GENETHA ANNE GRAY

Sandia National Laboratories
P.O. Box 969, MS 9159
Phone: (925)294-4957, Fax: (925)294-2234
e-mail: gagray@sandia.gov
http://www.csmr.sandia.gov/~gagray

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

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.

WORK EXPERIENCE

Sandia National Laboratories, Livermore, California *Aug 2002 - present*
Technical Staff Member (Jan 2004-present) and *Post Doc* (Aug 2002-Jan 2004) in the Computational Sciences and Mathematical Research Department. Involved in the following projects:

- Research of enemble classification methods for disparate data fusion (principal investigator).
- Implemention of a verification and validation process for an electrical circuit simulator; includes planning experimental tests, data analysis of computational and experimental results and code calibration.
- Investigation of optimization schemes that incorporate statistical Gaussian process models to improve sampling.
- Development and testing of a dynamic multifidelity-multilevel hybrid optimization scheme and its application to groundwater remediation problems.
- Maintenance, testing and revision of a C++ parallel optimization software code, Asynchronous Parallel Pattern Search (APPSPACK).
- Development of an integrated computational/experimental model to address questions of trans-membrane protein structure.
- Parameter identification for a computer simulation of a semiconductor bridge.

Sandia National Laboratories, Livermore, California *summer 1998*
Intern in the Scientific Computing Division. Worked with C code for solving large unconstrained minimization problems found in computational chemistry.

Bayer Laboratories, Berkeley, California *1995*
Biotechnician in the Recombinant Factor VIII Division. Responsible for carrying out FDA protocol designed to purify products used in the production of blood clotting drugs.

Calgene, Davis, California *1991-1994*
Research associate and *Intern* in the Tomato Research and Development Group. Carried out various bench top biology processes (westerns, southerns, PCR, and cloning) as well as sterile tissue culture and seed germination assays. Also participated in field trial studies and data collection and analysis.

TEACHING AND MENTORING EXPERIENCE

Rice University, Houston, Texas *1997-2000*
Teaching Assistant and *Grader:* taught recitation, held office hours, prepared homework solutions, and assisted with exam preparation and grading for undergraduate and graduate courses.

Alliance for Graduate Education and the Professoriate *summers 2000 and 2001*
Mentor for undergraduate and high school students in science, engineering, and math in the AGEP program held at Rice University.

California State University, Sacramento *1995-1997*
Instructor and *Tutor:* Responsible for preparing and delivering lectures and assigning and grading all homework and exams for undergraduate courses; Member of the staff at the drop in tutoring center provided for students taking undergraduate math courses.

RESEARCH INTERESTS AND SKILLS

- *Research interests:* Optimization, Computer Code Validation, Statistics, Computational Biology and Inverse Problems.
- *Platforms used:* Unix, Linux, Windows, and Macintosh environments.
- *Programming skills:* Fortran 90, C, C++, MPI, Matlab, LaTeX, C-shell scripts and html.

PAPERS AND TECHNICAL REPORTS

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, (also available as Sandia Technical Report SAND2004-6391).

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

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, Sept 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, Sept 2005.

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

G. A. Gray, T. G. Kolda, K. L. Sale, M. M. Young, "Optimizing an empirical scoring function for transmembrane protein structure determination," *INFORMS Journal on 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.

G.A. Gray, "A Variational Study of the Electrical Impedance Tomography Problem," doctoral thesis, Rice University, CAAM Department Technical Report, TR02-02, May 2002.

K. R. Kavanaugh, J. P. Reese, C. E. Kees, C. T. Kelley, C. T. Miller, A. J. Booker, J. E. Dennis, Jr, D. E. Finkel, M. W. Farthing, G. Couture, G. A. Gray, T. G. Kolda, "A comparison of Optimization Methods for Problems Involving Flow and Transport Phenomena in Saturated Subsurface Systems," in preparation for submission to *Advances in Water Resources*.

HONORS AND FUNDING AWARDED

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

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

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

Institute for Math and its Applications (IMA) at the University of Minnesota, Workshop on Career Options for Women in Mathematics, funded participant *Feb 2005*

Association for Women in Math (AWM), Workshop for recent Ph.D.s, funded participant *July 2004*

Proteomics: Sequence, Structure, Function, IPAM, UCLA, funded participant *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, funded participant *May 2003*

AWM Workshop for graduate students, funded participant *July 2002*

W.M. Keck Center for Computational Biology, predoctoral fellow *1999-2002*

George R. Brown Computational Engineering, fellow *2000-2001*

PRESENTATIONS

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 in progress)

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."

June 2006 University of Utrecht, The Netherlands, Geosciences Department Colloquium: "Verification, Validation, and Calibration of Simulators"

June 2006 Computational Methods in Water Resources (CMWR), Copenhagen, Denmark, invited talk: "Approaching the Groundwater Remediation Problem Using Multifidelity Optimization."

Apr 2006 Iterative Methods Conference, Copper Mountain, CO, presentation: "The Role of Optimization in the Verification, Validation, and Calibration Processes"

Feb 2006 Quantitative Methods for Defense and National Security, Santa Monica, CA, poster presentation: "Enhancing Information Extraction by Applying Ensemble Classification to Disparate Data Sets."

Dec 2005 Murray State University, Murray, KY, Phi Mu Epsilon banquet, keynote address: "Simulation Code Validation: Using Math to Find and Correct Mistakes."

Nov 2005 INFORMS Annual Meeting, San Francisco, CA, presentation: "Using APPSPACK to Identify Optimal Model Parameters," and presentation: "Ensemble Classification of Disparate Data Sets."

July 2005 SIAM Annual Meeting, New Orleans, LA, presentation: "Using Optimization to Approach the Transmembrane Protein Identification Problem"

June 2005 SIAM Confernce on Mathematical and Computational Issues in the Geosciences, Avignon, France, presenation: "Multifidelity Optimization Via Pattern Search and Space Mapping."

Mar 2005 California State University, Sonoma, Mathematics Department colloquium: "Using Simulation-Based Optimization Methods to Solve Groundwater Flow Problems."

Feb 2005 IMA Workshop, Career Options for Women in Mathematical Sciences, Minneapolis, MN, poster presentation: "Multifidelity Optimization Using Asynchronous Parallel Pattern Search and Space Mapping Techniques."

Jan 2005 UC Davis, Mathematics Department Biomathematics seminar: "Combining Experimental and Computational Techniques for the Identifications of Transmembrane Protein Structures."

July 2004 SIAM Annual Meeting, AWM Workshop, Portland, OR, presentation: "An Empirical Scoring Function for the Optimal Bundling of Transmembrane Helices."

Apr 2004 UCLA, Bioengineering Department, seminar: "An Integrated Computational Experimental Approach to the Transmembrane Protein Structure Determination Problem"

Apr 2004 IPAM, UCLA, seminar: "Optimal Bundling of Transmembrane Helices Using Sparse Distance Constraints"

Feb 2004 SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, poster presentation: "A Parallelized Method of Parameter Identification for Electrical Simulation Software"

Feb 2004 Biophysical Society Annual Meeting, Baltimore, MD, poster presentation: "Optimal Bundling of the Transmembrane Helices of Integral Membrane Proteins"

Jan 2004 The 5th Biennial Structural Biology Symposium, Membranes: A Challenge for Protein Magnetic Resonance, Florida State University, Tallahassee, FL, poster presentation: "Optimal Bundling of the Transmembrane Helices of Integral Membrane Proteins"

May 2003 Program for Women in Mathematics: Summer Session on Bio Math, Institute for Advanced Studies, Princeton, NJ, lecture: "Two Examples of Simulation Based Optimization"

May 2003 Tenth Anniversary Reunion of the Program for Women in Mathematics, Institute for Advanced Studies, Princeton, NJ, poster presentation: "Derivative-Free Optimization for Transmembrane Protein Structure Determination"

May 2003 CSU, Hayward, seminar: "Two Examples of Simulation Based Optimization"

Apr 2003 SAMSI, Simulation and Optimization Workshop, RTP, NC, poster presentation: "Derivative-Free Optimization for Transmembrane Protein Structure Determination"

Mar 2003 Fourth Bay Area Numerical Analysis Day, Stanford University, Palo Alto, CA, presentation: "Derivative-Free Optimization for Transmembrane Protein Structure Determination"

Feb 2003 SIAM Conference on Computational Science & Engineering, San Diego, CA, contributed talk: "Transmembrane Protein Structure Determination"

Jul 2002 SIAM Annual Meeting, Philadelphia, PA, minisymposium presentation: "A Variational Study of the Electrical Impedance Tomography Problem"

July 2002 AWM Workshop, SIAM Annual Meeting, Philadelphia, PA, poster presentation: "A Variational Study of the Electrical Impedance Tomography Problem"

June 2002 Free University, Brussels, Belgium, seminar: "A Variational Study of the Electrical Impedance Tomography Problem"

PROFESSIONAL LEADERSHIP AND VOLUNTEER WORK

AWM meetings committee for the SIAM Annual Meeting 2005	*2004-2005*
Science Buddies Advisor	*2002-present*
Sandia Math & Science Awards Banquet hostess and mentor	*2003, 2004*
SIAM committee on the annual meeting.	*2001-2003*
Rice University CAAM department graduate recruitment committee.	*1999-2000*
Judge for the Texas State Science Fair	*1999, 2000, & 2002*

PROFESSIONAL MEMBERSHIPS

Society for Industrial and Applied Mathematics (SIAM)

American Mathematical Society (AMS)

Association for Women in Mathematics (AWM)

Association for Computing Machinery (ACM)

Institution for Operations Research and the Management Sciences (INFORMS)