Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2006

Information Technology Laboratory
National Institute of Standards and Technology
Technology Administration
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INFORMATION TECHNOLOGY LABORATORY

NIST
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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 nine particular projects with accomplishments 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 2005 through December 2006.

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Cover photo. Mathematician Howard Hung experiences a quantum dot in MCSD's immersive visualization environment. This photo appeared in the photo gallery of the online interactive edition of June 2006 issue of *National Geographic* associated with the feature article "Nano's Big Future." See http://www7.nationalgeographic.com/ngm/0606/feature4/gallery2.html. Photo by Mark Thiessen / National Geographic Image Collection.

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

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Part I

Overview

Introduction

There is now very widespread recognition of the critical role of applied mathematics and computation to both the advancement of science and engineering and to industrial innovation. Indeed, a recent report[1] of the President's Information Technology Advisory Committee (PITAC) states

> *"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."*

In a similar vein, a report[2] prepared on behalf of the National Science Foundation 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."*

The importance to industry is also clear. According to the Council on Competitiveness[3], "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.

Information Technology at NIST. The mission of the National Institute of Standards and Technology (NIST) 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 nation's technology infrastructure and is needed by U.S. industry to continually improve products and services. The NIST Information Technology Laboratory (ITL) has the broad mission of supporting U.S. industry, government, and academia with measurements and standards that enable new computational methods for scientific inquiry, assure IT innovations for maintaining global leadership, and re-engineer complex societal systems and processes through insertion of advanced information technology. Through its efforts, ITL seeks to enhance productivity and public safety, facilitate trade, and improve the quality of life.

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[1] *Computational Science: Ensuring America's Competitiveness*, President's Information Technology Advisory Committee, June 2005.
[2] *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.
[3] *Study of US Industrial HPC Users*, Council on Competitiveness, 2004.

The other measurement science 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. In addition, an increasing number of NIST "products" are techniques, tools, and reference data to enable modeling, simulation, and data analysis in particular application domains.

To respond to the needs of its customers in industry, academia, government, and within NIST, ITL has developed a wide range of cross-cutting programs in areas such as information discovery, use, and sharing; complex systems; identity management; scientific discovery; and others. Applied mathematics and computational science plays an important role in these programs. This is clear from the four core competencies that ITL has identified as critical for it to carry out its work: (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.

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 engaged 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 particular 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 programs.

The technical work of the Division can be organized into eight general areas. We indicate overall goals and approach of each of these below. Of course, there is considerable overlap between these areas. Nevertheless, this breakdown provides a useful overview of Division thrusts.

<u>Mathematical Modeling of Mechanical Systems and Processes.</u>
Goals: Enable effective mathematical and computational modeling of mechanical processes and systems of critical importance to NIST programs. Improve the state-of-the-art in software for modeling and simulation of mechanical processes and systems.
Approach: Develop techniques and tools to enable accurate, reliable, and efficient modeling and simulation of mechanical processes and systems. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

<u>Mathematical Modeling of Electromagnetic Systems.</u>
Goals: Enable effective mathematical and computational modeling of electromagnetic and acoustic phenomena of critical importance to NIST programs. Improve the state-of-the-art in software for electromagnetic and acoustic modeling and analysis.
Approach: Develop techniques and tools to enable accurate, reliable, and efficient modeling and simulation of electromagnetic and acoustic phenomena. Work with external groups to improve the state-of-the-art in electromagnetic modeling through the use of benchmarks (challenge prob-

lems) and reference software. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

<u>Mathematical Modeling for Chemical and Biological Applications.</u>
Goals: Enable effective mathematical and computational modeling for chemical and biological applications of critical importance to NIST programs. Improve the state-of-the-art in software for chemical and biological modeling and analysis.
Approach: Develop techniques and tools to enable accurate, reliable, and efficient modeling and simulation of chemical and biological systems. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

<u>High Performance Computing</u>.
Goals: Improve the quality and rate of scientific discovery through the effective use of parallel and distributed computing resources.
Approach: Develop techniques and tools for parallel and distributed computing needed by NIST. Collaborate with NIST scientists in the application of high performance computing to high priority projects. Disseminate techniques and tools to the research community at large.

<u>High Performance Visualization.</u>
Goals: Develop an integrated environment that enhances scientific discovery at NIST by enabling fast, effective, and collaborative visual analysis of large-scale scientific data.
Approach: Develop visualization infrastructure to enable agile and flexible use of available visualization resources. Develop a virtual measurement laboratory based on an immersive visualization environment, enabling scientific exploration, discovery, and measurement science. Widely disseminate enabling tools for high-end visualization. Collaborate with NIST scientists in the application of high performance visualization to high priority NIST projects.

<u>Mathematics of Metrology.</u>
Goals: Develop effective methods for the solution to critical mathematical problems arising in metrological applications.
Approach: Anticipate needs of NIST in mathematical and computational methods for metrological applications, e.g. inverse and ill-posed problems, dynamical systems. Develop fundamental mathematical and computational techniques of widespread application. Galvanize interest within the applied and computational mathematics community for the study of problems occurring in measurement science.

<u>Quantum Information Theory.</u>
Goals: Develop fundamental understanding of potential of quantum mechanical systems for computation and communication.
Approach: Collaborate closely with the NIST Physics Lab and Electronics and Electrical Engineering Lab to demonstrate the information processing capabilities of quantum systems, including ion traps and optical systems. Develop architectural concepts for quantum information systems, including error control strategies promoting fault-tolerance. Develop techniques and tools enabling the analysis of behavior of quantum mechanical systems.

<u>Mathematical Knowledge Management</u>.
Goal: Enable the effective representation, exchange, and use of mathematical data.
Approach: Disseminate mathematical reference data for use by the technical research community. Develop technologies, tools, and standards to improve the presentation and exchange of mathematical reference data.

Fundamental Mathematical Software Development and Testing.
Goal: Improve the efficiency, reliability, ease-of-development, and portability of technical computing applications, and related commercial products.
Approach: Develop fundamental mathematical software components to ease development of efficient, reliable, and portable applications at NIST and in the technical computing community at large. Work with external groups to develop standard interfaces for mathematical software components to promote interoperability and performance portability. Develop test methods, data, and reference implementations to support testing and evaluation of mathematical software and underlying methods. Disseminate techniques and tools to the community at large.

Crosscutting Themes. Several crosscutting themes indicative of current industrial trends have emerged in the Division technical program. In particular, as NIST measurement science increasingly begins to focus on nanoscale phenomena, so have the modeling and simulation needs of NIST scientists. As a result, increasing numbers of Division projects are related to ***nanotechnology***. For example, MCSD staff members are developing techniques for the improvement of scanning electron microscope images, software for the modeling of nanomagnetic phenomena, and parallel computing and visualization techniques for models of optical properties of nanostructures.

A second crosscutting theme of MCSD research is ***virtual measurements***, i.e., the use of mathematical modeling and computational simulation to supplement, and even to replace, complex or expensive physical measurements. One example is the integration of computer simulation with physical measurement. Our OOF software for the finite element analysis of materials with complex microstructure enables analyses based on micrographs of real material samples, a capability useful in manufacturing quality control applications. We are also developing technologies to enable accurate interactive measurements during the analysis of data from physical measurement in immersive visualization environments. These tools have already seen application in the evaluation of prototype standard polymer scaffolds for the growth of human tissue. Looking further into the future, if computer models are to be used as a proxy for physical measurement, then it is necessary to be able to rigorously characterize the uncertainty in results from computer simulations, something that is rarely done today in any formal way. We are working to develop such methodologies in collaboration with NIST scientists.

Another recurring theme in our work is he need for the automated ***analysis of complex or large-scale scientific data*** sets, whether obtained from physical measurement or computer simulation. Often such data takes the form of images. In many cases the data is highly noisy. Recent areas of study here include object recognition in laser ranging (LADAR) data, sequence alignment problems in bioinformatics, and automated peak identification in mass spectral data. Visualization techniques provide an important means for scientists to make sense of large volumes of scientific data; our immersive scientific visualization lab, along with its associated software tools and environment, provide unique capabilities in this regard.

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. Details can be found in subsequent sections.

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.

Imaging and visualization technology and tools were behind a number of the Division's major accomplishments for the year. In some cases this involved the development of new imaging technologies themselves. For example, we worked with scientists in the NIST Electronics and Electrical Engineering Laboratory (EEEL) to evaluate the potential of optical coherence tomography as a diagnostic tool for cancer. One of the distinguishing features of this imaging modality is that both the intensity and phase fields can be measured. In a paper published in *Optics Express*, the team showed that optical phase offers potentially new diagnostic information on biological scatterers of interest in cancer detection. Algorithms and software tools for electromagnetic modeling developed by Andrew Dienstfrey of MCSD enabled the theoretical verification of these results.

Techniques for the post processing of image data to compensate for unwanted effects of imaging systems has long been a need for NIST measurement science, and MCSD has led in the development of such techniques. One particularly effective technique is the APEX method for real-time blind deconvolution developed by Alfred Carasso. It is blind in that the point-spread function (PSF) causing the blur is not known a priori. The PSF is taken from a class of 2-D heavy-tailed probability density functions whose parameters are estimated from the image itself. Once the PSF is determined, the deconvolution proceeds by marching a diffusion equation backwards in time. With FFTs as its computational kernel, it is highly efficient, even for large images. The method has been shown to be effective on a wide range of imagery, including medical images and scanning electron microscope images. In a paper published in the October 2006 issue of *Optical Engineering*, Carasso describes an extension of the technique to color imagery, which he applies to enhance a wide range of Hubble Space Telescope and other astronomical data. The journal editors featured one of these enhanced images on the October issue's cover.

Highly useful scientific data can be extracted from images in many other ways. The OOF (Object Oriented Finite element) system enables the direct computational study of structure-property relationships in materials with complex microstructures through highly sophisticated image analysis. When running OOF, a user assigns material properties to the features in an image of a material's microstructure, and then performs virtual experiments on the material (to obtain stress-strain fields, for example). Unlike commonly available commercial finite element codes, OOF features both a powerful suite of tools for adapting a finite-element mesh to the microstructural geometry of an image, and a modular and extensible scheme for adding new or customized property data to the underlying model. This year a major new version of OOF was released. With a design that is highly modular and extensible, OOF2 enables a much wider range of applications than the original. A workshop for OOF users held at NIST in September 2006 to introduce the new system attracted some 40 researchers from around the world. OOF2 was developed by Stephen Langer and Andrew Reid of MCSD, in cooperation with the NIST Materials Science and Engineering Laboratory (MSEL).

Other measurement science applications are not necessarily as amenable to completely automated processing. In these cases a more hands-on approach is necessary. We are pioneering the use of immersive visualization for the interactive measurement and analysis of properties of physical systems which have been captured using three-dimensional imaging technologies. In doing so we are developing the tools needed to create a true virtual measurement laboratory. For

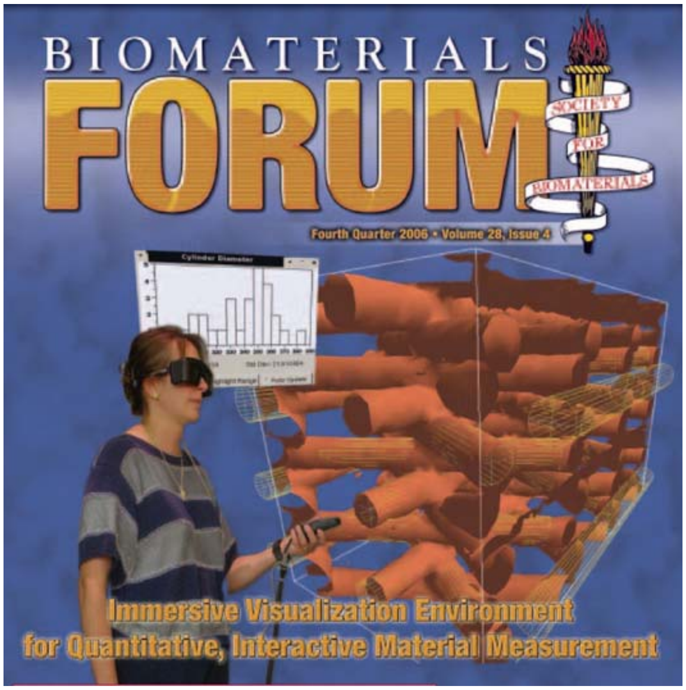


Figure 1. *MCSD work on quantitative interactive material measurement in an immersive visualization environment was featured on the cover of the 4th quarter 2006 issue of Biomaterials Forum. (This image used Courtesy of the Society for Biomaterials.)*

example, we have worked closely with MSEL scientists to characterize standard reference materials (e.g., polymer scaffolds) for the growth of tissue engineered products. To do so, three dimensional images that were generated with X-ray micro-computed tomography (μCT) were segmented and converted to a polygonal representation for the virtual environment. We then used interactive measurement and analysis tools we developed to compare an idealized "as designed" scaffold with an actual manufactured scaffold to determine differences in strut properties. This work was featured in a cover article in the fourth quarter 2006 edition of *Biomaterials Forum*.

Another type of virtual measurement is the prediction of physical properties of matter entirely through computation based on first principles. In a paper published this year in the *Journal of Chemical Physics*, James Sims of MCSD and Stanley Hagstrom of Indiana University announced a new high-precision milestone for the calculation of the disassociation energy of the hydrogen molecule (H_2). Accurate to 1 part in 100 billion, these are the most accurate energy values ever obtained for a molecule of that size, 100 times better than the best previous calculated value or the best experimental value. While very precise calculations have been done for systems of just three components such as helium (a nucleus and two electrons), Sims and Hagstrom are the first to reach this level of precision for H_2 with two nuclei and two electrons. The calculation requires solving an approximation of the Schrödinger equation using a series approximation. To make the problem computationally practical, Sims and Hagstrom merged two earlier algorithms for these calculations—one which has advantages in ease of calculation, and one which more rapidly achieves accurate results—into a hybrid with some of the advantages of both, known as the Hy-CI variational method. To enable the computation they developed specialized multi-precision arithmetic capabilities and a new parallel large-scale generalized matrix eigenvalue solver. The final calculations were run on a 147-processor parallel cluster at NIST over the course of a weekend—on a single processor it would have taken close to six months.

Large scale parallel computational methods developed by MCSD are also enabling the understanding of the properties of cement-based materials. William George and Judith Terrill of MCSD, along with Nicos Martys and Edward Garboczi of the NIST Building and Fire Research Laboratory were awarded 1,000,000 CPU hours on the 10,240-CPU Columbia supercomputer at NASA Ames Research Center for such work. The allocation was one of four awards of supercomputer time given out by NASA in a peer-reviewed competition for grand challenge computational science projects led by external researchers. The team is using NASA's supercomputer to study the flow, dispersion and merging of dense suspensions composed of rigid bodies having a wide range of size and shape under a variety of flow conditions. Access to the NASA machine will allow modeling at a level and range impossible with existing computing facilities available at NIST. The new realism of these models will significantly improve the scientific basis for prediction and measurement of the flow properties of concrete.

Finally, we are working closely with the NIST Physics Laboratory to begin to develop a measurement science infrastructure to enable computation based upon quantum mechanical systems. While quantum computers have the potential for significantly speeding up many useful algorithms, building quantum computers is challenging. Currently available quantum devices can realize computations with only a few quantum bits (qubits) and steps. Atomic qubits in ion traps are currently considered one of the leading candidates for realizing large quantum computers. A team led by David Wineland at NIST (PL, Boulder) has arguably the most advanced laboratory in the world for studying such systems. Manny Knill of MCSD is providing the theoretical underpinnings to enable the team to determine the potential of this technology. This year the team implemented two benchmark quantum subroutines for up to six atomic qubits and analyzed the error of the implementations. The first benchmark involved creating "Schrödinger cat states" of four to six qubits. The second demonstrated an entanglement purification protocol that is expected to play a key role in large scale implementations of quantum computers and quantum communication protocols. Each of these landmark accomplishments were reported in papers published in *Nature*.

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 50 articles appearing in peer-reviewed journals, including two published in *Nature*. 13 other invited articles and 14 papers in conference proceedings were published. Fourteen additional papers have been accepted and are awaiting publication, while 24 others have been submitted for review. Division staff members gave 28 invited technical talks and presented 19 others to conference 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 2006, the virtual server math.nist.gov satisfied nearly seven million requests for pages, or more than 19,000 per day. More than 1.7 Gbytes of data were shipped each day, and more than 539,000 distinct hosts were served. The virtual server gams.nist.gov, delivered 930,000 pages, or more than 2,500 per day. There have been nearly 115 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 2006 were: Template Numerical Toolkit (linear algebra using C++ templates): 15,310 downloads, Jama (linear algebra in Java): 13,656 downloads, and SparseLib++ (elementary sparse matrix manipulation in C++): 4,284 downloads.

Members of the Division are also active in professional circles. Nine staff members hold a total of 14 associate editorships of peer-reviewed journals. Three staff members served as guest editors organizing special journal issues. Staff members are also active in conference organization, two serving on organizing committees and four on program committees. Three staff members are organizing minisymposia for the upcoming International Congress on Industrial and Applied Mathematics (Zurich, 2007), four others organized sessions at meetings ranging from the SIAM Annual Meeting to 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 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 Vice-chair 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.

MCSD Student Interns - 2006				
Name	**Institution**	**Program**	**Mentor**	**Project Title**
Zachary Catlin	Purdue Univ.	SURF	S. Glancy	Characterization of quantum optical states.
Liuyuan Chen	Montgomery Blair High School	Student Volunteer	B. Rust	Wrote Fortran subroutines & made calculations with Fortran and Matlab
Michael Forbes	MIT	SURF	R. Kacker, D. Gilsinn	Combinatorial methods for software testing
Adam Lazrus	Charles E. Smith Upper School	Student Volunteer	J. Terrill	Distributed 3D Chemical Imaging: Porting a Serial Application to Screen Saver Science
Christine McKay	University of Maryland	SURF	W. George	A User Interface to a Distributed Computing Environment
David Warshawsky	Melvin J. Berman Hebrew Academy	Student Volunteer	J. Fong	Formulate simple framed structure design problem in 2D

SURF: NIST Student Undergraduate Student Fellowship Program.

Staff News

Howard Hung retired from NIST in July 2006 after more than 30 years of federal service. His long career featured many contributions to operations research, scientific computing, and visualization. He was most recently a member of the MCSD Scientific Applications and Visualization Group.

NIST/NRC Postdoctoral Associate Scott Glancy finished his two-year appointment in September 2006. He worked in the area of quantum information theory with Manny Knill in Boulder. Glancy was given a two-year extension on his appointment to continue this work. Christopher Schanzle, formerly of the NIST CIO Office joined MCSD in October 2005 to provide computer systems and programming support to Division staff. He serves as MCSD Computer Security Officer.

MCSD made two additional faculty appointments during FY 2006. These are made to full-time faculty members at local universities, who then typically spend about one day per week working in MCSD throughout the year. This year's new appointees were Daniel Anderson of George Mason University, an expert in mathematical modeling of fluid dynamics and materials phenomena, and Marc Olano of the University of Maryland Baltimore County, an expert in interactive 3D computer graphics.

Manny Knill of MCSD in Boulder was elevated to the status of NIST Fellow in September 2006. Designation as Fellow is the highest distinction given to NIST technical staff. There is a limit of 30 Fellows NIST-wide. Geoffrey McFadden of MCSD is the only other NIST Fellow in ITL.

Two MCSD staff members completed details at other government agencies at the end of FY 2006. Isabel Beichl participated in a sabbatical program within the Mathematics Research Group at the National Security Agency. She spent half of her time at the NSA as part of this program. Robert Bohn of MCSD completed a two-year assignment with NOAA's High Performance Computing and Communications Office.

MCSD provided support for six student staff members on summer appointments during FY 2006. Such appointments provide valuable experiences for students interested in careers in mathematics and the sciences. In the process, the students can make very valuable contributions to MCSD program. This year's students are listed in the table above.

Figure 2. *Three of MCSD's 2006 award winners. Left: Bradley Alpert, winner of the 2005 Arthur Flemming Award. Center: Dianne O'Leary, Fellow of the Association for Computing Machinery. Right: Manny Knill, Fellow of the American Physical Society.*

Awards

MCSD staff garnered a variety of awards and recognitions during the past year. Bradley Alpert was named a winner of the 2005 Arthur Flemming Award. Established by the Downtown Jaycees in 1948, the Flemming Awards honor outstanding federal employees with at most 15 years of service. The program is administered by the George Washington University in conjunction with the Flemming Award Commission. Twelve separate awards are made each year in three categories: administration, science, and applied science and mathematics. Alpert was recognized in the latter category for a sustained record of fundamental contributions to scientific computing, including the development of fast algorithms enabling the solution to heretofore intractable problems of computational physics. He is also cited for his extensive collaborations with scientists and engineers to apply innovative techniques to the solution of diverse problems of scientific and technological interest. Finally, the award recognizes Alpert's work as a mentor and leading proponent of careers in mathematics for students at the high school, undergraduate, graduate, and post-graduate levels. The award was conferred in ceremonies in Washington, DC on June 13, 2006. Alpert is the fourth MCSD staff member to receive the Flemming Award. Previous MCSD awardees were Anthony Kearsley (2001), Fern Hunt (2000), and Geoffrey McFadden (1989).

Emanuel (Manny) Knill was elected a Fellow of the American Physical Society (APS). This is a high honor in that Fellow status is granted to no more than one half of one percent of APS members. The selection was made by the APS Division of Atomic, Molecular and Optical Physics in recognition of Knill's outstanding contributions to physics. In particular, Knill was cited for “contributions to our understanding of the control and manipulation of quantum systems, including quantum error correction, determination of tolerable error rates, and linear optics quantum computing. Announcement of the fellowship occurred in the March 2006 issue of APS News. Knill is MCSD's second APS Fellow. Geoffrey McFadden was elected in 2001. Knill was also given the designation of NIST Fellow in September 2006.

Dianne O'Leary, an MCSD faculty appointee from the University of Maryland College Park was named a Fellow of the Association for Computing Machinery (ACM). The ACM Fellows Program was established in 1993 to recognize and honor outstanding ACM members for their achievements in computer science and information technology and for their significant contributions to the mission of the ACM. Fellow status is limited to at most 1% of ACM members. O’Leary will be recognized at ACM’s June 2007 award’s ceremony in San Diego.

Ronald Boisvert and Dianne O’Leary were also honored as Distinguished Scientists by the ACM. They 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 achieved a significant impact on the computing field.

Pete Stewart, an MCSD faculty appointee from the University of Maryland College Park was named a UMCP Distinguished University Professor. This formal title denotes an academic honor of highest distinction and is awarded to a limited number of the university's most accomplished professors.

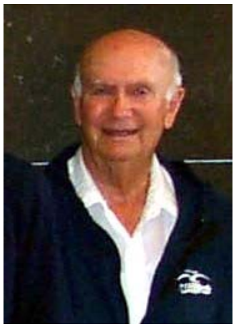
Finally, MCSD captured two of the four ITL Awards presented during 2006. Manny Knill was recognized with the ITL Best Journal Paper Award for "Quantum Computing with Realistically Noisy Devices," published as a feature article in *Nature*, volume 434, pages 39-44 (03 Mar 2005). MCSD’s Scientific Visualization Team, comprised of Judith Terrill, Terrence Griffin, John Hagedorn, Howard Hung, John Kelso, Yolanda Parker, Adele Peskin, and Steven Satterfield, were honored with the ITL Outstanding Contribution Award for “outstanding service as ambassadors of ITL, providing numerous demonstrations of ITL’s immersive scientific visualization capabilities which have led to widespread favorable recognition of NIST in the news media, as well as among stakeholders in Congress, industry, academia, and the general public”.

Passings

Eleazer Bromberg. Dr. Eleazer Bromberg, 92, was a mathematician at NBS/NIST from 1979 until his retirement in 1999, after which he continued as a guest researcher in MCSD for several years. At NIST he served as technical advisor to several Lab Directors in the area of high performance scientific computing. This was Lazer's second career, however. After receiving his Ph.D. in applied mathematics from the Courant Institute of Mathematical Sciences at New York University in 1950, he served as head of the Mechanics Branch of the Office of Naval Research. In 1953 he returned to NYU, where he remained until 1979, serving in a variety of roles including Professor, Administrative Director of the AEC Computing Center (1953-58), Assistant Director of the Courant Institute (1959-66), Vice Chancellor for Academic Affairs (1970-73), and Deputy Chancellor (1973-75). He also held visiting positions at the Los Alamos Scientific Laboratory and the IDA Center for Computing Sciences. He passed away on March 27, 2006 in Philadelphia.

Howland Fowler. Dr. Howland Auchincloss Fowler, 76, came to NBS in 1957 as an NRC Associate and spent his next 37 years as an NBS physicist specializing in low-temperature physics and applied mathematics. He served as scientific advisor to the directors of several major NIST organizations. In 1991 he became Leader of the Scientific Visualization Group in the NIST Computing and Applied Mathematics Laboratory. He was (co-)author of more than 30 scientific papers. He retired in 1994 but continued as a guest researcher in MCSD until 2000. He passed away on September 3, 2006 in Bethesda, MD.

André Deprit. Former NIST Fellow Dr. André Deprit, 81, was a NBS/NIST mathematician from 1979 until his retirement in 1999; he continued as a guest researcher in MCSD until 2003. André received a D.Sci. degree in mathematics from the University of Louvain in 1957. He held a professorship at Louvain before coming to the US in 1964 to work at Boeing. He had appointments at NASA Goddard and the University of Cincinnati before joining NBS. André was a leading expert in the mathematics of celestial mechanics, and a pioneer in the use of symbolic computing to tackle problems in that field. The author of more than 150 technical articles, his work was very highly regarded in the fields of space flight mechanics and astrodynamics, resulting in numerous awards, including the James Craig Watson Medal from the US National Academy of Sciences (1972), the Dirk Brouwer Award from the American Astronomical Society (1984), and the Department of Commerce Gold medal (1986). He passed away on November 7, 2006 in Gaithersburg, MD.



Morris Newman. Dr. Morris Newman, 82, was a research mathematician at NBS from 1952-1977. He was awarded a DOC Gold medal in 1966 for his work on algorithms for solving exactly integral linear systems using congruence techniques. In 1968 he wrote the book *Matrix Representations of Groups* and in 1972 the book *Integral Matrices,* which became a classic. Recently he served as an Associate Editor of the NIST Digital Library of Mathematical Functions while an emeritus professor at University of California at Santa Barbara. He passed away on January 4, 2007 in Santa Barbara, CA.