

Part I

# Overview



## **Introduction**

The mission of the Mathematical and Computational Sciences Division (MCSD) is to provide technical leadership within NIST in modern analytical and computational methods for solving scientific problems of interest to U.S. industry. Within the scope of our charter, we have set the following general goals.

- Enable scientific discovery and world-class metrology within the NIST Laboratories via the development and application of advanced mathematical and computational methods.
- Improve the environment for the computational science and engineering research community at large, with an emphasis on IT metrology.

With these goals in mind, we have developed a technical program in three broad areas.

1. Applied Mathematics
2. High Performance Computing and Visualization
3. Mathematical Software

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 in the computational sciences and engineering. In addition to these broad areas, we have identified two special focus areas.

4. Digital Library of Mathematical Functions
5. Quantum Information

These are being done in collaboration with other ITL Divisions, and other NIST Laboratories. The first is a large effort to construct a Web-based information base on the special functions of applied mathematics. The second is a special area of NIST-wide interest that we are growing.

Division 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 external organizations. We develop tools with the highest potential impact, and make resources easily available online. We provide consulting, as well as educational and training opportunities for NIST staff. We maintain a state-of-the-art scientific 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, nonlinear dynamics, and mathematical physics. We also provide expertise in parallel computing and scientific visualization and analysis. Application areas in which we have been actively involved 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. MCSD staff members also 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.

## **Technical Approach**

In this section we broadly characterize what the Division does based on the type of customer and the time horizon associated with the work.

### **Information Science Research**

ITL engages in a variety of mission-oriented research projects in the general area of information science. Such work is aimed at pushing the frontiers of science in anticipation of future needs of NIST measurement science programs. Such projects have time horizons in the range of 3-10 years.

**Strategic Drivers.** Within MCSD our efforts in information science are driven by future needs of NIST in mathematical and computational methods. As in most research organizations, there continues to be a growing use of modeling and simulation throughout the NIST Laboratories. In the long term, we foresee potential widespread use of virtual measurement systems transforming NIST metrology programs. Such systems determine physical property data by experimentally validated mathematical modeling and computational simulation systems. Finally, NIST's strategic focus areas of biosystems, nanotechnology, and public safety each provide new challenges for the mathematical and computational sciences.

**Goals.** ITL's principal goal in this area is to advance information science to enable metrology for future information systems as well as to enable overall NIST science and technology goals. Within MCSD our role is primarily to develop new and effective mathematical and computational techniques which anticipate needs of the NIST Laboratories. A particular strategic emphasis is the development of capabilities for modeling and simulation in nanotechnology, biosystems, and public safety. A important facet of NIST's nanotechnology program is its research in quantum information, and hence we are working to develop a world-class capability in quantum information theory.

**Example Projects.** The research in information science described in this report includes the development of

- Monte Carlo methods for estimating the solution to combinatorial counting problems
- Deconvolution methods, with application to blind image deblurring
- Optimization methods for problems with special structure, and problems with noisy data
- Methods of systems identification and parameter estimation
- Time-domain methods for electromagnetic modeling
- Computational techniques for bioinformatics-based data mining
- The Hy-CI method for the computation of atomic properties
- Architectures for quantum computers
- Methods for the synthesis of quantum circuits for arbitrary unitary operators
- Benchmarks for quantum information processing in ion trap and optical systems

### **Information Technology Research**

ITL engages in a wide spectrum of research and development of techniques and tools enabling metrology and standards with application in a time frame of roughly one to three years. Within MCSD, this work includes collaborative research with other NIST Laboratories to develop and apply mathematical and computational methods for problems associated with the development of measurements and standards in a wide variety of application domains. This work also includes the development of particular software tools for the solution of mathematical problems.

**Strategic Drivers.** The information technology research of MCSD is driven by the needs of NIST scientists and engineers to understand physical systems to enable the development of measurement

techniques and related instrumentation. Interdisciplinary research is becoming critical to the development of complex modern measurements systems, and the expertise in applied mathematics and scientific computing is a key ingredient. Modeling and simulation is increasingly critical in this regard. Such virtual laboratory technologies facilitate the understanding of physical systems necessary to the development of instrumentation. There is also a growing need to process and gain insight from large volumes of data, both from high-speed (combinatorial) experimental methods and from computer simulations. As theory and modeling become more sophisticated *virtual* measurement systems based primarily on computational simulation may ultimately emerge.

**Goals.** For MCSD, our overall goal in this area is to facilitate measurement technology development through applied research in the mathematical and computational sciences. We seek to accomplish this by engaging in peer-to-peer collaboration with NIST scientists and engineers in critical NIST programs, and by developing unique software tools that enable scientific discovery and technology development within NIST. As part of this latter goal, we work to develop state-of-the-art virtual laboratory technology.

**Example Projects.** The information technology research undertaken by MCSD includes the following collaborative work with other NIST Laboratories.

- Development and processing of models of physical objects from LADAR data to enable automation of construction sites (with BFRL)
- Computational modeling of the flow of concrete (with BFRL)
- Analysis of device response for high-speed waveform metrology (with EEEL)
- Modeling of resonant optical scattering by nanoscale periodic structures (with EEEL)
- Modeling and simulation of body armor and frangible bullets (with MEL)
- Optimization problems in smart machining systems (with MEL)
- Deconvolution of images from scanning electron microscopes (with MEL)
- Modeling of solidification processes in metals (with MSEL)
- Analysis of data from mass spectrographs (with MSEL)
- 3D chemical imaging at the nanoscale (with CSTL)
- Simulation and visualization of nanostructures and nano-optics (with PL)

In addition, MCSD's information technology research includes the development of the following computational science tools.

- OOF: a problem-solving environment for the modeling materials with complex microstructure
- OOMMF: a problem-solving framework for micromagnetic modeling
- PHAML: parallel adaptive multigrid methods and software for partial differential equations
- TNT: a toolkit for numerical computing based on C++ templates
- Screen Saver Science: a virtual computing environment based on Java and Jini
- Immersive visualization laboratory and software environment for visualization and analysis

## Technology Transition

This area includes all of the tests and evaluations, reference models and architectures required to effectively transition IT research products to mature technology products in the context of their applications.

**Strategic Drivers.** Many of the software tools developed by MCSD for use at NIST have widespread application externally. Thus, there is an excellent opportunity to transition NIST work to improve the environment for computational science at large. As computational science grows externally to NIST there is emerging a critical need for techniques of assessing the accuracy and reliability of modeling

and simulation tools and their underlying mathematical software components. Development and transition of measurement technologies of this sort is a typical role for NIST. Issues of portability and interoperability of scientific software and mathematical data are also emerging as critical in the external community, additional issues that a neutral party such as NIST can play a critical role.

**Goals.** ITL's goal in this arena is the transition of information technology innovations to applications through the development of information services, test sets, and automation tools. Within MCSD we aim to develop tools to assess the quality of mathematical modeling tools and mathematical software components. We seek to work with external groups to develop ad hoc standards for computational science tools and mathematical data to improve their portability and interoperability. Finally, we distribute software, test suites, and mathematical reference data to the public.

**Example Projects.** Technology transition projects within MCSD include the following.

- Guide to Available Mathematical Software
- Interoperable Message Passing Interface
- Reference implementation of the Sparse Basic Linear Algebra Subprograms standard
- SciMark benchmark for scientific computing in Java
- Matrix Market: test data sets for sparse linear algebra
- Benchmark problems and reference software for micromagnetic modeling
- Strong-sense benchmarks for verification of computer models for high consequence engineering systems
- Techniques and tools for semantic-based exchange of mathematical data

## Technology Insertion

Technology insertion is the process by which new technologies are adopted at large, becoming part of new and unique applications. This is the end of the spectrum closest to the user, and is work with potential immediate payoff.

**Strategic Drivers.** For MCSD our work in technology insertion is driven by needs of particular external communities. For example, there is a growing need for standardized mathematical reference data traceable to NIST. In addition, we respond to specific needs of other government agencies in areas in which we have unique expertise.

**Goals.** ITL enables the insertion of mature information technology into new application areas through the development of measurements, standards, and guidance. For example, MCSD works to generate and distribute mathematical reference data for the special functions of applied mathematics. In addition, we collaborate with other Federal agencies to apply NIST-developed technologies into mission-critical applications as requested.

**Example Projects.**

- Automated Raman and MALDI spectral searching for homeland security applications (FBI)
- Virtual Cement and Concrete Testing Laboratory (with BFRL)
- Device independent interaction framework for immersive scientific visualization (SBIR)
- Digital Library of Mathematical Functions

## **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.

Late 2004 marked the beta release of OOF2. The OOF Project, a collaboration between MCSD, MSEL's Ceramics Division and the Center for Theoretical and Computational Materials Science, and MIT, is developing software tools for analyzing real material microstructure. The microstructure of a material is the (usually) complex ensemble of polycrystalline grains, second phases, cracks, pores, and other features occurring on length scales large compared to atomic sizes. The goal of OOF is to use data from a micrograph of a real material to compute the macroscopic behavior of the material via finite element analysis. Originally released in 1999, OOF is intended to be a general tool, applicable to a wide variety of microstructures in a wide variety of physical situations, and has developed a substantial user base. OOF2 is a completely new version of the program, designed to be much more powerful and flexible than the original. The first release of OOF2 solves linear elasticity and thermal conductivity problems, but its new infrastructure allows it to be easily extended to a wide variety of other problems, such as chemical diffusion and reactions, piezoelectricity, and nonlinear effects. Stephen Langer of MCSD leads the project in collaboration with the NIST Center for Theory and Computation in Materials Science and MIT.

The Object-Oriented Micromagnetic Modeling Framework (OOMMF), developed by Michael Donahue and Donald Porter of MCSD, is another example of a very successful NIST problem-solving environment. OOMMF is an open, well-documented environment in which algorithms can be evaluated on benchmark problems by the micromagnetics research community. OOMMF also provides a fully functional micromagnetic modeling system, handling both two and three-dimensional problems, with sophisticated extensible input and output mechanisms. OOMMF has become an invaluable tool in the magnetics research community. In fiscal year 2004 alone, the software was downloaded more than 2,400 times, and use of OOMMF was acknowledged in more than 40 peer-reviewed journal articles. OOMMF is currently being extended to permit thermal modeling. Such capabilities are critical in the development of high sensitivity low field magnetic sensors, where performance is generally limited by thermal noise. This is the subject of a current NIST Competence project being undertaken jointly with EEEL.

MCSD computer scientists have developed powerful new techniques for the fusion and display of multiple sets of volumetric data from scientific instruments for display and exploration in an immersive environment. MCSD's Scientific Applications and Visualization Group is working with collaborators in MSEL who are gathering measured data using a variety of techniques, including optical coherence tomography and confocal fluorescence imaging. These measurement techniques provide multiple types of information on a sample, both structural and functional. When combined in a manner that is visually apparent, this can yield unprecedented insight towards the comprehension of complex relationships among large amounts of correlated data. MCSD's John Hagedorn, John Kelso, Adele Peskin, and Steve Satterfield have developed powerful new interactive visualization techniques for such data, which they have applied to the example of cell growth on polymer scaffolds. Measurement and visualization techniques of this type are expected to significantly accelerate the search for materials appropriate for tissue engineering applications.

MCSD is playing a key role in the development of a series of experimental benchmarks for quantum information processing. During 2004, Manny Knill of MCSD worked closely with David Wineland's group of PL in Boulder to realize two such benchmarks in ion trap systems. The first was

the first demonstration of quantum teleportation in an atomic system, which was described in the paper “Deterministic Quantum Teleportation of Atomic Qubits” which appeared in *Nature* on June 17. The second was a demonstration of error correction in an ion trap system. This was described in the paper “Realization of Quantum Error Correction” which appeared in the December 2, 2004 issue of *Nature*. Both accomplishments were widely noted in the press.

An MCSD mathematician has solved a key outstanding problem in the area of quantum circuit synthesis. This is the process by which an arbitrary quantum computation is mapped onto a collection of elementary operations (gates), resulting in a quantum circuit diagram. The problem, which is analogous to a classical problem in circuit design, has previously seen several solutions, but the new solution produces the smallest number of gates to date. Working with colleagues at the University of Michigan, Stephen Bullock of MCSD developed a new universal quantum circuit capable of implementing any unitary operator (mathematically, all quantum computations may be represented as operators of this type). The circuit has a top-down structure that concentrates components on the less significant qubits. The underlying algorithm, which is based on the so-called CS matrix decomposition, may be efficiently implemented using standard matrix analysis software. A theoretical analysis shows that the universal circuit is nearly optimal, that is, the number of gates for any given computation may be improved by at most a factor of two. It is the first to use fewer entangling gates than there are degrees of freedom in the matrix. The circuit adapts well to quantum computer architectures in which only nearest-neighbor interactions are possible, such as neutral atom or ion traps.

MCSD played a pivotal role in a recently released interagency report outlining a five-year plan for Federal investment in high end computing technologies. *The Federal Plan for High-End Computing*, which was released on May 10, 2004, lays out a five-year plan to improve how the Federal government fosters and exploits computing technologies for the nation’s most demanding computational problems. The report was developed by the High End Computing Revitalization Task Force (HECRTF), which was established by the Office of Science and Technology Policy under the auspices of the National Science and Technology Council. Participants included DoD (DARPA, ODUST (S&T), HPC Modernization Program, NSA), DOE (NNSA and Office of Science), EPA, NASA, NIH, NIST, NOAA, NSF, OMB, and OSTP. Judith Devaney of MCSD was a member of the core team that developed the report, serving as co-Chair of the HECRTF subcommittee on HEC Capability, Capacity, and Accessibility. The plan recommends (a) a coordinated, sustained research program over 10-15 years to overcome major technology barriers that limit effective use of high-end computer systems, (b) the creation of “leadership systems”, high capability computers that would enable U.S. scientists to solve challenging, high payoff, previously unsolvable problems, (c) a collaborative strategy to improve access to high end computers, and (d) improvement to the Federal procurement process for high end computing resources.

MCSD hosted a workshop on the Changing Face of Mathematical Software at George Washington University on June 3-4, 2004. The meeting provided a forum for commercial software vendors and academic and government researchers to discuss issues regarding the development, packaging, and dissemination of modern mathematical software libraries and systems. The workshop had 26 participants from six countries. Speakers included Brian Ford (NAG Ltd.), Tony Drummond (Lawrence Berkeley Laboratory), Wayne Enright (University of Toronto), Ian Gladwell (Southern Methodist University), Mo Mu (Hong Kong University of Science & Technology), Pete Stewart (University of Maryland), Abdou Youssef (George Washington University), as well as Michael Donahue, Stephen Langer, Bruce Miller, and Roldan Pozo of MCSD. The meeting was one of a yearly series of topical workshops sponsored by the International Federation for Information Processing’s (IFIP) Working Group 2.5 (WG 2.5). Chartered by UNESCO in 1961, IFIP is a multinational federation of professional and technical organizations fostering international cooperation in the field of information processing. Affiliated with IFIP’s Technical Committee 2 on Software Theory and Practice, WG 2.5 works to improve the quality of numerical computation by promoting the development and availability of sound numerical software. The group meets yearly to



exchange technical information and to plan joint projects. This year's meeting took place on June 1-2 at GWU. Ronald Boisvert of MCSD, who is the current Chair of IFIP WG 2.5, was the local organizer for the meeting and workshop. Further details can be found at the workshop website<sup>1</sup>.

## Staff News

MCSD welcomed a variety of new staff members this year. In November 2003 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. Scott Glancy joined the MCSD Boulder staff in September 2004 as an NRC Postdoctoral Fellow. A recent Ph.D. in Physics from the University of Notre Dame, Glancy will work with Manny Knill on the study of linear optics quantum computing.

Several new guest researchers also became associated with MCSD in 2004. Anoka Yimsiriwattana, a computer scientist from the University of Maryland Baltimore County is collaborating with MCSD's quantum computing project. Eduardo Martinez-Vecino of the University of Salamanca, Spain, spent two months visiting MCSD in 2004 where he studies discretization effects in modeling of thermal behavior of micromagnetic systems.

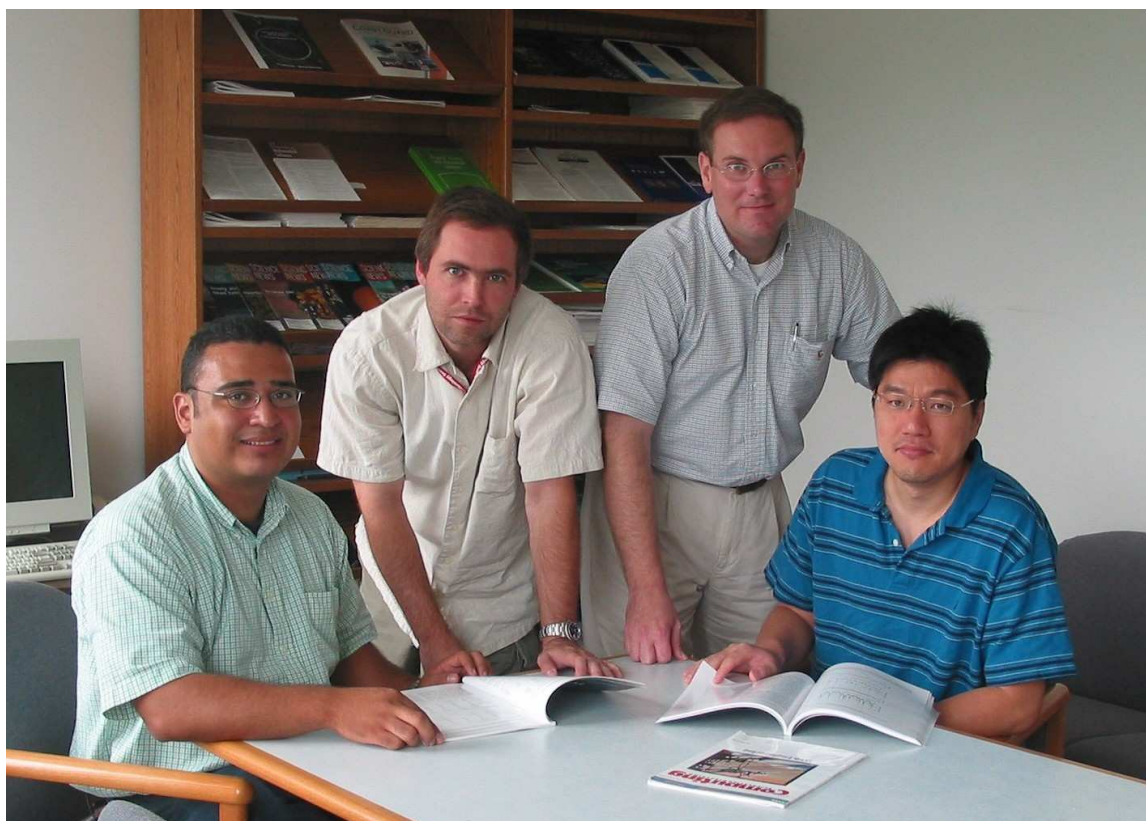
Two NRC Postdoctoral Fellows completed their tenure at MCSD in 2004. Luis Melara, who worked on materials modeling problems, took a position in the Mathematics Department at Colorado College. David (Daegene) Song, who works in quantum information theory, continues as a NIST guest researcher.

Friends and colleagues of Christoph Witzgall gathered at NIST on May 13, 2004 for a one-day symposium to celebrate his career-long contributions to the field of operations research. Witzgall retired from NIST in October 2003 after more than 30 years of Federal service. He was most recently a staff member of the ITL Mathematical and Computational Sciences Division, where he remains as a guest researcher. Twelve technical talks were presented at the symposium, which was entitled *Topics in Operations Research*. The talks spanned many of the areas in which Witzgall has made important contributions, including linear and quadratic programming, surface fitting, and computational geometry. Applications were described from areas as diverse as the optimal placement of facilities (e.g. post offices and fire stations), the routing of phone calls, the distribution of products to retail stores, and the determination of the sources of contaminants in buildings. Speaking at the symposium were Paul Boggs (Sandia National Laboratories), Jack Edmonds (University of Waterloo), Saul Gass (University of Maryland), Alan Goldman (Johns Hopkins University), Karla Hoffman (George Mason University), James Lawrence (George Mason University), Douglas Shier (Clemson University), Josef Stoer (Universitaet Wuerzburg), William Stone (NIST BFRL), and Francis Sullivan (Institute for Defense Analysis Center for Computing Sciences). A special issue of the *Journal of Research of NIST* will be devoted to proceedings of the workshop.



Christoph Witzgall of MCSD and Josef Stoer of Universitaet Wuerzburg

<sup>1</sup> <http://math.nist.gov/workshops/wg25-2004/>



MCS D actively participates in the NIST Postdoctoral Fellows Program administered by the National Research Council. Pictured above are four young researchers who participated in the program during FY 2004. (From left to right) Luis Melara and David Cotrell performed research in the area of mathematical modeling in materials science, while Stephen Bullock and Daegene Song did research in quantum information theory.



MCS D hosted five students in NIST's Summer Undergraduate Research Fellowship program in 2004. Pictured above are Angel Villalain-Garcia (*left*) of the University of Puerto Rico and Whitney Austin (*right*) of Jackson State University.

MCSD provided support for 10 student staff members on summer appointments during FY 2004. 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.

<b>Name</b>	<b>Institution</b>	<b>Program</b>	<b>Mentor</b>	<b>Project Title</b>
Whitney Austin	Jackson State University	SURF	S. Satterfield, J. Hagedorn	Tracker calibration for immersive visualization
Eric Baer	Carnegie Mellon University	Student	A. Kearsley	Computer programming
Shauntia Burley	Coppin State College	SURF	B. Saunders	Algorithms and software for interactive 3D graphics
Christopher Copeland	Vanderbilt University	Student	D. Gilsinn	Mathematical problems in construction metrology
Angel Villalain-Garcia	University of Puerto Rico	SURF	W. George	Authentication and authorization in a distributed compute server
Michael Huber	American University	SURF	B. Saunders	Algorithms and software for interactive 3D graphics
Elaine Kim	Stanford University	Student	B. Saunders	Graphics for DLMF Project.
Eric Ma	Montgomery Blair High School	Volunteer	S. Langer	Software development for the OOF2 microstructural analysis project.
Brandon Smith	University of Nebraska	SURF	A. Peskin	SAVG file tools.
Gaurav Thakur	The Learning Community International School	Volunteer	D. Lozier	Generalizations of the gamma function.

SURF: Summer Undergraduate Research Fellowship



## Awards



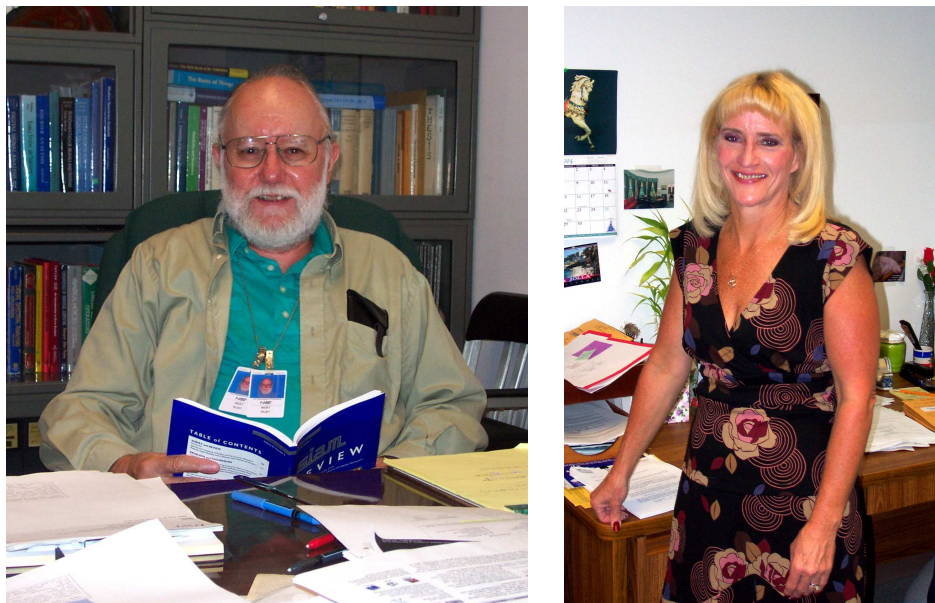
*Left:* Timothy Burns (center) with Debasis Basak and Richard Rhorer (MEL) in the NIST Kolsky Bar Lab. Burns and Rhorer were co-winners of the 2004 Allen V. Astin Measurement Science Award. *Right:* NIST Fellow Geoffrey McFadden.

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; McFadden is currently the only NIST Fellow from ITL.

Timothy Burns was one of a team of seven from MEL, MSEL, PL, and ITL to be awarded the 2004 *Allen V. Astin Measurement Science Award*. The Astin award is granted for outstanding achievement in the advancement of measurement science or in the delivery of measurement services. The team was cited for outstanding advancements in measurement science for dynamic material properties, leading to first ever measurement of the stress-strain relationship of a material under high strain-rate and heating-rate conditions prior to temperature-induced transformation.

G.W. (Pete) Stewart, an MCSD faculty appointee, has been elected to the *National Academy of Engineering*. Stewart is a Professor of Computer Science at the University of Maryland at College Park, as well as a Professor of the Institute for Advanced Computer Studies (UMIACS). Stewart was cited for development of numerical algorithms and software widely used in engineering computation. In particular, he is well known as an expert in algorithms and perturbation theory for matrix computation. His books on this subject have become standards in the classroom. He is one of the authors of the software package LINPACK, which helped transform the field of mathematical software into a discipline akin to engineering, and which spurred an explosion of mathematical software development in the 1980s. Stewart has been associated with NIST for nearly 25 years, passing on his expertise by teaching shortcourses here, consulting with NIST staff, and participating in the development of fundamental math software components.

MCSD staff captured two of the three annual ITL Awards for 2004. Bert Rust received the *ITL Outstanding Authorship Award* for a series of tutorial articles on data fitting published in *Computing in Science and Engineering*. Robin Bickel received the *ITL Outstanding Support Award* for outstanding initiative and dedication in the reorganization of the MCSD office functions, leading to substantial cost savings.



Two of three yearly ITL awards were won by MCSD staff in 2004. Bert Rust (*left*) won the Outstanding Authorship Award, while Robin Bickel (*right*) won the Outstanding Support Award.

## Technology Transfer

MCSD staff members continue to be active in publishing the results of their research. This year 53 publications authored by Division staff appeared, 43 in refereed journals. Thirteen additional papers have been accepted and are awaiting publication. Another 35 are under review. MCSD staff members were invited to give 53 lectures in a variety of venues and contributed another 31 talks in conferences and workshops. The Division lecture series remained very active, with 25 talks presented (six 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 12 such events. Among these were minisymposia at the SIAM Annual Meeting, the SIAM Image Science Conference, and the Joint Mathematics Meetings. MCSD hosted three local symposia in 2004, a Symposium on Topics in Operations Research (May 2004), a Workshop on the Changing Face of Mathematical Software (June 2004), and a Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems, each with approximately 40 attendees.

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. Several existing MCSD software packages saw new releases this year, including OOMMF (a problem-solving environment for micromagnetic modeling), TNT (Template Numerical Toolkit for numerical linear algebra in C), and OOF (a problem-solving environment for modeling of materials with complex microstructure). Many of our software packages experience substantial downloads. During the past 12 months, for example, OOMMF was downloaded 2,400 times. JAMA, the Java linear algebra package that we developed with the MathWorks registered 9,000 downloads, while TNT saw more than 10,500 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 80 million Web hits since its inception in 1994 as NIST's first Web server. More than 25 million of these hits occurred in the past year. The

Division server regularly handles more than 16,000 requests for pages each day, serving more than 55,000 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 was recently named Co-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. Fern Hunt serves on the Executive Committee of the Association for Women in Mathematics.

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).

During 2004 MCSD staff members served on technical review panels for Morgan State University, the IDA Center for Computing Sciences, as well as referees for some 35 journals and five funding agencies.