, UQ, OUU Algorithms
CSRI
Publications

Development:
Framework architect
DAKOTA 4.0 release

Impact: new algorithms in SBO/UQ/OUU/ROM, university collaborations, (invited) pubs/seminars

JAGUAR | AMPL | Library | Packages
Autotools | Docs | SQE

Deployment:
Use/access initiatives
External/internal impact
MESA: ASC L2, RF

DAKOTA 4.0 Release – May 12, 2006

- **Coordination: deliverables, timelines, library releases, SQE**
  (Internal: latest Acro, OPT++, DDACE, Surfpack, JEGA, Epetra)
  (External: latest PLplot, NLPQL, GSL)
- **Major usability initiatives:**
  - **Autotools deployment: autoconf/automake** [more scalable build support]
  - **JAGUAR GUI compatibility**
    - **Support for AMPL algebraic mappings**
  - **Library mode deployment: Xyce, SIERRA (Aria), Sage, et al.**
- **Many new capabilities** (in addition to package updates): **SBO, UQ, OUU, …**
- **Documentation: Manuals (3), release notes, Web pages, news notes, FAQ, …**
- **Deployments in process, Training sessions TBD**

Technical contributions: (~300 cvs commits)

- **Enable team development by extending core framework infrastructure**
- **Develop capabilities for ASC L2 milestone in UQ/RBDO + EE of MEMS**
- **Implementation of new algorithms from research activities**

Metrics:

- **SQE: FY05 NNSA audit, FY06 self assessment**
- **Approximately *3000 external, unique download registrations***

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Framework architect
DAKOTA 4.0 release

Impact: major usability release, reduce learning curve for next level of tool deployment

Deployment:
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MESA: ASC L2, RF

ASC Milestones | MESA

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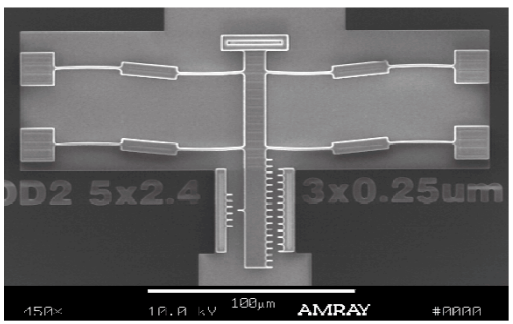
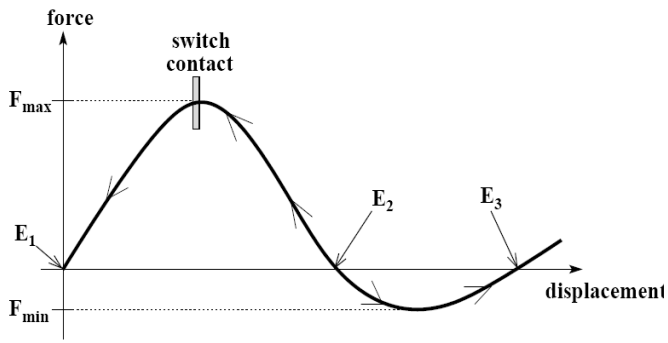
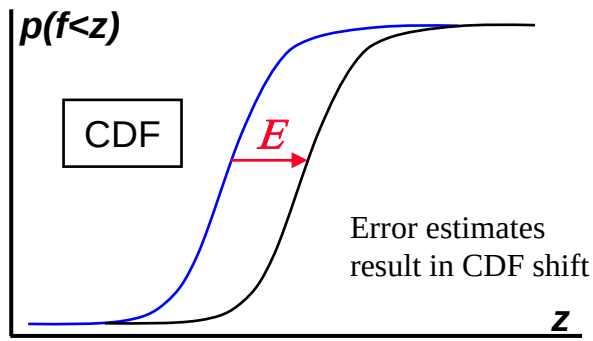
FY06 L1 & L2 Milestones

- **Apps/M&PM/V&V Level 1: W76-1/W80-3 Validation**
  - ***System level UQ and sensitivity analyses using DAKOTA to estimate design margins acknowledging uncertainties throughout the modeling process (QMU)***
  - ***Evidence that DAKOTA is managed to institutional software requirements (completed FY05 NNSA SQE review & FY06 SNL SA)***
  - ***Evidence of code verification (SQE)***
  - ***Demonstrated capability to perform ensemble computing w/ parallel codes and various platforms (multilevel parallelism)***
- **Algorithms Level 2: EE + UQ/RBDO**
  - **Shape optimization of compliant MEMS**
  - **Error-corrected reliability analysis (and RBDO)**
  - **Account for error or adapt mesh to control it**

Bi-stable MEMS Switch

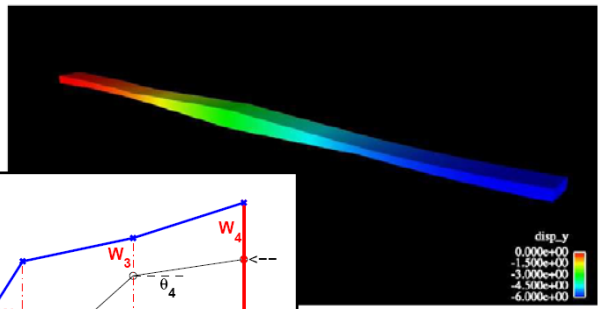


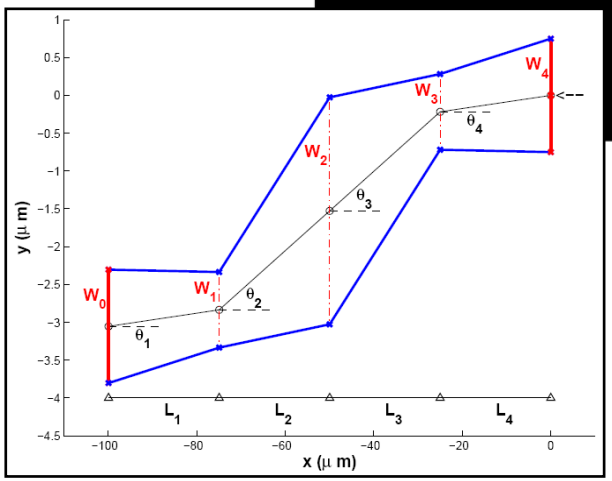




Bi-Stable MEMS Switch

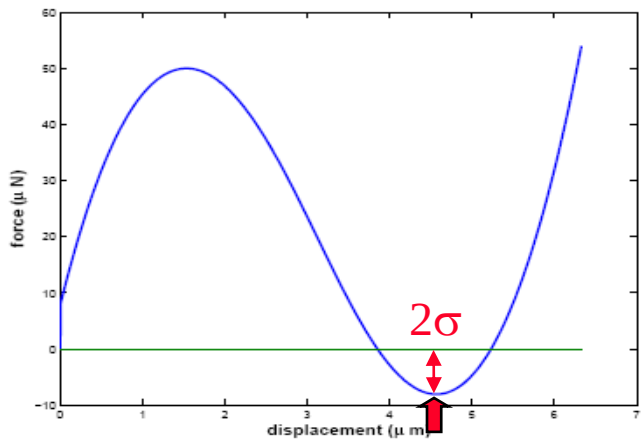
13 design vars:
W_i, L_i, θ_i





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

→ reliable + robust

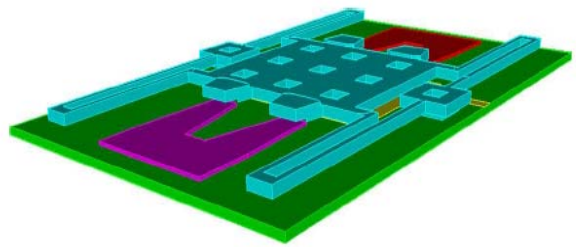


2 random vars:

variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

RF MEMS Switch:

Production MESA support
RBDO for reliable closure with control of damage energy



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MESA: ASC L2, RF

Impact: DP (ASC L1), MESA (ASC L2, RF), QASPR, NISAC, …

Service/Publications/Awards

Service:

- **1400 Service: ASC Algorithms PI team**
- **External Service:**
  - **Editorial Board: *Structure and Infrastructure Engineering***
  - **CU Boulder masters thesis committee (Weickum)**
  - **Vanderbilt PhD thesis committee (Bichon)**
  - **Accepted invitation to join AIAA NDA working group (pre-TC)**
  - **8 journal/conference manuscript reviews, REC2006 program committee**
- **Mentoring: LTEs, students**

Publications/Talks:

- **1 invited book chapter**
- **3 invited journal papers in press/in review**
- **9 conference papers/abstracts (5 presented)**
- **3 SAND report updates (DAKOTA 4.0 Manuals)**
- **4 invited lectures, seminars (3 accepted: MIT, USC, UA)**
- **5 other talks, including 1 VP-level briefing (Stulen, Kolhaas, et al.)**

Awards:

- **LLNL/SNL DPAE**

Closing Remarks

Very Busy Year

- Each of the 4 areas has increased activity
- Leadership: developing new opportunities
- Research: many CSRI collabs and joint pubs
- Development: 4.0 major release
- Deployment: ASC L1/L2 milestones, other MESA

Leadership:
Vision/program definition
Alignment/connectivity
New initiatives

Research:
Opt, UQ, OUU
CSRI
Publications

Development:
Framework architect
DAKOTA 4.0 release

Deployment:
Use/access initiatives
External/internal impact
MESA: ASC L2, RF

Technical excellence

- SBO: 1st filter SBO, 1st variable dim. multifidelity, E-ROM/S-ROM → 1st general ROM SBO
- UQ: AMV^2/AMV^2+, 2nd-order PMA, QN 2nd-order integrations, 2nd-order design sensitivities
- OUU: progression to 2nd-order TR-SB sequential RBDO, ~40 fn evals per limit state

Impact

- expanding mission space, high performing team
- class-leading algorithms in SBO/UQ/OUU/ROM, external recognition, well positioned for emerging ASC directions
- major usability release, next level of tool deployment
- Internal: DP (ASC L1), MESA (ASC L2, RF), QASPR, NISAC, …
- External: Tri-lab tool of choice, LM SSC/Aero, Goodyear, open source