**Part IV** 

# **Activity Data**

# **Publications**

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- 13. S. T. Erdogan, P. N. Quiroga, D. W. Fowler, H. A. Saleh, R. A. Livingston, E. J. Garboczi, P. M. Ketcham, J. G. Hagedorn, and S. G. Satterfield, "Three-dimensional Shape Analysis of Coarse Aggregates: New Techniques for and Preliminary Results on Several Different Coarse Aggregates and Reference Rocks," Cement and Concrete Research 36 (9) (September 2006), pp. 1619-1627.
- 14. H. Fang and D. P. O'Leary, "Stable Factorizations of Symmetric Tridiagonal and Triadic Matrices," *SIAM Journal on Matrix Analysis and Applications* **28** (2006), pp. 576-595.
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- 1. J. Bernal and C. Witzgall, "Integer Representation of Decimal Numbers for Exact Computations," *Journal of Research of the NIST* **111** (2) (March-April 2006).
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#### **Technical Reports**

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- 22. R. Somma, G. Ortiz, H. Barnum and E. Knill, "Efficient Solvability of Hamiltonians and Limits on the Power of Some Quantum Computational Models," *Physical Review Letters*.
- 23. B.J. Thijsse and B.W. Rust, "Freestyle Data Fitting and Global Temperatures," *Computing in Science & Engineering*.
- 24. W. E. Wallace, C. M. Guttman, K. M. Flynn, and A. J. Kearsley Numerical Optimization of Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry: Application to Synthetic Polymer Molecular Mass Distribution Measurement, Analytical Chemistry.

# **Presentations**

#### **Invited Talks**

- 1. I. Beichl, "Graphs and Matchings," National Security Agency, Fort Meade, MD, Sept., 19, 2006.
- T. Burns, "Steel Flow Stress Sensitivity to Temperature and Heating Rate: Recent Results from the NIST Pulse Heated Kolsky Bar," International Symposium on Plasticity, Halifax, Nova Scotia, Canada, July 17-22, 2006.
- 3. A. Carasso, "APEX Blind Deconvolution of Hubble Telescope Imagery and the Use of Levy Stable Laws," University of Minnesota School of Statistics Colloquium, October 20, 2005.
- A. Carasso, "APEX Blind Deconvolution of Hubble Space Telescope Imagery and Other Astronomical Data," Second International Conference on Scientific Computing and Partial Differential

- Equations and First East Asia SIAM Symposium, Hong Kong, China, December 12-16, 2005.
- A. Carasso, "Blind Deconvolution of Hubble Space Telescope Imagery," SIAM 2006 Image Science Meeting, Minisymposium on Variational and PDE Methods in Image Decomposition, Minneapolis, MN, May 17, 2006.
- M. J. Donahue, "Micromagnetics on Curved Geometries Using Rectangular Cells: Error Correction and Analysis," Micromagnetics: Experiments, Modeling, and Mathematical Theory Workshop, Bonn, Germany, Sept. 5, 2006.
- J. Fong, "NAS/NRC Postdoctoral Research Opportunities in Engineering and Mathematical Sciences at National Institute of Standards and Technology," Drexel University, Philadelphia, PA, Oct. 21, 2005.
- J. Fong, "Stochastic Modeling of Complex Structural System Failures and a Metrology-based Approach to V&V of Computer Simulations," Drexel University, Philadelphia, PA, Oct. 21 2005.
- J. T. Fong, "Scientific and Engineering Software (S&ES) Verification for Metrology and High-Consequence Engineering Applications," Computational & Statistical Science Seminar, Savannah River National Laboratory, Aiken, SC, April 27, 2006.
- J. Fong, "A Real-Time Non-Contact Direct-Measurement-based Reserve Capacity Modeling of an Earthquake Monitoring System," University of British Columbia, Vancouver, B.C., Canada, July 21, 2006.
- J. Fong, "A Reference-Benchmark Approach to Verification and Validation of High-Consequence Engineering System Simulations," University of British Columbia, Vancouver, B.C., Canada, July 28, 2006.
- 12. J. Fong, "Scientific and Engineering Software Verification for Metrology and High-Consequence Engineering Applications," Louisiana State University, Baton Rouge, LA., Sept. 29, 2006.
- J. Fong, "Stochastic Finite Element Method and Design of Experiments for Pressure Vessels & Piping Decision Making," ASME Pressure Vessels & Piping Conference, Vancouver, B.C., Canada, July 26, 2006.
- J. Fong, "Construction of a Helmholz Free Energy Function for an Isotropic Elastic-Viscoplastic Material," 2006 Meeting of the Society of Engineering Science, Penn State University, State College, PA, Aug. 14, 2006.

- 15. F. Hunt, "Visualizing the Frequency Patterns of DNA," New York University Faculty Resource Network Summer Program, New York, NY, June 16, 2006.
- S. Glancy, "Error Analysis For Encoding A Qubit In An Oscillator," Linear Optical Quantum Information Processing Workshop, Baton Rouge, Louisiana, April 9 - 12, 2006.
- 17. E. Knill, "Quantum Computing With Very Noisy Gates," Workshop on Trapped Ion Quantum Computing, NIST Boulder, February 21-24, 2006.
- E. Knill, "Fault-tolerant Architecture for Very Noisy Gates," University of Calgary, June 7, 2006.
- D. W. Lozier, "The DLMF Project: Lessons Learned and Future Directions," AMS Eastern Section Meeting, Bard College, Annandale-on-Hudson, NY, October 8, 2005.
- D. W. Lozier, "Math on the Web and the Digital Library of Mathematical Functions Project," SIAM Washington-Baltimore Section Meeting, Johns Hopkins University, Baltimore, MD, November 9, 2005.
- D. W. Lozier, "The Role of Computer Algebra in the DLMF Project," East Coast Computer Algebra Day, Drexel University, Philadelphia, PA, May 6, 2006.
- 22. G. McFadden, "Steady States and Oscillations in the p53/Mdm2 Network," NIH Laboratory of Molecular Pharmacology in the National Cancer Institute, Modeling Journal Club, October 18, 2005.
- 23. B. Miller, DLMF, "LaTeXML and Some Lessons Learned", Hot Topic Workshop on The Evolution of Mathematical Communication in the Age of Digital Libraries, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, December 8-9, 2006.
- D. P. O'Leary, "Matrix Factorizations for Information Retrieval," Stanford/Yahoo! Workshop on Modern Massive Datasets, Stanford, CA, June 2006.
- 25. D. Porter, Tcl Core Team Town Meeting, panel member, Portland, OR, October 26, 2005.
- B. Saunders, "Dynamic 3D Visualizations for the NIST Digital Library of Mathematical Functions," Twenty-first Willie Bee Rajanna Lecture, Department of Mathematics, Morgan State University, April 20, 2006.
- 27. A. Youssef, "Relevance Ranking and Hit packaging in Math Search," Hot Topic Workshop on The Evolution of Mathematical Communication in the Age of Digital Libraries, Institute for Mathematics

- and Its Applications, University of Minnesota, Minneapolis, December 8-9, 2006.
- 28. A. Youssef, "Roles of Math Search in Mathematics", 5th International Conference on Mathematical Knowledge Management, Wokingham, UK, August 11-12, 2006.

#### **Conference Presentations**

- D. M. Anderson, "Sharp-interface conditions for fluid-fluid systems undergoing phase transformation," American Physical Society, Division of Fluid Dynamics Annual Meeting, Tampa, FL, November 19-21, 2006.
- H. Bennett, A. Dienstfrey, L. Hudson, T. Oreskovic, T. Fuerst, and J. Sheppard, "Bone Mineral Density as a Biomarker for Assessing Bone Health: Bone Imaging," U.S.M.S. Workshop: Imaging as a Biomarker, NIST, Gaithersburg, Sept. 14-15, 2006.
- T. Burns, "Effect of Rapid Heating on the Flow Stress in a Carbon Steel of Interest in Manufacturing," 6th European Solid Mechanics Conference, Budapest, Hungary, August 28 - September 1, 2006.
- 4. M. J. Donahue and D. G. Porter, "Magnetization Normalization Methods for Landau-Lifshitz-Gilbert," MMM 2005, San Jose, California, Nov. 1, 2005.
- J. Dunkers, J. Hagedorn, A. Peskin, J. Kelso, J. Terrill, and L. Henderson, "Interactive, Quantitative Analysis of Scaffold Structure Using Immersive Visualization," poster presentation at 2006 Summer Bioengineering Conference, Amelia Island Plantation, Amelia Island, FL, June 21 - 25, 2006
- 6. W. George, J. Lancien, J. Terrill, "MPMD Program Model for Scientific Computing," Scatter/Gather Session II, Supercomputing 2005, Seattle, WA, Nov. 12-18, 2005.
- D. E. Gilsinn, M. A. McClain, and C. Witzgall, "Non-Oscillatory Splines on Irregular Data," SIAM Conference on Geometric Design and Computing, Phoenix, AZ, October 30-November 3, 2005.
- 8. S. Glancy, H. Vasconcelos, and E. Knill, "Production of Optical Coherent State Superpositions Using the Kerr Effect," Southwest Quantum Information and Technology, Albuquerque, NM, Feb. 16-19, 2006.
- 9. J. Hagedorn, J. Terrill, J. Kelso, and J. Dunkers, "Measurement of Tissue Engineering Scaffold

- Material," (video) DIVERSE Birds of a Feather session at the SIGGRAPH 2006 Conference, Boston, MA, August 2, 2006.
- R. Kacker, "Uncertainty Associated with Virtual Measurements from Computational Quantum Chemistry Models," National Conference of Standards Laboratories International (NCSLI) (www.ncsli.org), Nashville, TN, August 7-10, 2006.
- 11. A. Kearsley, "Recovery of Spheres from LADAR Data," IEEE Applied Imagery Pattern Recognition Workshop, Washington DC October 10, 2006
- 12. J. Kelso, "DIVERSE," DIVERSE Birds of a Feather (BOF) session; IEEE Visualization 2005 Conference, Seattle, WA, Nov. 12-18, 2005.
- 13. J. Lancien, W. George, and N. Martys, "Quaternion Dissipative Particle Dynamics," VCCTL Annual Meeting, NIST, Gaithersburg, MD, Nov. 29, 2005.
- 14. W .F. Mitchell, "The Addition of hp-Adaptivity to a Parallel Adaptive Finite Element Program," Twelfth SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, February 23, 2006.
- W.F. Mitchell, "PHAML: A Parallel hp-Adaptive Multigrid Program for 2D Elliptic Problems," Fifth International Conference on Scientific Computing and Applications, Banff, Alberta, Canada, May 18-21, 2006.
- S. Satterfield, "Shell Script VR," DIVERSE Birds of a Feather (BOF) session; IEEE Visualization 2005 Conference, Seattle, WA, Nov. 12-18, 2005.
- 17. B. Saunders, "From B-Spline Mesh Generation to Effective Visualizations for the NIST Digital Library of Mathematical Functions" Sixth International Conference on Curves and Surfaces, Avignon, France, June 29 July 5, 2006.
- J. Sims, G. Bryant, and H. Hung, "Excitons in Negative Band Gap Nanocrystals," American Physics Society March Meeting, Baltimore, MD, March 14, 2006.
- W. E. Wallace, C. M. Guttman, K. M. Flynn, and A. J. Kearsley, "Development of NIST SRM 2881, an Absolute Molecular Mass Distribution Polymer Standard," American Society for Mass Spectrometry Annual Meeting, Seattle, WA, May 28, 2006.

# **Software Released**

- J. Lancien, W. George, and N. Martys, Parallel QDPD code, Virtual Cement and Concrete Testing Laboratory.
- S. Langer, OOF2, Version 2.0 beta 8, Version 2.0.0, Version 2.0.1, <a href="http://www.ctcms.nist.gov/oof/oof2">http://www.ctcms.nist.gov/oof/oof2</a>
- 3. B. Miller, LaTeXML, Versions 0.4.1, 0.5.0, 0.5.1. <a href="http://dlmf.nist.gov/LaTeXML/">http://dlmf.nist.gov/LaTeXML/</a>
- 4. W. F. Mitchell, PHAML, Version 0.9.22, Version 0.9.23, Version 0.9.24, Version 0.9.25. <a href="http://math.nist.gov/tphaml">http://math.nist.gov/tphaml</a>
- W. F. Mitchell, f90gl, Version 1.2.11, Version 1.2.12. <a href="http://math.nist.gov/tf90gl">http://math.nist.gov/tf90gl</a>
- 6. W. F. Mitchell (co-developer), Zoltan, Version 2.0, Version 2.1. <a href="http://www.cs.sandia.gov/Zoltan/">http://www.cs.sandia.gov/Zoltan/</a>
- 7. D. Porter (release manager), Tcl/Tk, Version 8.4.12, Version 8.4.13, Version 8.5a4. http://www.tcl.tk/
- 8. R. Pozo, Sparse Basic Linear Algebra Subprograms (Sparse BLAS), ANSI C++ reference implementation. <a href="http://math.nist.gov/spblas/">http://math.nist.gov/spblas/</a>
- 9. R. Pozo, Template Numerical Toolkit (TNT), Version 3.0, Version 3.0.1, Version 3.0.2, Version 3.0.3. <a href="http://math.nist.gov/tnt">http://math.nist.gov/tnt</a>
- 10. R. Pozo, SciMark 2, Version 1.c (C version). http://math.nist.gov/scimark/
- 11. S. Satterfield, SAVG Visualization demos, <a href="http://math.nist.gov/mcsd/savg/demos/index.html">http://math.nist.gov/mcsd/savg/demos/index.html</a>

# **Conferences, Minisymposia, Lecture Series, Shortcourses**

#### **MCSD Seminar Series**

- 1. G.W. Stewart (MCSD), "Sparse Low-Rank Approximations to Sparse Matrices," October 12, 2005.
- J. Benedetto (University of Maryland), "Sigma-Delta Quantization and Finite Frames," November 2, 2005.
- B. Layton (Drexel University), "Nanometrology and Micrometrology in Biological Systems," November 29, 2005.

- 4. D. Tolani (Intelligent Automation, Inc.), "Symbolic Time Series Analysis (STSA) for Anomaly Detection," December 6, 2005.
- J. Boyar (University of Southern Denmark), "Scheduling Jobs on Grid Processors," Jan. 10, 2006
- S. Hagstrom (Indiana University), "Hylleraas-CI Calculations on the Beryllium Atom: A Progress Report," Jan. 24, 2006.
- C. Shakarji (MEL), "A Look at Mathematical and Computational Issues in Manufacturing Inspection Using Coordinate Measuring Machines," Jan. 31, 2006.
- 8. S. Dey (Naval Research Laboratory), "Recent Advances in Finite Element Methods for Structural Acoustics," Mar. 28, 2006.
- A. Varshney (University of Maryland), "Visual Computing: At the Crossroads of Realism, Modeling, and Perception," Apr. 12, 2006.
- C. Witzgall (ITL), G. Cheok (BFRL), A. Kearsley (ITL), "Recovery of Spheres from LADAR Data," May 23, 2006.
- J. Teresco (Williams College), "Parallel Adaptive Scientific Computation in Heterogeneous, Hierarchical, and Non-Dedicated Computing Environments," June 15, 2006.
- 12. B. Sneiderman (University of Maryland), "The Thrill of Discovery: Information Visualization for High Dimensional Spaces," Oct. 3, 2006.
- 13. M. Mascagni (Florida State University), "Using Simple Stochastic Differential Equations to Solve Complicated Partial Differential Equations," Oct. 18, 2006.
- 14. S. Bullock (IDA Center for Computing Sciences), "Projecting onto Qubit Irreps of Young Diagrams," Nov. 21, 2006.
- 15. B. Alpert (MCSD), "Sparse Representations and High Dimensional Geometry: What's the Excitement?" Dec. 5, 2006.

# **Local Events Organized**

- 1. S. Langer, Organizer, OOF2 Workshop, August 2006.
- A. Peskin, Member, Planning Board, Metrology for the Magnetic Data Storage Industry, USMS Workshop, October 20-21, 2005.
- J. Terrill, Member, Planning Board, Developing New Standards for Antibody Measurement: Bring-

ing Metrology to Serology, USMS Workshop, February 21-22, 2006.

### **External Events Organization**

- R. Boisvert, Organizing Committee, IFIP Working Conference on Grid-based Problem Solving Environments: Implications for Development and Deployment of Numerical Software, Prescott, Arizona, July 17-21, 2006.
- R. Boisvert, Co-organizer, Minisymposium on "Recent Advances in Software Tools for Scientific Computing", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
- 3. J. Fong, Co-developer, Panel Session, ASME Pressure Vessels and Piping Division Conference, July 23-27, 2006, Vancouver, Canada.
- 4. D. W. Lozier, Co-organizer, Minisymposium on "Computation and Application of Special Functions in Scientific Computing," SIAM Annual Meeting, Boston, MA, July 10-14, 2006.
- D.W. Lozier, Program Committee, Fifth International Conference on Mathematical Knowledge Management, Reading, UK, August 10-12, 2006.
- 6. D. W. Lozier, Co-organizer, Minisymposium on "Mathematical Knowledge Management", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
- 7. W. Mitchell, Scientific Committee, International Conference of Numerical Analysis and Applied Mathematics, Crete, Greece, September 2006.
- W. Mitchell, Program Committee, International Conference on High Performance Computing, Networking and Communication Systems, Orlando, FL, July 2007.
- F. Potra, Co-organizer, Minisymposium on "Interior Point Methods for Linear Programming", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
- S. Satterfield and J. Kelso, Co-organizers, Birds of a Feather Session on "DIVERSE", IEEE Visualization 2005 Conference, Minneapolis, MN, Oct. 23-28, 2005.
- 11. S. Satterfield and J. Kelso, Organizers, Birds of a Feather Session on "DIVERSE", SIGGRAPH 2006 Conference, Boston, MA, Aug. 2, 2006.

# **Other Professional Activities**

#### Internal

- R. Boisvert and Abbie O'Gallagher, ITL Diversity Committee.
- R. Boisvert, ITL representative, NIST Nanotechnology Strategic Working Group.
- 3. R. Boisvert, ITL representative, NIST Scientific Computing Steering Group.
- 4. D. Porter, MCSD representative, ITL Awards Committee.
- Staff members regularly review manuscripts for the Washington Editorial Review Board (WERB) and the Boulder Editorial Review Board (BERB), as well as proposals for the NIST ATP and SBIR programs.

#### **External**

#### **Editorial**

- 1. B. Alpert, Associate Editor, SIAM Journal on Scientific Computing.
- 2. I. Beichl, Column Editor, *Computing in Science & Engineering*.
- 3. R. Boisvert, Associate Editor, ACM Transactions on Mathematical Software.
- 4. R. Boisvert, Area Editor (Numerical Analysis, Mathematical Software, and Computational Engineering, Finance, and Science), Computing Research Repository (CoRR), <a href="https://www.arXiv.org">www.arXiv.org</a>.
- 5. D. Gilsinn, special issue editor, *Journal of Research of the NIST*, Vol. 111, no. 2, March-April, 2006.
- 6. D. Gilsinn, Associate Editor, ASME Journal of Computational and Nonlinear Dynamics.
- 7. R. N. Kacker, Member, Editorial Board, *Journal of Applied Statistics*.
- 8. R. N. Kacker, Member, Editorial Board, *Total Quality Management and Business Excellence*.
- 9. D. Lozier, Associate Editor, *Mathematics of Computation*.
- 10. G. McFadden, Associate Editor, *Journal of Crystal Growth*.
- 11. G. McFadden, Associate Editor, *Interfaces and Free Boundaries*.
- 12. G. McFadden, Associate Editor, SIAM Journal on Applied Mathematics.

- 13. W. Mitchell, Associate Editor, Applied Numerical Analysis and Computational Mathematics.
- 14. W. Mitchell, Associate Editor, Journal of Numerical Analysis, Industrial and Applied Mathematics
- 15. W. Mitchell, Associate Editor, International Journal of Applied Mathematics and Computational Science.
- 16. R. Pozo, Associate Editor, ACM Transactions on Mathematical Software.
- 17. J. Terrill, Special Issue Co-Editor (with Yang Cai of Carnegie Mellon University), Journal of Information Visualization (on Visual Analysis of Human Dynamics).

#### **Boards and Committees**

- R. Boisvert, Co-chair, Publication Board, Association for Computing Machinery (ACM).
- 2. R. Boisvert, Ex-Officio Member, ACM Council.
- R. Boisvert, Member, ACM Awards Committee.
- 4. R. Boisvert, Chair, International Federation for Information Processing's Working Group 2.5 (Numerical Software).
- R. Boisvert, Member, External Review Panel, Institute for Defense Analysis' Center for Computing Sciences.
- 6. F. Hunt, Member, Executive Committee, Association for Women in Mathematics.
- 7. F. Hunt, Organizer, Joint Association for Women in Mathematics and European Women in Mathematics Olga Taussky Todd Prize Committee.
- 8. D. Lozier, Vice Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
- 9. B. Miller, Member, Math Working Group, W3C (the World Wide Web Consortium).
- 10. D. Porter, Member, Tcl Core Team.
- 11. J. Terrill, OpenFPGA Working Group.
- 12. J. Terrill, Federal High End Computing Implementation Task Force.
- 13. J. Terrill, Federal High End Computing Research and Development, and Infrastructure Interagency Working Groups, Networking and Information Technology Research and Development Program.

#### Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including ACM Transactions on Mathematical Software, Applied Mathe-

matics Letters, ASME Journal of Computational and Nonlinear Dynamics, ASME Journal of Manufacturing Science and Engineering, Computing in Science and Engineering, IEEE Society for Signal Processing, IEEE Transactions on Magnetics, IEEE Transactions on Microwave Theory and Techniques, International Journal of Plasticity, International Journal of Information Visualization, International Journal of Plasticity, Journal of Computational and Nonlinear Dynamics, Journal for Computer-Aided Engineering and Software, Journal of Information Visualization, Journal of Magnetism and Magnetic Materials, Journal of Mass Spectroscopy, Journal of Mathematical Analysis and Applications, Journal of the Mechanics and Physics of Solids, Journal of Physics D: Applied Physics, Journal of Vibration and Control, Nonlinear Dynamics, Physical Review A, Physical Review B, Physical Review Letters, Physics Letters A, SIAM Journal on Optimization, SIAM Journal of Scientific Computing, Software - Practice and Experience, The International Journal for Human Computer Studies.

Staff members review proposals for the following research programs: Department of Energy, Department of Homeland Security, Engineering and Physical Sciences Research Council (EPSRC), and the NSF.

# **External Contacts**

MCSD staff members make contact with a wide variety of organizations in the course of their work. Examples of these follow.

#### **Industrial Labs**

3M 3Motion Project (UK) American Concrete Assoc. American Hydro Corp. Apple Computer Bank of America Borg Warner Transmission Systems Chesapeake Cryogenics

Cisco Systems

DrecWay

Dupont

Electro Science Technologies

Elligno Inc.

Fakespace

Ford Research Labs

GE Corporate R&D

GeoCap

IBM Research

Industrial Light and Magic Intelligent Automation, Inc.

Invensys JAMSTEC JP Engineering KTH Solid Mechanics

Landacorp Mac.com

Medical Media Lab Merck Pharmaceutical Northwest Numerics, Inc. O'Donnell Consulting Engineers

Proctor & Gamble

Pulsic Quovadx

Rationelle Software-Entwicklung

Raytheon Corp. RedOlive, Inc.

Roche Molecular Systems, Inc.

Schweitzer Engineering Laboratories, Inc.

Setterholm, Inc.

SGI Siemens

Siemans Westinghouse Power Corporation

Simplified Logic, Inc. The MathWorks, Inc. Timken Company Torrent Corp. (Spain)

UGS Corp.

United Technologies Research Center

Verari Systems

Xerox Xilinx

#### **Government/Non-profit Organizations**

Air Force Research Lab Army Research Lab

Catania Astrophysical Observatory

Hanscom Air Force Base Institute for Defense Analysis

J. Stefan Institute

N. Inst. Adv. Industrial Sci. Tech. (AIST, Japan)

Kirtland Air Force Base

Lawrence Livermore national Laboratory Los Alamos National Laboratory

Medical Res. Council Lab. of Molecular Biology (UK)

NASA

National Institutes of Health Naval Research Laboratory National Security Agency National Science Foundation Oak Ridge National Laboratory Ohio Supercomputer Center Sandia National Laboratories Savannah River National Laboratory

U.S. Department of Defense

#### Universities

A&T State University Arizona State University

Bard College Beloit College

Carnegie Mellon University California Institute of Technology

Columbia University

Dalhousie University (Canada)

Delft University of Technology (The Netherlands)

Dresden University (Germany)

Drexel University

Federal University of Parana (Brazil)

Florida State University

Georg August Universität Göttingen (Germany)

George Mason University Georgetown University George Washington University Hong Kong University (China)

Howard University Indiana University

Indiana University - Purdue University Indianapolis International University of Bremen (Germany)

Jackson State University Johns Hopkins University Louisiana State University Macalester College

Massachusetts Institute of Technology

Monash University (Australia)

Moscow State Technical University (Russia)

Penn State University

Polish Academy of Sciences (Poland)

Purdue University

Rudjer Boskovic Institute (Croatia) Russian Academy of Sciences (Russia)

San Diego State University

Siena College

Southern Methodist University

Stanford University

State University of New York

Technische Universität Berlin (Germany) Technische Universität Darmstadt (Germany) Technische Universität Munchen (Germany)

Tel Aviv University
Trinity University
Tufts University
Tulane University
U. Catolica de Valparaiso
University College London

Universidade Federal de Pernambuco (Brazil) Universidade Federal do Rio de Janeiro (Brazil)

Universitat GHS Essen

University of Abertay Dundee (UK) University of British Columbia University of California Los Angeles

University of Colorado

University of Edinburgh (IK) University of Erlangen (Germany)

University of Ferrara University of Florida

University of Kent at Canterbury (UK)

University of Houston

University of Illinois-Urbana/Champaign

University of Indiana University of Leeds University of Liverpool University of Maryland

University of Massachusetts Amherst

University of New Mexico

University of Maryland College Park University of Maryland Baltimore Country

University of Michigan University of Minnesota University of Modena (Italy) University of Pittsburgh

University of Sherbrooke (Canada) University of South Carolina University of Southern Denmark University of Strathclyde (Scotland)

University of Tech. Belfort-Montbeliard (France)

University of Tennessee

University of Texas at Arlington

Univ. of Texas, MD Anderson Cancer Ctr.

University of Tokyo (Japan) University of Torino (Italy) University of Toronto (Canada)

University of Warwick (United Kingdom)

University of Washington
University of Waterloo (Canada)
University of Western Australia
University of Windsor (Canada)
University of Wisconsin - Madison
University of Wisconsin - Milwaukee

Virginia Polytechnic Institute and State Univ.

Wake Forest University

Washington University (St. Louis) Wentworth Institute of Technology

Williams College

# Part V

# Appendices

# **Staff**

MCSD consists of full time permanent staff located at NIST laboratories in Gaithersburg, MD and Boulder, CO. This is supplemented with a variety of faculty appointments, guest researchers, postdoctoral appointments, and student appointments. The following list reflects all appointments held during FY 2006.

**Legend**: F = Faculty Appointee, GR = Guest Researcher, PD = Postdoctoral Appointee, S = Student, PT= Part time

#### **Division Staff**

Ronald Boisvert, *Chief*Robin Bickel, *Secretary*Jeffrey Fong

Roldan Pozo Christopher Schanzle David Warshawsky, S

# **Mathematical Modeling Group**

Geoffrey McFadden, Leader
Bradley Alpert (Boulder)
Timothy Burns
Alfred Carasso
Andrew Dienstfrey (Boulder)
Michael Donahue
Fern Hunt
Raghu Kacker
Anthony Kearsley
Peter Ketcham
Stephen Langer
Agnes O'Gallagher (Boulder)
Donald Porter

Mirit Aladjem, GR
Daniel Anderson, GR, F
Richard Braun, F
David Cotrell, GR
Michael Forbes, S
Katharine Gurski, GR
Seung-Ill Haan, GR
Sohyoung Kim, GR
Dianne O'Leary, F
Florian Potra, F
Sita Ramamurti, GR
Richard Yeh, G

# **Mathematical Software Group**

Daniel Lozier, Leader Marjorie McClain Bruce Miller William Mitchell Bert Rust Bonita Saunders Liuyan Chen, S

Joyce Conlon, GR Bruce Fabijonas, F Leonard Maximon, GR Frank Olver, GR G.W. Stewart, F Abdou Youssef, F

# **Optimization and Computational Geometry Group**

Ronald Boisvert, Acting Leader

Isabel Beichl Javier Bernal David Gilsinn

Emanuel Knill (Boulder)

Stephen Bullock, PD, GR

Zachary Catlin, S Theodore Einstein, GR Saul Gass, F

Scott Glancy, PD (Boulder)

James Lawrence, F David Song, GR Francis Sullivan, GR Christoph Witzgall, GR

AnochaYimsiriwattana, GR

# **Scientific Applications and Visualization Group**

Judith Terrill, Leader

Yolanda Parker, Office Manager

Robert Bohn William George Terence Griffin John Hagedorn Howard Hung

John Kelso

Adele Peskin (Boulder)

Steven Satterfield James Sims

Thomas Bugnazet, GR Julien Lancien, GR Adam Lazrus, S Christine McKay, S Marc Olano, F

# **Glossary of Acronyms**

ACL Association for Computational Linguistics ACM Association for Computing Machinery

ACS Advanced Camera for Surveys
ADI alternating direction implicit
AFM atomic force microscope

ANSI American National Standards Institute

APS American Physical Society

ASME American Society of Mechanical Engineers
ATP NIST Advanced Technology Program
BFRL NIST Building and Fire Research Laboratory

BLAS Basic Linear Algebra Subprograms

BMC BioMed Central BO Born-Oppenheimer

CEM computational electromagnetics
CIO NIST Chief Information Officer

CODATA Committee on Data for Science and technology
COLING International Committee on Computational Linguistics

CPU central processing unit CSS Calderbank-Shor-Steane

CSTL NIST Chemical Science and Technology Laboratory
CWI Centrum voor Wiskunde en Informatica (Amsterdam)
DARPA DOD Defense Advanced Research Projects Agency

DIVERSE Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (visualization

software)

DLMF Digital Library of Mathematical Functions (MCSD project)

DOD U.S. Department of Defense
DOE U.S. Department of Energy
DOJ U.S. Department of Justice
DPD dissipative particle dynamics
DSO distributed shared object

EEEL NIST Electronics and Electrical Engineering Laboratory

FEM finite element method FFT fast Fourier transform

FY fiscal year

GAMS Guide to Available Mathematical Software

GPU Graphics processing unit IDA Institute for Defense Analysis

IEEE Institute of Electronics and Electrical Engineers

IML++ Iterative Methods Library

IMPI Interoperable Message Passing Interface

IT information technology

ITL NIST Information Technology Laboratory

IV immersive visualization

IVE immersive visualization environment

IFIP International Federation for Information Processing

JAMA Java Matrix package LADAR laser detection and ranging

MALDI-TOF matrix-assisted laser desorption/ionization time-of-flight MCSD ITL Mathematical and Computational Sciences Division

MEL NIST Manufacturing Engineering Laboratory
MIT Massachusetts Institute of Technology
MKM mathematical knowledge management

MPI Message Passing Interface MRI magnetic resonance imaging MSEL NIST Materials Science and Engineering Laboratory

MV++ Matrix/Vector Library

μCT x-ray micro-computed tomography
 μmag Micromagnetics Activity Group
 NIH National Institutes of Health

NIST National Institute of Standards and Technology

NISTIR NIST Internal Report

NITRD Networking and Information Technology Research and Development

NASA National Aeronautics and Space Administration

NOAA National Oceanographic and Atmospheric Administration

NNSA National Nuclear Security Administration

NRC National Research Council
NSA National Security Agency
NSF National Science Foundation
OCT optical coherence tomography
ODE ordinary differential equation

OLES NIST Office of Law Enforcement Standards
OOF Object-Oriented Finite Elements (software package)

OOMMF Object-Oriented Micromagnetic Modeling Framework (software package)

PDE partial differential equation PET positron emission tomography

PHAML Parallel Hierarchical Adaptive Multi Level (software)
PITAC President's Information Technology Advisory Committee

PL NIST Physics Laboratory PSF point spread function

QDPD quarternion-based dissipative particle dynamics RAVE Reconfigurable Automatic Virtual Environment

S&E science and engineering

SAVG MCSD Scientific Applications and Visualization Group

SECB slow evolution from the continuation boundary SED NIST/ITL Statistical Engineering Division

SEM scanning electron microscope

SIAM Society for Industrial and Applied Mathematics SIGGRAPH ACM Special Interest Group on Graphics

SIMA NIAT Systems Integration for Manufacturing Applications Program

SOR successive overrelaxation

SPIE International Society for Optical Engineering

SRM standard reference material SSS Screen Saver Science

SURF Student Undergraduate Research Fellowship

TNT Template Numerical Toolkit

UMCP University of Maryland College Park

VCCTL Virtual Cement and Concrete Testing Laboratory

VRML virtual reality modeling language
W3C World Wide Web Consortium
XML Extensible Markup Language