Optimization and Uncertainty Estimation
9211
Department Review 2004

Delta from last year

Scott A. Mitchell

http://www.cs.sandia.gov/departments/9211/index.htm

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NNSA National Nuclear Security Administration

Sandia National Laboratories

New / Emerging Areas

- Take home message from last year's review
  - "Positioned to address emerging themes such as homeland security, multi-scale, multi-disciplinary" & multi-fidelity
- Major Research themes:
  - Water / Air homeland security (van Bloemen Waanders/Shadid)
    - Program growth, technical progress
  - Intrusive Optimization themes
    - Transients: Time Domain Decomposition (vBW/Bartlett/Collis)
    - TSFCore (Bartlett lead) impacting Trilinos and Optimization capability set-up
    - AD general tool plans (Gay/Phipps/Bartlett)
  - Multi-scale plans (Collis/Shadid/Christon/Lehoucq/Bochev/Hughes)
    - Collis program development story
  - DAKOTA multi-fidelity surrogate-based optimization corrections (Eldred/Giunta/CSRI)
  - Multi-disciplinary coupling via Sierra
  - Broader look at uncertainty, probability and statistics than just computational tools for propagating variability (Trucano)
    - Bayesian exploration under PRIDE LDRD, and MICS calibration under uncertainty (Swiler / Trucano / Heaphy / 8962)
    - Calibration / Validation / Predictability tradeoff (Trucano / Swiler)
    - Alternate forms of probability, epistemic uncertainty (Eldred/Trucano/CSRI).

Air and Water Homeland Security

- Programmatics
  - van Bloemen Waanders (vBW) initiated through 2002 LDRD
    - Big program, many excellent leaders and contributors…
  - Funding: LDRD 2002, DTRA 2003, DHS (air) 2003, EPA (water) 2004
- Goals and Challenges
  - Contaminant (attack) detection, clean-up, and effect mitigation
  - Source inversion (Where did attack originate? How strong was it?)
    - Both water and air capabilities
    - Intrusive gradient-based optimization of PDE-based simulations
    - DAKOTA / EPANet - water source inversion
    - Specialized direct QP solver for air inversion (Bartlett)
    - Intrusive Time Domain Decomposition methods underway for real-time
  - Risk assessment. Data w/ errors. (6500)
  - Sensor placement air (vBW) / water (Hart/Phillips)
- Air-contamination in interior spaces (e.g. airports)
  - Continuous space model. MPSalsa, Trilinos, DGM, Charon
- Water contamination of municipal water supplies
  - Discrete space model. EPANet + diffusion

Relations w/ other groups

- More projects with groups we already worked with, plus new ties to 6500, 6100, 15300, 1600
- CSRI instrumental
  - CMU, Rice, Notre Dame (long-term visitors), UIUC, …
  - OUU and TDD workshops
- 6000 water security, poroelasticity. (Finley, Hammond…)
- 8962 PRIDE LDRD, DAKOTA algorithms
- 8752 Multi-scale
- 9133
  - V&V program ties and funding
  - Collaborative uncertainty quantification research
    - Giunta, Red-Horse, Vicente Romero, Wojtkiewicz (9124), Gunzberger (CSRI)
- 9143 Adjoint Based Error Estimators, Optimization w/in Sierra
- 9113 MESA-tops microstructure optimization (Kempka, Bruns)
- Increased academic, NASA, LM, and Tri-labs (LLNL) DAKOTA use

Relations w/ other groups, ctd.

- More projects with groups we already worked with, plus new ties to 6500, 6100, 15300, 1600.
- 9200
  - 9210
    - 9215 Optimization algorithms, water security, mesh optimization, PRIDE - Bayesian design of experiments (Heaphy)
    - 9216 SEM JSF logistics, Agents, Sensitivity Analysis (15310, 9215)
    - 9214 Multi-scale
    - 9212 Parameter fitting for cell-system models (future)
  - 9230
    - 9233 Air security, multi-scale, Automatic Differentiation (plans), multi-fidelity (Entero)
    - 9235 Multi-scale, force field opt
    - 9232 DAKOTA Design Simulator applications, Opt, UQ, SA
    - 9231 Multi-scale, Alegra OUU capsule applications, V&V milestone (1674)
  - 9220 D2A

Staffing

- Last year green = joined, red = left, purple = both
  - OAA: Sandra Maestas - Kathryn Crowder (to Romig), Tanya Gallegos, Lydia Koch
  - Roscoe Bartlett
  - Shane Brown (LTE, no talk) – Mario Alleva (to Boeing SVS)
  - Scott Collis
  - Mike Eldred
  - David Gay
  - Mark Richards (6 month LTE) – Tony Giunta (to 9133)
  - Laura Swiler
  - Tim Trucano (rejoined from SEPR program office)
  - Bart van Bloemen Waanders

- Lot's o' changes … but everything's going well
  - Mike teaching & integration kudos
    - Transparent DAKOTA team swap-out

Dave Gay

- Joined SNL 6 Oct 2003, formerly Bell Labs DMTS
- Major technical areas
  - Automatic Differentiation (AD)
    - Semi-automatic, general purpose tool for analytic sensitivities for SNL PDE-based codes. Faster (usually) and more accurate than finite differences.
    - Backward (adjoint) & forward expression tree traversal
      - Similar to AMPL expression tree and AD experience
    - (Gay, Phipps, Bartlett - CSRF?)
  - Global optimization algorithm research
    - Branch & Bound-like technique for continuous optimization to provably find global optima.
    - Gay, Hart final-round LDRD
  - Problem expression
    - World-class leader on problem expression in AMPL
      - Develop capability to set-up optimization objectives and constraints w/in Sierra
    - Water security problem set-up
  - Mesh node placement optimization
    - MESQUITE optimization solver speedup, add gradient information w/ Knupp
  - Stochastic programming?
- Major partners
  - Bartlett, Phipps, Eldred, Hart, van Bloemen Waanders, Knupp

Scott Collis

- Joined SNL 21 July 2003, formerly Rice professor
- Major technical areas – "Prof. Multi"
  - Organizing Multi-scale effort
    - General mathematical framework, beyond materials
      - Transfer operators, VMS, LES
      - Bochev, Christon, Collis, Lehoucq, Shadid, Slepoy, Wagner
    - Large multi-scale LDRD in final round (Collis PI, Shadid PM)
      - Collis worked in technical area for years
      - Christon & Collis MICS proposal last June 2003
      - Laying groundwork for MICS multi-scale initiative response
  - Time-dependent air-flow multi-level preconditioners, inversion, DG, LES, sensitivities
  - Reduced Order Models (ROM) for use in Surrogate Based Optimization in DAKOTA (multi-fidelity)
- Major partners
  - van Bloemen Waanders, Bartlett, Christon, Wagner, Shadid, Lehoucq, Bochev, Slepoy, Eldred, Hassan+staff

Laura Swiler

- Joined dept 23 May 2003, formerly 15312
  - Was PI and main technical contributor for many 15300 projects came to 9200 to return to research roots (and PI our projects…)
  - Very quickly integrated into 9200
    - Represents DAKOTA project internally and externally
    - Ties to 9211, 9215, 9216, 9133, …
- Major contributor in many technical areas
  - Penetrator Reliability "PRIDE" LDRD
    - Bayesian updating of ranges in penetrator performance over uncertain target conditions. Multi-fidelity Pronto models.
    - Trucano & Martinez-Canales & Heaphy
  - MICS Calibration Under Uncertainty /w Trucano
  - Sensitivity Analysis of W-80 NEP Pad material parameters on component response (Salinas) – LEP Normal Environment analysis (Howard Walther)
  - Sensitivity Analysis of Support Enterprise Model for JSF logistics
    - Schoenwald & Watson
  - Statistical correlation metrics deployed in DAKOTA
  - Optimization Under Uncertainty
    - Providing technical leadership (summary papers) on importance sampling, Bayesian statistics. CSRF OUU PI since Giunta

Publications

- Editor, Conf. Committee, Professional offices
- Continued research and publication emphasis

	Journal Paper	Conference Paper or Talk	Invited Talk	SAND-only report	Editor of Journal	Conference Committee / Organizer	Professional Offices
Bartlett	1	3		1			
Collis	5	4	1			3	
Eldred	4	11	1	3	1	3	
Gay		2				2	1
Swiler		3		2		1	1
Trucano				1	1		
van Bloemen Waanders	2	7		2		4	

Technical Challenges

- Epistemic and Bayesian technology challenging research topics
  - Unique HPC and Simulation context
  - Predictability
- Transients (and uncertainty) in intrusive methods for air/water security and defense programs (DP)
  - Efficient parallel algorithm challenge

- Streamline capability development
  - Automatic Differentiation (right level of automation)
    - Demo problems successful
  - Progress - Sierra / Nevada integration simulation interfacing
- Streamline opt/UQ problem set-up
  - Progress - Dakota's Jaguar GUI developed by contractors
  - Sierra / Nevada integration problem specification

- "Blue skies ahead"

Personal Note

- **Hosting HMC student Susanna Ricco 2004**
  - **Shape “optimization” (matching) project**
    - **Incorporating MESQUITE**
    - **Closing DAKOTA design optimization loop**

Take-home messages

- Broad Center and lab-wide contribution
- New staff integration
- Exciting new work in
  - Homeland air and water security
  - Transient intrusive optimization
  - Multi-scale
  - Automatic Differentiation
  - “Uncertainty” (broadly defined)
    - Reliability-based optimization
    - Bayesian
    - Calibration and prediction