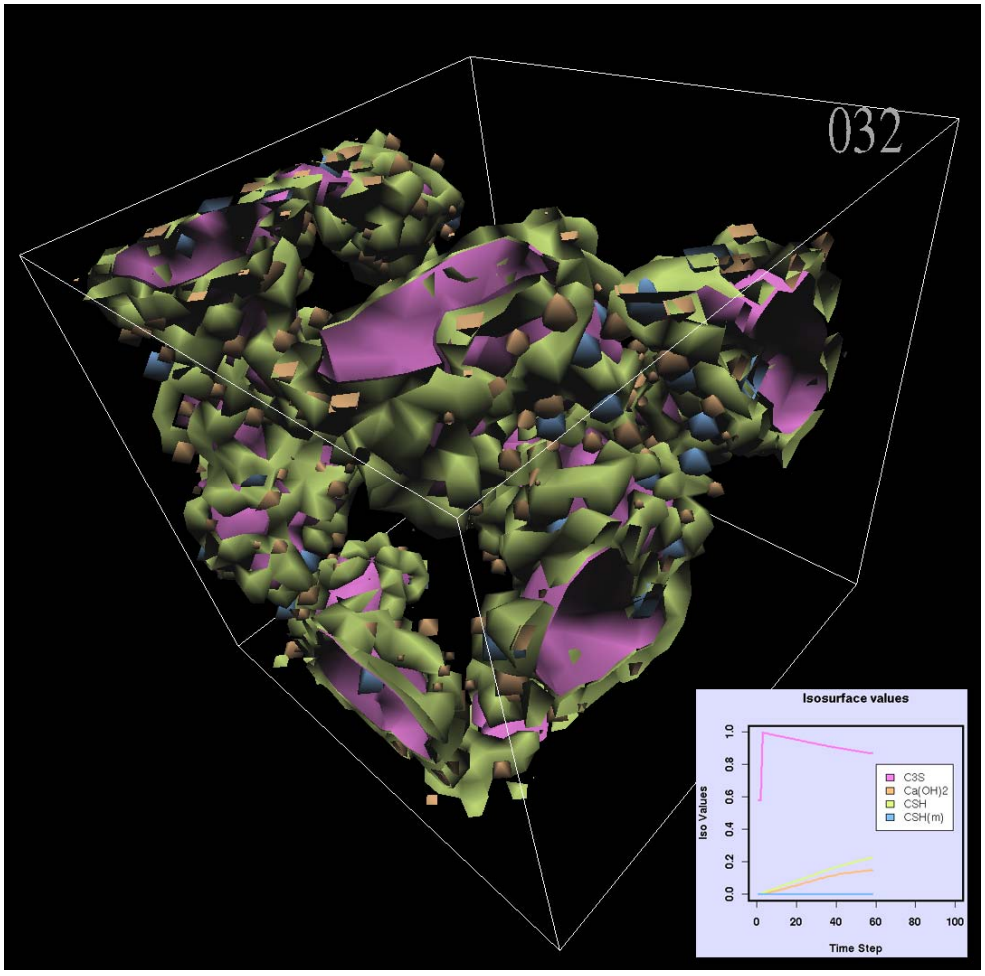
Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2007



Information Technology Laboratory
National Institute of Standards and Technology
U.S. Department of Commerce

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INFORMATION TECHNOLOGY LABORATORY

NIST National Institute of Standards and Technology U.S. Department of Commerce

Abstract

This report summarizes the technical work of the Mathematical and Computational Sciences Division (MCSD) of NIST's Information Technology Laboratory. Part I (Overview) provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II (Features) provides further details on eight particular projects of particular note this year. This is followed in Part III (Project Summaries) by brief summaries of all technical projects active during the past year. Part IV (Activity Data) provides listings of publications, technical talks, and other professional activities in which Division staff members have participated. The reporting period covered by this document is October 2006 through December 2007.

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Cover photo. Visualization and analysis of the microstructure a computational model of cement hydration showing four distinct phases. This is the result of research performed by William George, Steve Satterfield, and Edith Enjolras of MCSD in collaboration with Jeffrey Bullard of the NIST Building and Fire Research Laboratory.

Acknowledgement. We are grateful to Robin Bickel for collecting the information and organizing the first draft of this report.

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Part IV

Activity Data

Publications

Appeared

Refereed Journals

1. D.M. Anderson, P. Cermelli, E. Fried, M.E. Gurtin, and G.B. McFadden, "General Dynamical Sharp-interface Conditions for Two-phase Viscous Heat-conducting Fluids," *Journal of Fluid Mechanics* **581** (2007), pp. 323-370.
2. H. Bennett, A. Dienstfrey, L. Hudson, T. Oreskovic, T. Fuerst, and T. Shepherd, "Standards and Measurements for Assessing Bone Health--Workshop Report Co-sponsored by the International Society of Clinical Densitometry and the National Institute of Standards and Technology," *Journal of Clinical Densitometry* **9** (4) (2006), 399-405.
3. W. J. Boettinger, J. E. Guyer, C. E. Campbell, and G. B. McFadden, "Computation of the Kirkendall Velocity and Displacement Field in a 1-D Diffusion Couple with a Moving Interface," *Proceedings of the Royal Society of London* **463** (2007), pp. 3347-3373.
4. A. S. Carasso, "APEX Blind Deconvolution of Color Hubble Space Telescope Imagery and Other Astronomical Data," *Optical Engineering* **45** (October 2006), article 107004, 15 pages.
5. R. Dersimonian and R. Kacker, "Random-effects Model for Meta-analysis of Clinical Trials: An update," *Contemporary Clinical Trials* **28** (2007), pp. 105-114.
6. M. J. Donahue and R. D. McMichael, "Micromagnetics on Curved Geometries Rectangular Cells: Error Correction and Analysis," *IEEE Transactions on Magnetics* **43** (2007), pp. 2878-2880.
7. E. J. Garboczi, J. F. Douglas and R. B. Bohn, "A Hybrid Finite Element-analytical Method for Determining the Intrisic Elastic Moduli of Particles Having Moderately Extended Shapes and a Wide Range of Elastic Properties," *Mechanics of Materials* **38** (2006), pp. 786-800.
8. D. E. Gilsinn and F. A. Potra, "Integral Operators and Delay Differential Equations," *Journal of Integral Equations and Applications* **18** (3) (Fall 2006), pp. 297- 336.
9. D. E. Gilsinn, "Computable Error Bounds for Approximate Periodic Solutions of Autonomous Delay Differential Equations," *Nonlinear Dynamics* **50** (2007), pp. 73-92.
10. J. Hagedorn, S. Satterfield, J. Kelso, W. Austin, J. Terrill, and A. Peskin, "Correction of Location and Orientation Errors in Electromagnetic Motion Tracking," *Presence* **16** (4) (2008-8), pp. 352-366.
11. R. Kacker, B. Toman, and D. Huang, "Comparison of ISO GUM, Draft GUM Supplement 1, and Bayesian Statistics Using Simple Linear Calibration," *Metrologia*, **43** (2006), pp. S167-S177.
12. R. Kacker and J. Lawrence, "Trapezoidal and Triangular Distributions for Type B Evaluation of Standard Uncertainty," *Metrologia* **44** (2007), pp. 117-127.
13. A.J. Kearsley, "Algorithms for Optimal Signal Set Design," *Optimization Methods and Software* **21** (6) (December 2006), pp. 977-994.
14. A. Kearsley, L. Melara and R. Tapia "A Homotopy Method in the Regularization of Total Variation Denoising," *Journal of Optimization Theory and Applications* **133** (2) (2007), pp. 15-25.
15. A. Kearsley, W. Wallace, C. Guttman, and K. Flynn, "Numerical Optimization of Matrix-Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry: Application to Synthetic Polymer Molecular Mass Distribution Measurement," *Analytica Chimica* **604** (2007), pp. 62-68.
16. R. Kessel, R. Kacker, and M. Berglund "Coefficient of Contribution to the Combined Standard Uncertainty," *Metrologia* **43** (2006), pp. S189-S195.
17. E. Knill, "Protected Realizations of Quantum Information," *Physical Review A* **74** (Oct. 2006), Art. No. 042301.
18. E. Knill, G. Ortiz, and R.D. Somma, "Optimal Quantum Measurements of Expectation Values of Observables," *Physical Review A* **75** (Jan. 2007), Art. No. 012328.
19. D. Leibfried, E. Knill, C. Ospelkaus, D. J. Wineland, "Transport Quantum Logic Gates for Trapped Ions," *Physical Review A* **76** (Sept. 2007), Art. No. 032324.
20. Z. H. Levine, A. Volkovitsky, and H. K. Hung, "Alignment of Fiducial Marks in a Tomographic Tilt Series with an Unknown Rotation Axis," *Computer Physics Communications* **176** (April 2007), pp. 694-700.
21. G. B. McFadden, S. R. Coriell, K. F. Gurski, and D. L. Cotrell, "Onset of Convection in Two Liquid Layers with Phase Change," *Physics of Fluids* **19** (2007), Art. No. 104109.

22. W. F. Mitchell, "A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids," *Journal of Parallel and Distributed Computing* **67** (4) (2007), pp. 417-429.

23. P. Naidon, E. Tiesinga, W. F. Mitchell and P. S. Julienne, "Effective-range Description of a Bose Gas under Strong One- or Two-Dimensional Confinement," *New Journal of Physics* **9** (2007), p. 19.

24. D.P. O'Leary, G.K. Brennen, and S.S. Bullock, "Parallelism for Quantum Computation with Qudits," *Physical Review A* **74** (2006), Art. No. 032334.

25. J. Rehacek, Z. Hradil, E. Knill, A. I. Lvovsky, "Diluted Maximum-likelihood Algorithm for Quantum Tomography," *Physical Review A* **75** (Apr. 2007), Art. No. 042108.

26. R. Reichle, D. Leibfried, E. Knill, J. Britton, R. B. Blakestad, J. D. Jost, C. Langer, R. Ozeri, S. Seidelin, and D. J. Wineland, "Experimental Purification of Two-atom Entanglement," *Nature* **443** (Oct. 19, 2006), pp. 838-841.

27. J. S. Sims and S. A. Hagstrom, "Mathematical and Computational Science Issues in High Precision Hylleraas-configuration Interaction Variational Calculations II. Kinetic Energy and Electron-nucleus Interaction Integrals," *Journal of Physics B: Atomic, Molecular, and Optical Physics* **40** (2007), pp. 1575-1587.

28. J.S. Sims and S.A. Hagstrom, "High Precision Variational Born-Oppenheimer Energies of the Ground State of the Hydrogen Molecule," *Journal of Chemical Physics* **124** (9)(2006), pp. 094101-1 – 094101-7.

29. M. D. Stiles, W. M. Saslow, M. J. Donahue, and A. Zangwill, "Adiabatic Domain Wall Motion and Landau-Lifshitz Damping," *Physical Review B* **75** (2007), p. 214423.

30. R. Somma, H. Barnum, G. Ortiz, and E. Knill, "Efficient Solvability of Hamiltonians and Limits on the Power of Some Quantum Computational Models," *Physical Review Letters* **92** (Nov. 10 2006), Art. No. 190501.

31. Q. Wang, B. Saunders, and S. Ressler, "Dissemination of 3D Visualizations of Complex Function Data for the NIST Digital Library of Mathematical Functions," *CODATA Data Science Journal* **6** (2007), pp. S146-S154.

Journal of Research of NIST

1. A. Gaigalas, F. Hunt, and L. Wang, "Modeling of Photochemical Reactions in a Focused Laser Beam," *NIST Journal of Research* **112** (4) (July-August 2007), pp. 191-208.

2. J. Hagedorn, J. Dunkers, S. Satterfield, A. Peskin, J. Kelso, and J. Terrill, "Measurement Tools for the Immersive Visualization Environment: Steps Toward the Virtual Laboratory," *NIST Journal of Research* **112** (5) (Sept.-Oct. 2007), pp. 257-270.

3. A. Kearsley and D. Cotrell, "Flow Control Through the Use of Topography," *NIST Journal of Research* **112** (3) (2007), pp. 1-9.

4. Z. Levine, A. Kearsley, and J. Hagedorn, "Bayesian Tomography for Projections with an Arbitrary Transmission Function with an Application to Electron Tomography," *Journal of Research of NIST* **111** (6) (Nov.-Dec. 2006), pp. 411-417.

5. G.B. McFadden, S.R. Coriell, K. F. Gurski, and D. L. Cotrell, "Convective Instabilities in Two Liquid Layers," *NIST Journal of Research* **112** (5) (Sept.-Oct. 2007), pp. 271-281.

Other Invited Publications

1. I. Beichl, D.P. O'Leary, and F. Sullivan, "Your Homework Assignment: Monte Carlo Minimization," *IEEE Computing in Science and Engineering* **9** (1) (2007), pp 72-80.

2. I. Beichl, D.P. O'Leary and F. Sullivan, "Answers to Your Homework Assignment," *IEEE Computing in Science and Engineering* **9** (2) (2007), pp. 99-103.

3. J. Hagedorn, J. Dunkers, A. Peskin, J. Kelso, and J. Devaney Terrill, "Quantitative, Interactive Measurement of Tissue Engineering Scaffold Structure in an Immersive Visualization Environment," *Biomaterials Forum* **28** (4) (2006), pp. 6-9.

4. W. F. Mitchell, Review of "Understanding and Implementing the Finite Element Method," by Mark S. Gockenbach, *SIAM Review*, **49** (3) (2007), pp. 532-533.

5. J. Miltat and M. Donahue, "Numerical Micromagnetics: Finite Difference Methods," in *Handbook of Magnetism and Advanced Magnetic Materials*, Volume 2: Micromagnetism, (H. Kronmüller and S. Parkin, eds.), Wiley 2007.

Conference Proceedings

1. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, and D. Basak, "Recent Results from the NIST Pulse-Heated Kolsky Bar, in *Proceedings of the 2007 Society for Experimental Mechanics Annual Conference*, Springfield, MA, June 3-6, 2007.
2. T. Dennis, S. D. Dyer, and A. Dienstfrey, "Phase-Dispersion Light Scattering for Quantitative Size-Imaging of Spherical Scatterers," in *Proceedings of SPIE Photonics West 2007* **6446** (Feb. 2007), San Jose, CA, January 20-25, 2007.
3. S. D. Dyer, L. K. Street, S. M. Etzel, T. Dennis, A. Dienstfrey, V. Tsvankin, and W. Tan, "Characterization of Cell Samples from Measurements of Spectroscopic Scattering Phase-Dispersion," in *Proceedings of SPIE Photonics West 2007* **6446** (Feb. 2007), San Jose, CA, January 20-25, 2007.
4. J. T. Fong, J. J. Filliben, and R. J. Fields, "An Uncertainty & Risk-based Approach toward a Cost-Effective High-Temperature Material Property Database," in *Proceedings National Nuclear Security Administration (NNSA) Future Technologies Conference II, Track Three (Materials Technology Trends for Defense & National Security)*, Oct. 11-12, 2006, Washington, DC.
5. J. T. Fong, J. J. Filliben, W .F. Ranson, and P. V. Marcal, "A Real-Time Non-Contact and Direct-Measurement-based Fatigue Life Prediction Methodology with Uncertainty & Risk Analyses," in *Proceedings National Nuclear Security Administration (NNSA) Future Technologies Conference II, Track Four (Future Trends in Analysis and Characterization)*, Oct. 11-12, 2006, Washington, DC.
6. J. T. Fong, J. J. Filliben, and R .J. Fields, "Uncertainty Quantification of Material Properties of Two Types of Steels at Elevated Temperatures for Stochastic Modeling of Structures on Fire," in *Proceedings of a Three Metals Society (TMS) Symposium on Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World*, Orlando, FL, Feb. 25-Mar. 1, 2007
7. A. Gaigalas, F. Hunt, K. Cole, and L. Wang, "Interpretation of Photochemical Reactions in Focused Laser Beams," in *Proceedings of the 8th WSEAS Conference on Mathematics and Computers in Biology and Chemistry* (2007), pp. 85-89.
8. Y. Lei, R. Kacker, D. R. Kuhn, V. Okun, and J. Lawrence, "IPOG: A General Strategy for T-Way Software Testing," in *14th Annual IEEE International Conference on Engineering of Computer-Based Systems*, Tucson, AZ, 2007, pp. 549 – 556.
9. N. S. Martys, C. F. Ferraris, V. Gupta, J.H. Cheung, J. G. Hagedorn, A. P. Peskin, E. J. Garboczi, "Computational Model Predictions of Suspension Rheology: Comparison to Experiment," in *Proceedings of the 12th International Conference on the Chemistry of Cement*, Montreal, Canada, July 8-13, 2007.
10. R. Radebaugh and A. O'Gallagher, "Modeling a Fast Cooldown Technique for Pulse Tube Cryocoolers," in *Proceedings of the Beijing International Congress of Refrigeration* (Aug. 2007), paper no. ICR07-A1-1319.
11. B. Rust and B. Thijsse, "Data-Based Models for Global Temperature Variations," in *Proceedings of the 2007 International Conference on Scientific Computing* (2007), Las Vegas, NV, June 25-28, 2007, pp. 10-16.
12. B. Saunders and Q. Wang, "From B-Spline Mesh Generation to Effective Visualizations for the NIST Digital Library of Mathematical Functions," in *Curve and Surface Design, Proceedings of the Sixth International Conference on Curves and Surfaces*, Avignon, France, June 29 – July 5, 2006, pp. 235-243.

Technical Reports

1. I. Beichl and R. Boisvert, "Mathematical Foundations of Measurement Science for Information Systems: Report of a Planning Workshop," NISTIR 7465, October 24, 2007.
2. D. E. Gilsinn, "Approximating Periodic Solutions of Autonomous Delay Differential Equations," *NISTIR 7375,* November, 2006.
3. W. F. Mitchell, "PHAML User's Guide," NISTIR 7374, October, 2006.

Accepted

1. J. B. Bowles, J. T. Fong, R. deWit, and J. J. Filliben, "Verification of a Finite Element Cantilever Beam Vibration model of a Micro- and Nano-Measurement Problem using a Metrology-based Approach," *Proceedings of ASME Pressure Vessels & Piping Conference*, San Antonio, TX, July 22-26, 2007.
2. A. S. Carasso and A. E. Vladar, "Calibrating Image Roughness by Estimating Lipschitz Exponents, with Applications to Image Restoration," *Optical Engineering.*

3. Y. Chao, J. T. Fong, P. S. Lam, and R. deWit, "Uncertainties in Transferring Fracture Toughness from Laboratory to Large Scale Structures," *Proceedings of ASME Pressure Vessels & Piping Conference*, San Antonio, TX, July 22-26, 2007.

4. D. L. Cotrell, G. B. McFadden, and B .J. Alder, "Effect of an Axially-periodic Radius on the Linear Stability of Pipe Flow," *Proceedings of the National Academy of Sciences.*

5. T. Dennis, S. D. Dyer, A. Dienstfrey, S. Gurpreet, and P. Rice, "Analyzing Quantitative Light Scattering Spectra of Phantoms Measuremented with Optical Coherence Tomography," *Journal of Biomedical Optics.*

6. D. G. Edwards, J. T. Fong, R. deWit, and J. J. Filliben, "Verification of a Stochastic Finite Element Cylinder-Impact Model of a Crashworthiness Problem using Response Surface Methodology and Fractional Factorial Design," *Proceedings of ASME Pressure Vessels & Piping Conference*, San Antonio, TX, July 22-26, 2007.

7. J. T. Fong, W. F. Ranson, III, R. I. Vachon, and P. V. Marcal, "A Non-Contact NDE Methodology for Prediction of Fatigue Failure," *Proceedings of ASME Pressure Vessels & Piping Conference*, San Antonio, TX, July 22-26, 2007.

8. J. T. Fong, R. deWit, G. B. Sinclair, and J. J. Filliben, "Verification of a Stochastic Finite Element Frictionless Contact/Rigid Indentor Model using a Metrological Approach and two Finite Element Codes, ANSYS and ABAQUS," *Proceedings ASME Pressure Vessels & Piping Conference*, San Antonio, TX, July 22-26, 2007.

9. J. T. Fong, and O. F. Hedden, eds., "Engineering Safety, Applied Mechanics, and Nondestructive Evaluation (NDE)," *Proceedings of an ASME Symposium on NDE in honor of Dr. Spencer H. Bush (1920-2005), ASME 2007 Pressure Vessels & Piping Conference*, San Antonio, TX, July 25-26, 2007.

10. S. Glancy and H. M. Vasconcelos, Methods for Producing Optical Coherent State Superpositions, http://arxiv.org/abs/0705.2045, *Journal of the Optical Society of America B.*

11. N.K. Gupta, E.P. Shine, R.C. Tuckerfield, and J.T. Fong, "Validation of Computer Models for Nuclear Material Shipping Packages," *Proceedings ASME 2007 Pressure Vessels & Piping Conference*, San Antonio, TX, July 23-26, 2007, Paper No. PVP2007-26751.

12. F. Hunt, A. Gaigalas, and L. Wang, "Mathematical Derivation of a Model of the Frequency Domain Measurement Technique," *NIST Journal of Research*.

13. R. Kacker, "Comments on 'Bayesian Evaluations of Comparison Data' by Ignacio Lira," *Metrologia*.

14. R. Kacker, K.-D. Sommer, and R. Kessel, "Evolution of Modern Approaches to Express Uncertainty in Measurement," *Metrologia*.

15. A. Kearsley and W. Wallace, "New Approaches to Data Reduction in Mass Spectrometry," *MALDI and ESI Mass Spectrometry of Synthetic Polymers*, Liang Li (ed.), Wiley Interscience, 2007.

16. Y. Lei, R. Carver, R. Kacker, and D. Kung, "A Combinatorial Testing Strategy for Concurrent Programs," *Software Testing, Verification and Reliability*.

17. Y. Lei, R. Kacker, D. Kuhn, V. Okun, and J. Lawrence, "IPOG/IPOG-D: Efficient Test Generation for Multi-way Combinatorial Testing," *Software Testing, Verification and Reliability*.

18. L. A. Melara, A. J. Kearsley, and R. A. Tapia, "A Homotopy Method in the Regularization of Total Variation Denoising Problems," *Journal of Optimization Theory and Applications*.

19. B.R. Miller, "Creating Webs of Math Using LaTeX," *Proceedings 6th International Congress on Industrial and Applied Mathematics*, Zurich, Switzerland, July 17, 2007.

20. D. G. Porter and M. J. Donahue, "Precession Axis Modification to a Semi-analytical Landau-Lifshitz Solution Technique," *Journal of Applied Physics*.

21. A. C. E. Reid, R. C. Lua, R. E. Garcia, V. R. Coffman, and S. A. Langer, "Modeling Microstructures with OOF2," *International Journal of Materials and Product Technology*.

22. B. Rust and D. O'Leary, "Residual Periodograms for Choosing Regularization Parameters for Ill-Posed Problems," *Inverse Problems*.

23. B. Thijsse and B. Rust, "Freestyle Data Fitting and Global Temperatures," *Computing in Science and Engineering*.

24. J. Terrill, W. George, T. Griffin, J. Hagedorn, J. Kelso, M. Olano, A. Peskin, S. Satterfield, J. Sims, J. Bullard, J. Dunkers, N. Martys, A. O'Gallagher, and G. Haemer, "Extending Measurement Science to Interactive Visualization Environments," Chapter in *Trends in Interactive Visualisation: A-State-of-the-Art Survey*, edited by Elena Zudilova-Seinstra, Tony Adriaansen and Robert van Liere, to be published by Springer, UK.

25. A. Youssef, "Methods of Relevance Ranking and Hit-content Generation in Math Search," *Proceedings of Mathematical Knowledge Management (MKM 2007)*, RISC, Hagenberg, Austria, June 27-30, 2007.

Submitted

1. P. Barker, Y. Xiao, F. Hunt, and N. Glenn, "Whole Genome Amplification Improves FISH Hybridization with Bacterial Artificial Chromosome Cancer Biomarker Probes.
2. I. Beichl, S. Bullock, and D. Song, "A Quantum Algorithm Detecting Concentrated Maps."
3. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, and D. Basak, "Recent Results from the NIST Pulse-Heated Kolsky Bar."
4. R. J. Epstein, S. Sedelin, D. Leibfried, J. H. Wesenberg, J. J. Bollinger, J. M. Amini, R. B. Blakestad, J. Britton, J. P. Home, W. M. Itano, J. D. Jost, E. Knill, C. Langer, R. Ozeri, N. Shiga, and D. J. Wineland, "Simplified Motional Heating Rate Measurements of Trapped Ions."
5. D. E. Gilsinn, "On Algorithms for Estimating Computable Error Bounds for Approximate Periodic Solutions of an Autonomous Delay Differential Equation."
6. D. E. Gilsinn, "A Pseudospectral Approximation to the Fundamental Matrix of a Linear Delay Difffereential Equation with Periodic Coefficients."
7. C. M. Guttman, K. M. Flynn, and A. J. Kearsley, "Numerical Optimization of Matrix-Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry: Application to Synthetic Polymer Molecular Mass Distribution Measurement".
8. F. Y. Hunt, A. K. Gaigalas, and L. Wang, "Mathematical Derivation of a Model of the Frequency Domain Measurement Technique"
9. R. Kacker, "Classical and Bayesian Interpretation of the Birge Test of Consistency and Its Generalized Version in Interlaboratory Evaluations."
10. S. Kim, M. I. Aladjem, G. B. McFadden, and K.W. Kohn, "Fine Tuning of p53-Mdm2-MdmX Network by MdmX during DNA Damage Response."
11. E. Knill, D. Leibfried, R. Reichle, J. Britton, B. Blakestad, D. Jost, C. Langer, R. Ozeri, S. Seidelin, D. J. Wineland, "Randomized Benchmarking of Quantum Gates."
12. D. R. Kuhn, Y. Lei, R. Kacker, V. Okun, and J. Lawrence, "An Algorithm for Covering Arrays with Strength Larger than Three."
13. Y. Lei, R. Kacker, D. R. Kuhn, V. Okun, and J. Lawrence, "Two-deterministic Strategies for Multi-way Software Testing."
14. N. S. Martys, D. Lootens, W. George, S. Satterfield, J. Kelso, and P. Hebraud, "Spatial-Temporal Correlations in Concentrated Suspensions."
15. N. S. Martys, D. Lootens, W. George, S. Satterfield, J. Kelso, and P. Hebraud, "Stress Chains Formation Under Shear of Concentrated Suspensions."
16. S. P. Mates, R. L. Rhorer, E. P. Whitenton, T. J. Burns, and D. Basak, "A Pulse-Heated Kolsky Bar Technique for Measuring Flow Stress of Metals Subjected to High Loading and Heating Rates."
17. R. Radebaugh, Y. Huang, A. O'Gallagher, and J. Gary, "Calculated Regenerator Performance at 4 K with Helium-4 and Helium-3."
18. J. Sims, W. George, T. Griffin, J. Hagedorn, H. Hung, J. Kelso, M. Olano, A. Peskin, S. Satterfield, J. Terrill, G. Bryant, and J. Diaz, "Advancing Scientific Discovery through Parallelization and Visualization III. Tightbinding Calculations on Quantum Dots."

Presentations

Invited Talks

1. I. Beichl, "Using SIS to Speed Up MCMC," DIMACS Workshop on Markov Chain Monte Carlo: Synthesizing Theory and Practice, Trenton, NJ, June 5, 2007.
2. T. Burns, "Bifurcation in Material Flow During High-Speed Machining," Sixth International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16-20, 2007.
3. T. Burns, "Measurement and Modeling of Rapid Shear in High-Speed Machining," SHEAR 07, International Symposium on Shear Behavior and Mechanisms in Materials Plasticity, Nancy, France, September 4-7, 2007.
4. M. J. Donahue, "Overview and Outlook of the OOMMF Micromagnetic Modeling Package," IEEE Magnetism in Nanotechnology and Electronics Conference, Gaithersburg, MD, June 25, 2007.
5. J. Fong, **"**Verification and Validation of a Life-Prediction Model for Safety Assessment of Critical

Structures," Department of Mechanical Engineering Seminar, University of South Carolina, Columbia, SC, Oct. 4, 2006.

6. J. Fong, **"**An Uncertainty & Risk-based Approach toward a Cost-Effective High-Temperature Material Property Database," National Nuclear Security Admin (NNSA) Future Technologies Conference II, Track Three (Materials Technology Trends for Defense & National Security), Washington, DC, Oct. 11, 2006.
7. J. Fong, **"**A Real-Time Non-Contact and Direct-Measurement-based Fatigue Life Prediction Methodology with Uncertainty & Risk Analyses," National Nuclear Security Admin (NNSA) Future Technologies Conference II, Track Four (Future Trends in Analysis and Characterization), Washington, DC, Oct. 12, 2006.
8. J. Fong, "Verification of Finite Element Simulations of Progressive Failure of Structures on Fire," Department of Civil Engineering Seminar, Tufts University, Medford, MA, Oct. 27, 2006.
9. J. Fong, **"**On the Feasibility of Verification, Standardization, and Certification of a Library of Computational Models," 2007 High Level Simulation Languages and Application Conference of the Western MultiConference on Modeling and Simulation (WMC '07), San Diego, CA, Jan. 15, 2007.
10. J. Fong, **"**Verification of a Stochastic Finite Element Cylinder-Impact Model of a Crashworthiness Problem using Response Surface Methodology and Fractional Factorial Design," Department of Statistics Seminar, University of South Carolina, Columbia, SC, Jan. 29, 2007.
11. J. Fong, "Uncertainty Quantification of Material Properties of Two Types of Steels at Elevated Temperatures for Stochastic Modeling of Structures on Fire," Symposium on Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World, during the 2007 Annual Meeting of the Minerals, Metals, and Materials Society (TMS), Orlando, FL, Feb. 27, 2007.
12. J. Fong, **"**A Layered Software Approach using TrueGrid, Ls-Dyna, and Ls-Opt to Computational Modeling with Applications in Pressure Vessels and Piping Technology for Nuclear Waste Packaging and Transportation," DoD Savannah River National Laboratory, Aiken, SC, April 12, 2007.
13. J. Fong, "A Non-Contact NDE Methodology for Prediction of Fatigue Failure," ASME Symposium on Engineering Safety, Applied Mechanics, and Nondestructive Evaluation (NDE), 2007 Pressure Vessels and Piping Technology Conference, San Antonio, TX, July 25, 2007.
14. F. Hunt, "A Sample Path Result for a Class of Markov Decision Processes," Stochastic Control and Dynamics Workshop, Mathematical Sciences Research Institute, Univ. California, Berkeley, CA, Mar. 27, 2007.
15. F. Hunt, "A Markov Decision Process Result Motivated by a Multiple Sequence Alignment," Stochastic Dynamical Systems and Control Workshop, Berkeley, CA, April 5, 2007.
16. R. Kacker, "A Review of the Guide to the Expression of Uncertainty in Measurement," New Brunswick Laboratory, Argonne, IL Mar. 5-9, 2007.
17. R. Kacker, "Frequentist and Bayesian Statistics in the Context of Evaluating Uncertainty," New Brunswick Laboratory, Argonne, IL, Mar. 5-9, 2007.
18. E. Knill, "Randomization Hypothesis," When Matter Meets Information Workshop, Perimeter Institute, Waterloo Canada, June 25-29, 2007.
19. S. Langer, "OOF: Analyzing Material Microstructure," SIAM Conference on Computational Science and Engineering, Costa Mesa, CA, Feb. 19-23, 2007.
20. D.W. Lozier, "MKM and the DLMF," Mathematical Knowledge Management Workshop on Sustainability, Interoperability and Scalability, Dalhousie Distributed Research Institute and Virtual Environment (D-DRIVE), Dalhousie University, Halifax, Canada. April 26 - 29, 2007.
21. B. R. Miller, "DLMF, LaTeXML and some Lessons Learned," The Evolution of Mathematical Communications in the Age of Digital Libraries, IMA Workshop, Minneapolis, MN, Dec. 8-9, 2006.
22. D.P. O'Leary, "Parallel Matrix Computation: From the ILLIAC to Quantum Computing ," Stanford 50: State of the Art and Future Directions of Computational Mathematics and Numerical Computing, Stanford University, Stanford, CA, March 30, 2007.
23. D. Porter (panelist), "Open Discussion with the Tcl/Tk Core Team," Fourteenth Annual Tcl/Tk Conference, New Orleans, LA, September 26, 2007.
24. R. Radebaugh and A. O'Gallagher, "Modeling a Fast Cooldown Technique for Pulse Tube Cryocoolers," 22nd International Congress of Refrigeration, Beijing, China, Aug. 22-25, 2007.

Conference Presentations

1. R. Boisvert, "Special Functions, Reference Data and Mathematical Software," International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16, 2007.
2. G.W. Bryant, M. Zielinski, W. Jaskolski, J. Aizpurua, and J.S. Sims, "Controlling the Optical Properties of Self-Assembled Quantum Dots Using External Strain," Material Research Society Fall Meeting, Boston, MA., November 26-30, 2007.
3. A. Dienstfrey, R. Wittmann, and B. Rider, "Statistics of Electromagnetic Fields and Random Matrix Theory," (poster), Second CU-NIST Symposium, University of Colorado at Boulder, Mar. 22, 2007.
4. M. J. Donahue and R. D. McMichael, "Micromagnetics on Curved Geometries Using Rectangular Cells: Error Correction and Analysis," 10th Joint MMM/Intermag Conference, Baltimore, MD, Jan. 11, 2007.
5. M. J. Donahue, "Accurate Computation of the Demagnetization Tensor," 6th International Symposium on Hysteresis Modeling and Micromagnetics HMM-2007, Naples, Italy, 4-Jun-2007.
6. E. Enjolras, W. George, J. Bullard, and J. Terrill, "Parallelization of HydraticCA," VCCTL Bi-Annual Meeting, Gaithersburg MD, Nov. 13-14, 2007.
7. W. George, J. Lancien, N. Martys, J. Terrill, and E. Garboczi, "Large Scale Simulations of Suspensions," NASA Booth, Supercomputing 2007, Reno, NV, November 10-16, 2007.
8. S. Glancy, E. Knill, and H. Vasconcelos, "Entanglement Purification of Any Stabilizer State," Quantum Information Processing Workshop, Brisbane, Australia, Jan. 30, 2007.
9. S. Glancy, E. Knill, and H. Vasconcelos, "Entanglement Purification of Any Stabilizer State," American Physical Society March Meeting, Denver, CO, Mar. 5, 2007.
10. S. Glancy, "Entanglement Purification of Any Stabilizer State," Asian Conference on Quantum Information Science, Kyoto University, Kyoto, Japan, September 2-6, 2007.
11. F. Hunt, "Visualizing the Frequency Patterns in DNA," Pi Mu Epsilon ceremony at Mount St. Mary's University, Emmitsburg, MD, Nov. 19, 2006.
12. R. Kacker and J. Lawrence, "Trapezoidal and triangular distributions for Type B evaluation of standard uncertainty" PTB-BIPM Workshop on the Impact of Information Technology in Metrology, Berlin, Germany, June 5, 2007.
13. R. Kacker, R. Datla, and A. Parr, "Comments on the Evaluation of Key Comparison Data by Cox et al," (poster), PTB-BIPM Workshop on the Impact of Information Technology in Metrology, Berlin, Germany June 5-7, 2007.
14. E. Knill, "Randomized Benchmarking of Quantum Gates," American Physical Society March Meeting, Denver, CO, Mar. 14, 2007.
15. D.W. Lozier, "Utilizing the DLMF in Scientific Research," 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16, 2007.
16. N.S. Martys, C.F. Ferraris, V. Gupta, J.H. Cheung, J.G. Hagedorn, A.P. Peskin, E.J. Garboczi, "Computational Model Predictions of Suspension Rheology: Comparison to Experiment," 12th International Conference on the Chemistry of Cement, Montreal, Canada, July 11, 2007.
17. N.S. Martys, C.F. Ferraris, W. George, J. Lancien, J. Terrill, E. Garboczi, A.P. Peskin, J. Hagedorn, M. Olano, J. Kelso, S. Satterfield, H. Zhu, J.H. Cheung, B.-W. Chun, V. Gupta, D. Lootens, R. Flatt, and B. Descheneaux, "Computational Modeling of Suspensions: Recent Advances and Future Research Directions," VCCTL Bi-Annual Meeting, Gaithersburg, MD, Nov. 13-14, 2007.
18. B. R. Miller, "Creating Webs of Math Using LaTeX," 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 17, 2007.
19. B.R. Miller, "Why TeX and LaTeXML?," Joint Joining Educational Mathematics and OpenMath Meeting, Linz, Austria, June 26, 2007.
20. W. F. Mitchell and E. Tiesinga, "An h-p Adaptive Strategy with Limited p," SIAM Conference on Computational Science and Engineering, Costa Mesa, CA, Feb. 18-23, 2007.
21. M. O'Hara and D.P. O'Leary, "Adiabatic Quantum Computing and the Adiabatic Theorem in The Presence of Noise," GRID (Graduate Research Interaction Day), University of Maryland, College Park, MD April 12, 2007.
22. M. O'Hara and D.P. O'Leary, "Adiabatic Quantum Computing and the Adiabatic Theorem in The Presence of Noise," Gordon Research Conference on Quantum Information Science, Il Ciocco, Lucca (Barga), Italy, April 15-20, 2007.

23. M. Olano and S. Satterfield, "Non-photorealistic Visualization of Cement," OSG BOF at ACM SIGGRAPH, San Diego, August 8, 2007.
24. F. Potra, "Interior Point Methods for Linear Complementarity Problems," International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 18, 2007.
25. B. Rust, "Data-Based Models for Global Temperature Variations," CSC'07 - The 2007 International Conference on Scientific Computing," Las Vegas, NV, June 26, 2007.
26. S. Satterfield, J. Kelso, and M. Olano, "Diverse-Flexible Source VE API, Diverse BOF," ACM SIGGRAPH, San Diego, CA, August 8, 2007.
27. A. Youssef, "Recent Advances in Math Search," 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 17, 2007.

Software Released

1. S. Langer, OOF2: analysis of materials with complex microstructure, version 2.0.2 (Feb. 16, 2007), Alpha versions 2.0.4a1 through 2.0.4a3 (May-June 2007), Beta versions 2.0.4b1 and 2.0.4b2 (July-August, 2007).
   See http://www.ctcms.nist.gov/oof/oof2
2. S. Langer, gtklogger: creation and execution of regression tests for programs that use a graphical user interface, version 1.0 (August 2007), version 1.1 (September 2007).
   See http://www.ctcms.nist.gov/oof/gtklogger
3. W.F. Mitchell, PHAML: parallel hierarchical adaptive multi-level solver for partial differential equations, version 1.0 (May 4, 2007), version 1.1.0 (July 3, 2007).
   See http://math.nist.gov/phaml/
4. D. Porter, Tcl/Tk: tool control language and toolkit, version 8.4.14 (October 19, 2006), version 8.5a6 (October 20, 2006), version 8.4.15 (May 25, 2007), version 8.4.16 (September 24, 2007), version 8.5b1 (September 26, 2007).
5. R. Pozo, TNT: Template Numerical Toolkit, version 3.0.4, version 3.0.5, version 3.0.6, version 3.0.7, version 3.0.8.
   See http://math.nist.gov/tnt

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. B. Shneiderman (University of Maryland), "The Thrill of Discovery: Information Visualization for High-Dimensional Spaces," Oct. 3, 2006.
2. M. Mascagni (Florida State University), "Using Simple Stochastic Differential Equations to Solve Complicated Partial Differential Equations", Oct. 18, 2006.
3. S. Bullock (MCSD), "Projecting onto Qubit Irreps of Young Diagrams," Nov. 21, 2006.
4. B. Alpert (MCSD), "Sparse Representations and High-Dimensional Geometry: What's the Excitement?," Dec. 5, 2006.
5. T. Gill (Howard University), "Sufficiency Class for Global (in Time) Solutions to the Three-Dimensional Navier-Stokes Equations," Feb. 6, 2007.
6. E. Fried (Washington University, St. Louis), "Sharp-Interface Theory for Transitions Between the Isotropic and Uniaxial Nematic Phases of a Liquid Crystal," May 3, 2007.
7. J. Nakagawa (Nippon Steel Corp.), "Mathematics in Industry: How is a Hidden Rule Found from Operation Data?," May 25, 2007
8. L. Chen (University of Maryland), "Multigrid Analysis of H_1, H(curl) and H(div) Systems for Locally Adapted Grids," June 5, 2007.
9. D. Mijuca (University of Belgrade, Serbia), "On the Use of Fully Three Dimensional Multifield Mixed Finite Element Scheme in Multiscale Structural and Building Energy Efficiency Simulations," June 28, 2007.
10. A Youssef (MCSD), "Advances in Math Search: Summarization and Relevance Ranking of Math Hits," Sept. 21, 2007.
11. B. Miller (MCSD), "LaTeXML: Converting LaTex to XML and MathML," Sept. 28, 2007.
12. P.A. Lott (University of Maryland), "Efficient Numerical Simulation of Advection Diffusion Systems, Dec. 19, 2007.

Local Events Organized

1. T. Burns, Program Committee, International Conference on Smart Machining Systems, NIST, Gaithersburg, MD, March 13-15, 2007.
2. D. Gilsinn, Shortcourse, Numerical Analysis with Matlab, NIST, Gaithersburg, MD, Oct. 3, 4, Nov. 7, 8, and Dec. 4, 6, 2007.
3. S. Glancy, Quantum Information Journal Club, NIST, Boulder, weekly event.

External Events Organization

1. R. Boisvert and B. Ford (Oxford), Organizers, Minisymposium "Recent Advances in Software Tools for Scientific Computing," 6th International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, Switzerland, July 16, 2007.
2. M. Donahue, International Steering Committee, Hysteresis Modeling and Micromagnetics Symposium.
3. J. Fong, Organizer, Symposium on Nondestructive Evaluation (NDE), ASME 2007 Pressure Vessels and Piping Conference, San Antonio, Texas, July 25-26, 2007.
4. D. W. Lozier, B. Miller, and A. Youssef, Organizers, Minisymposium "Math on the Web: Content Development and Implementation," 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16-17, 2007.
5. W. F. Mitchell, Scientific Committee, International Conference of Numerical Analysis and Applied Mathematics (ICNAAM 2007), Corfu, Greece, Sept. 16-20, 2007.
6. W. F. Mitchell, Program Committee, International Conference on High Performance Computing, Networking and Communication Systems, Orlando, FL, July 9-12, 2007.
7. S. Satterfield, J. Kelso, and M. Olano, "DIVERSE Birds-of-a-Feather," ACM SIGGRAPH, San Diego, August 8, 2007.

Other Professional Activities

Internal

1. I. Beich, Director, ITL Student Undergraduate Research Fellowship (SURF) Program.
2. R. Boisvert, NIST Scientific Computing Steering Group.
3. B. Rust, ITL Awards Committee.
4. B. Rust, MCSD Seminar Chair.
5. 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, Editor, *IEEE Computing in Science and Engineering*.
3. R. Boisvert, Associate Editor, *ACM Transactions on Mathematical Software*.
4. R. Boisvert, Area Editor, (Numerical Analysis, Mathematical Software, and Computational Engineering, Finance, and Science), Computing Research Repository (CoRR), www.arXiv.org.
5. D. Gilsinn, Associate Editor, *ASME Journal of Computational and Nonlinear Dynamics*.
6. D. Gilsinn and Balakumar Balachandran (University of Maryland), and Tamas Kalmar-Nagy (Texas A&M), eds., *Delay Differential Equations: Recent Advances and New Directions*, Springer, to appear.
7. D. Lozier, Associate Editor, *Mathematics of Computation*.
8. G. McFadden, Associate Editor, *Journal of Crystal Growth* and *Interfaces and Free Boundaries*.
9. W. Mitchell, Associate Editor, *International Journal of Applied Mathematics and Computational Science, Journal of Numerical Analysis, Industrial and Applied Mathematics,* and *Applied Numerical Analysis and Computational Mathematics*.
10. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*.

11. J. Terrill, Editor, *Journal of Information Visualization, Special Issue on Visual Analysis of Human Dynamics*.

Boards and Committees

1. R. Boisvert, Co-chair, Publication Board of the Association for Computing Machinery (ACM).
2. R. Boisvert, Member, ACM Awards Committee.
3. R. Boisvert, Chair, International Federation for Information Processing's Working Group 2.5 (Numerical Software).
4. R. Boisvert, Member, Review Panel, U.S. Army's basic (6.1) research program in Mathematics, Modeling, Communications, Networks, and Information Sciences.
5. F. Hunt, Member, Executive Committee of the Association for Women in Mathematics.
6. D. Lozier, Vice Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
7. B. Miller, Member, Math Working Group, W3C (the World Wide Web Consortium).
8. D. Porter, Member, Tcl Core Team.
9. B. Saunders, Member, Selection Committee, Etta Z. Falconer Lecture.
10. J. Terrill, Member, Federal High End Computing Implementation Task Force.
11. J. Terrill, Member, Federal High End Computing Research and Development, and Infrastructure Interagency Working Group.

Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including *ACM Transactions on Mathematical Software, Applied Physics Letters, Engineering with Computers, High Performance Computing, Networking and Communication Systems, IEEE International Symposium on Information Theory*, *IEEE Transactions on Information Theory*, *IEEE Transactions on Microwave Theory and Techniques, International Journal of Computational Science and Engineering, International Journal of Computer Mathematics, Journal of Manufacturing Science and Engineering, Journal of Mathematical Analysis and Applications*, *Letters in Mathematical Physics, Nature*, *Nature Physics*, *Nonlinear Dynamics, Numerische Mathematik*, *Optics Communications, Optics Express, Physica B, Physics Letters A, Physical Review A, Physical Review A: Atomic, Molecular, and Optical Physics, Physical Review B*, *Physical Review Letters, Quantum Information and Computation*, *SIAM Journal of Scientific Computing*, *Transactions of the American Mathematical Society.*
2. Staff members review proposals for the following research programs: ACEnet Research Fellowships (Atomic Canada). ATP, Department of Energy, NIH, NIST Innovations in Measurement Science (IMS) Program, 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

ActiveState
Agilent Technologies
Bergen Scientific (Norway)
Chemical Abstracts Service
CWI Amsterdam (The Netherlands)
Design Science Inc.
Etnus
Fox TV
Gamma Logic
GE Research
Hewlett Packard
Hospira
IBM
Johnson Scientific
Mathworks, Inc.
Nippon Steel Corp.
Orbital Sciences Corp.
Plastic Technologies
Politecnico di Torino
Portland Cement Association
Proctor & Gamble Corp.
Raytheon
Rowan Williams Davies & Irwin Inc.
Simula Research Laboratory (Norway)
Simulistics
Stillwater Supercomputing Solutions
STMicroelectronics
Tech-EDV
UGS Corp.
Victoria Interrante
Viewray Inc.
Visual Numerics, Inc.

Government/Non-profit Organizations

AT&T Labs
Air Force Research Laboratory

Argonne National Laboratory
Army Intelligence Evaluation Center
Army Research Office
Council on Competitiveness
CWI (Amsterdam)
IDA Center for Computing Sciences
Institute for Systems Biology (Seattle)
Institut Laue Langevin (France)
International Federation for Information Processing
Jet Propulsion Laboratory
KTH Royal Institute of Technology (Sweden)
Lawrence Berkeley Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
NAG Ltd.
National Aeronautics and Space Administration
NASA Ames Research Center
National Center for Atmospheric Research
National Reconnaissance Office
National Science Foundation
National Security Agency
Naval Research Laboratory
Ohio Supercomputer Center
Sandia National Laboratories
Savannah River National Laboratory
U.S. Air Force Phillips Laboratory
World Wide Web Consortium

Universities

American University
California Institute of Technology
Carnegie Mellon University
Case Western Reserve University
Catholic University of Leuven (Belgium)
Cornell University
Dartmouth College
Dnippropetrovs'k University (Ukraine)
Drexel University
George Mason University
Georgetown University
George Washington University
Georgia Tech
Howard University
Illinois Institute of Technology
Indiana University
Iowa State University
Jacobs University (Bremen, Germany)
Johannes Kepler University (Linz, Austria)
Louisiana State University
MIT
New York University
North Carolina State University
Oregon State University
Penn State University
Purdue University
Rensselaer Polytechnic Institute
Russian Academy of Sciences (Russia)
Shaw University
Southeast University
Southern Methodist University
Stanford University
Technical University of Munich (Germany)
Texas A&M
Texas Tech
Trinity University
Tufts University
UCLA
Universidade Federal do Ceará, Brazil
Université Henri Poincare (France)
University of Aachen (Germany)
University of British Columbia
University of Bristol (UK)
University of California Davis
University of California San Diego
University of California Santa Barbara
University of Catolica de Valparaiso (Chile)
University of Colorado
University of Florida
University of Hanover
University of Helsinki (Finland)
University of Henri Poincare (France)
University of Karlsruhe (Germany)
University of Kent (UK)
University of Illinois Medical Center
University of Indiana
University of Linkoping (Sweden)
University of Magdeburg (Germany)
University of Maryland Baltimore County
University of Maryland College Park
University of Michigan
University of Minnesota
University of Natural Science (Vietnam)
University of Nevada Las Vegas
University of New Mexico
University of Nottingham (England)
University of Oxford (UK)
University of Patras (Greece)
University of Rovira I Virgili (Spain)
University of Saarland (Germany)
University of South Carolina
University of South Florida
University of Tennessee
University of Texas at Arlington
University of Texas at Austin
University of Toronto (Canada)
University of Utah
University of Vienna (Austria)
University of Washington
University of Western Ontario (Canada)
University of Wisconsin
Uppsala University (Sweden)
Utsunomiya University (Japan)
Virginia Tech

Yale University
Williams College

Part V

Appendices

Staff

MCSD consists of full time permanent staff located at NIST laboratories in Gaithersburg, MD and Boulder, CO. This is supplemented with a variety of faculty appointments, guest researchers, postdoctoral appointments, and student appointments. The following list reflects all appointments held during any portion of FY 2007.

Division Staff

Ronald Boisvert, *Chief* , Ph.D. (Computer Science), Purdue University, 1979
Robin Bickel, *Secretary*
Jeffrey Fong, Ph. D. (Applied Mechanics and Mathematics), Stanford University, 1966
Roldan Pozo, Ph.D. (Computer Science), University of Colorado at Boulder, 1991
Christopher Schanzle, B.S. (Computer Science), University of Maryland – Baltimore County, 1989

Guest Researchers
Barry Bernstein / Illinois Institute of Technology
Grant Erdmann, Commerce Science Fellow / Air Force Research Laboratory

Mathematical Modeling Group

Geoffrey McFadden, *Leader* , Ph.D. (Mathematics), New York University, 1979
Bradley Alpert (Boulder), Ph.D. (Computer Science), Yale University, 1990
Timothy Burns, Ph.D. (Mathematics), University of New Mexico, 1977
Alfred Carasso, Ph.D. (Mathematics), University of Wisconsin, 1968
Andrew Dienstfrey (Boulder), Ph.D. (Mathematics), New York University, 1998
Michael Donahue, Ph.D. (Mathematics), The Ohio State University, 1991
Fern Hunt, Ph.D. (Mathematics), New York University,
Raghu Kacker, Ph.D. (Statistics), Iowa State University, 1979
Anthony Kearsley, Ph.D. (Computational and Applied Mathematics), Rice University, 1996
Peter Ketcham. M.S. (Mathematics), University of Minnesota, 1997
Stephen Langer, Ph.D. (Physics), Cornell University, 1989
Agnes O'Gallagher (Boulder), M.S. (Applied Math), University of Colorado at Boulder, 1991
Donald Porter, Ph.D. (Electrical Engineering), Washington University, 1996

NRC Postdoctoral Associates
Valerie Coffman, Ph.D. (Physics), Cornell University, 2006

Contractors
Andrew C.E. Reid, Ph.D. (Physics), Queen's University, Kingston, Ontario, 1994

Faculty Appointees
Daniel Anderson / George Mason University
Dianne O'Leary / University of Maryland College Park
Florian Potra / University of Maryland Baltimore County

Guest Researchers
Mirit Aladjem / National Institutes of Health
Richard Braun / University of Delaware
David Cotrell / Lawrence Livermore National Laboratory
John Gary (Boulder)
Katharine Gurski / George Washington University

Seung-Ill Haan / University of Maryland Baltimore County
Sohyoung Kim / National Institutes of Health
Yu (Jeff) Lei / University of Texas at Arlington

Students
Kevin Dela Rosa / University of Texas at Arlington
Michael Forbes / MIT
Gillian Haemer / University of Southern California
Olga Kuznetsova / University of Maryland College Park

Mathematical Software Group

Daniel Lozier, *Leader,* Ph.D. (Applied Mathematics), University of Maryland, 1979
Marjorie McClain, M.S. (Mathematics), University of Maryland College Park, 1984
Bruce Miller, Ph.D. (Physics), University of Texas at Austin, 1983
William Mitchell, Ph.D. (Computer Science), University of Illinois at Urbana-Champaign, 1988
Bert Rust, Ph.D. (Astronomy), University of Illinois at Urbana-Champaign, 1974
Bonita Saunders, PhD (Mathematics), Old Dominion University, 1985

Contractors
Joyce Conlon, B.A. (Mathematics), University of Maryland Baltimore County, 1979

Faculty Appointees
Frank Olver / University of Maryland College Park
G.W. Stewart / University of Maryland College Park
Abdou Youssef / George Washington University

Guest Researchers
Leonard Maximon / George Washington University

Students
Liuyuan Chen (Montgomery Blair High School, Maryland)

Optimization and Computational Geometry Group

Ronald Boisvert, *Acting Leader*
Isabel Beichl, Ph.D. (Mathematics), Cornell University, 1981
Javier Bernal, Ph.D. (Mathematics), Catholic University, 1980
Brian Cloteaux, Ph.D. (Computer Science), New Mexico State University, 2007
David Gilsinn, Ph.D. (Mathematics), Georgetown University, 1969
Scott Glancy (Boulder), Ph.D. (Physics), University of Notre Dame, 2003
Emanuel (Manny) Knill (Boulder), Ph.D., (Mathematics), University of Colorado at Boulder, 1991

NRC Postdoctoral Associates
Bryan Eastin, Ph.D. (Physics), University of New Mexico, 2007

Faculty Appointees
Saul Gass / University of Maryland College Park
James Lawrence / George Mason University

Guest Researchers
Stephen Bullock / IDA Center for Computing Sciences
Sita Ramamurti / Trinity University, DC
David Song / Korea Institute for Advanced Study
Francis Sullivan / IDA Center for Computing Sciences
Christoph Witzgall, NIST Scientist Emeritus

Students

Kevin Costello / Carnegie Mellon University
Adam Meier / University of Colorado
Yanbao Zhang / University of Colorado

Scientific Applications and Visualization Group

Judith Devaney, *Leader*, Ph.D. (Information Technology), George Mason University, 1998
Yolanda Parker, *Office Manager*
Robert Bohn, Ph.D. (Physical Chemistry), University of Virginia, 1991
William George, Ph.D. (Computer/Computational Science), Clemson University, 1995
Terence Griffin, B.S. (Mathematics), St. Mary's College of Maryland, 1987
John Hagedorn, M.S. (Mathematics), Rutgers University, 1980
John Kelso, M.S. (Computer Science), George Washington University, 1984
Adele Peskin (Boulder), Ph.D. (Chemical Engineering), University of Colorado at Boulder, 1985
Steven Satterfield, M.S. (Computer Science), North Carolina State University, 1975
James Sims, Ph.D. (Chemical Physics), Indiana University, 1969

Faculty Appointees

Marc Olano (University of Maryland Baltimore County)

Guest Researchers

Dong Yeon Cho / Seoul National University, Korea
Edith Enjolra / Université Blaise Pascal, France
Cedric Houard / Université Blaise Pascal, France
Julien Lancien / France

Students

Aaron Jones / Hampton College
Omotunwase Olubayo / Hampton College
Sathish Ragappan / Quince Orchard High School, Maryland
Miguel Rois / University of Puerto Rico

Glossary of Acronyms

ACM	Association for Computing Machinery
ANSI	American National Standards Institute
API	application programmer's interface
ASME	American Society of Mechanical Engineers
ATP	NIST Advanced Technology Program
BFRL	NIST Building and Fire Research Laboratory
BLAS	Basic Linear Algebra Subprograms
BMD	bone mineral density
CCG	DoD Coordinated Calibration Group
CMM	coordinate measuring machine
CMU	Carnegie Mellon University
CODATA	Committee on Data for Science and technology
CPU	central processing unit
CSTL	NIST Chemical Science and Technology Laboratory
CT	computed tomography
CWI	Centrum voor Wiskunde en Informatica (Amsterdam)
DARPA	DOD Defense Advanced Research Projects Agency
DIVERSE	Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (visualization software)
DLMF	Digital Library of Mathematical Functions (MCSD project)
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOJ	U.S. Department of Justice
DPD	dissipative particle dynamics
DXA	dual-energy x-ray absorptiometry
EEEL	NIST Electronics and Electrical Engineering Laboratory
FDA	Food and Drug Administration
FFT	fast Fourier transform
FY	fiscal year
GAMS	Guide to Available Mathematical Software
GPU	Graphics processing unit
HPC	high performance computing
HTML	hypertext markup language
Hy-CI	Hylleraas-Configuration Interaction technique
ICIAM	International Congress on Industrial and Applied Mathematics
IDA	Institute for Defense Analysis
IEEE	Institute of Electronics and Electrical Engineers
IML++	Iterative Methods Library
ISCD	International Society of Clinical Densitometry
IT	information technology
ITL	NIST Information Technology Laboratory
IFIP	International Federation for Information Processing
JAMA	Java Matrix package
MALDI-TOF	matrix-assisted laser desorption/ionization time-of-flight
MCMC	Markov chain Monte Carlo
MCSD	ITL Mathematical and Computational Sciences Division
MEL	NIST Manufacturing Engineering Laboratory
MIT	Massachusetts Institute of Technology
MKM	mathematical knowledge management
MMM	magnetism and magnetic materials
MPI	Message Passing Interface
MRI	magnetic resonance imaging
MSEL	NIST Materials Science and Engineering Laboratory
MV++	Matrix/Vector Library

μmag	Micromagnetics Activity Group
NASA	National Aeronautics and Space Administration
NCSU	North Carolina State University
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NISTIR	NIST Internal Report
NITRD	Networking and Information Technology Research and Development
NNSA	National Nuclear Security Administration
NRC	National Research Council
NSF	National Science Foundation
OCT	optical coherence tomography
ODE	ordinary differential equation
OLES	NIST Office of Law Enforcement Standards
OOF	Object-Oriented Finite Elements (software package)
OOMMF	Object-Oriented Micromagnetic Modeling Framework (software package)
PDE	partial differential equation
PET	positron emission tomography
PHAML	Parallel Hierarchical Adaptive Multi Level (software)
PITAC	President's Information Technology Advisory Committee
PL	NIST Physics Laboratory
PREP	Professional research Experience Program
QDPD	quarternion-based dissipative particle dynamics
QKD	quantum key distribution
RAVE	Reconfigurable Automatic Virtual Environment
SAVG	MCSD Scientific Applications and Visualization Group
SECB	slow evolution from the continuation boundary
SHPB	split-Hopkinson pressure bar
SIAM	Society for Industrial and Applied Mathematics
SIGGRAPH	ACM Special Interest Group on Graphics
SIMA	NIST Systems Integration for Manufacturing Applications Program
SIS	sequential importance sampling
SOR	successive overrelaxation
SPIE	International Society for Optical Engineering
SRM	standard reference material
SSS	Screen Saver Science
SURF	Student Undergraduate Research Fellowship
SVD	singular value decomposition
TNT	Template Numerical Toolkit
UMBC	University of Maryland Baltimore County
UNLV	University of Nevada Las Vegas
URL	universal resource locator
VCCTL	Virtual Cement and Concrete Testing Laboratory
VRML	virtual reality modeling language
W3C	World Wide Web Consortium
XML	Extensible Markup Language