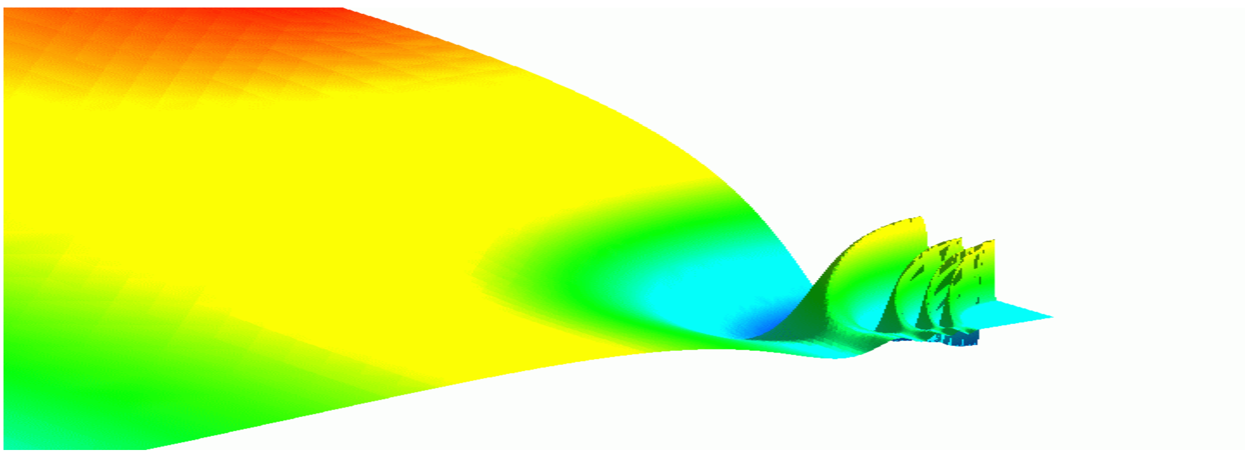
# Mathematical and Computational Sciences Division

## Summary of Activities for Fiscal Year 2003



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

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# Abstract

This report summarizes the technical work of the Mathematical and Computational Sciences Division of NIST's Information Technology Laboratory. Part I provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II provides additional details covering many of the research activities of the Division. Part III provides listings of publications, technical talks, and other professional activities in which Division staff members have participated.

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Thanks to Robin Bickel for collecting and organizing the information contained in this report.

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Part I

# Overview

# Introduction

The mission of the Mathematical and Computational Sciences Division (MCSD) is stated as follows.

> *Provide technical leadership within NIST in modern analytical and computational methods for solving scientific problems of interest to U.S. industry. The division focuses on the development and analysis of theoretical descriptions of phenomenon (mathematical modeling), the design of requisite computational methods and experiments, the transformation of methods into efficient numerical algorithms for high-performance computers, the implementation of these methods in high-quality mathematical software, and the distribution of software to NIST and industry partners.*

Within the scope of our charter, we have set the following general goals.

- Insure that sound mathematical and computational methods are applied to NIST problems.
- Improve the environment for computational science and engineering research community at large.

With these goals in mind, we have developed a technical program in five major areas.

1. Applied Mathematics
2. High Performance Computing and Visualization
3. Mathematical Software
4. Digital Library of Mathematical Functions
5. Quantum Information

The first area and second areas are accomplished primarily via collaborations with other technical units of NIST, supported by mathematical research in key areas. Projects in the third area are typically motivated by internal NIST needs, but have products, such as software, which are widely distributed. This work is also often done in conjunction with external forums whose goals are to promulgate standards and best practices. The fourth and fifth areas represent large special projects. These are being done in collaboration with other ITL Divisions, and other NIST Laboratories. Each of these is described in further detail below.

Our customers span all of the NIST Laboratories, as well as the computational science community at large. We have developed a variety of strategies to increase our effectiveness in dealing with such a wide customer base. We take advantage of leverage provided via close collaborations with other NIST units, other government agencies, and industrial organizations. We develop tools with the highest potential impact, and make online resources easily available. We provide routine consulting, as well as educational and training opportunities for NIST staff. We maintain a state-of-the-art visualization laboratory. Finally, we select areas for direct external participation that are fundamental and broadly based, especially those where measurement and standards can play an essential role in the development of new products.

Division staff maintain expertise in a wide variety of mathematical domains, including linear algebra, special functions, partial differential equations, computational geometry, Monte Carlo methods, optimization, inverse problems, and nonlinear dynamics. We also provide expertise in parallel computing, visualization, and a variety of software tools for scientific computing. Application areas in which we have been actively involved in this year include atomic physics, materials science, electromagnetics, manufacturing engineering, construction engineering, bioinformatics, and image analysis.

In addition to our direct collaborations and consulting, output of Division work includes publications in refereed journals and conference proceedings, technical reports, lectures, software packages, and Web services. In addition, MCSD staff members participate in a variety of professional activities, such as refereeing manuscripts and proposals, service on editorial boards, conference committees, and offices in professional societies. Staff members are also active in educational and outreach programs for mathematics and computer science students at all levels.

# Overview of Technical Areas

In this section we provide additional background on each of the Division's major program areas, including their impetus, general goals, and expected long-term outcomes. Details on the technical work that has been undertaken in each of these areas can be found in Part II.

## Applied Mathematics

**Impetus.** As computing resources become more plentiful there is increased emphasis on answering problems by "putting problems on the computer". Formulating the right questions, translating them into tractable computations, and analyzing the resulting output, are all mathematics-intensive operations. It is rare for a bench scientist to be expert both in their primary subject area and in the often deep and subtle questions of the mathematics that they engender. Thus, NIST needs a sustained cadre of professional mathematicians who can bring their expertise to bear on the wide variety of mathematics problems found at NIST. Often, the mathematics resulting from NIST problems is widely applicable outside, bringing added benefit to the work.

**Activities.** MCSD mathematicians engage in consulting and long-term collaboration with NIST scientists and their external customers. They also work to develop requisite mathematical technologies, including mathematical models, methods and software. The following are examples of such activities.

- Mathematical modeling of solidification processes
- Monte Carlo methods for combinatorial counting problems
- Micromagnetic modeling
- Modeling of complex material microstructures
- Modeling of high-speed machining processes
- Development and analysis of image sharpening methods
- Computational techniques in bioinformatics
- Mathematical problems in construction metrology

**Expected Outcomes.** Improved mathematical techniques and computational procedures will lead to more effective use of mathematical and computational modeling at NIST. Areas such as materials science, high-speed machining, and construction technology will see immediate improvements in methodology. Distribution of related methodology and tools will allow these benefits to accrue to the scientific community at large. Examples of the latter include (1) improved imagery from scientific instruments, and (2) improved accuracy and reliability of micromagnetic modeling software.

## High Performance Computing and Visualization

**Impetus.** The most demanding mathematical modeling and data analysis applications at NIST require resources that far exceed those routinely found on the scientist's desktop. In order to accomplish such computations in a reasonable amount of time, one must often resort to the use of parallel computers. The effective use of such high-end computers requires that computational algorithms be redesigned, often in a very fundamental way. Effecting these changes, and debugging the resulting code, requires expertise and a facility with specialized software tools that most working scientists do not possess. Hence, it is necessary to support the use of such facilities with specialized expertise and tools in these areas. Similarly, the use of sophisticated visualization equipment and techniques is necessary to adequately digest the massive amount of data that these high performance computer simulations can produce. It is not easy to become facile with the use of such tools, and hence specialized expertise in their use must also be provided. Finally, real-time interaction with massive data sets requires visualization facilities not available on the desktop, and hence the development of such facilities and tools must also be undertaken if NIST is to gain the benefits of state-of-the-art scientific visualization.

**Activities.** MCSD staff members collaborate with NIST scientists on the application of parallel computing to mathematical models of physical systems. In addition, they collaborate with NIST scientists on the application of advanced scientific visualization and data mining techniques. They develop and maintain supporting hardware and software tools, including a fully functional visualization laboratory. The following are examples of these activities.

- Grid computing
- Parallel computation of the ground state of atomic systems
- Parallel computing and visualization of the flow of suspensions
- Visualization of the molecular dynamics of shake gels
- Visible cement database
- Immersive visualization tools

**Expected Outcomes.** Working closely with NIST scientists to improve the computational performance of their models will lead to higher fidelity simulations, and more efficient use of NIST computing resources. New scientific discovery will be enabled through the insight provided by visualization and data mining. Finally, widespread dissemination of supporting techniques and tools will improve the environment for high performance computing and visualization at large.

## Mathematical Software

**Impetus.** Mathematical modeling in the sciences, engineering, and finance inevitably leads to computation. The core of computations is typically a series of well-defined recurring mathematical problems, such as the solution of a differential equation, the solution of a linear algebraic system, or the computation of a transform. Much mathematical research has focused on how to solve such problems efficiently. The most effective means of transferring this expertise to potential customers is by encapsulating it in reusable software components. Since much work at NIST relies on such computations, it has a natural interest in seeing that such components are developed, tested, and made available. The computational science community outside of NIST has similar needs. Programming methodologies and tools for developing efficient and reliable mathematical modeling codes in general, and for developing and testing reusable mathematical software components in particular, are also of interest.

**Activities.** MCSD staff members develop of mathematical algorithms and software in response to current and anticipated NIST needs. They are also involved in the development of standards for mathematical software tools, and in the widespread dissemination of research software, tools, testing artifacts, and related information to the computational science community at large. The following are examples of such activities.

- Numerical computing in Java
- The Sparse BLAS
- Template Numerical Toolkit
- Parallel adaptive multigrid methods and software
- Problem-solving environments for materials science and engineering
- Guide to Available Mathematical Software
- The Matrix Market

**Expected Outcomes.** Improved access to general-purpose mathematical software will facilitate the rapid development of science and engineering applications. In addition, the availability of community standards and testing tools will lead to improved portability, performance, and reliability of science and engineering applications.

## Digital Library of Mathematical Functions

**Impetus.** The special functions of applied mathematics are extremely useful tools in mathematical and computational modeling in a very wide variety of fields. The effective use of these tools requires access to a convenient source of information on the mathematical properties of these functions, such as series expansions, asymptotics, integral representations, relations to other functions, methods of computation, etc. For some 40 years the NBS *Handbook of Mathematical Functions* has served this purpose. However, this book is now greatly out of date. Many new properties of these functions are known, many new functions have come into widespread use, many new scientific applications have emerged, and current computational methods are completely different than those of the 1950s. Finally, today there are new and more effective means of presenting the information: online, Web-based, highly interactive, and visual.

**Activities.** The purpose of this project is to develop a freely available, online, interactive resource for information on the special functions of applied mathematics known as the Digital Library of Mathematical Functions (DLMF). With the help of some 40 outside technical experts, we are surveying the technical literature, extracting the essential properties of interest in applications, and packaging this information in the form of a reference compendium. To support the presentation of such data on the Web, we are developing semantic-based source markup, mathematics-aware search tools, indices, thesauri, and interactive Web-based visualizations.

**Expected Outcomes.** Widespread access to state-of-the-art data on the special functions will improve mathematical modeling in many areas of science, statistics, engineering, and finance. The DLMF will encourage standardization of notations and normalizations for the special functions. Users of the special functions will have an authoritative reference to cite the functions they are using, providing traceability to NIST for standardized mathematical objects.

## Quantum Information

**Impetus.** Quantum information networks have the potential of providing the only known provably secure physical channel for the transfer of information. Quantum computers have potential for speeding up previously intractable computations. Such technology remains in its infancy, having only been demonstrated in laboratory settings. A solid measurement and standards infrastructure is needed to move this into the technology development arena. ITL is supporting the work in the NIST Physics and Electronics and Electrical Engineering Laboratories to develop quantum processors, memory, and communication systems, concentrating on the critical areas of quantum computer architecture, error correction, secure protocols, algorithms, and benchmarking.

**Activities.** This project is an ITL-wide effort with participants in four Divisions. ITL is working to develop a quantum communications test bed facility for the DARPA QuIST program as part of a larger effort to develop a measurement and standards infrastructure to support quantum communications. MCSD is further supporting the NIST Quantum Information program through collaborative research with the NIST Physics Laboratory and Electronics and Electrical Engineering Laboratory related to quantum information theory. A five-year competence program award from the NIST Director's Office supports the latter work. Within MCSD we are working on issues related to novel architectures for quantum computers, the modeling of neutral atom traps as quantum processors, the benchmarking of quantum processes, and the development and analysis of quantum algorithms and protocols.

**Expected Outcomes.** We expect that the development of an open, measurement-focused test bed facility will allow a better understanding of the practical commercial potential for secure quantum communication and serve the development of standardized network protocols for this new communications technology. By working closely with staff members of the NIST Physics Laboratory, who are working to develop quantum processors, we expect that early processor designs will be more capable and useable.

# Highlights

In this section we provide examples of some of the major accomplishments of the Division over the past year. 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.

In the course of his efforts to improve scanning electron microscope imagery in use for NIST metrology, A. Carasso has developed a new, highly effective real-time image deblurring procedure capable of recovering fine details, i.e. texture, in images. The procedure is based upon a new metric for characterizing the degree of smoothness of an image. The metric determines the particular Lipschitz space in which the image lies, which can be determined by manipulating the image itself. Using singular integrals based upon this Lipschitz space information, Carasso has created an entirely new cost functional for image deblurring. Most significantly, this new cost functional has the property that its minimum can be found explicitly in the Fourier transform domain. Therefore, using fast Fourier transform algorithms, the deblurred image can be obtained directly by inverse transforming this closed form Fourier expression. This provides an enormous computational advantage over existing methods for large size images. The procedure has been demonstrated on a wide variety of image types. The smoothness metric itself may have important applications in calibrating or monitoring the performance of imaging systems. A paper describing these new methods has been accepted by the *SIAM Journal on Applied Mathematics*, and a patent application is in process.

This year saw the first release by MCSD of a major new software package for the solution to elliptic boundary-value problems on parallel computers. PHAML, developed by W. Mitchell, is the culmination of several years of research on parallel adaptive multigrid methods. Adaptive grid refinement allows the computational grid to evolve automatically, becoming finest where solution gradients are steepest. This ensures the most effective use of computational resources, enabling the solution of otherwise impossibly difficult problems. Unfortunately, both multigrid methods and adaptive methods are notoriously challenging to parallelize effectively due to complex and changing communication patterns. Mitchell has made very significant contributions to the study of such algorithms in recent years, and these are now available to the scientific community in PHAML. Mitchell has also worked closely with staff of the NIST Physics Lab to apply PHAML to solve Schrödinger's equation relevant to the study of neutral atoms confined in optical traps. Understanding the interactions of atoms corresponding to qubits of a quantum gate requires the computation of multiple eigenvalues in the middle of the spectrum, whose eigenstates have very sharp gradients, a very challenging computation. An extension of the PHAML software was successfully applied to a model of interacting Cesium atoms in a trap with a grid of 1.5 million vertices on eight processors. Mitchell gave four talk at conferences on this topic this year, two of which were invited plenary lectures, and four papers were written and submitted to refereed journals.

The modeling of neutral atom trap quantum systems is but one aspect of a newly expanded quantum information research program being undertaken by MCSD. This work was encouraged with the awarding of NIST Director's Competence Program funding at the start of FY 2003. The focus of the MCSD program is architectures and algorithms for quantum computing. The first result of this work was a description by D. Song and colleagues in the NIST Physics Lab for an architecture for lattice-based quantum computers that supports operations between distant qubits using entanglement swapping. Termed a "quantum bus,' news of the study, which appeared in *Physics Review A*, was picked up by several on-line technology information outlets. The MCSD program was strengthened further in late FY 2003 with the addition of two new researchers: Manny Knill, a senior quantum information theorist, and Stephen Bullock, an NRC postdoctoral fellow specializing in quantum circuit synthesis.

MCSD helped shape the future of classical high end computing this year through its pivotal role in the Federal High End Computing Revitalization Task Force (HECRTF). Authorized by wording in the FY 2003 Federal budget, the OSTP and OMB commissioned a government-wide study to determine the needs for high-end computing resources by government agencies. The HECRTF was asked to develop a plan for Federally sponsored high-end computing R&D, as well as plans for ensuring accessibility to high-end computing resources to meet needs of the agencies. J. Devaney of MCSD served as co-Chair of the HECRTF subcommittee on HEC Capability, Capacity, and Accessibility. The HECRTF report is expected to be released soon.

Within NIST, MCSD continued to provide leadership in the application of high performance parallel computing and visualization technologies to the solution of critical Institute problems. An illustrative example was this year's application of the MCSD immersive visualization facility to the study of "smart gels". Scientists in the NIST Chemical Science and Technology Laboratory (CSTL) are studying particular materials called shake gels. Through some as yet unknown process, these watery mixtures of clays and polymers firm up into gels when shaken, and then relax again to the liquid phase after some time has passed. S. Satterfield collaborated with C. Gonzalez of CSTL to develop immersive visualizations of the output of numerical simulations of shake gels for molecular display. The 3D visualization enabled the scientists see that it is the water's oxygen atoms, instead of the hydrogen atoms as previously thought, that attach to the clay to enable the gel processes. The striking visualizations from this project have received a great deal of notoriety, being featured in HPCwire (an online news outlet), the local Washington, DC Fox TV news outlet, as well as the NEXT @ CNN Saturday science feature on the CNN TV network.

## Staff News

MCSD welcomed a variety of new staff members this year. Dr. Emanuel Knill assumed a full-time appointment in MCSD/Boulder in late September 2003. An expert in quantum information theory, Dr. Knill will be the senior researcher on the ITL/PL Quantum Information Theory and Practice Competence project. His previous position was at the Los Alamos National Laboratory. Dr. Jeffrey Fong, who retired from MCSD in 1997, was rehired to participate in BFRL's investigation of the World Trade Center disaster. In November 2003 Dr. Florian Potra of the University of Maryland Baltimore County joined MCSD as a faculty appointee to strengthen the Division's research program in applications of mathematical optimization methods.

Two new NRC Postdoctoral Fellows began two-year appointments this year. Stephen Bullock joined MCSD in June 2003. He received a Ph.D. in mathematics from Cornell University in 2001. Most recently he held a postdoctoral appointment at the University of Michigan. At NIST he will be participating in the quantum information program, specializing in quantum circuit synthesis. A second NRC Postdoctoral Fellow, David Cotrell also joined the Division in September 2003. He recently received a Ph.D. in Mechanical Engineering from the University of Illinois at Urbana-Champaign, and will be working on flow problems in materials science with G. McFadden and colleagues in MSEL.

Two new guest researchers became associated with MCSD in 2003. Dr. Barry Bernstein of the Illinois Institute of Technology is collaborating with J. Fong on finite element analysis of structures. Dr. Sam Lomonaco of the University of Maryland Baltimore County is collaborating with MCSD's quantum computing project.

MCSD mathematician Dr. Christoph Witzgall retired from NIST after more than 30 years of government service in October 2003; he remains associated with MCSD as a guest researcher to continue his collaborations with BFRL. Peggy Liller, a group secretary with MCSD, also retired in April 2003. NRC Postdoctoral Fellow Dr. Katherine Gurski completed her appointment in January 2003; she is now a faculty member at George Washington University, retaining guest researcher status at NIST.

MCSD provided support for 12 student staff members on summer appointments during FY 2002. 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 were as follows.

| Name | Institution | Program | Mentor | Project Title |
|---|---|---|---|---|
| Eric Baer | Carnegie Mellon Univ. | Student | A. Kearsley | A method for predicting the behavior of Lagrange Multipliers in highly nonlinear problems |
| Christian Brown | Montgomery Blair H.S. | Volunteer | | Glyph Toolbox |
| Harry Bullen | Montgomery Blair H.S. | Volunteer | S. Satterfield | Glyph Toolbox |
| Joshua Chang | Montgomery Blair H.S. | Student | F. Hunt | Methods of determining model parameters when training data is sparse relative to the size of the model sample space. |
| Christopher Copeland | Vanderbilt Univ. | Student | | Nonlinear dynamics |
| Sean Kelly | Montgomery Blair H.S. | Volunteer | S. Satterfield | Glyph Toolbox |
| Elaine Kim | Stanford Univ. | Student | B. Saunders | Development of graphics and visualizations for the DLMF Project. |
| Eric Ma | Montgomery Blair H.S. | Volunteer | S. Langer | Software development for the OOF2 microstructural analysis project. |
| Shirin Mehraban | Univ. of Maryland | SURF | F. Hunt | Constructing alignments based on solving the dual linear programming problem. |
| Sheehan Olver | Univ. of Minnesota | SURF | B. Saunders | Development of graphics and visualizations for the DLMF Project. |
| Samuel Small | College of William & Mary | SURF | S. Satterfield | Glyph Toolbox |
| Robert Xiao | Montgomery Blair H.S. | Volunteer | S. Satterfield | Glyph Toolbox |

## Awards

**External.** Ronald Boisvert received the 2002 Keene State College ***Alumni Achievement Award*** at ceremonies held in Keene, NH on May 29, 2003. The award is given to "one whose professional achievement in his/her chosen field brings honor to him or herself and Keene State College." Boisvert is the 32nd recipient of the award, which has been given out yearly since 1971.


Left: NIST 2002 Bronze Medal winners Michael Donahue and Donald Porter. Right: Ronald Boisvert, winner of the 2002 Keene State College Alumni Achievement Award.

**Internal.** Michael Donahue and Donald Porter of MCSD, along with Robert McMichael of the NIST Materials Science and Engineering Laboratory, received the NIST ***Bronze Medal*** in December 2002 for scientific and engineering achievement in the advancement of computational techniques for simulating the behavior of micromagnetic materials. According to the citation, they "demonstrated exemplary initiative and creativity in pioneering the development of frameworks and tools for the intercomparison of micromagnetic modeling software". The citation goes on to say, "By fostering new levels of reliability for predictive models, this work is eliminating a critical barrier to the development of a new generation of magnetic devices that operate at a submicron scale".


Left: NIST Fellow Geoffrey McFadden. Right: Isabel Beichl, winner of the 2003 Outstanding Contribution to ITL Award.

Geoffrey McFadden of MCSD has been elevated to the position of ***NIST Fellow***. He was recognized for his prolific and high impact collaborative research in the mathematics of materials science, especially for his contributions to the theory of phase transitions. NIST Fellow status is conferred on less than 1% of NIST staff.

Isabel Beichl was the winner of the 2003 ***Outstanding Contribution to ITL Award***. Beichl was cited for her initiative and dedication in the development and operation of the ITL Student Undergraduate Research Fellowship (SURF) program.

## Technology Transfer

MCSD staff members continue to be active in publishing the results of their research. This year 47 publications authored by Division staff appeared, 32 in refereed journals. Twenty-five additional papers have been accepted and are awaiting publication. Another 33 are under review. MCSD staff members were invited to give 31 lectures in a variety of venues and contributed another 26 talks to conferences and workshops. The Division lecture series remained very active, with 28 talks presented (nine by MCSD staff members); all were open to NIST staff.

MCSD staff members also organize workshops, minisymposia, and conferences to provide forums to interact with external customers. This year, staff members were involved in organizing 13 external events. Among these are the ACM Java Grande ISCOPE Conference, the Hysteresis and Micromagnetic Modeling 2003 Symposium, the Blackwell-Tapia Award Conference, and the SIAM National Meeting.

Software continues to be a by-product of Division work, and the reuse of such software within NIST and externally provides a means to make staff expertise widely available. The package PHAML, a parallel adaptive multigrid solver for elliptic boundary value problems had its initial public release. It is a Fortran 90 package utilizing MPI and OpenGL graphics. Several existing MCSD software packages saw new releases this year, including OOMMF (a problem-solving environment for micromagnetic modeling) and TNT (Template Numerical Toolkit for numerical linear algebra in C). Many of our software packages experience substantial downloads. During the past 12 months, for example, OOMMF was downloaded 2,000 times. OOF, our object-oriented finite element system for the modeling of materials with complex microstructures, was downloaded some 2,300 times. JAMA, the Java linear algebra package that we developed with the MathWorks registered 4,500 downloads, while TNT saw more than 10,000 downloads.

Web resources developed by MCSD continue to be among the most popular at NIST. The MCSD Web server at math.nist.gov has serviced more than 50 million Web hits since its inception in 1994 as NIST's first Web server. 12 million of these hits occurred in the past year. The Division server regularly handles more than 10,000 requests for pages each day, serving more than 43,000 distinct hosts on a monthly basis. Altavista has identified more than 8,500 external Web links to the Division. Seven MCSD sites are listed among ITL's top 10:

1. NIST Math Portal, http://math.nist.gov/
2. Matrix Market, http://math.nist.gov/MatrixMarket/
3. Guide to Available Mathematical Software: http://gams.nist.gov/
4. Division home page: http://math.nist.gov/mcsd/
5. ACM Transactions on Mathematical Software: http://math.nist.gov/toms/
6. Digital Library of Mathematical Functions: http://dlmf.nist.gov/
7. Template Numerical Toolkit: http://math.nist.gov/tnt/

## Professional Activities

Division staff members continue to make significant contributions to their disciplines through a variety of professional activities. R. Boisvert serves as Chair of the International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software). He also serves as Vice-Chair of the ACM Publications Board. D. Porter serves on the Tcl Core Team, which manages the development of the Tcl scripting language. D. Lozier serves as chair of the SIAM Special Interest Group on Orthogonal Polynomials and Special Functions.

Division staff members serve on journal editorial boards of nine journals: *ACM Transactions on Mathematical Software* (R. Boisvert and R. Pozo), *Computing in Science & Engineering* (I. Beichl), *IEEE Transactions on Information Science* (E. Knill), *Interfaces and Free Boundaries* (G. McFadden), *Journal of Computational Methods in Science and Engineering* (M. Donahue), *Journal of Crystal Growth* (G. McFadden), *Journal of Numerical Analysis and Computational Mathematics* (I. Beichl and W. Mitchell), *Mathematics of Computation* (D. Lozier), *SIAM Journal of Applied Mathematics* (G. McFadden), *SIAM Journal of Scientific Computing* (B. Alpert).

Division staff members also work with a variety of external working groups. R. Boisvert and Roldan Pozo chair the Numerics Working Group of the Java Grande Forum. R. Pozo chairs the Sparse Subcommittee of the BLAS Technical Forum. M. Donahue and D. Porter are members of the Steering Committee of muMag, the Micromagnetic Modeling Activity Group.