



Optimization and Uncertainty Estimation

9211

Department Review 2005

Trends and Positioning

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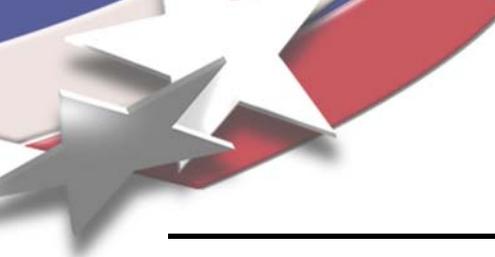
www.cs.sandia.gov/optimization/

Sandia National Laboratories, 2005-3646P



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9211 Dept Review Outline

- **Strategic planning**
- **Technical Scope**
 - Enabling, bridging, end use
- **Emerging Areas**
 - MESA, system model, verification
- **External funding**
- **Staffing Changes**
 - FY05
 - FY06 sneak peek
- **FY05 budget and what it means**



Strategic Planning

- **9210 planning exercise**
- **9211 planning exercise**



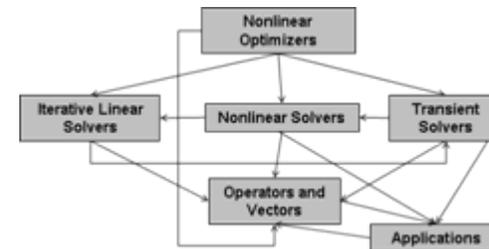
9210 Strategic Planning

- **Position for broadening mission**
 - Echoed for Sandia at Spring Managers Conference
- **Algorithms as enabling technology**
 - We need to bridge
 - We're the ones that care whether we're relevant
- **Advocacy of Modeling and Simulation (M&S) as way of life. Broaden “market” for M&S for all of us.**

9211 Strategic Planning

- 9211

- End use as design optimization and assessment
- Bridge to other activities as an enabling technology
 - 9211 responsible to bridge gap
 - Ongoing bridges
 - Solvers and Simulators,
 - SAND / intrusive optimization, AD, multi-scale, interior point inequality constraints
 - Homeland security, water and air systems
 - Verification & validation
 - New bridges
 - Microsystems
 - Bio / nano molecular simulations
 - Cell system modeling
 - “Social” system modeling



Motto: “optimization is central”

- Consequence – need staff spanning technical areas, bridging to other depts, not “just” technically excellent
- Socialize our role

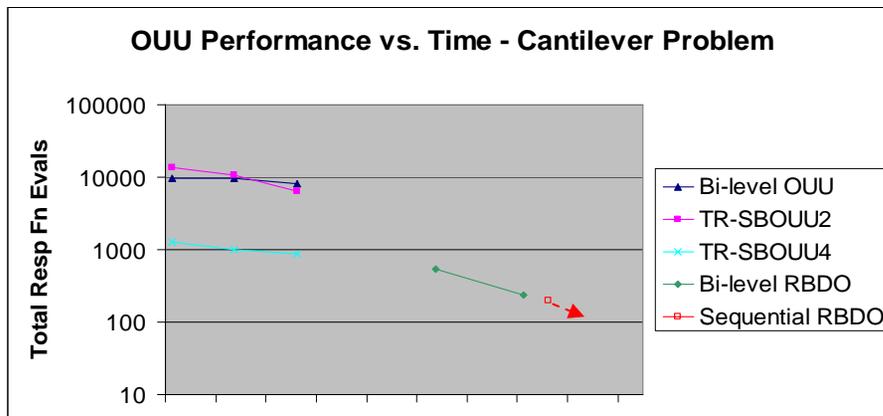


Emerging Areas

- **MESA**
 - **“Cultural distance”**
 - Part of team, horizontal technical integration
 - not consulting or capabilities
 - Earn credibility by producing parts on schedule
 - “Let me join MESA so I can do capability R&D” a non-starter
 - Demonstrate value on applications as a pre-requisite for seeing the need for 9200 M&S
 - **Bridge through**
 - From the top, 9200 management advocating M&S
 - Grass-roots, 9200 staff joining design teams, demonstrating M&S contributions to what MESA values, MESA staff will use and eventually ask for what is useful to them.
 - **Thomas**
 - Technical microsystem design optimization (with product deadlines)
 - MESA program funding, plus specific projects (FY06)!
 - Ambassador for 9200 capabilities
 - Help 9237, 9226 insertion
 - ... and traditional 9200-style research
 - **Eldred**
 - MEMS Design Optimization ASC milestone
 - Teach MESA-TOPS staff to use DAKOTA
 - **van Bloemen Waanders w/ 8962**
 - Topology optimization for microfluidics and microstructures capability

Emerging Areas

- **Verification Methods Research (Trucano sub-program)**
 - **Method of Manufactured Solutions (Knupp ½ time)**
 - **Prediction and Confidence (Swiler)**
 - **Not caring about verification means you don't care about the credibility of your calculation; the message is your calc is not important**
 - The opposite of advocacy of M&S as a way of life
- **Efficacy of Bayesian for HPC simulations conclusions (Swiler, single-author, 60 pages)**
- **Optimization for simultaneous reliability and performance**



$$\hat{u}_z(y(x)) = x' \hat{\beta}$$

$$\hat{\sigma}_z^2(y(x)) = (\hat{\gamma} + \hat{\Delta}'x)'V(\hat{\gamma} + \hat{\Delta}'x) + \hat{\sigma}_\varepsilon^2$$

$$(\hat{\gamma} + \hat{\Delta}'x) = \frac{\partial \hat{y}}{\partial z} = l(x)$$

Emerging Areas

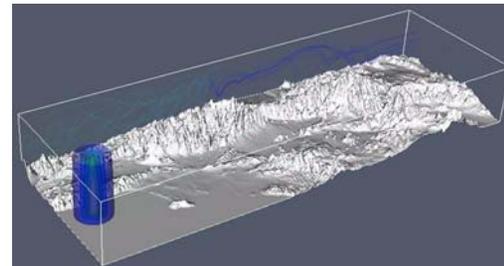
- **Non-engineering systems**

- **Cognition and Uncertainty in complex Decisions.**
May be agent-based models.
V&V (Trucano)



- **Modeling and analysis of social or bio cell systems (FY06 LTE)**
 - optimal parameter selection
 - dynamical system behavior optimization

- **Time-dependent multi-grid preconditioners for homeland security**





External funding

- **To be strategically valuable, external funding needs to support research and development *supporting Sandia's mission***
 - not “developers for hire” or “training on demand”
- **Examples**
 - EPA IAG – renewed for two more years, \$1.5m/year
 - LM-SV – expanded, \$250k/year CY2004, 05
- **Both are right types.**
NASA training classes wrong type, turned down.
- **Challenge: turn “product” interest in DAKOTA into the right type of funding (or a collaboration)**



Staffing

- FY05, green = joined, red = left, net +1 by transfers
 - Roscoe Bartlett
 - Shane Brown (LTE)
 - **Scott Collis**
 - **Andrei Draganescu (LTE)**
 - Mike Eldred
 - David Gay
 - **Pat Knupp**
 - **Mark Richards (LTE, pursuing PhD)**
 - Laura Swiler
 - **Steve Thomas**
 - Tim Trucano
 - Bart van Bloemen Waanders
- Tony Giunta (9133, DAKOTA Product Manager, best ally & advocate imaginable)
- FY06
 - **Brian Adams (LTE)**
 - **System modeling and optimization, e.g. cell networks, agent-based simulations**
 - **Parameter estimation**
 - **Danny Dunlavy (LTE, von Neumann Fellow)**
 - **Optimization and homotopy algorithms, projects w/ three departments**
 - **Judy Hill (LTE, CSGF Howes Award)**
 - **Intrusive optimization and transient inversion**
 - **Multi-scale, materials**



Staffing

- The “new” people

Pat Knupp

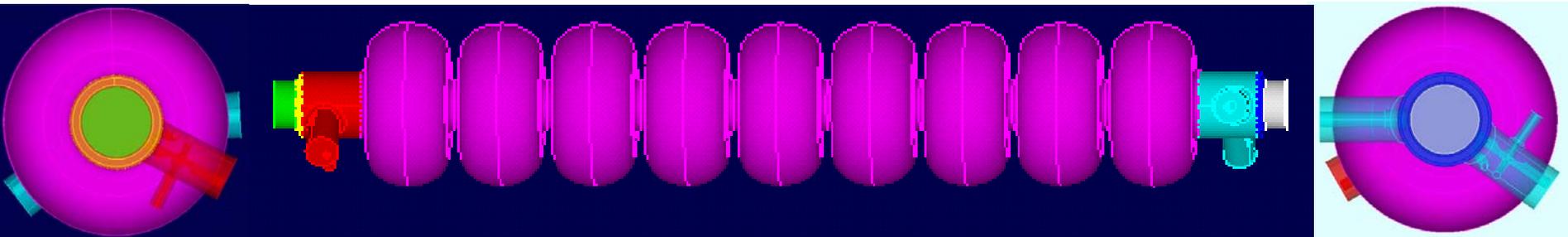


- **DMTS**

- Icon of 9200, SNL 8 years
- June 2004 moved from 9215 to 9211
- 1/2 time on Verification for second year

- **Interests**

- **Verification – Method of Manufactured Solutions**
 - Authored MMS book in 2002 w/ LANL
 - Spontaneous adoption of MMS by 3 code teams FY04
 - “Twenty four open questions in Manufactured Solutions” and ASC V&V project to answer them for HPC context -> “credible M&S” advocacy
- **Design Optimization – Mesh Smoothing**
 - Sandia Lead for TSTT SciDAC multi-lab project on SLAC design optimization
 - ILC is DoE’s number 2 objective



- **Mesh smoothing R&D**

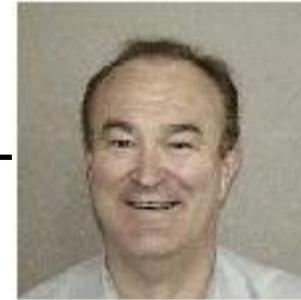
- An enabling technology for shape opt, Alegra

- **Partners**

- **Mesh Smoothing: LANL, LLNL**
- **Verification: Oberkampf, Trucano**

$$\sigma = \frac{3(\alpha\sqrt{2})^{2/3}}{\frac{3}{2}(\lambda_{11} + \lambda_{22} + \lambda_{33}) - (\lambda_{12} + \lambda_{23} + \lambda_{31})}$$

Steve Thomas

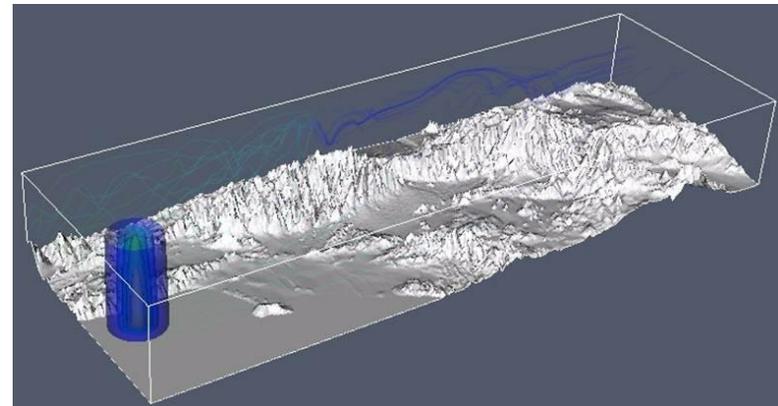


- **PMTS**
 - SNL 3 years
 - March 2004, moved from 8962 to 9211
- **Experience**
 - Inventing algorithms and computational systems
 - CIS LDRD IAT, 8962 manager
 - Bell Labs, large-scale optimization of weapons systems.
 - Exxon/Mobil research, large-scale decision analysis of seismic data, data systems design optimization, information theory applications, 3D seismic interpretation systems.
 - PhD CS and MS EE Cornell
- **Interests include**
 - Design Optimization, 9200-style R&D
 - MESA
 - Design optimization R&D&A
 - Capability ambassador
 - Program development
 - Verification research
 - Hierarchical decomposition of component “errors” to system verification
- **Partners**
 - MESA: Kempka, Massad, Keifer,...tbd
 - Algorithms R&D: Gay, Swiler, Trucano

Andrei Draganescu



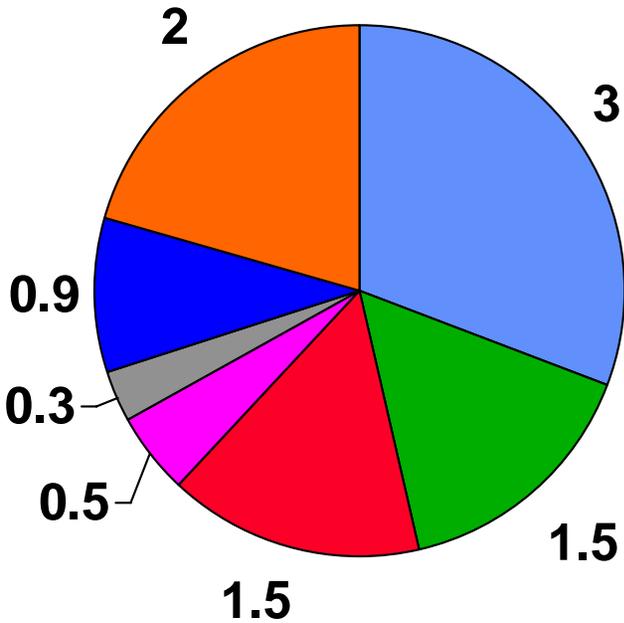
- **LTE**
 - October 2004
 - PhD Math Univ. Chicago, Flash Center, Argonne
- **Current Research**
 - **Enabling next level of parallel efficiency**
 - Multigrid preconditioners for large scale source inversion
 - Multigrid algorithms for velocity inversion constrained by Stokes flow
- **Future Research**
 - Velocity inversion constrained by Navier Stokes
 - Large scale optimization for gas dynamics
- **Partners**
 - van Bloemen Waanders, Collis, Hill, Eldred
 - Dupont, Ghattas, Akclelik, Biros



FY05 Budget Meaning

Spend

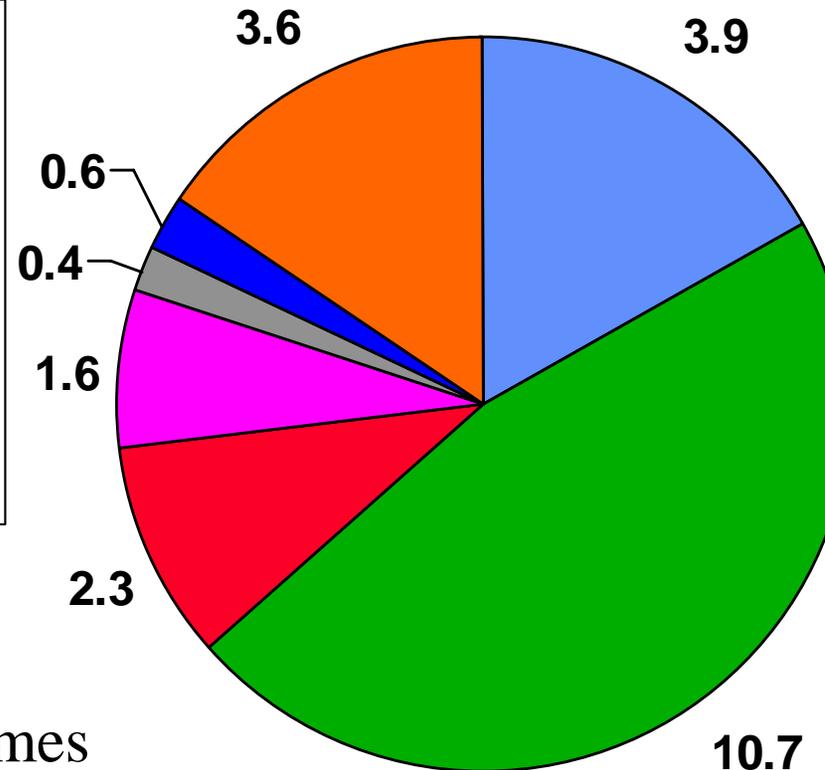
9.7 "FTE" staff + contractors



62% ASC
21% LDRD
12% WFO
5% DoE OS

Lead

23.1 "FTE" the staff PI or PM



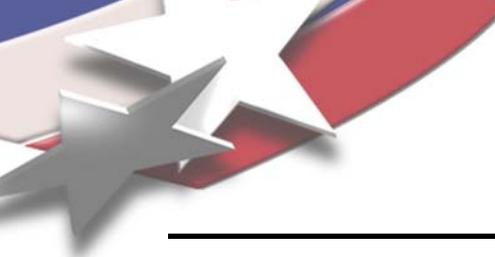
- Lead 2.4 (or 1.6) times what we spend on ourselves
- Work on projects we don't lead, too

no double counting, i.e being PM and PI only counts once
counts 10.7 tgruca V&V methods PI
else 1.7 pknupp & silver V&V PI, right pie is 14 FTE
counts lpswile PRIDE PI for 0.5 year
doesn't count swthoma pre-9211
doesn't count samitch
doesn't count collis post-9211



Staff Leadership

- Define research directions, inspire others, ...
- Some easily measurable evidence
 - Whitepaper, panel roles for M&S advocacy
 - Program development / generate funding
 - Including Steve MESA program funding
 - Project leadership: every single xMTS in 9211 leads at least one cross-organization project,
 - Except Steve who just arrived and unloaded PM 😊



Take-home messages

- **Bridging, lab-wide leadership and M&S advocacy**
 - **MESA**
 - **Non-engineering simulations, cell (FY06) and social**
 - **Enabling optimization:**
 - **Automatic Differentiation**
 - **Mesh movement for geometric design optimization**
 - **Solvers (Thyra in Trilinos)**
- **Deepening**
 - **Verification**
 - **Robust-Optimization algorithms in DAKOTA**
 - **Transient intrusive optimization**
 - **Prediction**