Part III

Activity Data

Publications

Appeared

Books and Book Chapters

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2. S.E. Russek, R.D. McMichael, M.J. Donahue and S. Kaka, "High-speed switching and rotational dynamics in small magnetic thin-film devices," in *Spin Dynamics in Confined Magnetic Structures II (Topics in Applied Physics)* **87**, Burkard Hillebrands and Kamel Ounadjela (Eds.), Springer-Verlag, 2003.
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3. A. Andreas and I. Beichl, "Estimating the Work in Integer Partitioning," *IEEE Computing in Science and Engineering* **5** No. 1 (Jan.-Mar. 2003), pp. 48-56.
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5. H.S. Bennett and H. Hung, "Dependence of Electron Density on Fermi Energy in N-Type Gallium Antimonide," *Journal of Research of the National Institute of Standards and Technology* **108**, Number 3 (May-June 2003), pp. 193-198.
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11. M.J. Donahue, G. Vertesy, and M. Pardavi-Horvath, "Defect Related Switching Field Reduction in Small Magnetic Particle Arrays," *Journal of Applied Physics* **93** (2003), pp. 7038-7040.
12. B.R. Fabijonas, D.W. Lozier and J.M. Rappoport, "Algorithms and Codes for the Macdonald Function: Recent Progress and Comparisons," *Journal of Computational and Applied Mathematics* **161** (1) (November 15, 2003), pp. 179-192.
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14. D. Gilsinn, H. Bandy and A. Ling, "A Spline Algorithm for Modeling Cutting Errors on Turning Centers," *Journal of Intelligent Manufacturing* **13** (2002), pp. 391-401.
15. D. Gilsinn, "Estimating Critical Hopf Bifurcation Parameters for a Second-Order Delay Differential Equation with Application to Machine Tool Chatter," *Nonlinear Dynamics* **30** (2002), pp. 103-154.
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17. P. Huang and R. Kacker, "Repeatability and Reproducibility Standard Deviations in the Measurement of Trace Moisture Generated Using Permeation Tubes," *Journal of Research of the National Institute of Standards and Technology* **108** (2003), pp. 235-240.

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30. D. Song, G. Brennen, and C. Williams, "Quantum Computer Architecture Using Nonlocal Interactions," *Physical Review A* **67** (2003), p. 050302.

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2. J.E. Devaney and J.G. Hagedorn, "Discovery in Hydrating Plaster Using Multiple Machine Learning Methods," *Lecture Notes in Computer Science* **2534** (November 2002), pp. 47-58.

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7. G. McFadden, "Phase-field Models of Solidification," in *Contemporary Mathematics*, Recent Advances in Numerical Methods for Partial Differential Equations and Applications **306**, Knoxville, TN, May 10-12, 2001, X. Feng and T.P. Schulze (Eds.), (American Mathematical Society, Providence, RI, 2002), pp. 107-145.

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3. D.E. Gilsinn, G.S. Cheok, D.P. O'Leary, "Deconvolving LADAR Images of Bar Codes for Construction Site Object Recognition," NISTIR 7044, September 2003.

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3. G. Cheok, W. Stone, and C. Witzgall, "Some Issues Relating to Performance Evaluation of LADARs," Sept. 17, 2003, *Proceedings of PerMIST-03*.

4. M. J. Donahue and D. G. Porter, "Exchange Energy Formulations for 3D Micromagnetics," *Physica B*.

5. M.J. Donahue and D.G. Porter, "Simulation of Transverse Domain Wall Dynamics," *Journal of Applied Physics*.

6. D.E. Gilsinn and A.V. Ling, "Comparative Statistical Analysis of Test Parts Manufactured in Production Environments," *ASME Journal of Manufacturing Science and Engineering*.

7. D.E. Gilsinn, G.S. Cheok, D.P. O'Leary, "Deconvolving LADAR Images of Bar Codes for Construction Site Object Recognition," *Journal of Automation in Construction*.

8. D.E. Gilsinn, "Approximating Limit Cycles of a Van der Pol Equation with Delay," *Proceedings of Dynamic Systems and Applications*.

9. J.E. Guyer, W.J. Boettinger, J. A. Warren, and G.B. McFadden, "Phase-field Modeling of Electrochemistry: Equilibrium," *Physical Review E*.

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14. A. Kearsley, "An Optimization Approach to Multiple Sequence Alignment," *Applied Mathematics Letters*.

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16. A.J. Kearsely and L.A. Melara, Jr., "Simulation of an Austenite-twinned-Martensite Interface," *NIST Journal of Research*.

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1. D. Basak, H.W. Yoon, R. Rhorer, T. Burns, T. Matsumoto, "Temperature Control of Pulse Heated Specimens in a Kolsky Bar Apparatus Using Microsecond Time-Resolved Pyrometry," *Proceedings of the Fifteenth Symposium on Thermophysical Properties*, Boulder, CO, June 22-27, 2003.

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9. G. Cheok and C. Witzgall, "TIN Methods for Surface Generation," NISTIR.

10. J. Douglas, N. Martys, and J. Hagedorn, "Breakup of a Fluid Thread in a Confined Geometry: Droplet-Plug Transition, Perturbation Sensitivity, and Kinetic Stabilization with Confinement," *Physical Review E*.

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19. R. Kacker, "Combining Information from Interlaboratory Studies Using Random Effects Model," *Technometrics*.
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24. S. Satterfield, Quicktime video of the Smart Gel immersive visualization demo, SC2003.
25. T.L. Schmitz, J.C. Ziegert, T.J. Burns, B. Dutterer, and W.R. Winfough, "Tool Length-dependent Stability Surfaces," *Society of Manufacturing Engineer's (SME) Journal of Manufacturing Processes*.
26. J.S. Sims and N.S. Martys, "Simulation of Sheared Suspensions with a Parallel Implementation of QDPD," *Computer Physics Communications*.
27. Y. Son, K. Migler, N. Martys, and J. Hagedorn, "The Effect of Confinement on the Capillary Instability of a Polymer Thread: An Experimental and Numerical Study," *Macromolecules*.
28. D. Song, G. Brennen, and C. Williams, "Quantum Computer Architecture," *Proceedings of Quantum Communication, Measurement and Computing*.
29. D. Song, "Post-measurement Nonlocal Gates," *Journal of Optics B: Quantum and Semiclassical Optics*.
30. D. Song, "Secure Key Distribution by Swapping Quantum Entanglement," *Physical Review Letters*.
31. D. Wheeler, I.P, Moffett, G.B. McFadden, S.R. Coriell, and D. Josell, "Influence of a Catalytic Surfactant on Roughness during Film Growth," *Journal of the Electrochemical Society*.
32. R. C. Wittmann, B. K. Alpert, and M. H. Francis, "Near-Field, Spherical-Scanning Antenna Measurements Using Nonideal Measurement Locations," *IEEE Transactions on Antennas and Propagation*.
33. C. Witzgall, G. Cheok, and J. Bernal, "TIN Techniques for Data Analysis and Surface Construction," *NISTIR*.

In Process

1. I. Beichl, M. Robinson, D. Song, and F. Sullivan, "A Quantum Algorithm for Determining if a Function is One to One."
2. I. Beichl and F. Sullivan, "Grover's Algorithm: Lower Bounds on Quantum Complexity."
3. H.S. Bennett and H. Hung, "Dependence of Electron Density on Fermi Energy in N-type Gallium Antimonide."
4. C. Brown, H. Bullen, S. Kelly, R. Xiao, S. Satterfield, J. Hagedorn, J. Devaney, "Visualization and Data Mining in a 3D Immersive Environment: Summer Project 2003."
5. T.J. Burns and T.L. Schmitz, "Receptance Coupling Analysis for Prediction of Tool-Point Frequency Response."
6. K. S. Downs, M. A. Hamstad and A. O'Gallagher, "Wavelet Transform Signal Processing to Distinguish Different Acoustic Emission Sources."
7. W.L. George, "Constructing a Distributed Parallel Computing Environment using Jini and JavaSpaces," *IEEE Computing in Science and Engineering*.
8. W.L. George, A. Lumsdaine, J. Squyres, J. Hagedorn, J. Devaney, "Interoperable MPI," *IEEE Transactions on Parallel and Distributed Systems*.
9. K.F. Gurski, G.B. McFadden, and M.J. Miksis, "The Effect of Contact Lines on the Rayleigh Instability with Anisotropic Surface Energy."
10. M. A. Hamstad, K. S. Downs and A. O'Gallagher, "Practical Aspects of Acoustic Emission Source Location by a Wavelet Transform."

11. F. Hunt, "Sample Path Optimality for a Markov Optimization Problem."
12. R. Kacker, R. Datla, and A. Parr, "Response to Comments on Combined Result and the Associated Uncertainty from Interlaboratory Evaluations."
13. R. Kacker and R. Dersimonian, "Quantification of Uncertainty in Meta-analysis."
14. R. Kacker, R. Datla, and A. Parr, "Statistical Interpretation of Key Comparison Reference Value, Degrees of Equivalence, and Their Associated Uncertainties."
15. R. Kacker, R. Datla, and A. Parr, "Statistical Analysis of CIPM Key Comparisons Based on the ISO Guide."
16. A.J. Kearsley and L.A. Melara, Jr., "Computational Simulation of Twinned-Martensite Using Symmetric P_2 Finite Element Mesh."
17. A.J. Kearsley, L.A. Melara Jr., and M.C. Villalobos, "Numerical Experiments with Total Variation Denoising Problems."
18. D. Matheu, C. Gonzalez and R. Kacker, "Uncertainty Associated with Reaction Barrier of Transition State in Bi-molecular Reactions."
19. W.F. Mitchell, "A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids".
20. B. Rust and D. O'Leary, "A Truncated Singular Component Method for Ill-Posed Problems."
21. B. Rust and B. Thijsse, "Spline Fits to Conventional Smoothing Spline Fits and Parameterized Model Fits to Measured Time Series Data."
22. J.S. Sims and S.A. Hagstrom, "Math and Computational Issues in High Precision Hy-CI Variational Calculations."
23. J. Slutsker, A.L. Roytburd, W.J. Boettinger and J.A. Warren, G.B. McFadden, K. Thornton, P. Voorhees, "Phase-field Modeling of Solidification Under Stress."
24. C. Witzgall, J. Bernal, and G. Cheok, "Assessing the Accuracy of Just Meshing."

Visualizations Published

1. T. Griffin, P. Ketcham, D. Feder, S. Satterfield, C. Clark, and J. Devaney, "Animation of a Bose-Einstein condensate visualization," in "From Terabytes to Insights," shown at the opening session of the Supercomputing 2002 conference, November 19, 2002, Baltimore, MD.
2. P. Ketcham, "Image of a Bose-Einstein Condensate," appeared on a poster by the Research and Development Centre on Bose-Einstein Condensation, Trento, Italy, announcing the Inauguration Meeting and Celebration of Lev Pitaevskii's 70th Birthday, March 14-15, 2003.
3. P. Ketcham, "Animation of a morphing cement aggregate", appeared in presentations given by Edward Garboczi (861) at the Virtual Cement and Concrete Testing Laboratory (VCCTL), Bi-Annual Consortium Meeting, Dusseldorf, Germany, Dec 2-3, 2002.
4. T. Griffin and J. Sims, "Movies of cement flow under various conditions including density variations, flow through rebars, and in rheometers", Virtual Cement and Concrete Testing Laboratory (VCCTL), Bi-Annual Consortium Meeting, Dusseldorf, Germany, December 2-3, 2002.

Presentations

Invited Talks

1. R.F. Boisvert, "A Handbook of Special Functions for the Digital Age," British Applied Mathematics Colloquium, University of Southampton, UK, April 8, 2003.
2. R.F. Boisvert, "A Handbook of Special Functions for the Digital Age," International Workshop on Numerical and Symbolic Scientific Computing, St. Wolfgang, Austria, June 17, 2003.
3. S. Bullock, "An Arbitrary Quantum Computation in 23 Gates," Quantum Information and Bose-Einstein Condensate Seminar, NIST Physics Laboratory, Gaithersburg, MD, August 8, 2003.
4. S. Bullock, "Symmetry Groups of the n-tangle and Maximal Concurrence," Institute for Defense Analysis, Center for Computing Sciences, Bowie, MD, Sept. 8, 2003.

5. S. Bullock, "Quantum Circuit Design and the Word Problem on $SU(2^n)$," Workshop on Locally Symmetric Spaces, Mathematische ForschungsInstitut Oberwolfach, Baden-Würtemburg, Germany, October 1, 2003.
6. A.S. Carasso, "The APEX Method in Image Sharpening and Heavy-Tailed Point Spread Functions," National Institutes of Health, November 14, 2002.
7. M.J. Donahue, "Exchange Energy Formulations for 3D Micromagnetics," Applied Math Lab Seminar, New York University, New York, NY, Apr 10, 2003.
8. J. Fong, "Mathematical Modeling of Structures on Fire: Deterministic or Stochastic," Division of Mechanics and Computation, Dept. of Mech. Engineering, Stanford University, Stanford, CA, June 13, 2003.
9. D.E. Gilsinn, "Approximating Limit Cycles of a Van der Pol Equation with Delay," 4th International Conference on Dynamic Systems and Applications 4, Atlanta, GA, May 20, 2003.
10. K. Gurski, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability," Department of Mathematics and Statistics Seminar, University of Maryland Baltimore County, October 28, 2002.
11. K. Gurski, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability, Department of Engineering Sciences and Applied Mathematics Colloquium, Northwestern University, Chicago, IL, November 4, 2002.
12. K. Gurski, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability, Materials Science and Engineering Lab Brown Bag Lunch Seminar, NIST, October 17, 2002.
13. F. Hunt, "An Introduction to Genetic Sequence Alignment" Mathematical Association of America New Jersey Section, Fairleigh Dickinson University, Newark, NJ, October 26, 2002.
14. F. Hunt, "Progress on a Linear Program Based Algorithm for Multiple Sequence Alignment," Bioinformatics Institute and Mathematics Department of the University of Maryland, Baltimore County, February 13, 2003.
15. F. Hunt, "A Proposed Multiple Sequence Alignment Scheme Based on solving a Linear Programming Problem," National Library of Medicine, Computational Biology Division, NIH, April 30, 2003.
16. R. Kacker, "Uncertainty in Virtual Measurements," DOE/NSF/SIAM Workshop on Predictability of Complex Phenomena, Los Alamos National Laboratory, Santa Fe, NM, December 16-18, 2002.
17. A. Kearsley, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," Workshop on Methods for Mass Spectroscopy, NIST, November 7, 2002.
18. A. Kearsley, "An Infeasible Point Method for Solving an Interesting Class of 0/1 Programming Problems," Department of Mathematics and Statistics Colloquium, University of Maryland, Baltimore. MD, April 4, 2003.
19. S.A. Langer, "Object Oriented Modeling of Microstructural Physics," Colloquium of the Laboratory for Computer Design of Materials, George Mason University, March 26, 2003.
20. S.A. Langer and E.R. Fuller, "Object Oriented Modeling of Microstructural Physics," Distinguished Lecture Series on Computational Materials Science and Engineering, Cornell University, Ithaca, NY, November 19, 2002.
21. S.A. Langer, "Modeling the Mechanical Properties of Materials using OOF," 14th Advanced Cement-Based Materials/NIST Computer Modeling Workshop, June 12, 2003.
22. D.W. Lozier, "Toward a New (and New-Age) Abramowitz and Stegun," Centre for Experimental and Constructive Mathematics, Simon Fraser University, Vancouver, Canada, January 24, 2003.
23. G. McFadden, "Interfacial Boundary Conditions and Phase-field Models of Solidification, Nonequilibrium Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales," Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD, October 20, 2003.
24. L. Melara, "Computational Modeling of Austenite-Martensite Interface," Tenth Annual Sigma Xi Post-Doctoral Poster Presentation, National Institute of Standards and Technology, Gaithersburg, MD, February 27, 2003.
25. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Department of Mathematics, George Mason University, Fairfax, VA, May 2, 2003.
26. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Department of Computational and Applied Mathematics, Rice University, Houston, TX, May 6, 2003.
27. G. McFadden, "Analysis of Hydrodynamic and Interfacial Instabilities during Cooperative Monotectic Growth," 41th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, January 8, 2003.
28. R. Pozo, "High Performance Java Computing," Joint ACM JavaGrande and International Symposium on Computing in Object-oriented Parallel Environments (ISCOPE) Conference, Seattle, WA, November 4, 2002.

29. B. Saunders, "3D Graphics and the NIST Digital Library of Mathematical Functions," Howard University, March 31, 2003.
30. B. Saunders, "Numerical Grid Generation and Effective 3D Visualizations for the NIST Digital Library of Mathematical Functions," American University, October 22, 2002.
31. B. Saunders, "3D Graphics on the World Wide Web: Visualizations for the NIST Digital Library of Mathematical Functions," MAA MD-DC-VA Section Meeting, Norfolk State University, Norfolk, VA, April 12, 2003.

Conference Presentations

1. B. Alpert, "A Representation of Waves in Unbounded Domains," Virtual Electromagnetic Testrange Program Review, DARPA Applied and Computational Mathematics Program, Wright-Patterson Air Force Base, OH, October 8-10, 2002.
2. T.J. Burns (Tony L. Schmitz, Department of Mechanical and Aerospace Engineering, University of Florida, co-author), "Receptance Coupling for High-Speed Machining Dynamics Prediction," SIAM Conference on Applications of Dynamical Systems, Snowbird, UT, May 27-31, 2003.
3. J.E. Devaney and John G. Hagedorn, Discovery in Hydrating Plaster Using Multiple Machine Learning Methods, Fifth International Conference on Discovery Science, DS 2002, Lubeck, Germany, November 24-26, 2002.
4. J.E. Devaney, "Federal Funding of High End Computing (HEC) at the National Institute of Standards and Technology," Supercomputing 2002 "Birds of a Feather" on Federal Funding of High End Computing, Baltimore, MD, November 19, 2002.
5. A. Dienstfrey, "Kramers-Kronig Analysis, Analytic Continuation, and Singular Value Expansions," Joint Mathematics Conference, Baltimore, MD, January 16, 2003.
6. M. J. Donahue and D. G. Porter, "Comparison of Exchange Energy Formulations for 3D Numerical Micromagnetics," MMM 2002, Tampa, FL, November 2002.
7. M. J. Donahue, G. Vertesy, and M. Pardavi-Horvath, "Defect Related Switching Field Reduction in Small Magnetic Particle Arrays," MMM 2002, Tampa, FL, November 2002.
8. M.J. Donahue and D.G. Porter, "Exchange Energy Formulations for 3D Micromagnetics," HMM 2003, Salamanca, Spain, May 28, 2003.
9. D. E. Gilsinn, "Approximating Limit Cycles of a Van der Pol Equation with Delay", 4th International Conference on Dynamic Systems and Applications, Atlanta, GA, May 20, 2003.
10. A. Kearsley, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," 51st Annual Mass Spectrometry and Applied Topics Conference, Montreal, Canada, June 10, 2003.
11. D.W. Lozier, "Digital Library of Mathematical Functions: Technical Issues," Centre for Experimental and Constructive Mathematics, Simon Fraser University, Vancouver, Canada, January 24, 2003.
12. D.W. Lozier, "Toward a New (and New-Age) Abramowitz and Stegun," SIAM Annual Meeting, Montreal, Canada, June 19, 2003.
13. N. Martys and J.S. Sims, "The Role of Aggregate Shape and Size in the Rheology of Concrete," Biannual Meeting of VCCTL, Dusseldorf, Germany, December 2-3, 2002.
14. N. Martys and J.S. Sims, "Self compacting Concrete," ACBM Conference on Self Compacting Concrete, November 2002. Chicago.
15. G. McFadden, "Phase-Field Models of Solidification and Electrochemistry," Department of Materials Science and Engineering Department Seminar, Rensselaer Polytechnic Institute, Troy, NY, October 30, 2003.
16. G. McFadden, "Phase-Field Modeling of Electrochemistry," Department of Mathematical Sciences Department Seminar, New Jersey Institute of Technology, Newark, NJ, November 14, 2003.
17. W.F. Mitchell, "PHAML: A Parallel Adaptive Multilevel Program for Elliptic PDEs," Eleventh Copper Mountain Conference on Multigrid Methods, Boulder, CO March 29, 2003.
18. W.F. Mitchell, "Parallel Adaptive Multilevel Methods with Full Domain Partitions," First International Conference on Numerical Analysis and Computational Mathematics, Cambridge, MA, May 25, 2003.
19. W.F. Mitchell, "Adaptive Grid Refinement for a Model of Two Confined and Interacting Atoms", Adaptive Methods for Partial Differential Equations and Large-Scale Computation, Troy, NY, October 12, 2003.

20. W.F. Mitchell and E. Tiesinga, "On Preconditioners for Interior Eigenvalues of Schrödinger's Equation", 2003 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, Napa, CA, October 28, 2003.
21. D.P. O'Leary, "8 Rules for Career Success," ALL-Women in Engineering Symposium, IEEE Women in Engineering Washington Area Affinity Group, Lanham, MD, May 2003.
22. D.P. O'Leary, "Blind Deconvolution Algorithms," IPAM/SIAM/EMS Conference on Applied Inverse Problems, Lake Arrowhead, CA, May 2003.
23. B. Rust, "Separating Signal from Noise in Global Warming," 35th Symposium on the Interface: Computing Science and Statistics, in Salt Lake City, UT, March 14, 2003.
24. E. Tiesinga and W.F. Mitchell, "Adaptive Grid Modeling of Two Interacting Atoms," 34th Meeting of the Division of Atomic, Molecular and Optical Physics, May 2003. (poster presented by E. Tiesinga Div. 842).
25. C. Witzgall, G. Cheok, and D. Gilsinn, "Terrain Characterization from Ground-Based LADAR", PerMIS 2003, National Institute of Standards and Technology.
26. L. Yanik, E. Della Torre, and M. J. Donahue, "A Test Bed for a FDTD Micromagnetic Program with Eddy Currents," HMM 2003, Salamanca, Spain, May 28, 2003.

Software Released

1. f90gl version 1.2.7, February 25, 2003 (W. Mitchell).
2. Glyph Toolbox (H.W. Bullen, IV, J.S. Chang, A.V. Harn, S.P. Kelly, S.G. Satterfield, P.M. Ketcham, and J.E. Devaney)
3. Immersive visualization tools (A. Peskin and S. Satterfield).
4. Jama/C++, version 1.2 (R. Pozo).
5. OOMMF, version 1.2.0.3, October 30, 2002 (M. Donahue and D. Porter).
6. PHAML, version 0.9, March 2003 (W. Mitchell).
7. Tcl/Tk, version 8.4.2, March 3, 2003, (D. Porter).
8. Tcl/Tk, version 8.4.3, May 20, 2003 (D. Porter).
9. Tcl/Tk, version 8.4.4, July 22, 2003 (D. Porter).
10. Template Numerical Toolkit (TNT), version 1.2 (R. Pozo).

Conferences, Minisymposia, Lecture Series, Short-courses

MCSD Seminar Series

1. F. Potra (UMBC), "Interior Point Methods," Sept. 30, 2003.
2. S. Bullock, "Quantum Computations and Unitary Matrix Decompositions," Sept. 23, 2003.
3. M. Donahue, "Micromagnetics Exchange Energy Formulations," Sept. 16, 2003.
4. P. Black (Software Diagnostics and Conformance Testing Division, NIST ITL), "Simulating Quantum Computing and Communication," Sept. 9, 2003.
5. I. Reid (Numerical Algorithms Group, UK), "An Underpinning Numerical Software Environment for Metrology," Aug. 15, 2003.
6. R. Madhavan (NIST MEL), "Iterative Registration of 3D LADAR Data for Autonomous Navigation," June 24, 2003.
7. B. Braams (Courant Institute of Mathematical Sciences), "Two Approaches to Fitting the Potential Energy Surface," June 18, 2003.
8. B. Braams (Courant Institute of Mathematical Sciences), "Reduced Density Matrices and Semidefinite Optimization," June 17, 2003.
9. D. Jamrog (Lincoln Laboratory, Massachusetts Institute of Technology), "A New Global Optimization Strategy for the Molecular Replacement Problem from X-ray Crystallography," May 27, 2003.
10. L. Rossi (University of Delaware), "High Spatial Order Vortex Methods and Lagrangian Techniques Using Deforming Basis Functions," May 20, 2003.

11. J. Williams (NIST Physics Laboratory), "Simulating Spin Waves in Ultra-cold Quantum Gases," May 8, 2003.
12. M. Rojas (Wake Forest University), "Large-Scale Optimization Techniques for the Regularization of Ill-Posed Problems," May 1, 2003.
13. G.W. Stewart (University of Maryland and MCSD), "MATWRAP: A Fortran 95 Wrapper for Matrix Operations," April 30, 2003.
14. C. Villalobos (University of Texas-Pan American), "The Sphere of Convergence of Newton's Method on Two Equivalent Systems from Linear and Nonlinear Programming," April 23, 2003.
15. B. Li (University of Maryland), "Theory and Computation of Matensitic Microstructure," March 25, 2003.
16. W.F. Mitchell, "A Preview of Fortran 2000," Gaithersburg, March 18, 2003, Boulder, March 27, 2003.
17. A. Reid (Drexel University, NIST MSEL, and MCSD), "Computational Materials Science Using Object Oriented Finite-elements," March 11, 2003.
18. Q. Ding (Pennsylvania State University Harrisburg), "Data Mining on Spatial Data," February 25, 2003.
19. R. McMichael (NIST MSEL), "Magnetization Dynamics and Random Matrices," January 28, 2003.
20. D. Torney (Los Alamos National Laboratory), "A Complete System of Orthogonal Step Functions," January 14, 2003.
21. M. Byrd (Harvard University), "Quantum Computation and Error Protection: Fantasy and Myth," December 11, 2002.
22. R. Book (CNA Corp.), "Public Research Funding and Private Innovation: The Case of the Pharmaceutical Industry," December 3, 2002.
23. E. Edwards (SAIC Technology Solutions), "LAPACK3E – A Fortran 90-enhanced Version of LAPACK," November 14, 2002.
24. J. Engel (retired), "Turing Computability and Related Topics Re-visited," November 12, 2002.
25. L. Curfman McdInnes (Argonne National Laboratory), "Scalable Solution of PDE-based Applications Using PETSc," November 5, 2002.
26. R. Pozo, "High Performance Java for Scientific and Technical Computing," October 29, 2002.
27. D. Anderson (George Mason University and MCSD), "Modeling the Solidification of Temary Alloys in Mushy Layers," October 15, 2002.
28. W. George, "Screen Saver Science: Parallel Distributed Computing and Java/Jini/JavaSpaces," October 1, 2002.

DLMF Seminar Series

1. D. Jeffrey (University of Western Ontario), "Multivalued Inverse Functions: Mathematical Treatment and Implementation in Computer Algebra Systems," February 10, 2003.
2. A. Youssef (George Washington University and MCSD), "Search and Retrieval System for Math Equations and Text," January 10, 2003.

Local Events Organized

1. R. Boisvert, Co-organizer, *Workshop on Instrumentation and Metrology for Nanotechnology*, NIST, Gaithersburg, January 26-28, 2004.
2. D.E. Gilsinn, Co-organizer, *Topics in Operations Research*, NIST Symposium in Honor of Christoph Witzgall, May 13, 2004.
3. S. Satterfield and Y. Parker, Sponsors, NIST presentation by James River Technical on SGI Visualization and Servers, Dec. 12, 2002.

External Event Organization

1. R. Boisvert, Co-organizer, *Workshop on the Changing Face of Mathematical Software*, Washington, DC, June 3-4, 2004.
2. R. Boisvert, Co-organizer, International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software) Meeting, Washington, DC, June 1-2, 2004.

3. R. Boisvert, Program Committee, *ACM Java Grande/ISCOPE Conference*, Seattle, WA, November 3-5, 2002.
4. R. Boisvert, Co-organizer, *International Workshop on Numerical and Symbolic Scientific Computing*, St. Wolfgang, Austria, June 16-21, 2003.
5. A. Carasso, Co-organizer, Mini-symposium, *SIAM Image Science Conference*, Salt Lake City, May 2004. The mini-symposium, which will focus on the loss and recovery of fine structure in image processing, will feature eight speakers in two sessions.
6. M. Donahue, Program Committee, *Hysteresis and Micromagnetic Modeling 2003 Symposium*, Salamanca, Spain, May 28-30 2003.
7. D. Gilsinn, Co-organizer, Minisymposium on Delay Differential Equations, *SIAM Annual Meeting*, Portland, OR, July 2004.
8. F. Hunt, Member, Organizing Committee, Blackwell-Tapia Prize Conference, Mathematical Sciences Research Institute, Berkeley, CA, November 1-2, 2003.
9. A.J. Kearsley and L. Melara, Co-organizers, Minisymposium on Computational and Mathematical Modeling of Microstructures, *Fifth International Congress on Industrial and Applied Mathematics*, Sydney, Australia, July 7-12, 2003.
10. D. Lozier, Organizing Committee, Minisymposia on Special Functions: Computational Methods and Applications, *SIAM National Meeting*, Montreal, Canada, June 15-19, 2003.
11. D.W. Lozier, Co-organizer, AMS-SIAM Special Session on "Classical and Nonlinear Special Functions and Their Applications," *Joint Mathematics Meetings*, Phoenix, Arizona, January 9, 2004. The session will have 14 speakers.
12. W.F. Mitchell, Scientific Committee, First International Conference on Numerical Analysis & Computational Mathematics, Cambridge, UK, May, 2003.
13. D.P. O'Leary, Member, Organizing Committee, SIAM 2004 Annual Meeting.
14. S. Satterfield and J. Kelso, Co-organizers, Birds of a Feather (BOF) Session "DIVERSE: Open-Source VR and Simulation API," SIGGRAPH 2003.

Other Professional Activities

Internal

1. R. Boisvert and J. Bernal, Members, ITL Diversity Committee.
2. R. Boisvert, Member, NIST People Council.
3. A. Dienstfrey, Member, NIST Research Advisory Committee.
4. A. Kearsley, Chair, MCSD Seminar Series.
5. A. O'Gallagher, Member, ITL Awards Committee.
6. B. Rust, Member, NIST Research Library Advisory Board.

External

Editorial

1. B. Alpert, Associate Editor, *SIAM Journal on Scientific Computing*.
2. I. Beichl, Member, Editorial Board, *IEEE Computing in Science and Engineering*.
3. I. Beichl, Associate Editor, *Applied Numerical Analysis & Computational Mathematics*
4. R. Boisvert, Editor-in-Chief, *ACM Transactions on Mathematical Software*.
5. M. Donahue, *Journal of Computational Methods in Sciences and Engineering*
6. E. Knill, Associate Editor, *IEEE Transactions on Information Theory*.
7. G. McFadden, Associate Editor, *Journal of Crystal Growth*.
8. G. McFadden, Associate Editor, *Interfaces and Free Boundaries*.
9. G. McFadden, Associate Editor, *SIAM Journal on Applied Mathematics*.
10. W. Mitchell, Associate Editor, *Applied Numerical Analysis & Computational Mathematics*

11. D.P. O'Leary, Member Editorial Board, SIAM book series on "Fundamentals of Algorithms".
12. D.P. O'Leary, Associate Editor, *SIAM Journal on Matrix Analysis and Applications*.
13. D.P. O'Leary, Associate Editor, *Linear Algebra and Its Applications*,
14. D.P. O'Leary, Member, Editorial Board, *Computing in Science and Engineering*.
15. D.P. O'Leary, Column Editor, "For Your Homework," *Computing in Science and Engineering*.
16. D. Lozier, Associate Editor, *Mathematics of Computation*.
17. R. Pozo, Associated Editor, *ACM Transactions on Mathematical Software*.

Boards and Committees

1. R. Boisvert, Vice-Chair, ACM Publications Board.
2. R. Boisvert, Member, Ad-hoc Search Committee for Editor-in-Chief, *ACM Transactions on Modeling and Computer Simulation (TOMACS)*.
3. R. Boisvert, Member, Ad-hoc Search Committee for Editor-in-Chief, *ACM Journal of Experimental Algorithmics*.
4. R. Boisvert, Member, Ad-hoc Search Committee for Editor-in-Chief, *Journal of the ACM*.
5. R. Boisvert, Member, Ad-hoc Search Committee for Editor-in-Chief, *ACM Transactions on Design Automation for Electronic Systems*.
6. R. Boisvert, Chair, International Federation for Information Processing Working Group 2.5 (Numerical Software).
7. J. Devaney, NIST Representative, High End Computing Group, National Coordination Office for Information Technology Research and Development.
8. J. Devaney, Task Co-Chair, High-End Computing Revitalization Task Force.
9. F. Hunt, Member, Executive Board, Association for Women in Mathematics.
10. S. Langer, Member, Ph.D. Thesis Committee, Department of Materials Science and Engineering, MIT.
11. D. Lozier, Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
12. D. Porter, Member, Tcl Core Team.
13. B. Saunders, Member, External Advisory Council, School of Computer, Mathematical and Natural Sciences, Morgan State University.

Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including *Applied Mathematics Letters*, *Cambridge University Press*, *Computers and Mathematics with Applications*, *Computing Prescriptions, Concurrency and Computation: Practice and Experience*, *Electronic Transactions on Numerical Analysis*, *IEEE Transactions on Magnetics, International Journal of Plasticity, Journal for Automation in Construction*, *Journal of Applied Physics, Journal of Computational Physics, Journal of Computational and Applied Mathematics, Journal of Magnetism and Magnetic Materials, Journal of Manufacturing Science and Technology, Mathematical and Computer Modeling, Mathematics of Computation*, *MIT Presence, Nonlinear Dynamics*, *Physica B, Physical Review E, Physical Review Letters*, *SIAM Journal on Applied Mathematics*, *SIAM Journal on Scientific Computing*, *Thin Solid Film*.
2. Staff members review proposals for the following research programs: NIST ATP, DOE, NSF, EPSRC (UK).

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

ADI Limited   Ball Aerospace
ARINC   Cadence Design Systems
Atrenta, Inc.   Certegy Card Services

Coreco Imaging, Inc.
Delta Add-Power Systems
Electronic Arts
Eastman Kodak Co.
Fakespace Systems
Ford Motor Company
Harris Corporation
High Performance Computing Center (Germany)
Inetcam Inc.
Intel Corporation
Legerity
Lehman Brothers
Lucent Technologies
Mentor Graphics

Microsoft
Mil-tach, Inc.
Nationale Superieure des Telecommunications
   (France)
OmegaComputer.com
Panoptic Computer Network
Raytheon
Redpoint Consulting
Seagate
Tokyo Institute of Technology
Visage Inc.
Visory Group
X-Tek Corporation

Government/Non-profit Organizations

Brookhaven National Lab
Department of Defense (DoD)
Federal Bureau of Investigation
Georgia Tech. Research Institute
Institute for Defense Analyses
Jet Propulsion Laboratory
Los Alamos National Laboratory

National Institutes of Health (NIH)
National Library of Medicine
Naval Research Laboratory
Sandia Laboratory
Sandia Livermore Laboratory
U.S. Army Soldier Biological Chemical
   Command

Universities

American University
Bowie State University
Brown University
Carnegie Mellon University
Chinese Academy of Sciences
City University of New York
Duke University
Emory University
George Mason University
Georgetown University
Indiana University
King Faisal University (Saudi Arabia)
Louisiana Tech University
Massachusetts Institute of Technology
Morehouse College
Norfolk State University
North Carolina A&T University
Northwestern University
Oregon State University
Pennsylvania State University
Rensselaer Polytechnic Institute
Rice University
Spelman College
Stanford University

St. Olaf College
Technion (Israel)
Temple University
The College of William and Mary
Tougaloo College
Trinity College
Universidad Nacional Autonoma de Mexico
University of Arizona
University of Bretagne (France)
University of California – Los Angeles
University of California – San Diego
University of Colorado
University of Florida
University of Maryland
University of Nebraska
University of Newcastle Medical School (UK)
University of New Mexico
University of North Carolina
University of Southampton (UK)
University of South Carolina
University of Trieste (Italy)
University of Utah
University of Wisconsin
Xavier University