GENETHA ANNE GRAY

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EDUCATION

Rice University, Houston, Texas *Aug 1997 - May 2002*

Ph.D., Computational and Applied Mathematics (CAAM), May 2002.

- *thesis:* "A Variational Study of the Electrical Impedance Tomography Problem"
- *advisors:* Dr. Liliana Borcea and Dr. Yin Zhang
- Fellow, Keck Center for Computational Biology

M.A., Computational and Applied Mathematics, May 2001.

California State University, Sacramento *Aug 1995 - May 1997*
M.A., Mathematics, May 1997.

University of California, Davis *Sept 1989 - June 1993*
B.S., Mathematics, June 1993.

POST-GRADUATE WORK EXPERIENCE

Sandia National Laboratories, Livermore, CA, *Technical Staff Member* (Jan 2004-present) and *Post Doc* (Aug 2002-Jan 2004). Accomplishments include:

- Development of a parallel hybrid optimization scheme. In this research project, I investigated a sampling approach that combines a statistical Gaussian process model and an optimization pattern search. I created prototype software, HOPSPACK and demonstrated improved efficiency and robustness both for test problems and real applications problems in the areas of electrical engineering and groundwater. I received funding from the American Institute of Mathematics to lead a workshop on this topic in Oct 2008.
- Improvement of calibration and parameter estimation schemes for numerical simulators. To meet the needs of internal customers, I developed an automated procedure to improve the accuracy of numerical simulations. This work included developing appropriate objective functions, linking optimization and simulation codes, and analyzing results. The approach was applied to simulators for semiconductor bridges, groundwater flow, cardiovascular control, and mechanical systems.
- Principal investigator for ensemble classification methods project. Over a 3-year span, I led a multi-disciplinary research team, secured funding, scoped project to disparate data fusion, planned project milestones, presented implementation and execution progress to stakeholders on an annual basis, generated peer-reviewed papers on research innovation, and delivered results as major deliverable to Sandia grand challenge project focused on immune system response to pathogens.
- Verification and validation process lead for a radiation-hardened circuits project. In this role, I planned experimental tests for multiple radiation facilities, analyzed experimental data, developed new code calibration methods, developed faster simulation processes, calibrated simulation codes, analyzed simulation data, and maintained frequent update and synchronization meetings with geographically-dispersed teams.
- Maintenance, testing and revision of a C++ parallel optimization software code, Asynchronous Parallel Pattern Search (APPSPACK). As part of the APPSPACK code development team, I made changes to the software to reduce the minimum number of processors needed to run the code in parallel, worked on the release of the version of the code containing this change, produced documentation and performed extensive testing.

- Development of an integrated computational/experimental model to address questions of transmembrane protein structure. I used my training in biology to interact with biologists and implement software to predict protein structures given experimental data from chemical cross-linking.
- Demonstration of a multi-level, multi-fidelity method of optimization. As part of the team, I investigated, implemented, tested, and documented an approach to an optimization using surrogates and space mapping. The software was demonstrated on a mechanical engineering and a groundwater remediation problem

OTHER WORK EXPERIENCE

Rice University, Houston, TX, Teaching Assistant, Computational & Applied Mathematics Department, 1997-2000.

Sandia National Laboratories, Livermore, CA, Intern, Scientific Computing Division, summer 1998.

California State University, Sacramento, Instructor, Mathematics Department, 1995-1997

Bayer Laboratories, Berkeley, CA, Biotechnician, Recombinant Factor VIII Division, 1995.

Calgene, Davis, CA, Research associate (1993-1994), Intern (1991-1993), Tomato Research & Development Group.

RESEARCH INTERESTS AND SKILLS

- *Research interests:* Optimization, Computer Code Validation, Uncertainty Quantification, Decision Making, Statistics, Computational Biology and Inverse Problems.
- *Platforms used:* Unix, Linux, Windows, and Macintosh.
- *Programming skills:* Fortran 90, C, C++, MPI, Matlab, LaTeX, C-shell scripts and html.
- Department of Energy clearance.

REFEREED PAPERS

K. R. Fowler, G. A. Gray, M. Olufsen, "Modeling Heartrate Regulation- Part II: Parameter Identification," *J. Cardiovascular Engineering*, vol. 8, no. 2, Jun 2008.

K. R. Fowler, J. P. Reese, C. E. Kees, J. E. Dennis, Jr., C. T. Kelley, C. T. Miller, C. Audet, A. J. Booker, G. Couture, R. W. Darwin, M. W. Farthing, D. E. Finkel, J. M. Goblansky, G. A. Gray, T. G. Kolda, "A Comparison of Derivative-free Optimization Methods for Water Supply and Hydraulic Capture Community Problems," *Advances in Water Resources*, vol. 31, issue 5, pp. 743–757, May 2008.

G. A. Gray, P. J. Williams, K. L. Sale, W. M. Brown, and J-L. Faulon, "Disparate Data Fusion for Protein Phosphorylation Prediction," *Annals of Operations Research* Special Volume on Data Mining, in press.

G. A. Gray, M. Martinez-Canales, C. Lam, B. E. Owens, C. Hembree, D. Beutler, C. Coverdale, "Designing Dedicated Experiments to Support Validation and Calibration Activities for the Qualification of Weapons Electronics," Proceedings of the 14th NECDC, Jan 2007.

G. A. Gray, M. Taddy, M. Martinez-Canales, H. K. H. Lee, "Enhancing Parallel Pattern Search Optimization with a Gaussian Process Oracle," Proceedings of the 14th NECDC, Jan 2007.

G. A. Gray, T. G. Kolda, "APPSPACK 4.0: Asynchronous Parallel Pattern Search for Derivative-Free Optimization," *ACM TOMS*, vol. 32, no. 3, Sept 2006.

G. A. Gray, K. R. Fowler, "Approaching the Groundwater Remediation Problem Using Multifidelity Optimization," Proceedings XIV Conference on Computational Methods in Water Resources, June 2006.

G. A. Gray, T. G. Kolda, K. L. Sale, M. M. Young, "Optimizing an empirical scoring function for transmembrane protein structure determination," *INFORMS J. Computing*, Special Issue on Computational Biology, vol. 16, no. 4, pp. 406–418, 2004.

K. L. Sale, J-L. Faulon, G. A. Gray, J. Schoeniger, M. M. Young, "Optimal bundling of the transmembrane helices of integral membrane proteins using sparse distance constraints," *Protein Science*, vol. 13, no. 10, pp. 2613–2627, 2004.

L. Borcea, G. A. Gray, Y. Zhang, "Variationally Constrained Numerical Solution of Electrical Impedance Tomography," *Inverse Problems*, vol. 19, pp. 1159–1184, 2003.

PUBLICATIONS IN PREPARATION, UNDER REVIEW, AND UNREFEREED

G. A. Gray, J. Griffin, "HOPSPACK: Hybrid Optimization Parallel Pattern Search," User's Manual, in preparation.

T. Lowry, S. James, M. Grace, D. Arnold, G. A. Gray, M. Ahlmann, "Development of a Deterministic Site Characterization Tool Using Multi-Model Ranking and Inference," Technical Report SAND2008-5438, Sandia National Laboratories, Jul 2008.

H. K. H. Lee, M. Taddy, G. A. Gray, "Selection of a Representative Sample," submitted *J Classification*, Jun 2008, available as Sandia National Labs Report SAND2008-3857J.

G. A. Gray, M. Taddy, J. D. Griffin, M. Martinez-Canales, H. K. H. Lee, "Hybrid Optimization: A Tool for Model Calibration," in preparation for *IEEE*, available as Sandia National Labs Report SAND2008-0145J.

M. Taddy, H. K. H. Lee, G. A. Gray, J. D. Griffin, "Bayesian Guidance for Robust Parallel Pattern Search Optimization," submitted to *Technometrics*, Jan 2008, available as Sandia National Labs Report SAND2008-0104J.

G. A. Gray, P. J. Williams, K. L. Sale, G. S. Davidson, "Datapipelining for Heterogeneous Data Fusion," Technical Report SAND2007-6092, Sandia National Laboratories, Sept 2007.

G. A. Gray, K. L. Sale, P. J. Williams, "Disparate Data Fusion for Protein Phosphorylation Prediction," Proceedings of the AI/DM Pre-Conference Workshop at the INFORMS Annual Meeting, Nov 2006.

J. P. Castro, G. A. Gray, A. A. Guinta, P. D. Hough, "Developing a Computationally Efficient Dynamic Multilevel Hybrid Optimization Scheme using Multifidelity Model Interactions," Technical Report SAND2005-7498, Sandia National Laboratories, Livermore, CA, Nov 2005.

D. Brown, G. A. Gray, "Implementation of a Data Fusion Algorithm for RODS, a Real-time Outbreak and Disease Surveillance System," Technical Report SAND 2005-6007, Sandia National Laboratories, Livermore, CA, Sep 2005.

G. A. Gray, "Parameter Identification for the Electrical Modeling of Semiconductor Bridges," Technical Report SAND2005-0940, Sandia National Laboratories, Livermore, CA, Feb 2005.

CAREER DEVELOPMENT AWARDS

Statistical and Applied Mathematical Sciences Institute (SAMSI), Program on Risk Analysis, Extreme Events, and Decision Theory *2007*

American Institute of Mathematics (AIM), Workshop on Short-term Cardiovascular-Respiratory Control Mechanisms *Oct 2006*

Statistical and Applied Mathematical Sciences Institute (SAMSI), Program on the Development, Assessment, and Utilization of Complex Computer Models *2006-07*

Mathematical Issues and Challenges in Data Assimilation for Geophysical Systems: Interdisciplinary Perspectives, Institute for Pure and Applied Math (IPAM), *Feb 2005*

Proteomics: Sequence, Structure, Function, IPAM, UCLA, *spring 2004*

Computational Biophysics Summer School, Beckman Institute, UIUC, Urbana-Champaign, IL *June 2003*

Institute for Advanced Studies Women's Program in Mathematics, Bio Math Summer Session, *May 2003*

RECENT PRESENTATIONS

Jul 2008 Computational Methods in Water Resources, San Francisco, CA, presentation: "The Applicability of Hybrid Optimization for Solving the Plume Contaminant Problem"

May 2008 SIAM Conference on Optimization, Boston, MA, presentation: "Some Considerations in Evaluating Derivative-Free Methods for Simulation Based Optimization Problems"

Apr 2008 Iterative Methods Conference, Copper Mountain, CO, presentation: "Hybrid Optimization: Combining the Best to Overcome the Worst"

Nov 2007 INFORMS Annual Meeting, Seattle, WA, presentation: "Derivative-Free Optimization as a Tool for Simulator Calibration."

Aug 2007 International Conference on Continuous Optimization, Hamilton, ON, presentation: "Optimization as a Tool for the Calibration of an Electrical Circuit Simulator."

June 2007 SIAM Conference on Control and its Applications, San Francisco, CA, presentation: "Parameter Estimation for a Model of Baroreflux Regulation of Heartrate."

May 2007 Statistics Spring Research Conference, Ames, IA, presentation: "Dedicated Experiments to Support Model Validation and Calibration"

Apr 2007 Clarkson University, Potsdam, NY, Mathematics Colloquium: "Some Considerations for Evaluating the Predictive Capabilities of Xyce, An Electrical Circuit Simulator."

Jan 2007 INFORMS Computing Science Meeting, Coral Gables, FL, presentation: "A Hybridization of Direct Search Optimization and Treed Gaussian Process"

Nov 2006 INFORMS Annual Meeting, Pittsburgh, PA, presentation: "Designing a Database to Support Electrical Circuit Validation."

Nov 2006 Workshop on Artificial Intelligence and Data Mining, Pittsburgh, PA, presentation: "Disparate Data Fusion for Protein Phosphorylation Prediction."

Oct 2006 NECDC Annual Meeting, Los Alamos National Lab, NM, plenary talk: "Designing Dedicated Experiments to Support Validation and Calibration Activities for the Qualification of Weapons Electronics," and presentation: "Enhancing Parallel Pattern Search Optimization with a Gaussian Process Oracle." (Corresponding proceedings papers)

Sept 2006 NC State University, Raleigh, NC, Numerical Analysis Colloquium: "Derivative-Free Methods for Simulation-Based Optimization."

Sept 2006 SAMSI Kickoff Workshop for the Program in Development, Assessment, and Utilization of Complex Computer Models, RTP, NC, invited talk: "Verification, Validation, and Calibration of an Electrical Circuit Simulator" and poster presentation: "Designing Dedicated Experiments for Validation Activities of an Electrical Circuit Simulator."