Part III

Activity Data

Publications

Appeared

Refereed Journals

- 1. B. Alpert, L. Greengard, and T. Hagstrom, "Nonreflecting Boundary Conditions for the Time-Dependent Wave Equation," *Journal of Computational Physics* **180** (2002), pp. 270-296.
- B. Alpert, G. Beylkin, D. Gines, and L. Vozovoi, "Adaptive Solution of Partial Differential Equations in Multiwavelet Bases," *Journal of Computational Physics* 182 (2002), pp. 149-190.
- 3. A.L. Ankudinov, J.J. Rehr, J.S. Sims, C.E. Bouldin, H.K. Hung, "Rapid Calculation of X-ray Absorption Near Edge Structure Using Parallel Computing," *Journal of X-ray Spectroscopy* **30** (2001), pp. 431-434.
- 4. A. Ankudinov, C.E. Bouldin, J.S. Sims, H.K. Hung, J.J. Rehr, "Parallel Calculation of Electron Multiple Scattering using Lanczos Algorithms," *Physical Review B* **65**, 104107 (2002).
- 5. I. Beichl and F. Sullivan, "It's Bound to be Right," *Computing in Science and Engineering* **4**, No. 2, (2002), pp. 86-90.
- 6. I. Beichl, "Dealing with Degeneracy in Triangulation" *Computing in Science and Engineering* **4**, No. 6, (2002), pp. 70-74
- 7. A. Andreas and I. Beichl, "Estimating the Work of Integer Partitioning," *Computing in Science and Engineering* **5**, No. 1, (2003), pp. 48-56.
- D.P. Bentz, S. Mizell, S. Satterfield, J. Devaney, W. George, P. Ketcham, J. Graham, J. Porterfield, D. Quenard, F. Vallee, H. Sallee, E. Boller and J. Baruchel, "The Visible Cement Dataset," *NIST Journal of Research* 107 No. 2 (March-April, 2002), pp. 137-148.
- 9. A. Carasso, "The APEX Method in Image Sharpening and the Use of Low Exponent Lévy Stable Laws," *SIAM. Journal of Applied Mathematics* **63** (2002), pp. 593-618.
- 10. A. Carasso, D. Bright, and A. Vladar, "The APEX Method and Real-time Blind Deconvolution of Scanning Electron Microscope Imagery," *Optical Engineering* **41** (2002), pp. 2499-2514.
- 11. S. Coriell and G. McFadden, "Applications of Morphological Stability Theory," *Journal of Crystal Growth* 237-239P1 (2002), pp. 12-17.
- 12. M. J. Donahue and D. G. Porter, "Analysis of Switching in Uniformly Magnetized Bodies," *IEEE Transactions on Magnetics* **38** (2002), pp. 2468-2470.
- 13. W. George and J.A. Warren, "A Parallel 3D Dendritic Growth Simulator Using the Phase-field Method," *Journal of Computational Physics* **177** (2002), pp.264-283.
- D.E. Gilsinn, M.A. Davies, B. Balachandran, "Stability of Precision Diamond Turning Processes That Use Round Nosed Tools," *Journal of Manufacturing Science and Engineering* 123 (November, 2001), pp. 747-748.
- 15. D.E. Gilsinn, H.T. Bandy, A.V. Ling, "A Spline Algorithm for Modeling Cutting Errors on Turning Centers," *Journal of Intelligent Manufacturing* **13** (2002), pp. 391-401
- 16. D.E. 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.
- 17. K. Gurski and R. Pego, "Normal Modes for a Stratified Viscous Fluid Layer," *Royal Society of Edinburgh* **132A** (2002), pp. 1-15.
- 18. M. Hamstad, J. Gary, and A. O'Gallagher, "Effects of Lateral Plate Dimensions on Acoustic Emission Signals from Dipole Sources," *Journal of Acoustic Emission* **19** (2001), pp. 258-274.
- 19. R. Kacker, R. Datla, and A. Parr, "Combined Result and the Associated Uncertainty from Interlaboratory Evaluations Based on the ISO Guide," *Metrologia* **39** (2002), pp. 279-293.
- 20. A.J. Kearsley, L. C. Cowsar, R. Glowinski, M. F. Wheeler and I. Yotov, "Optimization Approach to Multiphase Flow," *Journal of Optimization Theory and Applications* **111**, No. 3. (2001), pp. 473-488.
- A. Kearsley and A.M. Reiff, "Existence of Weak Solutions to a Class of Non-strictly Hyperbolic Conservation Laws with Non-interacting Waves," *Pacific Journal of Mathematics* 205 Issue 1 (2002), pp. 153-170.

- 22. P. Ketcham and D. Feder, "Visualization of Bose-Einstein Condensates," *Computing in Science and Engineering* 5, No. 1 (2003), pp. 86-89.
- 23. G. McFadden and A. Wheeler, "On the Gibbs Adsorption Equation for Diffuse Interface Models," *Proceedings of the Royal Society (London) A* **458** (2002), pp. 1129-1149.
- 24. C.S. O'Hern, S.A. Langer, A.J. Liu, and S.R. Nagel, "Random Packings of Frictionless Particles," *Physical Review Letters* 88 (Feb. 2002), p. 075507.
- 25. I.K. Ono, C.S. O'Hern, D.J. Durian, S.A. Langer, A. J. Liu, and S.R. Nagel, "Effective Temperatures of a Driven System Near Jamming," *Physical Review Letters* **89** (Aug. 2002), p. 095703.
- 26. S. Blackford, J. Demmel, J. Dongarra, I. Duff, S. Hammarling, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petitet, R. Pozo, K. Remington, and C. Whaley, "An Overview of the Sparse Basic Linear Algebra Subprograms: the New Standard from the BLAS Technical Forum," ACM Transactions on Mathematical Software 28, No. 2 (June 2002), pp. 135-151.
- 27. R. Pozo, M.A. Heroux and I.S. Duff, "An Updated Set of Basic Linear Algebra Subprograms (BLAS)," *ACM Transactions on Mathematical Software* 28, No. 2 (June 2002), pp. 206-238.
- 28. B. Rust, "Fitting Nature's Basic Functions Part II: Estimating Uncertainties and Testing Hypotheses," *Computing in Science and Engineering* **3**, No. 6 (Nov./Dec. 2001) pp. 60-64.
- 29. B. Rust, "Fitting Nature's Basic Functions Part III: Exponentials, Sinusoids and Nonlinear Least Squares," *Computing in Science & Engineering* (July-August 2002), pp. 72-77.
- 30. J.S. Sims, W.L. George, S.G. Satterfield, H.K. Hung, J.G. Hagedorn, P.M. Ketcham, T.J. Griffin, S.A. Hagstrom, J.C. Franiatte, G.W. Bryant, W. Jaskolski, N.S. Martys, C.E. Bouldin, V. Simmons, O.P. Nicolas, J.A. Warren, B.A. am Ende, J.E. Koontz, B. J. Filla, V.G. Pourprix, S.R. Copley, R.B. Bohn, A.P. Peskin, Y.M. Parker, and J.E. Devaney, "Accelerating Scientific Discovery Through Computation and Visualization II," *NIST Journal of Research* 107 (3) (May-June, 2002), pp. 223-245.
- 31. J.S. Sims and S.A. Hagstrom, "High Precision Hy-CI Variational Calculations for the Ground State of Neutral Helium and Heliumlike Ions," *International Journal of Quantum Chemistry*, **90** Issue 6 (2002), pp. 1600-1609.
- V.R. Vedula, S.J. Glass, D.M. Saylor, G.S. Rohrer, W.C. Carter, S.A. Langer, and E.R. Fuller, "Residual-Stress Predictions in Polycrystalline Alumina," *Journal of the American Ceramic Society* 84 (Dec. 2001), p. 2947.
- 33. H. Westlund, G. Meyer, and F. Hunt, "The Role of Rendering in Measurement Science for Optical Reflections," *Journal of NIST Research* **107** No. 3 (May-June 2002), pp. 247-259.

Conference Proceedings

- 1. B.A. am Ende, M.W. Cresswell, R.A. Allen, T.J. Headley, W.F. Guthrie, L.W. Linholm, E.H. Bogardus, and C.E. Murabito, "Measurement of the Linewidth of Electrical Test-Structure Reference Features by Automated Phase-Contrast Image Analysis," in *Proceedings of the IEEE International Conference on Microelectronic Test Structures*, April 8-11, 2002.
- D. Anderson, G. McFadden, and A. Wheeler, "A Phase-Field Model with Convection: Numerical Simulations," in *Interfaces for the 21st Century: New Research Directions in Fluid Mechanics and Materials Science*, (eds. Marc K. Smith, Michael J. Miksis, Geoffrey B. McFadden, G. Paul Neitzel, David R. Canright), Imperial College Press, London, 2002, pp. 213-230.
- 3. D. Anderson, G. McFadden, A. Wheeler, "A Phase-field Model of Convection with Solidification," Paper AIAA 2002-0891, *Proceedings of the 40th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, January 14-17, 2002.
- R. Braun, J. Zhang, J. Cahn, G. McFadden, and A. Wheeler, "Model Phase Diagrams for an FCC Alloy," in Interfaces for the 21st Century: New Research Directions in Fluid Mechanics and Materials Science, (eds. Marc K. Smith, Michael J. Miksis, Geoffrey B. McFadden, G. Paul Neitzel, David R. Canright), Imperial College Press, London, 2002, pp. 131-145.
- M.W. Cresswell, E.H. Bogardus, J.V. Martinez de Pinillos, M.H. Bennett, R.A. Allen, W.F. Guthrie, C.E. Murabito, B.A. am Ende, L.W. Linholm, "CD Reference Materials for Sub-Tenth Micrometer Applications," in *Proceedings of the SPIE Microlithography Conference 4689*, March 3-8, 2002.
- N. Dao, F.J. Castano, C.A. Ross, M.J. Donahue, and S.L. Whittenburg, "Micromagnetics Simulation of Asymmetric Pseudo-Spin Valve Dots," *Materials Research Society Symposia Proceedings* 731 (2002), pp. 291-296.

- 7. J.E. Devaney and J.G. Hagedorn, "The Role of Genetic Programming in Describing the Microscopic Structure of Hydrating Plaster," in *Late Breaking Papers, Genetic and Evolutionary Computing Conference*, GECCO 2002, New York, July 8-13, 2002, pp. 91-98.
- K. Furlani, D. Latimer, M. Kincaid, D. Gilsinn, and A. Lytle, "Prototype Implementation of an Automated Tracking Structural Steel Tracking System," ISARC 2002, 19th International Symposium on Automation and Robotics in Construction, *NIST Special Publication 989*, (ed. W.C. Stone), Gaithersburg, MD, September 23-25, 2002, pp. 467-473.
- D. E. Gilsinn, J.E. Lavery, "Shape-preserving, Multiscale Fitting of Bivariate Data by Cubic L₁ Smoothing Splines," in *Approximation Theory X: Wavelets, Splines, and Applications*, (eds. C. K. Chui, L. L. Schumaker, J. Stockler), Vanderbilt University Press, Nashville, TN 2002, pp. 283-293.
- D.E. Gilsinn, G.S. Cheok, and D.P. O'Leary, "Reconstructing Images of Bar Codes for Construction Sight Object Recognition," in ISARC 2002, 19th International Symposium on Automation and Robotics in Construction, *NIST Special Publication 989*, (ed. W.C. Stone), September 23-25, 2002, pp. 363-368.
- F. Hunt, E. Marx, G. Meyer, T. Vorburger, P. Walker, and H. Westlund, "A First Step Toward Photorealistic Rendering of Coated Surfaces and Computer Based Standards of Appearance," in *Service Life Prediction Methodology and Metrologies*, ACS Symposium Series 805, (eds. J.W. Martin and D. Bauer), 2001, pp. 437-451.
- 12. R. Kacker, R. Datla, and A. Parr, "Combined Result and Uncertainty from Interlaboratory Evaluations Based on the ISO Guide (Abstract and Presentation)," in *Proceedings of the Measurement Science Conference*, Session I-D, January 2002.
- 13. J. Kelso, L.E. Arsenault, S.G. Satterfield, and R.D. Kriz, "DIVERSE: A Framework for Building Extensible and Reconfigurable Device Independent Virtual Environments," in *Proceedings of Virtual Reality 2002 Conference*, Orlando, March 24-27, 2002, pp. 183-190.
- 14. J. E. Lavery and D E. Gilsinn, "Representation of Natural Terrain by Cubic L₁ Splines," in *Trends in Approximation Theory*, (eds. K. Kopotun, T. Lyche, and M. Neamtu), Vanderbilt University Press, Nashville, TN, 2001, pp. 235-242.
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- N. S. Martys, J. G. Hagedorn, J. E. Devaney, "Pore Scale Modeling of Fluid Transport Using Lattice Boltzmann Methods," in *Ion and Mass Transport in Cement-Based Materials*, American Ceramic Society, 2002, pp. 239-252.
- 17. G. McFadden, S. Coriell, and B. Murray, "Convective and Morphological Instabilities during Crystal Growth," in *Proceedings of the 2002 NASA Microgravity Materials Science Conference*, Huntsville, Alabama, June 24-26, 2002.
- G. McFadden, "Phase-Field Models of Solidification," in *Recent Advances in Numerical Methods for Partial Differential Equations and Applications*, (eds. X. Feng and T.P. Schulze), Contemporary Mathematics 306 (2002), American Mathematical Society, Providence, RI, pp. 107-145.
- 19. W.F. Mitchell, "The Design of a Parallel Adaptive Multi-Level Code in Fortran 90," in *Proceedings of the 2002 International Conference on Computational Science*.
- 20. E. Shirley, R. Kacker, and R. Datla, "Diffraction Corrections in Radiometry: A Proposed Method to Estimate Uncertainties," in *Proceedings of the Measurement Science Conference*, Session I-D, January 2002.
- 21. W.C. Stone, G.S. Cheok, K.M. Furlani, and D. Gilsinn, "Object Identification Using Bar Codes Based on LADAR Intensity," in *International Symposium for Automation and Robotics in Construction (ISARC)* 2001, Krakow, Poland, Sept. 10-11.
- C. Witzgall and G. Cheok, "Experiences with Point Cloud Registration," in *ISARC 2002, 19th International Symposium on Automation and Robotics in Construction*, NIST Special Publication 989, (ed. W.C. Stone), September 23-25, 2002, pp. 349-355.

Technical Reports

- H.T. Bandy, M.A. Donmez, D.E. Gilsinn, C.S. Han, M.D. Kennedy, A.V. Ling, N.D. Wilkin, K.W. Yee, "A Methodology for Compensating Errors Detected by Process-Intermittent Inspection", NISTIR 6811, October, 2001.
- 2. D.E. Gilsinn and A.V. Ling, "Comparative Statistical Analysis of Test Parts Manufactured in Production Environments," NISTIR 6868, June 2002.
- 3. K. Gurski and G. McFadden, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability," NISTIR 6892.
- 4. M. Michel, "Contribution au Transfert de Donnees: Application à MPI," Ph.D Thesis, University Henri Poincare, UMR 7503, October 2001.
- 5. R. Pozo, "NIST Sparse BLAS User's Guide," NISTIR 6744.

Accepted

- 1. J. Bernal, A. Kearsley, C. Guttman, W. Wallace, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," *Proceedings of the 50th ASMS Conference*.
- 2. R.F. Boisvert, "Mathematical Software: Past, Present, and Future," in *Computational Science, Mathematics, and Software*, (eds. R.F. Boisvert and E.N. Houstis, Eds.), Purdue University Press.
- 3. R.F. Boisvert and E.N. Houstis, eds., *Computational Science, Mathematics, and Software*, Purdue University Press, 2003.
- 4. C.E. Bouldin, J.S. Sims, H.K. Hung, J.J. Rehr, A. Ankudinov, "Parallel Calculation of Electron Multiple Scattering using Lanczos Algorithms," *Physical Review B*.
- 5. J.E. Devaney and J.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, *Lecture Notes in Artificial Intelligence*, Springer-Verlag, Heidelberg.
- 6. H. Fowler, J. Devaney, and J. Hagedorn, "Growth Model for Filamentary Streamers in an Ambient Field," *IEEE Transactions on Dielectrics and Electrical Insulation*.
- 7. W.L. George, J. Hagedorn, and J. Devaney, "Parallel Programming with IMPI," Dr. Dobb's Journal.
- 8. J. Guyer, W. Boettinger, J. Warren, and G. McFadden, "Model of Electrochemical 'Double Layer' Using the Phase Field Method," in *Design and Mathematical Modeling of Electrochemical Systems*, (eds. J.W. Van Zee, M.E. Orazem, T. Fuller, and C.M. Doyle), Electrochemical Society, Pennington, NJ, 2002.
- 9. F.Y. Hunt, A.J. Kearsley, and Wan H., "A Linear Programming Approach to Multiple Sequence Alignment," *Applied Mathematics Letters*.
- 10. R. Kacker and N.F. Zhang, "On-line Control Using Integrated Moving Average Model for Manufacturing Errors," *International Journal of Production Research*.
- 11. A. Kearsley, P.T. Boggs, and J.W. Tolle, "Hierarchical Control of a Linear Diffusion Equation," *Proceedings of the 1st Sandia Workshop on PDE-constrained Optimization.*
- 12. A. Kearsley, F. Hunt, and H. Wan, "An Optimization Approach to Multiple Sequence Alignment," *Applied Mathematics Letters*.
- 13. A. Kearsley, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," in *Proceedings of the 50th ASMS Conference*.
- 14. D.W. Lozier, "Digital Library of Mathematical Functions Project," Annals of Mathematics and Artificial Intelligence.
- 15. N. Martys, J. Hagedorn, and J. Devaney, "Lattice Boltzmann Simulations of Single and Multi-Component Flow in Porous Media," in *Mesoscopic Modeling: Techniques and Applications*, (eds. Nicolaides and Bick), Marcel Dekker.
- 16. N. Martys and J. Hagedorn, "Modeling Fluid Flow in Porous Media Using the Lattice Boltzmann Method," *Materials Science of Concrete*, (ed. Jacques Marchand).
- 17. B.R. Miller and A. Youssef, "Technical Aspects of the Digital Library of Mathematical Functions," *Annals of Mathematics and Artificial Intelligence*.
- 18. 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*, Springer-Verlag.

- 19. T.L.Schmitz and T.J. Burns, "Receptance Coupling for High-Speed Machining Dynamics Prediction," *Proceedings of IMAC-XXI: A Conference & Exposition on Structural Dynamics*, Kissimmee, Florida, February 3-6, 2003.
- 20. C. Williams, B. Alpert, U. Arz, and D. Walker, "Causal Characteristic Impedance of Planar Transmission Lines," *IEEE Transactions on Advanced Packaging*.

Submitted

- 1. R.A. Allen, B.A. am Ende, M.W. Cresswell, C.E. Murabito, T.J. Headley, W.F. Guthrie, L.W. Linholm, C.H. Ellenwood, and E.H. Bogardus, "Test Structures for Referencing Electrical Linewidth Measurements To Silicon Lattice Parameters Using HRTEM," *IEEE Transactions on Semiconductor Manufacturing*.
- 2. B. Alpert and Y. Chen, "A Representation of Acoustic Waves in Unbounded Domains."
- 3. D. Basak, H.W. Yoon, R. Rhorer, T. Burns, "Microsecond Time-Resolved Pyrometry During Rapid Resistive Heating of Samples in a Kolsky Bar Apparatus," in *Proceedings of the 8th Symposium on Temperature, Its Measurement and Control in Science and Industry*, Chicago, IL, October 21-24, 2002.
- 4. R.F. Boisvert and R. Pozo, "Java," Handbook of Accuracy and Reliability in Scientific Software.
- 5. A. Dienstfrey and H. Jingfang, "Integral Representations for Elliptic Functions," *Transactions of the American Mathematical Society.*
- 6. M.J. Donahue, G. Vertesy, and M. Pardavi-Horvath, "Defect Related Switching Field Reduction in Small Magnetic Particle Arrays," *Journal of Applied Physics*.
- 7. B.R. Fabijonas, D.W. Lozier and F.W.J. Olver, "Algorithm: Airy Functions," ACM Transactions on Mathematical Software.
- 1. 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*.
- 8. D. E. Gilsinn, A. V. Ling, "Comparative Statistical Analysis of Test Parts Manufactured in Production Environments", *ASME Journal of Manufacturing Science and Engineering*.
- 9. K.F. Gurski and G.B. McFadden, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability," *Proceedings of the Royal Society (London) A.*
- 10. K. Gurski, R. Kollar, and R. Pego, "Slow Damping on Internal Waves in a Stably Stratfied Fluid," *Proceedings of the Royal Society of London.*
- 11. J. Guyer, W. Boettinger, J. Warren, and G. McFadden, "Model of Electrochemical 'Double Layer' Using the Phase Field Method," *Physica D*.
- 12. M. A. Hamstad, A. O'Gallagher, and J. Gary, "Examination of the Application of a Wavelet Transform to Acoustic Emission Signals: Part 1. Source Identification," *Journal of Acoustic Emission*.
- 13. M. A. Hamstad, A. O'Gallagher, and J. Gary, "Examination of the Application of a Wavelet Transform to Acoustic Emission Signals: Part 2. Source Location," *Journal of Acoustic Emission*.
- 14. R. Kacker, "Combining Information from Interlaboratory Studies Using Random Effects Model,"
- 15. G.B. McFadden, S.R. Coriell, T.P. Moffat, D. Josell, D. Wheeler, W. Schwartzacher, and J. Mallett, "A Mechanism for Brightening: Curvature Enhanced Surfactant Concentration," *Journal of the Electrochemical Society*.
- 16. I.K. Ono, S. Tewari, S.A. Langer, and A.J. Liu, "Velocity Fluctuations in a Steadily Sheared Model Foam," *Physical Review E.*
- 17. J.S. Sims and N.S. Martys, "Simulation of Sheared Suspensions with a Parallel Implementation of QDPD," *Computer Physics Communications*.
- 18. 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*.
- 19. G. Tanoglu, R. Braun, J. Cahn, and G. McFadden, "A1-L1₀ Phase Boundaries and Anisotropy Via Multiple-order-parameter Theory for an FCC Alloy," *Acta Materialia*.
- 20. R. Wittmann, B. Alpert, M. Francis, "Spherical Near-Field Antenna Measurements Using Nonideal Measurement Locations," in *Proceedings of the Antenna Measurement Techniques Association*, 2002.

In Process

- 1. I. Beichl, J. Carlson, and F. Sullivan, "Approximating Numbers of Independent Sets of a Graph with Application to the Hard-Square Entropy Constant".
- 2. I. Beichl, M. Robinson, D. Song, and F. Sullivan "A Quantum Algorithm for Determining If a Function is One to One".
- 3. I. Beichl and F. Sullivan, "Applications of Sinkhorn Balancing: the Monomer-Dimer Problem."
- 4. H.W. Bullen IV, J.S. Chang, A.V. Harn, Sean P. Kelly, S.G. Satterfield, P.M. Ketcham, and J.E. Devaney, "A Glyph Toolbox for Immersive Scientific Visualization."
- 5. M. J. Donahue and D. G. Porter, "Comparison of Exchange Energy Formulations for 3D Numerical Micromagnetics."
- 6. W.L. George, "C-DParLib Reference Manual".
- 7. W.L. George, "C-DParLib User's Guide".
- 8. K. Gurski, G. McFadden and M. Miksis, "The Effect of Contact Lines on the Rayleigh Instability with Anisotropic Surface Energy".
- 9. J. Guyer, W. Boettinger, J. Warren, and G. McFadden, "Phase Field Modeling of Electrochemicistry."
- 10. P. Huang and R. Kacker, "Repeatability and Reproducibility Uncertainty in Measurement of Humidity Produced by Permeation-Tube Moisture Generators".
- 11. R. Kacker, "Combining Information from Independent Similar Studies using Random Effects Model".
- 12. R. Kacker, R. Datla, and A. Parr, "More on Combined Result and the Associated Uncertainty".
- 13. R. Kacker and A. Jones, "On Use of Bayesian Statistics to Make Guide to the Expression of Uncertainty in Measurement Coherent."
- 14. A. Kearsley and C. Lawrence, "A New Matrix-free Interior Point Algorithm for Large-scale Spherically Constrained Quadratic Programs".
- 15. A. Kearsley and G. Cornuejouls, "An Infeasible Point Method for Solving 0/1 Integer Programming Problems".
- 16. N. Martys, J. Douglas, and J. Hagedorn, "Breakup of a Fluid Thread in a Confined Geometry: Transition from Bulge Instability and Kinetic Stabilization with Confinement."
- 17. B. Rust, "A Threshold Singular Component Method for Ill-Posed Problems."
- 18. B. Rust, "Fitting Nature's Basic Functions Part IV: The Variable Projection Algorithm," *Computing in Science & Engineering.*
- 19. B. Rust and W. Johnson, "Nonlinear Regression on Time-Domain Signals from Pulsed Excitation of Multiple Resonant Modes."
- 20. B. Rust and D. O'Leary, "A Truncated Singular Component Method for Ill-Posed Problems."

Visualizations Published

- 1. C. Clark, D. Feder, P.M. Ketcham, S.G. Satterfield. "Bose-Einstein Condensates," appeared in: the opening video of the SC2002 (Super Computing) conference, Baltimore MD, Nov 16-22, 2002.
- 2. P. Ketcham, BEC image, appeared in: "Bose-Einstein Condensation of Atomic Gases," *Nature* **416** (6877) (March 14, 2002), pp. 211-218.
- 3. P. Ketcham, High-resolution BEC image, appeared in: Exhibition on the Philosophy of Physics, Oxford University Reunion, March 27, 2002, New York.
- 4. P. Ketcham, animation of a morphing cement aggregate, appeared in: E. Garboczi, "CCTL: A Web-Based Virtual Cement and Concrete Testing Laboratory," Portland Cement Association Meeting, Chicago, IL, Sept. 16, 2002.
- 5. P. Ketcham, animation, appeared in: N. Martys, "Modeling Complex Fluids Using Lattice Boltzmann and Dissipative Particle Dynamics Methods," Levich Institute, City College, City University of New York, Sept. 10, 2002.

Presentations

Invited Talks

- 1. B. Alpert, "Geometry Representation and Quadrature for Computational Electromagnetics," DARPA Virtual Electromagnetics Testrange (VET) Kickoff Meeting, Breckenridge, CO, October 16, 2001.
- 2. B. Alpert, "Quadratures for Mostly-Uniform Discretizations of Regular and Singular Functions," Fast Algorithms Seminar, University of Colorado, Boulder, February 19, 2002.
- R. Boisvert, "Building the DLMF: Information Technology Issues," Workshop on Special Functions in the Digital Age, Institute for Mathematics and Its Applications (IMA), University of Minnesota, Minneapolis, MN, July 22, 2002.
- 4. A. Carasso, "The APEX Method in Image Sharpening and Heavy-tailed Point Spread Functions," National Institutes of Health, November 14, 2002.
- 5. J.E. Devaney, J.G. Hagedorn, S.G. Satterfield, P.M. Ketcham, and H.K. Hung, "Glyphs, Interestingness, and Data Mining," Gordon Conference on Combinatorial and High Throughput Materials Science, Meriden, NH, June 30 July 5, 2002.
- 6. A. Dienstfrey, "Multipole Methods for Photonic Crystal Computations," Fast Algorithms Seminar, University of Colorado at Boulder, February 27, 2002.
- 7. A. Dienstfrey, "Integral Representations for Elliptic Functions," University of North Carolina Analysis Seminar, March 20, 2002.
- 8. A. Dienstfrey, "Multipole Methods for Photonic Crystal Computations," University of North Carolina Applied Math Seminar, March 22, 2002.
- 9. 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.
- 10. K. Gurski, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability," Department of Engineering Sciences and Applied Mathematics Colloquium, Northwestern University, November 4, 2002.
- 11. K. Gurski, "An HLLC-type Approximate Riemann Solver for Magnetohydrodynamics," Department of Mathematical Sciences, George Mason University, November 9, 2001.
- 12. F. Hunt, "A Tutorial On Multiple Genetic Sequence Alignment," Conference for African American Researchers in the Mathematical Sciences, Princeton University, June 19, 2002.
- 13. F. Hunt, "Visualizing the Frequency Patterns of DNA," Morgan State University, Baltimore, MD, September 19, 2002.
- 14. R. Kacker, "Combined Result and Uncertainty from Interlaboratory Evaluations Based on the ISO Guide," Measurement Science Conference, Anaheim, CA, January 2002.
- 15. R. Kacker, "Combined Result and the Associated Uncertainty from Interlaboratory Evaluations Based on the ISO Guide," Eighth International Conference on New Developments & Applications in Optical Radiometry, Gaithersburg, MD, May 20-24, 2002.
- 16. A. Kearsley, "An Infeasible Point Method for a Class of Discrete Optimization Problems," Department of Mathematics, University of Maryland, November 30, 2001.
- 17. A. Kearsley, "An Infeasible Point Method Applied to the Cornuejols-Dawande Instance of Zero-one Programs," Center for Nonlinear Analysis, Carnegie Mellon University, Pittsburgh, PA, January 16, 2002.
- 18. A. Kearsley, "An Infeasible Point Method for a Class of Binary Programming Problems," Weekly Colloquium, University of North Carolina, Chapel Hill, April 3, 2002.
- 19. A. Kearsley, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," 50th ASMS Conference, Orlando, FL, June 3, 2002.
- 20. A. Kearsley, "Hierarchical Control Problems of Systems Governed by Differential Equations," Sandia Livermore National Labs, Livermore, CA, June 19, 2002.
- 21. A. Kearsley, "Optimality Conditions for Hierarchical Control Problems, Equations," Sandia Livermore National Labs, Livermore, CA, June 26, 2002.
- 22. D.W. Lozier, "Development of a New Handbook and Web Site of Properties of Special Functions," IMA Summer Program on Special Functions in the Digital Age, University of Minnesota, July 22, 2002.
- 23. D.W. Lozier, "Development of a New Handbook of Properties of Special Functions," Workshop on Foundations of Computational Mathematics, University of Minnesota, August 5, 2002.

- 24. D.W. Lozier, "The Digital Library of Mathematical Functions: A Comprehensive New Web Site and Handbook for the Special Functions of Applied Mathematics," Workshop on Electronic Information and Communication in Mathematics, Tsinghua University, Beijing, China, August 30, 2002.
- 25. G. McFadden, "Modeling of Flow During Coupled Monotectic Growth," 40th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 15, 2002.
- 26. G. McFadden, "Analytic Solution of Non-Axisymmetric Isothermal Dendrites," 2002 SIAM 50th Anniversary and Annual Meeting, Philadelphia, PA, July 9, 2002.
- 27. G. McFadden, "The Effect of Surface Tension Anisotropy on the Rayleigh Instability in Material Systems," 2002 SIAM 50th Anniversary and Annual Meeting, Philadelphia, PA, July 10, 2002.
- 28. G. McFadden, "The Effect of Surface Tension Anisotropy on Quantum Wires," Workshop on the Evolution and Self-assembly of Quantum Dots, Northwestern University, Evanston, IL, August 27, 2002.
- 29. B. Miller, "Representation, Display and Manipulation of Mathematics on the Web," Workshop on Special Functions in the Digital Age, Institute for Mathematics and Its Applications (IMA), University of Minnesota, Minneapolis, MN, August 1, 2002.
- 30. D.P. O'Leary, "Toward Understanding the Convergence of Krylov Subspace Methods," Symposium on Iterative Solvers for Large Linear Systems, Eidgenössische Technische Hochschule (ETH), Zurich, February 18, 2002.
- 31. F.W.J. Olver, "Error Bounds, Hyperasymptotics, and Uniform Asymptotics," Workshop on Special Functions in the Digital Age, Institute for Mathematics and Its Applications (IMA), University of Minnesota, Minneapolis, MN, July 22, 2002.
- 32. R. Pozo, "Java and Scientific Computing," Joint Workshop of the Organisation Associtave du Parallelisme (ORAP), and the Swiss Forum for High-Performance Computing (SPEEDUP) in Lyon, France, October 25, 2001.
- 33. R. Pozo, "Java and Scientific Computing," University of Tennessee, Knoxville, TN, February 22, 2002.
- 34. R. Pozo, "Java and Scientific Computing," Sandia National Laboratories, Albuquerque, NM, March 14, 2002.
- 35. B. Saunders, "Effective 3D Visualizations for the NIST Digital Library of Mathematical Functions," Mathematical Association of America, Maryland, D.C., Virginia Section Meeting, Virginia Tech, Blacksburg, VA, October 19, 2001.
- 36. B. Saunders, "Interactive 3D Visualizations of High Level Functions in a Mathematical Digital Library," IMA 2002 Summer Program: Special Functions in the Digital Age, University of Minnesota, August 1, 2002.
- 37. D. Song, "Entanglement Swapping," University of Maryland at Baltimore County, May 2002.
- 38. F. Sullivan, "Applications of Sinkhorn Balancing: Low Cost Approximations for Hard Problems," Annual Meeting of the American Mathematical Society, San Diego, CA, January 16, 2002.
- A. Youssef, "Search Systems for Mathematical Equations," Workshop on Special Functions in the Digital Age, Institute for Mathematics and Its Applications (IMA), University of Minnesota, Minneapolis, MN, July 31, 2002.

Conference Presentations

- 1. B. Alpert, "Quadratures for Mostly-Uniform Discretizations of Regular and Singular Functions," SIAM Annual Meeting, Philadelphia, PA, July 10, 2002.
- 2. B.A. am Ende, M.W. Cresswell, R.A. Allen, T.J. Headley, W.F. Guthrie, L.W. Linholm, E.H. Bogardus, and C.E. Murabito, "Measurement of the Linewidth of Electrical Test-Structure Reference Features by Automated Phase-Contrast Image Analysis," IEEE International Conference on Microelectronic Test Structures, Midas, Ireland, April 8-11, 2002.
- 3. G.W. Bryant, J. Aizpurua, Rui-Hui Xie, J. Franiatte, J.E. Devaney, W. Jaskolski, M. Zielinski, S. Lee, J. Kim, L. Jonsson, and J.W. Wilkins, "Designing the Nanoworld: Atomic Scale Simulations of Nanostructures and Nanodevices," Poster Presentation, Nanotechnology Open House, NIST, June 20, 2002.
- T. Burns, "Impact-Oscillator Model for Low Radial Immersion," 14th U.S. National Congress of Theoretical and Applied Mechanics, Virginia Polytechnic Institute and State University, Blacksburg, VA, June 23, 2002.
- 5. A. Carasso, "Blind Deconvolution and the APEX Method," SIAM Conference on Imaging Science, Boston MA, March 5, 2002.

- M.W. Cresswell, E.H. Bogardus, J. V. Martinez de Pinillos, M.H. Bennett, R.A. Allen, W.F. Guthrie, C.E. Murabito, B.A. am Ende, L.W. Linholm, "CD Reference Materials for Sub-Tenth Micrometer Applications," SPIE Microlithography Conference, Santa Clara, CA, March 3-8, 2002.
- 7. M.J. Donahue and D.G. Porter, "High Resolution Study of Discretization Effects in muMAG Standard Problem No. 1," MMM 2001, Seattle, WA, November 13, 2001.
- 8. M.J. Donahue and D.G. Porter, "Analysis of Switching in Uniformly Magnetized Bodies," Intermag Europe 2002, Amsterdam, The Netherlands, May 2, 2002.
- W.L. George and J. Scott, "Screen Saver Science: Realizing Distributed Parallel Computing with Jini and JavaSpaces," 2002 Conference on Parallel Architectures and Compilation Techniques, PACT2002), ACM SIGARCH, Charlottesville, VA, September 22-25, 2002.
- D. E. Gilsinn, "Estimating Critical Hopf Bifurcation Parameters for a Second Order Delay Differential Equation with Application to Machine Tool Chatter," SIAM Annual Meeting, Philadelphia, PA, July 8–12, 2002.
- D. E. Gilsinn, G. S. Cheok, D. P. O'Leary, "Reconstructing Images of Bar Codes for Construction Site Object Recognition", ISARC 2002, 19th International Symposium on Automation and Robotics in Construction, NIST, Gaithersburg, MD, September 23, 2002.
- 12. K. Gurski, "Modeling a Quantum Wire: The Effect of Anisotropic Surface Energy on the Rayleigh Instability," American Mathematical Society and Mathematical Association of America Southeastern Sectional Meeting, Atlanta, GA, March 9, 2002.
- 13. F. Hunt, "A Linear Programming Approach to Multiple Sequence Alignment," Bioinformatics Spring Workshop, National Center for Genomic Research, Santa Fe, New Mexico, March 12, 2002.
- 14. S. Langer, "Modeling the Elastic Properties of Materials using OOF," 13th ACBM/NIST Computer Modeling Workshop, Building and Fire Research Laboratory, NIST, June 13, 2002.
- 15. D.W. Lozier, "The Digital Library of Mathematical Functions Project," SIAM Annual Meeting, Philadelphia, PA, July 8, 2002.
- 16. D.W. Lozier, "Development of a New Handbook of Properties of Special Functions," International Congress of Mathematicians, Beijing, China, August 23, 2002.
- 17. G. McFadden, "Effect of Flow Due to Density Change on Eutectic Growth," 2001 APS Division of Fluid Dynamics Annual Meeting, San Diego, CA, November 19, 2001.
- 18. W.F. Mitchell and E. Tiesinga, "Computing Interior Eigenvalues of a Schroedinger Equation, Seventh Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, March 25-29, 2002.
- 19. W.F. Mitchell, "The Design of a Parallel Adaptive Multi-Level Code in Fortran 90," International Conference on Computational Science (ICCS2002), Workshop on PDE Software, Amsterdam, The Netherlands, April 23, 2002.
- 20. W. Mitchell, "Parallel Adaptive Grid Refinement in PHAML," IMACS Workshop on Adaptive Methods for Partial Differential Equations, Toronto, CA, August 7, 2002.
- 21. B. Rust, "The Truncated Singular Component Method for Ill-Posed Problems," SIAM 2002 Annual Meeting, Philadelphia, PA, July 2002.
- 22. D. Song, "Quantum Bus and Efficient Nonlocal Operations," The 6th International Meeting on Quantum Communication, Measurement and Computing (QCMC 2002), MIT, July 23, 2002, Cambridge, MA.
- 23. D. Song, "Quantum Bus and Efficient Nonlocal Operations," Advanced Research and Development Activity (ARDA), Army Research Office (ARO) meeting, Nashville, TN, August 23, 2002.
- 24. C. Witzgall and G. Cheok, "Experiences with Point Cloud Registration" ISARC (International Society for Automation and Robotics in Construction), NIST, September 24, 2002.

Presentations Given at NIST

- 1. A. Carasso, "Direct Blind Deconvolution and Lévy Densities," NIST Center for Neutron Research, Gaithersburg MD, January 30, 2002.
- J. E. Devaney, B. Am Ende, H. K. Hung, J. Hagedron, "Informatics for Microwave-Frequency Microscopy in High Throughput Materials Analysis," 2001 ATP Program Review: Combinatorial Methods for Materials Research, NIST, Gaithersburg, October 19, 2001.
- 3. J. E. Devaney, J. G. Hagedorn, "From Data to Models Using Multiple Machine Learning Methods," Poster Presentation, Nanotechnology Open House, NIST, June 20, 2002.

- 4. J. E. Devaney, J. G. Hagedorn, "Plaster From a Machine Learning Perspective," Virtual Cement and Concrete Testing Laboratory Meeting, NIST, Gaithersburg, May 9-10, 2002.
- 5. M. Donahue, "Micromagnetic Modeling," Poster Presentation, Nanotechnology Open House, NIST, June 20, 2002.
- 6. M. Donahue, "The OOMMF Micromagnetics Modeling Package," NIST Magnetics Video Seminar, August 20, 2002.
- 7. J.C. Franiatte, J.E. Devaney, G.W. Bryant, S.G. Satterfield, and W.L. George, "Building Nanostructures Interactively in an Immersive Visualization Environment," Poster Presentation, Nanotechnology Open House, NIST, June 20, 2002.
- 8. D.E. Gilsinn, G.S. Cheok, D.P. O'Leary, and W.C. Stone, "Enhanced Construction Object Recognition Through Sensor Fusion," NIST LADAR Lecture Series, June 18-20, 2002.
- 9. K. Gurski, "Modeling a Quantum Wire: The Effect of Anisotropic Surface Energy on the Rayleigh Instability," Sigma Xi Postdoctoral Poster Presentations, NIST, February 28, 2002.
- 10. K. Gurski, "The Effect of Anisotropic Surface Energy on the Rayleigh Instability," Material Science Department Bag Lunch Seminar, NIST, October 17, 2002.
- 11. A. Kearsley, "Advanced Numerical Methods for Polymer Mass Spectral Data Analysis," Polymer Division Seminar Series, July 24, 2002.
- 12. B. Rust, "Fitting Nature's Basic Functions," NIST Summer Undergraduate Research Fellowhip Seminar Series, July 26, 2002.
- 13. J. Scott and W. George, "Distributed Computing in Java: The Screen Saver Science Project," 2002 SURF Colloquium, NIST, August 15, 2002.
- 14. C. Witzgall, "Meshing," NIST LADAR Lecture Series, June 19, 2002.
- 15. C. Witzgall, "Registration," NIST LADAR Lecture Series, June 19, 2002.

Conferences, Minisymposia, Lecture Series, Short-courses

MCSD Seminar Series

- 1. Manil Suri (University of Maryland Baltimore County), "The p and hp Finite Element Modeling of Thin Structures," Oct. 30, 2001.
- 2. Barbara A. am Ende (MCSD), "Visualizing a Sub-Aqueous, Subterranean Cave," Nov. 6, 2001.
- 3. Katharine F. Gurski (MCSD), "An HLLC-type Approximate Riemann Solver for Ideal Magnetohydrodynamics," Nov. 13, 2001.
- Raghu Kacker (MCSD), "Analysis of Uncertainty in Interlaboratory Evaluations Based on the ISO Guide," Nov. 27, 2001.
- 5. James Lawrence (MCSD and George Mason University), "Some Problems of Combinatorial Geometry," Dec. 4, 2001.
- 6. Michael Mascagni (Florida State University), "First and Last Passage Random Walk Algorithms," Dec. 10, 2001.
- 7. Jon Tolle (University of North Carolina), "Hierarchical Control Problems," Dec. 11, 2001.
- 8. Fredrick R. Phelan Jr. (Multiphase Material Group, Polymer Division, NIST), "Microstructure Modeling of Polymer Blends in Complex Flows," Dec. 18, 2001.
- 9. Guillermo Sapiro (University of Minnesota), "Image and Video Inpainting," Jan. 23, 2002.
- 10. Fern Hunt (MCSD), "A Linear Programming Approach to Multiple Sequence Alignment," Jan. 29, 2002.
- 11. Alex Tolstoy (A. Tolstoy Sciences), "Underwater Acoustics and the Hunt for Red October," Feb. 12, 2002.
- 12. Anthony Kearsley (MCSD), "An Infeasible Point Method for Solving a Class of Binary Programming Problems," Feb. 19, 2002.
- 13. Javier Bernal (MCSD), "REGTET: A Program for Computing Regular Tetrahedralizations," Feb. 27, 2002.
- 14. Daniel Gottesman (University of California at Berkeley), "Private Key and Public Key Quantum Cryptography," March 5, 2002.
- 15. Mila Nikolova (CNRS, France), "Critical Features of the Minimizers of Non-smooth Cost-functions: Application to Image Processing," March 8, 2002.

- 16. Kirsi Majava (University of Jyvaskyla, Finland), "SAC Semi-adaptive, Convex Optimization Methodology for Image Restoration," March 12, 2002.
- 17. William Mitchell (MCSD), "Parallel Adaptive Multigrid Software for Elliptic PDEs and Eigenvalue Problems," March 19, 2002.
- 18. Susan Minkoff (University of Maryland Baltimore County), "Staggered In-time Coupling of Fluid Flow and Geomechanical Deformation Modeling for 4D Seismic," March 28, 2002.
- 19. Arlin Stoltzfus (Center for Advanced Research in Biotechnology, NIST), "Amino Acid Exchangeability from Experimental Data," April 9, 2002.
- 20. Nicos Martys (BFRL), "Modeling Complex Fluids Using Lattice Boltzmann and Dissipative Particle Dynamics Methods," April 16, 2002.
- 21. Troy Marusich (Third Wave Systems, Inc., Minneapolis, MN), "Modeling of Production Metal Cutting Processes," April 18, 2002.
- 22. Arthur Pittenger (University of Maryland Baltimore County), "Quantum Computation and the Separability Problem," April 24, 2002.
- 23. Barbara Keyfitz (University of Houston), "Singular Shocks in a Two-Fluid Model for Bubbly Flows," April 29, 2002.
- 24. Barry Bernstein (Illinois Institute of Technology), "An Expository Talk on Theory of Bifurcations with Numerical Examples," May 3, 2002.
- Anastase Nakassis (Advanced Network Technology, ITL), "Cryptography and Quantum Cummunications," May 16, 2002.
- 26. Nico Temme (CWI, Amsterdam, The Netherlands), "New Software for a Class of Special Functions," May 22, 2002.
- 27. Donald Porter (MCSD), "Programming Advantages of an Embedded Command Language," May 28, 2002.
- 28. Michael Trosset (College of William and Mary), "On the Use of Second-Order Information in Distance Geometry and Multidimensional Scaling," June 4, 2002.
- 29. Andries van Dam (Brown University), "Immersive VR for Scientific Visualization: A Progress Report," June 11, 2002.
- 30. Bruce Fabijonas (MCSD/Southern Methodist University), "The Craik-Criminale Class of Solutions to the Incompressible Navier-Stokes and Similar Equations," June 25, 2002.
- 31. G. Pestka, "Hylleraas-Cl Approach to Dirac-Coulomb Eigenvalue Problem: Ground States of Helium-like Atoms," July 2, 2002.
- 32. D. Song (MCSD), "Introduction to Quantum Algorithms," July 16,2002.
- 33. P. Williams, "Using Indicators in Finite Termination Procedures," Aug. 1, 2002.
- 34. D. E. Gilsinn (MCSD), "Estimating Critical Hopf Bifurcation Parameters for a Second Order Delay Differential Equation with Application to Machine Tool Chatter," Sept. 26, 2002.

DLMF Seminar Series

- 1. P. Clarkson (University of Kent), "The Painlevé Equations Nonlinear Special Functions," Nov. 20, 2001.
- 2. B. Verdonk (University of Antwerp), "Contribution to a Digital Library of Special Functions," Nov. 21, 2001.
- 3. M. Kohlhase (Carnegie Mellon University), "Administration, Visualization and Distribution of Mathematical Knowledge in the Internet Era," Dec. 3, 2001.
- 4. S. Casey (American University), "Complex Mappings From an Evolutionary Viewpoint," April 2, 2002.
- 5. N. Temme (CWI, The Netherlands), "New Software for a Class of Special Functions," May 22, 2002.

Local Events Organized

Shortcourses

- 1. J. Filla (organizer), "Hands-on Introduction to LabVIEW, using LV 6," NIST (Boulder), March 28-29.
- 2. H. Hung, "Basic Unix", NIST, December 4 and 5 and December 11 and 12, 2001.

Workshops

- 1. J. Filla arranged and hosted a LabVIEW Workshop NIST (Boulder) on November 2, 2001. Included were a users meeting, a LabVIEW 6 presentation, and a hands-on LabVIEW networking seminar taught by Ed McConnell of National Instruments.
- 2. MCSD presented an Open House for ITL staff in Gaithersburg on May 16, 2002. A poster and demo format was used. Some 60 staff attended. The following posters were presented.
 - a. Micromagnetic Modeling, Michael Donahue and Donald Porter
 - b. Digital Library of Mathematical Functions, Daniel Lozier, Bruce Miller, and Bonita Saunders
 - c. Combinatorial Counting Problems, Isabel Beichl
 - d. Modeling of Quantum Wires, Katherine Gurski and Geoffrey McFadden
 - e. Deconvolution of LADAR Scans, David Gilsinn
 - f. Parallel Adaptive Grid Refinement, William Mitchell
 - g. Blind Image Deblurring, Alfred Carasso
 - h. Modeling of Material Microstructure, Stephen Langer
 - i. Cement Modeling and Visualization, Judith Devaney and John Hagedorn
 - j. RAVE Immersive Visualization Facility, Steve Satterfield and Terrence Griffin

External Event Organization

- 1. R. Boisvert, Program Committee, ACM Java Grande/ISCOPE Conference, Seattle, WA, November 3-5, 2002.
- 2. R. Boisvert, Program Committee, Iterative Solvers for Large Linear Systems: Celebrating 50 Years of the Conjugate Gradient Method, Zurich, February 18-20, 2002.
- 3. R. Boisvert, Co-organizer, *Workshop on the Mathematics of Mathematical Software*, June 3-4, 2002, Portland, Oregon. The meeting was sponsored by the IFIP Working Group 2.5 (Numerical Software) and Intel.
- 4. R. Boisvert, Co-organizer, International Workshop on Numerical and Symbolic Scientific Computing, St. Wolfgang, Austria, June 16-21, 2003.
- 5. D. Lozier, Organizing Committee, IMA Summer Program: *Special Functions in the Digital Age*, Institute for Mathematics and Its Applications, University of Minnesota, July 22 August 2, 2002.
- 6. D. Lozier, Organizing Committee, *International Conference on Special Functions and their Applications*, Institute of Mathematical Sciences, Madras, India, September 23-27, 2002.
- 7. D. Lozier, Organizing Committee, Minisymposia on Special Functions: Computational Methods and Applications, *SIAM National Meeting*, Montreal, June 2003.
- 8. B. Miller, Program Committee, *MathML International Conference*, Chicago, June 28-30, 2002.

Software Released

- 1. DIVERSE Graphics Modules (DSOs), http://math.nist.gov/mcsd/savg/software/.
 - Screen Contact Alert DSO (J.C. Franiatte, S.G. Satterfield, and J.G. Hagedorn)
 - TurnTableNode DSO (A.P. Peskin and S.G. Satterfield)
 - ABswitch DSO (A.P. Peskin and S.G. Satterfield)
 - TIM (Things in Motion) DSO (A.P. Peskin and S.G. Satterfield)
- 2. OOMMF, 1.1 beta 1, October 2, 2001, http://math.nist.gov/oommf/, (M. Donahue and D. Porter).
- 3. PHAML, Version 0.9, April 18, 2002, http://math.nist.gov/phaml/, (W.Mitchell).
- 4. Tcl/Tk 8.3.3 binary for the Windows NT 4/Alpha platform, October 2, 2001, http://www.tcl.tk/, (D. Porter).
- 5. Tcl/Tk 8.4.0, September 14, 2002, <u>http://www.tcl.tk/</u>, (D. Porter).
- 6. Tcl package "control" version 0.0, in tcllib 1.1, October 21, 2001, <u>http://www.tcl.tk/</u>, (D. Porter).
- 7. Tcl package "control" version 0.1, in tcllib 1.2, January 20, 2002, <u>http://www.tcl.tk/</u>, (D. Porter).
- 8. Template Numerical Toolkit (TNT), Version 1.1, August 2002, http://math.nist.gov/tnt/, (R. Pozo).

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

Acuity Research Air Products and Chemicals Inc. Altair Engineering American Superconductor Analog Devices Inc. Baker-Hughes Inc. Boeing Aerospace BP Center for Visualization Catalyst Group Centre National de la Recherche Scientifique (France) Cisco Systems CWI (The Netherlands) Ecole Nationale de la Statistique et de L'Analyse de L'Informatique (ENSAI) (France) Electronic Development Labs Inc. Excellatron Solid State LLC Exxon Mobile Research and Engineering Ford Fujitsu System Integration Laboratories (Japan) German Cement Assoc. Illumina Intel International Science and Technology Center (ISTC) (Moscow) Johnson Scientific Group Inc.

Government/Non-profit Organizations

Association for Computing Machinery American Chemical Society American Mathematical Society Argonne National Laboratory Army Research Laboratory Army Research Office (ARO) Association for Women in Mathematics Commonwealth Scientific and Industrial Research Organization (CSIRO) (Australia) Department of Defense (DoD) Department of Energy (DoE) Food and Drug Administration Federal Highway Administration **IEEE Computer Society** Institute of Mathematical Sciences (India) International Atomic Energy Agency (Austria) Massively Parallel Technologies MatrixOne Metacomp Technologies MPI Software Technology National Center for Genomic Research Nebule.com Nikkoa.com Nonlinear Dynamics Nortel Networks Nuclear Physiology Laboratory (Brazil) Portland Cement Association Printers Integrated Color Solutions R.R. Donnelly and Sons Company SAS Institute Science and Technology Center (STCU) (Ukraine) Sematech SGI Siemens Sun Microsystems SuSE Linux Teledyne Solutions Inc. Third Wave Systems, Inc. Three Mile Island Vympel Corporation (Russia) Weidlinger Associates Xerox Palo Alto Research Center

International Society for Automation and Robotics in Construction (ISARC) Joint Warfare Analysis Center Kirtland Air Force Base Los Alamos National Laboratory National Institutes of Health (NIH) National Science Foundation (NSF) Natural Sciences and Engineering Research Council (NSERC) of Canada Naval Surface Warfare Center (NSWCCD) Office of Naval Research Sandia National Laboratory Society for Industrial and Applied Mathematics (SIAM) U.S. Department of Energy (DoE) U.S. Office of Personnel Management U.S. Treasury

Universities

American University Bowie State University Brown University Capital University of Medical Sciences (China) Carnegie Mellon University Chelyabinsk State University (Russia) City University of New York College of William and Mary Colorado School of Mines Columbia University Cornell University Delft University of Technology (The Netherlands) Duke University Eidgenössische Technische Hochschule (ETH) (Switzerland) Florida State University George Mason University George Washington University Harvard University Hong Kong University of Science and Technology Illinois Institute of Technology Indiana University Marymount University Massachusetts Institute of Technology (MIT) Morgan State University National University of Malaysia New York University Nicolas Copernicus University of Torun (Poland) Northwestern University Osaka University (Japan) Oxford University Penn State University Princeton University **Rice University RWTH Mathematical Institute (Germany)** Sienna College Southern Methodist University Stanford University Tel Aviv University Tsinghua University (China) **UBS** Warburg Universita degli di Salerno (Italy) University of Antwerp (Belgium) University of Bristol (UK) University of California at Berkeley University of California at Irvine University of Chicago University of Colorado University of Connecticut Health Care Center University of Delaware University of Florida University of Geneva (Switzerland) University of Houston University of Kent (UK)

University of Manchester (UK) University of Maryland University of Michigan University of Minnesota University of Montreal University of North Carolina University of Pittsburgh University of San Sebastian University of South Carolina University of Southampton (UK) University of Southern California University of Stuttgart University of Tennessee University of Trento (Italy) University of Utah University of Wisconsin Vietnam National University Virginia Polytechnic Institute and State University Wake Forest University Washington University

Other Professional Activities

Internal

- 1. I. Beichl served as co-director of the ITL Student Undergraduate Research Fellowship (SURF) program.
- 2. R. Boisvert and J. Bernal serve on the ITL Diversity Committee.
- 3. R. Boisvert serves on the NIST Scientific Computing Working Group.
- 4. A. Dienstfrey served on the NIST Research Advisory Committee.
- 5. J. Filla served as the NIST 2010 Strategic Planning People-Strategic Focus Area point-of-contact for ITL.
- 6. A. Kearsley served as colloquium chair for the MCSD.
- 7. A. O'Gallagher served as a member of the ITL Awards Committee.
- 8. B. Rust served as ITL representative to the NIST Research Information Center Advisory Committee.
- 9. B. Rust serves on the NIST Library Advisory Committee.
- 10. 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

- 1. B. Alpert served as Associate Editor for SIAM Journal on Scientific Computing.
- 2. I. Beichl served on the editorial board of *Computing in Science and Engineering*.
- 3. Isabel Beichl and W. Mitchell serve on the editorial board of the new *Journal of Numerical Analysis and Computational Mathematics*.
- 4. R. Boisvert serve as Chair of the International Federation for Information Processing's Working Group 2.5 on Numerical Software.
- 5. R. Boisvert served as Editor-in-Chief of the ACM Transactions on Mathematical Software.
- 6. R. Boisvert served as Vice-Chair of the ACM Publications Board.
- 7. J. Devaney served on an applicant selection panel for the Financial Crimes Enforcement Network of the U.S. Treasury.
- 8. M. Donahue serves on the editorial board of the *Journal of Computational Methods in Science and Engineering*.
- 9. F. Hunt served on an NIH review panel for proposals submitted to the Algorithms, Adapters and Data Distribution program for of biomedical images associated with the Visible Human Project Insight Toolkit.
- 10. D. Lozier served as Associate Editor of Mathematics of Computation.
- 11. D. Lozier served as Chair of the SIAM Activity Group on Orthogonal Polynomials and Special Functions.
- 12. G. McFadden served on the editorial boards of the SIAM Journal of Applied Mathematics, the Journal of Crystal Growth, and Interfaces and Free Boundaries.
- 13. D. Porter served as a leading member of the Tcl Core Team.
- 14. R. Pozo served as Associate Editor for the ACM Transactions on Mathematical Software.
- 15. B. Saunders served on the selection committee for the John Smith Award for Distinguished College or University Teaching Award sponsored by the MD-DC-VA Section 9if the Mathematical Association of America.
- 16. Division staff members referee manuscripts for a wide variety of journals including Acta Metallurgica, Applied and Computational Harmonic Analysis, Applied Mathematics Letters, Computers and Mathematics with Applications, Computing in Science and Engineering, Fluid Dynamics Research, IEEE Computing in Science and Engineering, IEEE Transactions on Antennas and Propagation, IEEE Transactions on Circuits and Systems (Part I), IEEE Transactions on Magnetics, Institute of Statistical Mathematics, International Journal of Electronics, International Journal of Nonlinear Mechanics, Journal of Applied Physics, Journal of Computational and Applied Mathematics, Journal of Computational and Applied Mathematics, Journal of Computational and Physics, Journal of Computational and Graphical Statistics, Journal of Computational Physics, Journal of Crystal Growth, Journal of Fluid Mechanics, Journal of Lightwave Technology, Journal of Manufacturing Science and Engineering A, Mathematical and Computer Modeling, Mathematical Reviews, Mathematics of Computation, NIST Journal of Research, Nonlinear Science, Numerical Algorithms,

Parallel Computing, Physica D, Physica D, Physical Review, Physical Review B, Physics of Fluids, SIAM Journal on Applied Mathematics, SIAM Journal on Numerical Analysis, SIAM Journal of Scientific Computing, and Springer-Verlag.

- 17. Division staff members referee manuscripts for a wide variety of conferences including ASME Design Engineering Technical Conference, Java Grande/ISCOPE Conference, SC2001 (Super Computing), the 3rd International Conference on Large-Scale Scientific Computations, and the Fifteenth TOYOTA Conference on Scientific and Engineering Computations for the 21st Century.
- 18. Staff members review proposals for the following research programs: American Chemical Society, AFOSR, ARO, DARPA, DOE, NASA, NSF, and the W.M. Keck Foundation.