Optimization and Uncertainty Estimation 1411 Department Review 2006

"Men wanted for hazardous journey. Small wages, bitter cold, long months of complete darkness, constant danger, safe return doubtful. Honour and recognition in case of success."



Advertisement for Antarctic trip by Sir Ernest Shackleton (apocryphal)

Scott A. Mitchell www.cs.sandia.gov/optimization/

SAND2006-3639P



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Outline

- Strategy
- Trends
- Staffing & Budget





Current strategy and issues

- Current strategy, articulated last year, demonstrated this year
 - Broaden to engage with emerging areas.
 - Enabling ubiquitous optimization/UQ and M&S.
 - Changing Applications
 - Other than NW hardware assessment $\ensuremath{\uparrow}$
 - Demonstrating value of MS&O in microsystems 1
 - Partner across 14x0, 1500, 1700, 2600, 8900
 - Broad University, industry, tri-lab engagement
 - Technologies
 - Derivatives (Sacado FAD / RAD) for complex SNL C++ PDE
 - Trilinos enabler for semi-intrusive opt
 - DAKOTA as end-use tool
 - Multi-fidelity (reduced order modeling)
 - Multi-scale & multi-physics (decontamination of biofilms)
- Work to ensure people not spread too thin



- Labs changing → three trends highlighted
- 1411 expertise central to defining many emerging National, ASC, Lab, Center themes
 - We're enabling technology so fairly easy to latch onto new "application" areas
 - Red in following slides = will be discussed in staff talks



Program Trends

1411 Activity

Trend

Verification toolkit (Knupp)

DAKOTA for UQ and Validation Calibration ASC Leadership (Trucano)

Exxon Mobile (Wheeler collab w/ vBW)

Predictive Credibility

LDRD

not just simulation, enabling *predictive* simulation

CSRF Simulation Capabilities Intrinsic Quality V&V; simulation for design, hooks for sensitivities

ASC Alg

Intrinsic UQ combination of intrusive UQ, numerical analysis, stochastic simulations, stochastic modeling ASC Weapons QMU milestones

DoE Headquarters V&V Emphasis Predictive Science Panel PSP V&V Center of Excellence Alliance recompete

ASC V&V Verification Research



Program Indicators

Program Trends



Trend

Indicators

Program

Program Trends



Info Science & Decision Support

CSRF Information Science optimization-like exploration of design spaces validation-like analysis of results

National Security mission

ISE sampling strategy



Looking outside



- WFO changing
 - EPA, LM-SV future, GY
- Series of "line-of-sight" workshops
 - SNL-NW, SNL microelectronics & microsystems
 - Not about throwing better tools over the wall; (potential) SNL missions want committed partners
 - Partnerships take time
 - SNL "impact" in tension with "research"
 - DoE / SC



Staffing

- FY06, green = joined, red = will leave
 - Brian Adams (LTE)
 - Roscoe Bartlett
 - Shane Brown (LTE)
 - Andrei Draganescu (LTE, to UMBC faculty)
 - Danny Dunlavy (LTE, von Neumann Fellow)
 - Mike Eldred
 - David Gay
 - Judy Hill (LTE, CSGF Howes Award)
 - Pat Knupp
 - Laura Swiler
 - Steve Thomas
 - Tim Trucano
 - Bart van Bloemen Waanders
- See http://www.cs.sandia.gov/optimization/ Department Review 2006, LTE talk slides
- FY07
 - No change anticipated





FY06 Budget

- DOE ASC slight downturn
- DOE Office of Science increase
 - would like further SC growth, e.g. SciDAC-2



Take-home messages

- Broad engagement
- Trends we are positioned for
 - Predictive Credibility aka simulation intrinsic quality / UQ / confidence / sensitivities
 - Simulation for design (vs. just assessment)
 - Stockpile & national security decision support
- Changing NW focus to application partnership vs. customer
- Many lab trends unclear, but we're relatively flexible, and can help define the future.



"Autumn Sunset" painted by Sir Ernest Shackleton

