Daniel M. Dunlavy

Optimization and Uncertainty Estimation
Sandia National Laboratories
P.O. Box 5800, MS 1318
Albuquerque, NM 87185-1318 USA

Phone: 505.284.6092
Fax: 505.845.7442
Email: dmdunla@sandia.gov
http://www.cs.sandia.gov/~dmdunla

Research Interests

- Applied Mathematics and Computational Science
- Optimization, Numerical Linear Algebra, and Numerical Analysis
- Computational Molecular Biology and Information Retrieval

Education

University of Maryland, College Park, MD
Ph.D., Applied Mathematics and Scientific Computation — August 2005
M.S., Applied Mathematics and Scientific Computation — December 2003
Advisor: Dianne O'Leary, Department of Computer Science

Western Michigan University, Kalamazoo, MI
M.S., Applied Mathematics — April 2001
Advisor: Niloufer Mackey, Department of Mathematics

Northwestern University, Evanston, IL
B.A., Computer Studies — June 1994

Research Positions

Sandia National Laboratories, Albuquerque, NM
John von Neumann Postdoctoral Fellow — 2005–present
Collaborators: Michael S. Eldred, and Andrew G. Salinger, Tamara G. Kolda
Projects: Simulation-based optimization using surrogates (DAKOTA)
Space-time solvers and preconditioners for large-scale PDEs (Trilinos)
Linear and multilinear algebra algorithms for informatics

University of Maryland, College Park, MD
Graduate Research Assistant — 2001–2005
Advisor: Dianne O'Leary, Department of Computer Science
Projects: Homotopy optimization methods and protein structure prediction
Query-based multi-document clustering and summarization

Center for Computing Sciences, Bowie, MD
Student Intern — 2002–2004
Advisor: John Conroy, Research Staff
Project: Named-entity extraction and cross-document co-referencing

Sandia National Laboratories, Livermore, CA
Student Intern — Summer 2001
Advisor: Tamara Kolda, Computational Sciences & Mathematics Research
Project: Surrogate models in derivative-free optimization

Western Michigan University, Kalamazoo, MI
Graduate Research Assistant 2000–2001
Advisor: Niloufer Mackey, Department of Mathematics
Project: Structure-preserving eigensolvers

Institute for Mathematics and Its Applications, Minneapolis, MN
Visitor in Residence Summer 2000
Advisor: Robert Melville, Lucent Technologies
Project: Numerical solution of DAE's for RF circuits

Northwestern University, Evanston, IL
Research Assistant 1992–1993
Advisor: Gil Krulee, Electrical Engineering and Computer Science
Project: Online tutorial system for library databases

Teaching

Western Michigan University, Kalamazoo, MI *Teaching Assistant* 1999–2001
Math 110: Algebra I (4 sections)
Sole classroom contact, prepared and graded all homework/quizzes
Developed pilot program for computer-based testing system

Other Professional Experience

Sylvan Learning Center, Stevensville, MI, *Math Tutor* 1998–1999

Lakeshore Public Schools, Stevensville, MI, *Computer Instructor* 1998–1999

Sperling Sampson West, San Francisco, CA, *Computer Programmer* 1995–1998

DechTar Direct, Inc., San Francisco, CA, *Computer Technician* 1994–1995

Northwestern University, Evanston, IL, *Computer Technician* 1993–1994

GD Searle, Skokie, IL, *Computer Programmer* 1991–1993

Service

Referee, AIAA Multidisciplinary Analysis and Optimization Conference 2006–present

Referee, SIAM Review 2005–present

Referee, SIAM Journal on Numerical Analysis 2005–present

Panel Member, CSE Education Panel, SIAM Conference on Computational Science and Engineering, Orlando, FL February 2005

Student Representative, AMSC Graduate Committee, University of Maryland 2004-2005

President, AMSC Student Council, University of Maryland 2004-2005

Graduate Student Mentor, AMSC Program, University of Maryland 2002–2004

Scribe, DOE Multiscale Mathematics Workshop May 2004

Volunteer, Graph Theory, Combinatorics, Algorithms and Applications Conference 2000

Journal Articles

Daniel M. Dunlavy, Dianne P. O'Leary, John M. Conroy, and Judith D. Schlesinger, "QCS: A System for Querying, Clustering, and Summarizing Documents", *Information Processing & Management*, accepted October 2006.

Daniel M. Dunlavy, Dianne P. O'Leary, Dmitri Klimov, and Devarajan Thirumalai, "HOPE: A Homotopy Optimization Method for Protein Structure Prediction", *Journal of Computation Biology*, 12(10):1275-1288, December 2005.

D. Steven Mackey, Niloufer Mackey, and Daniel M. Dunlavy, "Structure Preserving Algorithms for Perplectic Eigenproblems," *Electronic Journal of Linear Algebra*, 13:10-39, 2005.

Conference Proceedings

Michael S. Eldred and Daniel M. Dunlavy, "Formulations for Surrogate-Based Optimization with Data Fit, Multifidelity, and Reduced-Order Models", AIAA-2006-7117, *Proceedings of the 11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*, September 2006.

John M. Conroy, Daniel M. Dunlavy and Dianne P. O'Leary, "From TREC to DUC to TREC Again," *Proc. Text Retrieval Conference (TREC)*, November 2003.

Daniel M. Dunlavy, John M. Conroy, Judith D. Schlesinger, Sarah A. Goodman, Mary Ellen Okurowski, Dianne P. O'Leary, and Hans van Halteren, "Performance of a Three-Stage System for Multi-Document Summarization," *Proc. Document Understanding Conference (DUC)*, June 2003.

Daniel M. Dunlavy, John M. Conroy, and Dianne P. O'Leary, "QCS: A Tool for Querying, Clustering, and Summarizing Documents" *Proc. Human Language and Technology – North American Association of Computational Linguists (HLT-NAACL)*, June 2003.

Technical Reports

Daniel M. Dunlavy, Dianne P. O'Leary, John M. Conroy, and Judith D. Schlesinger, "QCS: A System for Querying, Clustering, and Summarizing Documents", SAND2006-5000, Sandia National Laboratories, Albuquerque, NM, October 2006.

Eldred, M.S., Brown, S.L., Adams, B.M., Dunlavy, D.M., Gay, D.M., Swiler, L.P., Giunta, A.A., Hart, W.E., Watson, J.-P., Eddy, J.P., Griffin, J.D., Hough, P.D., Kolda, T.G., Martinez-Canales, M.L. and Williams, P.J., "DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 4.0", Sandia National Laboratories Technical Reports, Albuquerque, NM, September-October 2006. Users Manual (SAND2006-6637), Developers Manual (SAND2006-4056), Reference Manual (SAND2006-4055).

Daniel M. Dunlavy, Tamara G. Kolda, W. Philip Kegelmeyer, "Multilinear Algebra for Analyzing Data with Multiple Linkages," SAND 2006-2079, Sandia National Laboratories, Albuquerque, NM, April 2006.

Daniel M. Dunlavy and Dianne P. O'Leary, "Homotopy Optimization Methods for Global Optimization", SAND 2005-7495, Sandia National Laboratories, Albuquerque, NM, December 2005.

Daniel M. Dunlavy, "Homotopy Optimization Methods and Protein Structure Prediction", PhD thesis, AMSC Program, University of Maryland, August 2005.

Daniel M. Dunlavy, "QCS: An Information Retrieval System for Improving Efficiency in Scientific Literature Searches", *M.S. Scholarly Paper*, Applied Mathematics and Scientific Computation Program, University of Maryland, December 2003.

D. Steven Mackey, Niloufer Mackey, and Daniel M. Dunlavy, "Structure Preserving Algorithms for Perplectic Eigenproblems," *Numerical Analysis Report No. 427*, Manchester Centre for Computational Mathematics, Manchester, England, May 2003.

Danny Dunlavy, Sookhyung Joo, Runchang Lin, Roummel Marcia, Aurelia Minut, and Jianzhong Sun, "Numerical Steady-State Solutions of Non-Linear DAE's Arising in RF Communication Circuit Design," *IMA Preprint Series* 1752-1, February 2001.

Other Publications

Danny Dunlavy, Chris Danforth, Aaron Lott, and Bob Shuttleworth, "Survival Guide for Graduate Students in Scientific Computation," Applied Mathematics and Scientific Computation Program, University of Maryland, Fall 2004.

Daniel M. Dunlavy, "Constitution of the Applied Mathematics and Scientific Computation Student Council", University of Maryland, August 2004.

Software Projects

DAKOTA: Design Analysis Kit for Optimization and Terascale Applications
`http://endo.sandia.gov/DAKOTA`

Trilinos: Parallel solver algorithms for large-scale, complex multi-physics applications
`http://software.sandia.gov/Trilinos`

QCS: Query, Cluster, Summarize information retrieval engine
`http://stiefel.cs.umd.edu:8080/qcs`

Talks/ Lectures

"Global Optimization: For Some Problems, There's HOPE," *Ninth Copper Mountain Conference on Iterative Methods*, Copper Mountain, CO, April 2006.

"Preconditioners for the Space-Time Solution of Large-Scale PDE Applications," *SIAM Conference on Parallel Processing*, San Francisco, CA, February 2006.

"A Homotopy Method for Predicting Low Energy Conformations of Proteins," *SIAM Conference on Computational Science and Engineering*, Orlando, FL, February 2005.

"A Homotopy Method for Finding Low Energy Conformations of Polypeptides," *SIAM Conference on the Life Sciences*, Portland, OR, July 2004.

"Clustering and Summarizing MEDLINE Abstracts," *Biomedical Information Science and Technology Initiative (BISTI) Symposium*, Bethesda, MD, November 2003.

"Structure Preserving Eigensolvers," *SIAM Applied Linear Algebra Meeting*, Williamsburg, VA, July 2003.

"A Homotopy Method for Predicting the State of Minimal Energy for Chains of Charged Particles," *Spotlight on Graduate Research Winner's Lecture*, Department of Mathematics, University of Maryland, February 2003.

"A Homotopy Method for Predicting the State of Minimal Energy for Chains of Charged Particles," *Graduate Research Interaction Day*, University of Maryland, April 2002.

"Mathematical Modeling in Industry: Notes from a Graduate Workshop," *Pi Mu Epsilon Colloquium Series*, Western Michigan University, January 2001.

Posters

"A Homotopy Method for Potential Energy Minimization of a Protein Model," *Bioscience Research and Technology Review Day*, University of Maryland, 2004.

"A Homotopy Method for Predicting the State of Minimal Energy for Chains of Charged Particles," *Bioscience Research and Technology Review Day*, University of Maryland, 2002.

"Structure Preserving Eigen- solvers," *SIAM Annual Meeting*, San Diego, CA, 2001.

Conferences

SIAM Conference on Science and Engineering, Costa Mesa, CA, February 2007. (*Minisymposium Organizer and Speaker.*)

AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Portsmouth, VA, September 2006. (*Contributed Paper.*)

Ninth Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, April 2006. (*Contributed Talk.*)

SIAM Conference on Parallel Processing, San Francisco, CA, 2006. (*Contributed Talk.*)

SIAM Conference on Science and Engineering, Orlando, FL, February 2005. (*Contributed Talk.*)

SIAM Conference on the Life Sciences, Portland, OR, 2004. (*Contributed Talk.*)

NLM Annual Training Meeting, Indianapolis, IN, 2004.

Digital Biology: Emerging Paradigm (BISTI), Bethesda, MD, 2003. (*Poster.*)

SIAM Conference on Applied Linear Algebra, Williamsburg, VA, 2003. (*Contributed Talk.*)

Document Understanding Conference, Edmonton, AL, 2003.

Human Language and Technology – North American Association of Computational Linguists, Edmonton, AL, 2003. (*Software Demonstration.*)

SIAM Conference on Optimization, Toronto, ON, 2002.

SIAM Annual Meeting, San Diego, CA, 2001. (*Poster.*)

Great Lakes Symposium on Applied Statistics, Kalamazoo, MI, 2000.

Graph Theory, Combinatorics, Algorithms and Applications, Kalamazoo, MI, 2000. (*Volunteer.*)

Professional Affiliations

Society of Industrial and Applied Mathematics (SIAM)

American Institute of Aeronautics and Astronautics (AIAA)

Pi Mu Epsilon

Phi Kappa Phi

Honors awards

John von Neumann Postdoctoral Fellowship, Sandia National Laboratories, 2005–2007.

Spot Recognition Award, Sandia National Laboratories, September 2006.

Biomedical Informatics Fellowship, National Library of Medicine, 2003–2005.

SIAM Student Travel Award, SIAM Conference on the Life Sciences, July 2004.

SIAM Student Travel Award, Applied Linear Algebra Conference, July 2003.

Winner, Spotlight on Graduate Research, University of Maryland, February 2003.

Graduate Resarch Assistantship, University of Maryland, 2001–2003.

Block Fellowship, University of Maryland, 2001–2003.

Graduate Teaching Assistantship, Western Michigan University, 2001–2003.

Phi Kappa Phi Honor Society, WMU, 2001.

Travel Award, Yousef Alavi Endowment Fund, 2000.

Joseph Blazek Engineering Scholarship, 1989–1994.

Marquette National Bank Scholarship, 1989.

SKILLS

Programming: C, C++, HTML, Java, Matlab, Maple, Pascal, Perl
Systems: Unix(SunOS,Linux), PC(Windows95/98/NT/2000/XP,DOS), Mac

REFERENCES

Available upon request.