Part III

Activity Data

Publications

Appeared

Refereed Journals

1. M.D. Barrett, J. Chiaverini, T. Schaetz, J. Britton, W. M. Itano, J. D. Jost, E. Knill, C. Langer, D. Leibfried, R. Ozeri, and D. J. Wineland, "Deterministic Quantum Teleportation of Atomic Qubits," *Nature* **429** (June 17, 2004), pp.737-739.
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5. S.S. Bullock and I.L. Markov, "Smaller Circuits for Arbitrary n-qubit Diagonal Computations," *Quantum Information and Computation* **4** (1)(2004), pp. 027-047.
6. S.S. Bullock and G.K. Brennen, "Canonical Decompositions of n-qubit Quantum Computations and Concurrence," *Journal of Mathematical Physics* **45** (6) (2004), pp. 2447-2467. Also selected for inclusion in the *Virtual Journal of Nanoscale Science and Technology* **9** (21) and *Virtual Journal of Quantum Information* **4** (6).
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10. M.A. Davies, H.W. Yoon, T.L. Schmitz, T.J. Burns, and M.D. Kennedy, "Calibrated Thermal Microscopy of the Tool-Chip Interface in Machining," *Machining Science and Technology*, **7** (2) (2003), pp. 167-190.
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12. M. J. Donahue and D. G. Porter, "Exchange Energy Formulations for 3D Micromagnetics," *Physcia B* **343** (2004), pp. 177-183.
13. K.S. Downs, M.A. Hamstad and A. O'Gallagher, "Wavelet Transform Signal Processing to Distinguish Different Acoustic Emission Sources," *Journal of Acoustic Emission* **21** (2003), pp. 52-69.
14. 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.
15. B.R. Fabijonas, D.W. Lozier and F.W.J. Olver, "Computation of Complex Airy Functions and Their Zeros Using Asymptotics and the Differential Equation," *ACM Transactions on Mathematical Software* **30** (4) (December 2004), pp. 471-490.
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3. J.E. Devaney, S.G. Satterfield, and J.G. Hagedorn, "Science at the Speed of Thought," *Proceedings of the Workshop on Ambient Intelligence for Scientific Discovery*, Vienna, Austria, April 25, 2004.
4. J.T. Fong, "From Kane to World Trade Center: A 40-Year Journey in Computational Mechanics and Applied Physics," *Proceedings of the Stanford Mechanics Alumni Club -- Stanford Symposium on Topics in Analytical Dynamics and Applied Mechanics*, Stanford University, Stanford, CA, March 5, 2004, pp. 127-136.
5. T. Insperger, T.L. Schmitz, T.J. Burns, and G. Stepan, "Comparison of Analytical and Numerical Simulations for Variable Spindle Speed Turning," *Proceedings of IMECE '03*, 2003 ASME International Mechanical Engineering Congress, Washington, D.C., November 16-21, 2003, CD #IMECE2003-41809.
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2. M.E. Ali and G.B. McFadden, "Linear Stability of Cylindrical Couette Flow in the Convection Regime," *Physics of Fluids*.
3. W. Austin, J. Hagedorn, and S. Satterfield, "Immersive Visualization Tracker Calibration," NISTIR.
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6. J. Bernal, "Integer Representation of Decimal Numbers for Exact Computations," NISTIR.
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2. I. Beichl and F. Sullivan, "Grover's Algorithm: Lower Bounds on Quantum Complexity".
3. I. Beichl, M. Robinson, D. Song, and F. Sullivan "A Quantum Algorithm for Determining If a Function is One to One."
4. I. Beichl and F. Sullivan, "Contextuality and Its Relation to Quantum Computing."
5. B. Bernstein, J.T. Fong, J. Tang, and H.F. Brinson, "Adiabatic Tensile Creep Test of a Nonlinearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 327-336..
6. M. D. Bowdrey, J. A. Jones, E. Knill, R. Laflamme, "Compiling Gate Networks on an Ising Quantum Computer."
7. H.F. Brinson, J.T. Fong, and B. Bernstein, "Adiabatic Tensile Stress Relaxation Test of a Linearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 317-326.
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10. R. deWit, R., and J.T. Fong, "Bending of a Cantilever Beam," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 287-296.
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28. R. Kacker and R. Dersimonian, "Quantification of Uncertainty in Meta-analysis."
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46. J.S. Sims and S.A. Hagstrom, "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations II. Four-electron Integrals."
47. 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."
48. R.W. Swindeman, J.T. Fong, B. Bernstein, and R.J. Fields, "Adiabatic Tensile Stress Relaxation Test of a Visco-plastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 357-366.
49. A. Tabiei, J.T. Fong, H.F. Brinson, and B. Bernstein, "Adiabatic Tensile Creep Test of a Linearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 307-316.
50. J. Tang, J.T. Fong, R.J. Fields, and B. Bernstein, "Adiabatic Tensile Test of an Elastic-plastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 297-306.
51. D.C. Venerus, J.T. Fong, B. Bernstein, and H.F. Brinson, "Adiabatic Tensile Stress Relaxation Test of a Nonlinearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 337-346.
52. Q. Wang and B. Saunders, "Web-Based 3D Visualization in a Digital Library of Mathematical Functions," NISTIR.

Visualizations Published

1. S. Satterfield, Animation of Smart Gel, Opening video of the SC (Supercomputing) 2003 Conference, Phoenix Arizona, November, 2003.
2. D. Feder and P. Ketcham, Three Bose-Einstein Condensate images, p. 22, "Networking and Information Technology Research and Development: Advanced Foundations for American Innovation," Oct 2003 Supplement to the President's FY 2004 budget.

R. Boisvert giving a presentation on the Digital Library of Mathematical Functions Project at the Symposium on Software Environments for Numerical Problems held in Gent, Belgium, in November 2004.

Presentations

Invited Talks

International

1. R. Boisvert, "A Handbook of Special Functions for the Digital Age," Department of Computer Science Distinguished Lecture, University of Toronto, Toronto, Canada, October 7, 2003.
2. R. Boisvert, "A Handbook of Special Functions for the Digital Age," Symposium on Software Environments for Numerical Problems, University of Gent, Belgium, November 18, 2004.
3. Bruce R. Miller, "Digital Library of Mathematical Functions: LaTeX, MathML and ... OpenMath?" 10 Years of OpenMath Workshop, Helsinki, Finland, May 21-22, 2004.
4. R. Pozo, "The Role of Virtual Machines in Scientific Computing," Cluster and Computational Grids for Scientific Computing (CCGSC 2004) Conference, Faverges de la Tour, France, Sept. 26-29, 2004.

Domestic

5. B. Alpert, "Nonreflecting Boundary Conditions for Time-Domain Acoustic and Electromagnetic Wave Propagation," Computational and Applied Mathematics Seminar, Purdue University, West Lafayette, Indiana, September 17, 2004.
6. S. Bullock, "Time Reversal and n-qubit Canonical Decompositions," Gordon Conference on Quantum Computing, Ventura, CA, February 25, 2004.
7. S. Bullock, "Cartan Involutions and Entanglement Dynamics," Cornell University Department of Mathematics Lie Theory Seminar, Ithaca, NY, March 5, 2004.

8. J. Fong, "A SAP-to-LSDYNA Translator," Applied Research Associates, Mountain View, California, Nov. 10, 2003.
9. J. Fong, "From Kane to World Trade Center: A 40-Year Journey in Computational Mechanics and Applied Physics," SMAC-Stanford Symposium on Topics in Analytical Dynamics and Applied Mechanics, Stanford University, Stanford, CA, March 5, 2004.
10. J. Fong, "The Role of Metrological Research and the Application of Design of Experiments in Verification and Validation of Computer Solutions," Applied Research Associates, Inc., Littleton, CO, Aug. 2, 2004.
11. J. Fong, "The Role of Metrological Research and the Application of Design of Experiments in Verification and Validation of Computer Solutions," Sandia National Laboratories, Albuquerque, NM, Aug. 5, 2004.
12. D. Gilsinn, M. McClain, and C. Witzgall, "Using Nonoscillatory Splines to Model Urban Environments," SIAM Conference on Geometric Design and Computing, Seattle, WA, November 10-13, 2003.
13. F. Hunt, "Constructing Sequence Alignments from a Markov Decision Model with Estimated Parameter Values," Biological Language Conference, University of Pittsburgh, Pittsburgh, PA., November 21, 2003.
14. F. Hunt, "Markov Decision Processes and a Potential Application to Biological Sequence Alignment," American Mathematical Society Southeastern Section meeting, Tallahassee, FL, March 13, 2004.
15. A. Kearsley "Managing Explicit Nuclear Magnetic Resonance (NMR) Nonlinear Constraints on the Interatomic Distances"', DIMACS Working Group on New Algorithms for Inferring Molecular Structure from Distance Restraints, Rutgers University, New Brunswick, New Jersey, January 19, 2004.
16. E. Knill, "Postselected Quantum Computation," Quantum Information and Control Conference, Toronto, Ontario, Canada, July 22, 2004.
17. E. Knill, "Quantum Computing with Linear Optics," SPRC Annual Meeting, Stanford University, Stanford, CA, Sept 13, 2004.
18. D. Lozier, "MKM and the NIST Digital Library of Mathematical Functions," 2nd North American Workshop on Mathematical Knowledge Management, Phoenix, AZ, January 6, 2004.
19. G. McFadden, "Phase-Field Models of Solidification and Electrochemistry," Department of Materials Science and Engineering Seminar, Rensselaer Polytechnic Institute, Troy, NY, October 30, 2003.
20. G. McFadden, "Phase-Field Modeling of Electrochemistry," Department of Mathematical Sciences Department Seminar, New Jersey Institute of Technology, Newark, NJ, November 14, 2003.
21. G. McFadden, "Phase-Field Modeling of Elastic Effects During Phase Transitions," 3rd Annual Workshop on the Evolution and Self-Assembly of Quantum Dots, Northwestern University, Evanston, IL, August 16-17, 2004.
22. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Department of Mathematical Sciences, University of Delaware, Newark, DE, November 11, 2003.
23. L. Melara, "Introduction to the Finite Element Method," Department of Mathematics, Colorado College, Colorado Springs, CO, January 26, 2004.
24. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Colloquium, Department of Mathematics, Colorado College, Colorado Springs, CO, January 27, 2004.
25. L. Melara, "Introduction to the Finite Element Method," Department of Mathematics, Union College, Schenectady, NY, February 9, 2004.
26. L. Melara, "Simulation of an Austenite-Twinned-Martensite Interface, a PDE Optimization Problem," Computational Sciences and Mathematics Research, Sandia National Laboratories, Livermore, CA, June 7, 2004.
27. W.F. Mitchell, "A Parallel Adaptive Multilevel Method for Elliptic Boundary Value and Eigenvalue Problems, Rensselaer Polytechnic Institute, Troy, NY, February 4, 2004.

Local Area

28. I. Beichl, "Fast Methods for Sampling from a Dynamic PDF Part I: Fast Methods, Some Up-Front Cost," University of Maryland, Oct. 16, 2003.
29. I. Beichl, "Approximate Counting with Stratified Sampling: the 3D Hard Sphere Entropy Constant," Mathematics Research Division, NSA, Fort Meade, MD, April 7, 2004.
30. I. Beichl, "Counting, the Monte Carlo Way," NIST SURF Summer Seminar Series, July 3, 2004.
31. S. Bullock, "Time Reversal Symmetry and Concurrence Dynamics," NIST Quantum Information and Bose Einstein Condensate Seminar (QIBEC,) April 21, 2004.
32. S. Bullock and G. Brennen, "Time Reversal Symmetry and Entangled Eigenstates," Quantum Information and Coherence Seminar, University of Maryland, College Park, MD, May 4, 2004.

33. S. Bullock, "Matrix Decompositions and Quantum Circuit Design," Second Feynman Festival, University of Maryland College Park Physics Department, August 21, 2004.
34. S. Bullock, "Some Results on Quantum Circuits Design," UMBC Electrical Engineering and Computer Science Seminar, Sept. 17, 2004.
35. A. Carasso, "Singular Integrals and Recovery of Texture in Image Deblurring," Department of Mathematics, University of Maryland, College Park, MD, February 5, 2004.
36. J. Devaney, "Science at the Speed of Thought," The Coalition for Academic Scientific Computation Meeting, Washington, DC, March 4, 2004.
37. M. J. Donahue, "Standard Problems and Public Code for Micromagnetics," IFIP Workshop on the Changing Face of Mathematical Software, Washington, DC, June 3, 2004.
38. J. Fong, "An ISO-compliant Reference Benchmark Approach to Verification & Validation of Virtual Prototyping," DOD Defense Modeling & Simulation Office, Arlington, VA, July 15, 2004.
39. J. Fong, "The Role of Metrological Research and the Application of Design of Numerical Experiments (DNEX) in Verification and Validation of Virtual Prototyping," Office of Nuclear Regulatory Research, U. S. Nuclear Regulatory Commission, Rockville, MD, Sept. 13, 2004.
40. W. George, "A Java Based Parallel and Distributed Computing Environment," Bowie State University, Feb 26, 2004.
41. F. Hunt, "Visualizing the Frequency Patterns of DNA sequences," 4th Virtual Bioinformatics Research Conference, Ballston, VA, Sept. 21, 2004.
42. A. Kearsley, "An Infeasible Point Method for Solving a Class of Multidimensional Scaling Problems," University of Maryland, College Park, MD, Sept. 21, 2004.
43. J. Kelso, "Virtual Environments Using DIVERSE," Virginia Tech, Blacksburg, VA, August 16, 2004.
44. E. Knill, "Linear Optics Approaches," Quantum Information Science, Engineering, and Technology Workshop, Boulder, CO, April 30, 2004.
45. S. Langer, "Object Oriented Modeling of Microstructural Physics," Workshop on Nonequilibrim Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales, Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD, October 27, 2003.
46. S. Langer, "OOF: Object-Oriented Finite Element Analysis for Materials Scientists," Physics Colloquium, Georgetown University, Washington DC, February 17, 2004.
47. S. Langer, "Object Oriented Modeling of Microstructural Physics," Mechanical Engineering Colloquium, University of Maryland Baltimore Country, April 9, 2004.
48. S. Langer, "OOF: Object Oriented Modeling of Material Microstructure," IFIP Workshop on the Changing Face of Mathematical Software, Washington, DC, June 3, 2004.
49. D. Lozier and B. Miller, "A Handbook of Special Functions for the Digital Age," SIMA Technical Seminar, NIST, Gaithersburg, MD, February 24, 2004.
50. 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.
51. B. Miller, "Representing Mathematical Knowledge in the Digital Library of Mathematical Functions," IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 4, 2004.
52. R. Pozo, "The Role of Java in High Performance Computing," IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 3, 2004.
53. A. Youssef, Search in Mathematical Databases, IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 4, 2004.

Conference Presentations

International

1. S. Bullock, "Quantum Circuit Design and the Word Problem on the Unitary Group," Conference on Locally Symmetric Spaces, Mathematisches Forschungsinstittut Oberwolfach, Oberwolfach Germany, Oct. 1, 2003.
2. S. Bullock, "Gaussian Weighted L_2 Cohomology of Locally Symmetric Spaces," Conference on Locally Symmetric Spaces, Mathematisches Forschungsinstittut Oberwolfach, Oberwolfach Germany, Oct. 1, 2003.

3. T .J. Burns (with M.A. Davies, R.L. Rhorer, D. Basak, H.W. Yoon, R.J. Fields, L.E. Levine, E.P. Whitenton, M.D. Kennedy, and R. Ivester), "Influence of Heating Rate on Flow Stress in High-Speed Machining Processes," *7th CIRP International Workshop on Modelling of Machining Operations*, Cluny, France, May 4, 2004.
4. J. Devaney (with S. Satterfield and J. Hagedorn), "Science at the Speed of Thought" at the Workshop on Ambient Intelligence for Scientific Discovery, Vienna, Austria, April 25, 2004.

Domestic

5. B. Alpert, "Successes and Sticky Issues for Nonreflecting Boundary Conditions," International Conference on Spectral and High-Order Methods (ICOSAHOM), Providence, RI, June 22, 2004.
6. I. Beichl, "Approximate Counting with Stratified Sampling: the 3D Hard Sphere Entropy Constant," SIAM Workshop on Combinatorial Scientific Computing (CSC04), San Francisco, CA, February 28, 2004.
7. S. Bullock, "Entanglement Capacity of n-qubit Quantum Computations," SPIE Symposium, Orlando, FL, April 14, 2004.
8. A. Carasso, "Singular Integrals and Recovery of Texture in Image Deblurring," SIAM Conference on Imaging Science, Salt Lake City, UT, May 5, 2004.
9. D. Cotrell and A. J. Pearlstein, "Computation of Flow between a Rotating Screw and a Coaxial Circular Cylinder," American Physical Society Division of Fluid Dynamics Meeting, Rutherford, NJ, November 23-25, 2003.
10. J. Devaney, "Cement and Concrete: Parallel Computing, Scientific and Information Visualization," VCCTL (Virtual Cement and Concrete Testing Laboratory) Annual Meeting, November 20-21, 2003.
11. M. Donahue, "OOMMF: Where Is It, Where Is It Going?" muMAG meeting, Anaheim, CA, January 7, 2004.
12. M. Donahue, "Motion of Magnetic Domain Walls in Thin, Narrow Strips," SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, CA, May 23, 2004.
13. D. Gilsinn, M. McClain, C. Witzgall., "Experiences Using L_1 Splines in Modeling Urban Environments," SIAM Geometric Design and Computing Conference, Seattle, WA, Nov. 12-14, 2003.
14. D. Gilsinn, "Integral Equation Methods of Estimating Characteristic Multipliers for Linear DDEs with Periodic Coefficients" 2004 SIAM Annual Meeting, Portland, OR, July 10-16, 2004.
15. K. Irikura, R. Johnson, and R. Kacker, "Uncertainty Associated with Virtual Measurements from Computational Chemistry Models," Measurement Science Conference 2004, Anaheim, CA, Jan. 15-16, 2004.
16. R. Kacker, "Penal Discussion: ISO Guide to the Expression of Uncertainty in Measurement: Conventional vs. Bayesian Statistical Methods," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
17. R. Kacker, "Statistical Interpretation of Key Comparison Reference Value and Degrees of Equivalence," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
18. R. Kacker, "Combining Information from Interlaboratory Evaluations using Random Effects Model," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
19. J. Kelso and S. Satterfield, "DIVERSE: Open-Source VR and Simulation API," Birds of a Feather Session, SIGGRAPH '04, Los Angeles, CA, August 12, 2004.
20. D. Lozier, "Digital Library of Mathematical Functions: A Project Report," AMS-SIAM Special Session on Classical and Nonlinear Special Functions, Joint Mathematics Meetings, Phoenix, AZ, January 8, 2004.
21. L. Melara, "Simulation of Twinned-Martensite as a PDE Optimization Problem," Sixth Joint AMS-SMM International Meeting, Houston, TX, May 15, 2004.
22. B. Miller, "Authoring Mathematical Knowledge," 2nd North American Workshop on Mathematical Knowledge Management, Phoenix, AZ, January 6, 2004.
23. W. Mitchell, "Adaptive Grid Refinement for a Model of Two Confined and Interacting Atoms," Adaptive Methods for Partial Differential Equations and Large-Scale Computation Conference, Troy NY, October 12, 2003.
24. W. Mitchell and E. Tiesinga, "On Preconditioners for Interior Eigenvalues of Schroedinger's Equation," 2003 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, Napa, CA, October 28, 2003.

25. W. Mitchell and E. Tiesinga, "A Parallel Multigrid Method Applied to Schroedinger's Equation," The Eleventh Conference on Parallel Processing for Scientific Computing, San Francisco, CA, February 26, 2004.
26. A. Pearlstein and D. Cotrell, "Computation of Pressure-Driven Flow between a Nonrotating Screw and an Outer Coaxial Circular Cylinder," American Physical Society Division of Fluid Dynamics Meeting, Rutherford, NJ, November 23-25, 2003.
27. D. Porter, "OOMMF 1.1b2 Release," MicroMagnetic Modeling Activity Group Meeting, Anaheim, CA, January 8, 2004.
28. D. Porter and M.J. Donahue, "Velocity of Tranverse Domain Wall Motion Along Thin, Narrow Strips," 9th Joint MMM/Intermag Conference, Anaheim, CA, January 6, 2004.
29. B. Saunders and Q. Wang, "Mesh Generation for Effective 3D Visualizations in a Digital Library of Mathematical Functions," 13th International Meshing Roundtable, Williamsburg, VA, September 19-22, 2004.
30. D. Song, "Entanglement Swapping Based Quantum Key Distribution," DARPA Quantum Information Science and Technology (QuIST) Review Meeting, Chicago, IL, May 4-6, 2004."

Local Area

31. R. Kacker, "Combining Information from Interlaboratory Studies Using Random Effects Model," Eleventh Spring Research Conference on Statistics in Industry and Technology, American Statistical Association and the Institute of Mathematical Statistics, NIST, Gaithersburg, MD, May 19-21, 2004.

Software Released

1. M. Donahue and D. Porter, OOMMF 1.1.1.2, January 15, 2004.
2. D. Porter contributed to Tcl/Tk releases 8.4.5 (November 24, 2003), 8.4.6 (March 1, 2004), 8.5a1 (March 3, 2004), and 8.4.7 (July 29, 2004).
3. J. Kelso, visualization DSOs and utilities: tim.2 (Things In Motion, version 2), xwand, printScenegraph, smallFeatureCull DSO, dtk-writeShm, lodScale DSO, sgb (Scene Graph Builder) file loader, ifl (Instancing File loader), lod (Level Of Detail) file loader, m4 pseudo loader, flatten pseudo loader, clean" pseudo loader.
4. S. Langer, OOF2 version 2.0.b2.
5. A. Peskin, ABCDswitch DSO.
6. R. Pozo, Sparse Basic Linear Algebra Subprograms (BLAS) in ANSI C, preliminary version.
7. R. Pozo, SparseLib++ Version 1.6.
8. R. Pozo, Matrix Market Matlab input/output code update.
9. R. Pozo, Template Numerical Toolkit (TNT), Version 1.2.1 and Version 1.2.2.

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. D. Gilsinn (ITL), "Approximating Limit Cycles of an Autonomous Delay Differential Equation," September 28, 2004.
2. S. Bullock (ITL), "Matrix Decompositions and Quantum Circuit Design," September 15, 2004.
3. K. Mills (ITL), "Considering Emergence in Global Information Systems," July 27, 2004.
4. E. Shirley (PL), "Intrinsic Birefringence in Cubic Crystalline Optical Materials," June 10, 2004.
5. A. Sandu (Virginia Polytechnic Institute and State Univ.), "KPP: A Software Environment for Modeling Chemical Kinetics," May 25, 2004.
6. T. Schulze (Univ. of Tennessee), "Some New Tools for Simulating Nano-Scale Crystal Growth," May 10, 2004.

7. R. Nochetto (Univ. of Maryland), "Finite Element Methods for Surface Diffusion and Applications to Stressed Epitaxial Films," May 4, 2004.
8. K. Irikura, R. Johnson (CSTL) and R. Kacker (ITL), "Uncertainty from Bias in Virtual Measurements and the NIST Computational Chemistry Comparison and Benchmark Database," April 20, 2004.
9. J. Hubbard (CSTL), "Hydrodynamics, Electrostatics, and Brownian Motion: Some Rigorous, Tight Bounds," April 6, 2004.
10. C. Williams (PL), "An Introduction to Quantum Computing," March 23, 2004.
11. H. Elman (Univ. of Maryland), "Preconditioning Strategies for Models of Incompressible Flow," March 15, 2004.
12. R. Mountain (CSTL), "Molecular Dynamics Simulations and Sources of Uncertainty in Virtual Measurements," February 24, 2004.
13. T. Wanner (George Mason Univ.), "Pattern Formation in Cahn-Hilliard-Type Models," February 17, 2004.
14. A. Rukhin (ITL and UMBC), "Balanced Randomization Designs and Classical Probability Distributions," February 3, 2004.
15. K. Prasad (BFRL), "Coupled Fire Dynamics and Thermal Response of Complex Building Structures," January 20, 2004.
16. A. Carasso, "Singular Integrals, Image Smoothness, and the Recovery of Texture in Image Deblurring," December 16, 2003.
17. V. Torczon, "Generating Set Search for Nonlinear Programming," December 9, 2004.
18. R. Rainsberger, "Mesh Generation for Non-linear Finite Element Analysis," December 4, 2003.
19. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface" November 18, 2003.
20. D.L. Cotrell, "Linear Stability of Spiral Poiseuille Flow and Comparison to Experiments," November 4, 2003.
21. L. Giraud, "Sparse Iterative Techniques for the Solution of the 3D Maxwell Equations in Boundary Element Formulation," October 31, 2003.
22. T. Burns, "Subcritical Flip Bifurcation in High-Speed Machining," October 22, 2003.
23. B. Schneider, "The Discrete Variable Method for the Time Dependent and Time Independent Schroedinger Equation, Part II," October 15, 2003.
24. B. Schneider, "The Discrete Variable Method for the Time Dependent and Time Independent Schroedinger Equation, Part I," October 14, 2003.
25. M. Mascagni, "Computational Infrastructure for Parallel, Distributed, and Grid-based Monte Carlo Computations," October 9, 2003.

Local Events Organized

1. R. Boisvert, Organizing Committee, NIST Workshop on Metrology and Instrumentation for Nanotechnology, Gaithersburg, January 27-28, 2004.
2. R. Boisvert, Organizer, Workshop on the Changing Face of Mathematical Software, International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software), Washington, DC, June 3-4, 2004.
3. J. Fong, Chair, Organizing Committee, NIST Workshop on the Verification and Validation of Computer Models of High-Consequence Engineering Systems, Nov. 8-9, 2004.
4. D. E. Gilsinn, Organizer, Symposium on Topics in Operations Research, NIST Gaithersburg, May 13, 2004. Held in honor of the retirement of Christoph Witzgall.

IFIP Working Group 2.5 on Numerical Software meets in Washington in June 2004. From left to right: Wayne Enright, Bill Gropp, Bo Einarsson, Michael Thune, Craig Douglas, Ian Gladwell, Mladen Vouk, Brian Ford, Jim Pool, Ulrich Kulisch, and Mo Mu.

External Events Organization

1. R. Boisvert, Program Committee, *International Symposium on Symbolic and Algebraic Computation*, Beijing, China, July 2005, http://www.mmrc.iss.ac.cn/~issac2005.
2. R. Boisvert, Co-chair, Program Committee, *Symposium on Scientific Computing and Mathematical Software in Emerging Sciences and Technology*, Hong Kong, China, June 2005, http://www.math.ust.hk/~mamu/IFIP/Announce.html.
3. A. Carasso, Co-Organizer, Minisymposium on Loss and Recovery of Fine Structure in Image Processing, SIAM Image Science Conference, Salt Lake City, May 2004.
4. J. Devaney, Program Committee, Government and Industrial Track, Knowledge Discovery in Databases Conference.
5. M. Donahue, Program Committee, 49th Conference on Magnetism and Magnetic Materials, Washington DC, July 18-19, 2004.
6. J. Fong, Co-Chair, Symposium on Topics in Analytical Dynamics and Applied Mechanics, Stanford University, March 5, 2004.
7. D. E. Gilsinn, Chair, Minisymposium on Recent Developments in Methods of Solving Delay Differential Equations, SIAM 2004 Annual Meeting, Portland, OR, July 12-16, 2004.
8. D.W. Lozier, Organizing Committee, AMS-SIAM Special Session on Classical and Nonlinear Special Function, Joint Mathematics Meetings, Phoenix, AZ, January 7-10, 2004.
9. D.P. O'Leary, Organizing Committee, 2004 SIAM National Meeting.

Other Professional Activities

Internal

1. I. Beichl, Co-coordinator, ITL Summer Undergraduate Research Fellowship (SURF) Program
2. R. Boisvert and Abbie O'Gallagher, ITL Diversity Committee.

3. R. Boisvert, NIST People Council.
4. R. Boisvert, NIST Nanotechnology Strategic Working Group.
5. R. Boisvert, NIST Scientific Computing Steering Group.
6. D. Porter, ITL Awards Committee.
7. 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, Editorial Board, *Computing in Science & Engineering*.
3. I. Beichl, Associate Editor, *Journal of Numerical Analysis and Computational Mathematics*
4. R. Boisvert, Editor-in-Chief, *ACM Transactions on Mathematical Software*.
5. M. Donahue, *Journal of Computational Methods in Science and Engineering*
6. E. Knill, *IEEE Transactions on Information Science*
7. D. Lozier, Associate Editor, *Mathematics of Computation*.
8. G. McFadden, Associate Editor, *Journal of Crystal Growth.*
9. G. McFadden, Associate Editor, *Interfaces and Free Boundaries.*
10. G. McFadden, Associate Editor, *SIAM Journal on Applied Mathematics.*
11. W. Mitchell, Associate Editor, *Journal of Numerical Analysis and Computational Mathematics*
12. D. O'Leary, Editorial Board, *Computing in Science & Engineering*.
13. D. O'Leary, Editorial Board, SIAM Book Series on Fundamentals of Algorithms.
14. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*

Boards and Committees

1. R. Boisvert, ACM Publications Board.
2. R. Boisvert, Chair, International Federation for Information Processing Working Group 2.5 (Numerical Software)
3. R. Boisvert, Technical Review Committee, Institute for Defense Analysis Center for Computing Sciences.
4. J. Devaney, High End Computing Group, National Coordination Office for Information Technology Research and Development.
5. J. Devaney, High End Computing Revitalization Task Force.
6. F. Hunt, Executive Committee, Association for Women in Mathematics.
7. D. Lozier, Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
8. D. O'Leary, SIAM/AMS/ASA/AWM/IMS/MAA/NCTM Joint Committee on Women
9. D. Porter, Tcl Core Team.
10. B. Saunders, 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

American Mathematical Monthly
ASME Journal of Manufacturing Science and Engineering
Computers and Mathematics with Applications
Computers in Engineering
IEEE Transactions on Antennas and Propagation
IEEE Transactions on Computer Aided Design (TCAD)
IEEE Transactions on Electromagnetic Compatibility
IEEE Transactions on Instrumentation and Measurement
IEEE Transactions on Magnetics

IEEE Transactions on Parallel and Distributed Computing
International Journal of Numerical Methods in Engineering
International Journal of Plasticity
Journal of Computational and Applied Mathematics
Journal of Computational Physics
Journal of Computational Statistics
Journal of Magnetism and Magnetic Materials
Journal of Physics A: Mathematical and General Physic
Journal of Physics B: Atomic, Molecular, and Optical Physics
Journal of Rheology
Metrologia
Physical Review A
Physical Review B
Physical Review Letters
Precision Engineering
Radio Science
SIAM Journal on Applied Mathematics
SIAM Journal on Numerical Analysis
SIAM Journal on Optimization
SIAM Journal of Scientific Computing
Theoretical Computer Science
Total Quality Management and Business Excellence

2. Staff members review proposals for the following research programs: Kentucky Science and Engineering Foundation (KSEF), Civilian Research and Development Foundation, University of California Microelectronics Innovation and Computer Research Opportunities (MICRO) Program, Dutch National Science Foundation (NWO), and the National Science Foundation (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

Absoft Corporation
Altera Corporation
American Hydro Corp.
Applied Research Associates, Inc.
Atrenta, Inc.
Cisco Systems
Computers and Structures, Inc.
Cray, Inc.
Delta Add-Power Systems
Ether Media
Fuji Electric Advanced Tech., Co., Ltd.
General Electric Research Labs
Institute for Electronic Design Automation
Integral Systems, Inc.
Integrity Applications, Inc.
Intel Corporation
Invensys Systems, Inc.
Lick Observatory
Livermore Software Technology Corp.
Lucent Technologies
Mallett Technology, Inc.
Open Tech Inc.
Optimization Partner Stockholm AB
Raytheon
Rockwell Collins
SAC Capital
SIGOS
Superior Methods
System Planning Corp.
Targacept
Well Code Software
XYZ Scientific Applications, Inc.

Government/Non-profit Organizations

Association for Computing Machinery (ACM)
American Mathematical Society (AMS)
Air Force Office of Scientific Research
Army Research Office
DARPA
European Southern Observatory
FBI
IDA Center for Computing Sciences
Japan Aerospace Exploration Agency
Jet Propulsion Laboratory
Los Alamos National Laboratory
Mayo Clinic
National Institutes of Health
National Coordination Office for IT R&D
NASA
National Security Agency
NOAA
National Science Foundation (NSF)
Office of Naval Research
Office of Science and Technology Policy (OSTP)
Ohio Supercomputer Center
Research Org. for Info. Science & Tech. (Japan)
Sandia National Laboratory
Senate Appropriations Committee
Society for Industrial and Applied Mathematics (SIAM)
The Canadian Space Agency
U.S. Army Night Vision Laboratory
U.S. Department of Energy
U.S. Department of Defense
U.S. Joint Forces Command
U.S. Nuclear Regulatory Commission
Walter Reed Army Institute of Research

Universities

Abilene Christian University
American University
American University of Beruit Medical Center
Boston University
Bowie State University
Brown University
Cachan University (France)
Chinese Academy of Sciences
Colorado College
Coppin State University
Cornell University
Delaware State University
Drexel University
Duke University
George Mason University
George Washington University
Georgetown University
Graz University (Austria)
Illinois Institute of Technology
Innsbruck University (Austria)
Instituto Nazionale per las Fisica della Materia (Spain)
International University of Bremen (Germany)
Iowa State University
Jackson State University
New Mexico State University
Millersville University
Mississippi State University
MIT
Morgan State University
Northwestern University
Penn State University
Princeton University
Purdue University
Rensselaer Polytechnic Institute
Saarland University (Germany)
San Jose State University
Sienna College
Stanford University
Technion (Israel)
Tel-Aviv University (Israel)
Union College
University of Alaska
University of California
University of Cambridge
University of Cincinnati
University of Erlangen-Nurenberg (Germany)
University of Houston
University of Idaho
University of Illinois
University of Indiana
University of Iowa
University of Kentucky
University of Maryland
University of Minnesota
University of Mons (Belgium)
University of New Mexico
University of North Carolina
University of Puerto Rico
University of San Diego
University of Southhampton (United Kindom)
University of Tokyo
University of Valparaiso (Chile)
University of Verlangen (Germany)
University of Washington
University of Wisconsin

Utrecht University (The Netherlands)
Virginia Tech
Williams College