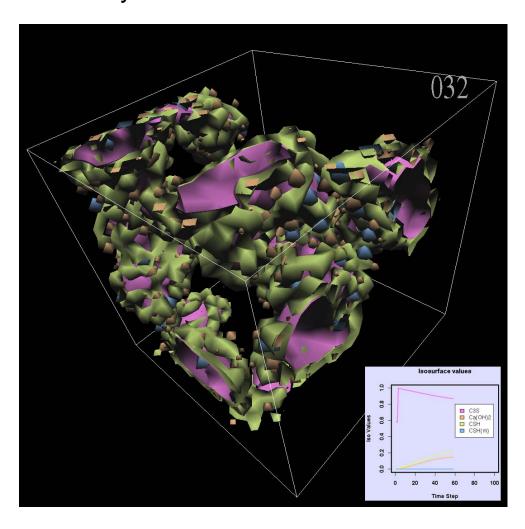
Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2007



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

January 2008





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.

For further information, contact Ronald F. Boisvert, Mail Stop 8910, NIST, Gaithersburg, MD 20899-8910, phone 301-975-3812, email boisvert@nist.gov, or see the Division's web site at http://math.nist.gov/mcsd/.

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.

Disclaimer. All references to commercial products in this document are provided only to document how results have been obtained. Their identification does not imply recommendation or endorsement by NIST.

Table of Contents

Part I. Overview	9
Introduction	11
Highlights	
Technical Accomplishments	
Technology Transfer and Professional Activities	
Staff News	17
Recognition	
Passings	20
Part II. Features	21
Parallel Adaptive Multilevel Finite Elements	23
Computable Error Bounds for Delay Differential Equations	25
Making Optical "Schrödinger Cat" States	
Modeling the Rheological Properties of Suspensions	
Computation, Visualization of Nano-structures and Nano-optics	
Error Correction for Electromagnetic Motion Tracking Devices	
Automated Combinatorial Testing for Software Systems	
Math Search	
Part III. Project Summaries	43
Mathematics of Metrology	45
Computable Error Bounds for Delay Differential Equations	
The Lipschitz Exponent as an Image Metrology Tool	
Systems Identification and Parameter Estimation	
Sparse Representations in High Dimensional Geometry	
Sequential Importance Sampling and the Markov Chain Monte Carlo Method	
Quantum Information	
Making Optical "Schrödinger Cat" States	
Quantum Computing With Ion Traps	
Quantum Computing Theory Preparing Ancillary States for Quantum Computation	
Adaptive Finite Element Modeling of Two Confined and Interacting Atoms	
Fundamental Mathematical Software Development and Testing	
Parallel Adaptive Multilevel Finite Elements	
OOF: Finite Element Analysis of Material Microstructures	
Sparse BLAS Standardization	
TNT: Object Oriented Numerical Programming	
SciMark, a Web-based Benchmark for Numerical Computing in Java	53
Mathematical Knowledge Management	55
Math Search	55
Digital Library of Mathematical Functions	55

Cultivating (Legacy) Mathematical Data	57
Visualization of Complex Function Data	58
High Performance Computing	59
Modeling the Rheological Properties of Suspensions	
Computation, Visualization of Nano-structure and Nano-optics	
High Precision Hy-CI Variational Calculations on Small Atomic Systems	59
Screen Saver Science	60
Computational Modeling of Cement Paste Hydration and Microstructure Development	60
Physics Models for Transport in Compound Semiconductors	61
High Performance Visualization	63
Error Correction for Electromagnetic Motion Tracking Devices	63
Computation, Visualization of Nano-structure and Nano-optics	
Virtual Cement and Concrete Testing Laboratory	
Visualization of Cement Paste Hydration and Microstructure Development	
Three-D Desktop	
Visualization of Network Dynamics	
Monitoring Change in Lung Tumors	
Mathematical Applications: Mechanical Systems and Processes	
Application of Optimization Techniques to Design for Multi-Hazard Conditions	
Instability in Pipe Flow	69
Materials Data and Metrology for Applications to Machining Processes, Frangible	
Ammunition, and Body Armor	
Mathematical Applications: Electromagnetic Systems	
Micromagnetic Modeling	
Time-Domain Algorithms for Computational Electromagnetics	
Laser Pulse Shape Measurement for Laser Guidance and Range Finding	
Modeling of Optical Spectra	
Mathematical Applications: Chemistry and Biology	
Modeling of Photochemical Reactions in a Focused Laser Beam	
Optical Coherence Tomography for Biomedical Imaging	
Accuracy and Standards for X-ray Measurements of Bone Mineral Density	
Monitoring and Modeling Change in Lung Tumors	
Computational Biology and Cell Imaging	
Mathematical Applications: Information Technology	
Automated Combinatorial Testing for Software Systems	
Foundations of Measurement Science for Information Systems	
Methods for Characterizing Massive Networks	
Standard Reference Data for Complex Network Research	
Standard Reference Data for Complex Network Research	04
Part IV. Activity Data	. 87
Publications	
Appeared	
Accepted	
Submitted	93

Presentations	93
Invited Talks	
Conference Presentations	
Software Released	96
Conferences, Minisymposia, Lecture Series, Shortcourses	96
MCSD Seminar Series	
Local Events Organized	97
External Events Organization	97
Other Professional Activities	97
Internal	97
External	97
External Contacts	98
Part V. Appendices	101
Staff	103
Glossary of Acronyms	106

Part I

Overview

Introduction

Applied mathematics and computation are critical to the advancement of science and engineering, which is, in turn, the principal fuel for industrial innovation. Indeed, a 2006 National Science Foundation report¹ states

"Simulation-based engineering science ... is a discipline indispensable to the nation's continued leadership in science and engineering. It is central to advances in biomedicine, nanomanufacturing, homeland security, microelectronics, energy and environmental sciences, advanced materials, and product development. There is ample evidence that developments in these new disciplines could significantly impact virtually every aspect of human experience."

A 2005 report² of the President's Information Technology Advisory Committee (PITAC) concludes further that

"Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation."

The connection to economic innovation has been emphasized by the Council on Competitiveness³ which has stated that "high performance computing is not only a key tool to increasing competitiveness, it is also a tool that is essential to business survival."

The disciplines of applied mathematics, statistics, and computer science are the foundation for computational science and engineering. Research in mathematical and statistical analysis, numerical algorithms, software tools, high performance computing, and visualization provide the basis for mathematical modeling, computational simulation, and data analysis in all fields. In this regard, close cooperation between mathematicians, computer scientists, and application scientists are critical. As the PITAC report states, "the 21st century's most important problems ... are predominantly multidisciplinary, multi-agency, multisector, and collaborative." Indeed, much of the most innovative research is now occurring at the intersection of mathematics, computer science, and applications, e.g., in areas like nanotechnology, bioinformatics, and quantum information.

NIST. The National Institute of Standards and Technology (NIST) plays a central role in the infrastructure for science and technology. Its mission is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life. In particular, the NIST Measurement and Standards Laboratories conduct research that advances the technology infrastructure needed by U.S. industry to continually improve products and services. Unveiled in 2006, the American Competitiveness Initiative underlines the importance of NIST in these efforts. Its report⁴ identifies the following examples of critical roles for NIST in the coming years:

¹ Simulation-based Engineering Science: Revolutionizing Engineering Science Through Simulation, Report of the National Science Foundation Blue-Ribbon Panel on Simulation-based Engineering Science, February 2006.

² Computational Science: Ensuring America's Competitiveness, President's Information Technology Advisory Committee, June 2005.

³ Study of US Industrial HPC Users, Council on Competitiveness, 2004.

⁴ American Competitiveness Initiative: Leading the World in Innovation, US Office of Science and Techology Policy, February 2006.

- World-class capability and capacity in nanofabrication and nanomanufacturing that will help transform current laboratory science into a broad range of new industrial applications for virtually every sector of commerce, including telecommunications, computing, electronics, health care, and national security (NSF, DoE, NIST)
- Chemical, biological, optical, and electronic materials breakthroughs critical to cutting edge research in nanotechnology, biotechnology, alternative energy, and the hydrogen economy through essential infrastructure such as the National Synchrotron Light Source II and the NIST Center for Neutron Research (DoE, NIST)
- Overcoming technological barriers to the practical use of quantum information processing to revolutionize fields of secure communications, as well as quantum mechanics simulations used in physics, chemistry, biology, and materials science (DoE, NIST, NSF)
- Overcoming technological barriers to efficient and economic use of hydrogen, nuclear, and solar energy through new basic research approaches in materials science (DoE, NSF, NIST)
- Addressing gaps and needs in cyber security and information assurance to protect our IT-dependent economy from both deliberate and unintentional disruption, and to lead the world in intellectual property protection and control (NSF, NIST)
- Development of manufacturing standards for the supply chain to advance and accelerate the development and integration of more efficient production practices (NIST)
- Enhanced response to international standards challenges, which impact U.S. competitiveness and limit export opportunities for American businesses by acting as technical barriers to trade (NIST)

ITL Programs

Begun FY 2007

Complex Systems

Complex Systems are composed of large interrelated, interacting entities which taken together, exhibit a macroscopic behavior which is not predictable by examination of the individual entities. The Complex Systems Program seeks to understand the fundamental science of these systems and develop rigorous descriptions (analytic, statistical, or semantic) that enable prediction and control of their behavior. Initially focused on the Internet and Grid Computing, this Program will facilitate predictability and reliability in these areas and other complex systems such as biotechnology, nanotechnology, semiconductors, and complex engineering.

Identity Management Systems

Identity management systems are responsible for the creation, use, and termination of electronic identities which are routinely used to access logical and physical resources, and have become a ubiquitous part of our national infrastructure. The Identity Management Systems Program is pursuing the development of common models and metrics for identity management, critical standards, and interoperability of electronic identities. These efforts will improve the quality, usability, and consistency of identity management systems while protecting privacy.

Information Discovery, Use, and Sharing

Society is awash in data - our ability to amass data has outpaced our ability to use it. Extracting knowledge, information, and relationships from this data is one of the greatest challenges faced by the scientists in the twenty-first century. The data can be as diverse as biological research data, medical images, automated newswire, speech, or video. The Information Discovery, Use, and Sharing Program fosters innovation throughout the information life cycle by developing the measurement infrastructure to enhance knowledge discovery, information exchange, and information usability. The Program enables novel computational approaches to data collection and analysis to be combined with improved interoperability techniques to effectively extract needed information from the wealth of available data.

Planned Startups in FY 2008

Cybersecurity

Cybersecurity is focused on ensuring three security objectives of information technology systems: confidentiality, integrity, and availability. The Cybersecurity Program creates a balance between our statutory responsibilities and a basic and applied research program. The Program addresses long-term scientific issues in some of the building blocks of IT security - cryptography, security testing and evaluation, security metrics, and security properties - providing a more scientific foundation for cybersecurity, while maintaining a focus on near-term issues.

(continued)

Enabling Scientific Discovery

Modern scientific research has become more and more dependent on mathematical, statistical, and computational tools for enabling discovery. The Enabling Scientific Discovery Program promotes the use of these tools to dramatically advance our ability to predict the behavior of a broad range of complex scientific and engineering systems and enhance our ability to explore fundamental scientific processes. This Program focuses on interdisciplinary scientific projects that involve novel computational statistics and the development of simulation methods and software. These efforts will have a foundational impact on scientific discovery throughout U.S. industry, government, and academia.

Pervasive Information Technologies

Pervasive information technology is the trend towards increasingly ubiquitous connected computing sensors, devices, and networks that monitor and respond transparently to human needs. The Pervasive Information Technologies Program facilitates the creation of standards for sensor communication, networking interoperability, and sensor information security. The Program enables the use of pervasive information technologies to enhance personal and professional productivity and quality of life.

Trustworthy Networking

The Trustworthy Networking Program's research encompasses the security, reliability, scalability, robustness, adaptability, and performance of networking technologies. The Program includes long-term fundamental research that is vetted against existing networking protocols. These efforts provide commercially viable techniques to test, measure, and improve the trustworthiness of networking technologies at the earliest stages of development.

Trustworthy Software

Trustworthy software is software that performs as intended for a specific purpose, when needed, with operational resiliency and without unwanted side effects, behaviors, or exploitable vulnerabilities. The Trustworthy Software Program will improve the ability to model, produce, measure, and assess trustworthiness in software through new and innovative technologies, models, measurement methods, and software tools. The resulting technologies, models, methods, and tools will reduce the cost and time of building in or assessing software trustworthiness in applications and systems.

Virtual Measurement Systems

A virtual measurement is a quantitative result and its uncertainty, obtained primarily by a nontrivial computer simulation or computer-assisted measurements, for example, computational models of physical systems. The Virtual Measurement Systems Program introduces metrology constructs, standard references, uncertainty characterization, and traceability into scientific computation and computer-assisted measurements. Uncertainty characterization and traceability in modeling will result in predictive computing with quantified reliability.

(This text is taken from the October 2007 ITL brochure edited by Elizabeth Lennon.)

- Accelerated work on advanced standards for new technologies (NIST)
- Advances in materials science and engineering to develop technologies and standards for improving structural performance during hazardous events such as earthquakes and hurricanes (NIST, NSF)

Information Technology at NIST. As one of the major operating units at NIST, the Information Technology Laboratory (ITL) promotes US innovation and industrial competitiveness by advancing measurement science, standards, and technology through research and development in IT, mathematics, and statistics. The importance of applied mathematics and computational science to ITL's work is clear from the four core competencies that it has identified:

- 1. IT measurement and testing,
- 2. Mathematical and statistical analysis for measurement science,
- 3. Modeling and simulation for measurement science, and
- 4. IT standards development and deployment.

To respond to the needs of its customers in industry, academia, and government, ITL has developed a set of cross-cutting and interdisciplinary programs. See the sidebar for a brief description of each.

The other laboratories and research centers within NIST are also important customers of ITL. Indeed, NIST's measurement science research program has been transformed by the advent of computational science and engineering. Nearly every NIST project, both theoretical and experimental, typically now has critical computational components. An increasing number of NIST "products" are techniques, tools, and reference data to enable modeling, simulation, and data analysis in particular application domains. As a result, the expertise of applied mathematicians and computer scientists are in high demand within NIST.

Mathematics and Computational Science at NIST. The Mathematical and Computational Sciences Division (MCSD) is one of six technical Divisions within ITL. MCSD provides leadership within NIST in the solution to challenging mathematical and computational problems. In particular, we seek to ensure that the best mathematical and computational methods are applied to the most critical problems arising from the NIST measurement science program. In addition, we also engage in highly leveraged research and development efforts to improve the environment for computational science and engineering at large.

To accomplish these goals, MCSD staff members engage in the following types of activities: (a) peer-to-peer collaboration with NIST scientists and engineers in a wide variety of critical applications, (b) targeted outreach efforts with selected external communities to advance the state-of-the-art in their subfield, (c) development and dissemination of unique mathematical and computational tools, and (d) research in targeted areas of applied mathematics and computer science of high relevance to future NIST measurement programs.

In Part III of this document we provide descriptions of most ongoing technical projects of the Division. These are organized under the following broad topic areas:

Mathematical Research

- a. Mathematics of Metrology
- b. Quantum Information
- c. Fundamental Mathematical Software Development and Testing
- d. Mathematical Knowledge Management
- e. High Performance Computing
- f. High Performance Visualization

Mathematical Applications

- g. Mechanical Systems and Processes
- h. Electromagnetic Systems
- i. Chemistry and Biology
- j. Information Technology

We expect that expertise in these areas will have considerable bearing on many of the nascent ITL Programs. In Part III (Project Summaries) we identify specific projects which are part of the three programs started in FY 2007: Complex Systems; Information Discovery, Use and Sharing; and Identity Management. Startup of projects associated with the ITL programs forming in FY 2008 is currently in process.

Highlights

In this section we identify some of the major accomplishments of the Division over the past year. We also provide news related to MCSD staff.

Technical Accomplishments

MCSD has made significant technical progress in a wide variety of areas during the past year. Here we highlight a few examples. Further details are provided in Part II (Features) and Part III (Project Summaries) of this document.

This year MCSD undertook a significant new initiative with the title *Mathematical Foundations of Measurement Science for Information Systems*. This was enabled by \$1.3M in new funding from the 2007 NIST Cyber Security Initiative, part of the American Competitiveness

Initiative. Conceived as a long-term basic research program in mathematics, the goal of this effort is the understanding, and ultimately the measurement, of fundamental properties of information systems which relate to the reliability and security of our cyber infrastructure. A one-day invitational workshop for senior leaders in the field was held at NIST on May 29, 2007 to assess the potential for a mathematical research program in this area, to consider intermediate-level technical goals, and to identify external research programs with which collaboration would be appropriate. A panel of eight external experts was assembled for wide-ranging discussion with some 15 NIST staff. A workshop report has been issued.

An important goal of this program will be to identify and characterize fundamental measurable properties of complex information systems that are indicators of the inherent level of security (i.e., resilience to threats both known and unknown). The program will develop and analyze abstract mathematical models of information system structure and information flow. Initially, this fundamental work will be applied to the study of complex information systems, such as computer networks and distributed systems, i.e., the area of study which has come to be known as network science. Relevant models will be studied using the theory of discrete random processes, graph theory, queuing theory, and modern Monte Carlo based computational approaches. We will study emergent behavior in large-scale networks, network reliability theory, and the analysis and development of self-healing (homeostatic) systems. The projects started up as part of this effort are described in Part III (Project Summaries) in the subsection entitled Mathematical Applications: Information Technology.

Results of MCSD research on the flow of suspensions (mainly concrete), carried out with a 2006 NASA award of 1,000,000 CPU hours on the Columbia supercomputer at the NASA Ames Research Center, were demonstrated at the NASA and NIST booths at the SC 2007 conference held in Reno, NV on November 10-16, 2007. This is the main conference in the US showcasing research enabled by massively parallel computing ("supercomputing"). The computational models developed use dissipative particle dynamics (DPD) to simulate the flow and interaction of solid particles in a fluid matrix. State-of-the-art real-time visualization based on non-photorealistic rendering and graphical processing unit (GPU) programming facilitated exploration of the rheology simulation output. At the NASA booth, these visualizations were shown on a large 3x3 array of monitors. The results demonstrated advances in understanding the influence of finite size effects, stress transmission, time scales, and system equilibration for both spherical particles and real-shape particles of gravel and sand. This work was carried out by a team of researchers in the NIST Building and Fire Research Laboratory and MCSD, led by Nicos Martys and Edward Garboczi (BFRL), and William George and Judith Terrill (MCSD).

As follow-on to this effort, the team was awarded an additional 400,000 CPU hours on the NASA supercomputer for 2008 to work on the chemistry (hydration) of cement as well as the flow of suspensions. In January 2008 the team was also awarded 750,000 CPU hours on the Blue Gene/P system at Argonne National Laboratory. The allocation is one of 55 awards of supercomputer time given in a peer-reviewed competition known as the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The new CPU time will enable more detailed modeling of the rheological properties of suspensions, as well as new work on a model simulating the three-dimensional changes in structure and chemical composition of aqueous mineral systems, such as those found in environmental geochemistry, ceramic processing, and cement-based materials.

During FY 2007 William Mitchell of MCSD released Version 1.0 of his PHAML system for the solution of elliptic partial differential equations. Such problems are found in a wide variety of models of physical phenomena, from the diffusion of heat in metal to the energy levels of atoms, and hence their efficient solution is of high interest. The core of PHAML is designed to

solve linear self-adjoint elliptic problems on general two dimensional domains, but hooks are provided which enable the solution to a much wider class, including eigenvalue, nonlinear, and time-dependent problems. PHAML stands for Parallel Hierarchical Adaptive Multi-Level, which characterizes the methods upon which the software is based. The package is the culmination of a decade of research on advanced solution methods, including high order finite elements, adaptive mesh refinement, multigrid solution techniques, dynamic load balancing, and parallel computing. Earlier beta releases of the program have been used for a variety of purposes, including solution of scientific and engineering applications, a platform for the investigation of new numerical methods and approaches to programming parallel computers, and a classroom tool for studying numerical methods or parallel computing. At NIST, PHAML has been used, for example, for the solution of a very challenging instance of the Schrödinger equation related to a model of interacting atoms representing qubits in a neutral-atom-based quantum computer.

Researchers in academia and industry are now developing a variety of useful technologies that exploit quantum optics phenomena. Some examples include quantum computation, quantum key distribution, interferometry, and lithography. Creating and maintaining superpositions of states of many photons and entangling them are critical capabilities needed for many such applications. However, because of the extreme fragility of quantum systems, producing them is still very challenging. As part of a NIST Innovations in Measurement Science project, we are working with scientists in the NIST EEEL to develop strategies for optical state preparation, manipulation, and measurement. This year Scott Glancy, working with guest researcher H. M. Vasconcelos, completed a thorough analysis of schemes for making a class of optical states called "Schrödinger cat" states. These states contain an equal superposition of two coherent states of opposite phase. This work is providing critical guidance for EEEL researchers who are working to create such states in the laboratory.

Finally, completion is finally in sight for the Digital Library of Mathematical Functions, the online successor to the classic NBS *Handbook of Mathematical Functions* (M. Abramowitz and I. Stegun, 1964). All 36 chapters are in the final stages of validation, and the full DLMF is expected to be released this calendar year. Look for a pre-release sample of chapters on the DLMF web site, http://dlmf.nist.gov/.

Technology Transfer and Professional Activities

The volume of technical output of MCSD remains high. During the last 18 months, Division staff members were (co-)authors of 31 articles appearing in peer-reviewed journals, including a paper published in *Nature*. Five other invited articles and 12 papers in conference proceedings were also published. Twenty-five additional papers have been accepted and are awaiting publication, while 18 others have been submitted for review. Division staff members gave 25 invited technical talks and presented 27 others to conferences and workshops.

MCSD continues to maintain an active Web site with a variety of information and services, including the Guide to Available Mathematical Software, the Matrix Market, and the SciMark Java benchmark. During calendar year 2007, the division web server satisfied nearly six million requests for pages, or more than 13,000 per day. More than 1.2 Gbytes of data were shipped each day. More than 500,000 distinct hosts were served. There have been more than 130 million "hits" on MCSD Web servers since they went online as NIST's first web servers in 1994.

Among our most popular software downloads for calendar year 2007 were: Template Numerical Toolkit (linear algebra using C++ templates): 17,779 downloads, JAMA (linear algebra in Java): 16,422 downloads, LAPACK++ (dense linear algebra in C++) 6,975 downloads, and SparseLib++ (elementary sparse matrix manipulation in C++): 5,726 downloads. Another

indication of the successful transfer of our technology is references to our software in refereed journal articles. Our OOMMF software for modeling of micro- and nano-magnetic phenomena was cited in 103 such papers which were published in calendar 2007 alone.

Members of the Division are also active in professional circles. Staff members hold a total of 11 associate editorships of peer-reviewed journals. They are also active in conference organization, serving on four organizing/steering/program committees. Staff members organized three minisymposia for the International Congress on Industrial and Applied Mathematics (Zurich, 2007), as well as a Birds-of-a-Feather session at SIGGRAPH.

Service within professional societies is also prevalent. Ronald Boisvert serves as Co-Chair of the Publications Board of the Association for Computing Machinery (ACM) and is a member of the ACM Council, the association's board of directors. Fern Hunt serves on the Executive Committee of the Association for Women in Mathematics. Daniel Lozier serves as Vicechair of the Society for Industrial and Applied Mathematics (SIAM) Activity Group on Orthogonal Polynomials and Special Functions. Staff members are also active in a variety of working groups. Ronald Boisvert serves as Chair of the International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software, Donald Porter is a member of the Tcl Core Team, and Bruce Miller is a member of W3C's Math Working Group. Judith Terrill represents NIST on the High End Computing Interagency Working Group of the Federal Networking and Information Technology Research and Development (NITRD) Program.

For further details, see Part IV (Activity Data) of this document.

Staff News

MCSD welcomed three new Postdoctoral Associates during this period. Brian Cloteaux joined MCSD in August 2007 from New Mexico State University, where he did research on analysis of abstract models of computation. At NIST he is working with Isabel Beichl on Monte Carlo methods for the estimation of properties of large-scale graphs. In September 2007 Bryan Eastin joined MCSD in Boulder from the University of New Mexico, where he did research on the relationship between error models and thresholds for fault-tolerant quantum computing. At NIST he will continue his investigations with Manny Knill. Finally, in January 2008, Valerie Coffman joined MCSD from Cornell University where she utilized finite element modeling to study the relationship between microscopic defects and the mechanical properties of polycrystals. At NIST she will be working with Stephen Langer on 3D image-based analysis of materials with complex microstructures.

During 2007 MCSD served as host to Grant Erdman, a research mathematician in the Information Operations and Special Programs Division of the Human Effectiveness Directorate of the Air Force Research Laboratory in San Antonio. As part of the Commerce Science Fellowship program, Erdman spent nine-months at NIST to learn of the organization and structure of the NIST measurement and science labs, while participating in technical projects related to his expertise in mathematical optimization.

Three guest researchers joined MCSD's Scientific Applications and Visualization Group this year to contribute to projects in high performance computing and scientific visualization. They are: Dr. Dong Yeon Cho of the School of Computer Science and Engineering of the Seoul National University (Korea), an expert in machine learning, genetic programming, and applications to bioinformatics, and Edith Enjolras and Cedric Houard, students at the College of Engineering in Computer Science, Modeling and Applications at the Blaise Pascal University in Clermont-Ferrand, France

During the summer of 2007 MCSD hosted 11 student interns working on a wide variety of projects, from image processing to quantum computer simulation; see the table for details.

MCSD Student Interns - 2007						
Name	Institution	Pro- gram	Mentor	Project Title		
Liuyuan Chen	Montgomery Blair High School	Student Volunteer	B. Rust	Wrote Fortran subroutines & made calculations with Fortran and Matlab		
Kevin Costello	Carnegie Mellon University	SURF	S. Glancy	Quantum computer simulation.		
Kevin Dela Rosa	University of Texas- Arlington	SURF	R. Kacker	Integrate improved algorithm into Fire-Eye.		
Michael Forbes	MIT	SURF	R. Kacker	Improving IPOG algorithm to yield smaller covering arrays.		
Gillian Haemer	University of Southern California	Student Volunteer	A. O'Gallagher	Image processing in an immersive visualization environment.		
Aaron Jones	Hampton College	SURF	J. Terrill	Visualizing nanostructures.		
Olga Kuznetsova	University of Maryland	SURF	S. Langer	Object-oriented finite elements for analyzing material microstructure.		
Adam Meier	University of Colorado	PREP	E. Knill	Simulating Fault Tolerant Architectures.		
Omotunwase Olubayo	Hampton College	SURF	A. Peskin	Image processing and virtual reality.		
Sathish Ragappan	Quince Orchard High School	Student Volunteer	J. Terrill	Curvature		
Miguel Rios	University of Puerto Rico	SURF	J. Terrill	Physics Models for Transport in Compound Semiconductors.		

SURF: NIST Student Undergraduate Student Fellowship Program. PREP: Professional Research Experience Program

Recognition

Anthony Kearsley was selected as part of a four-person team to receive the Department of Commerce Bronze Medal for work on matrix assisted laser desorption/ionization-time of flight-mass spectroscopy (MALDI-TOF-MS). The team was cited for work which enabled the wide-spread use of MALDI as a quantitative measurement tool. In particular, they developed a comprehensive online resource that includes an automated, operator-independent data analysis tool (MassSpectator), a consolidated collection of sample preparation methods, and polymer mass spectroscopy workshop reports. The citation states "Because of their enormous value to industrial, academic, and government researchers, the database and the accompanying tools exemplify the highest level of service to those engaged in mass spectroscopy." The co-recipients of the award were William Wallace, Charles Guttman, and Kathleen Flynn of MSEL. The Bronze Medal is the highest honorary recognition presented at the annual NIST awards ceremony.

During FY 2007 two MCSD mathematicians were honored as Distinguished Scientists by the Association for Computing Machinery (ACM). Ronald Boisvert and Dianne O'Leary, a faculty appointee from the University of Maryland, were included in a group of 49 professionals in ACM's inaugural class of distinguished members. The ACM Distinguished Membership Program recognizes members with at least 15 years of professional experience who have significant accomplishments or who have achieved a significant impact on the computing field. Founded in 1947, ACM is the world's oldest and largest educational and scientific computing society.



Recipients of the 2007 Department of Commerce Bronze Medal (from left to right): Anthony Kearsley (MCSD), William Wallace (MSEL), Kathleen Flynn (MSEL), and Charles Guttman (MSEL).

Ronald Boisvert was co-author of a paper named as winner of the ITL Outstanding Conference Paper for 2007. The paper recognized was

Xiao Tang, Lijun Ma, Alan Mink, Anastase Nakassis, Hai Xu, Barry Hershman, Joshua Bienfang, David Su, Ronald F. Boisvert, Charles Clark, Carl Williams "Quantum key distribution system operating at sifted-key rate over 4 Mbit/s," in *Proceedings of SPIE* **6244**, pp. 62440P-1-62440P-8 (April 2006).

The paper describes the design of the NIST high-speed quantum key distribution (QKD) system and the innovations in photonics, high-speed electronics, and information algorithms and protocols that were required to bring this system to fruition. With these techniques, the NIST QKD system significantly exceeded the world performance record for speed of key generation and exchange.

Also recognized with ITL Awards this year were Robin Bickel and David Gilsinn for their efforts in organizing the Division's move from NIST North back to the NIST main campus during the summer of 2006.



Andre Deprit

Former NIST Senior Fellow and MCSD Guest Researcher André Deprit was inducted into the NIST Gallery of Distinguished Scientists, Engineers and Administrators in ceremonies held in Gaithersburg on October 19, 2007. He was cited for pioneering the use of symbolic computing to solve outstanding problems in celestial mechanics, including the theory of integrable dynamical systems with applications to the motion of artificial satellites. André passed away on November 7, 2006. He was represented at the ceremony by his son Etienne.

MCSD mathematician Bonita Saunders was selected to serve as a distinguished presenter at the 2007 Awards Gala of the Benjamin Banneker Institute for Science and Technology which was held in Washington, DC on November 7, 2007. The annual Awards Gala recognizes those making significant contributions to the Institute's mission, "to increase access to, and

participation and performance in science and math related professions and academic pursuits by African Americans." Six awards were presented, recognizing excellence in grade school, high school, college, graduate school, PhD. pursuits, and life. Saunders presented the Grade School Award. Speakers at the event included NPR Journalist Juan Williams and TV personality Bill Cosby.

Passings



Joyce E. Conlon, 50, a systems programmer for MCSD since 1999, died in Rockville, Md., on Nov. 14, 2007, after suffering a stroke. Born April 30, 1957, in Richmond, Va., Conlon grew up in suburban Baltimore and attended the University of Maryland-Baltimore County where she earned a Bachelor of Arts degree in mathematics in 1979. Conlon worked as a computer programmer for the Defense Mapping Agency from 1980 to 1985. She began her career at NIST in the fall of 1985 as a computer specialist in the Computer Services Division. Seeing her way through several division name changes, Conlon was reassigned to the ITL High Performance Systems and Services Division and finally to the MCSD in

1999. She retired in July 2005. While at the MCSD, she provided technical computing support to MCSD staff, served as MCSD Computer Security Officer, and was an integral member of the team working to develop the NIST Digital Library of Mathematical Functions (DLMF), the 21st century successor to the NBS Handbook of Mathematical Functions. She continued her work on the DLMF as a guest researcher and contractor until the time of her death. [This text was adapted from an article in *NIST Connections*.]