Part I

Overview

Introduction

The Mathematical and Computational Sciences Division (MCSD) of NIST's Information Technology Laboratory (ITL) provides leadership within NIST in the solution to mathematical and computational problems arising from the NIST measurement science program. In doing so, we seek to ensure that the best mathematical and computational methods are applied to the most critical problems at NIST, and, through appropriate technology transfer efforts, to improve the environment for computational science and engineering at large. To accomplish these goals, MCSD staff members engage in the following general activities.

- Peer-to-peer collaboration with NIST scientists and engineers in a wide variety of critical applications.
- Development of unique general-purpose mathematical and computational tools.
- Research in targeted areas of applied mathematics and computer science of high relevance to future NIST programs.

The technical work of the Division is organized into seven general areas. In each case we indicate overall goals and approach.

Mathematical Knowledge Management.

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 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.

High Performance Computing.

Goals: Improve the quality and rate of scientific discovery through the 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.

Virtual Measurement Laboratory.

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 virtual laboratories. Collaborate with NIST scientists in the application of high performance visualization to high priority NIST projects

Mathematical Modeling of Mechanical Systems and Processes.

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.

Mathematical Modeling of Electromagnetic Systems.

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 .

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 and acoustic modeling through the use of benchmarks (challenge problems) and reference software. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

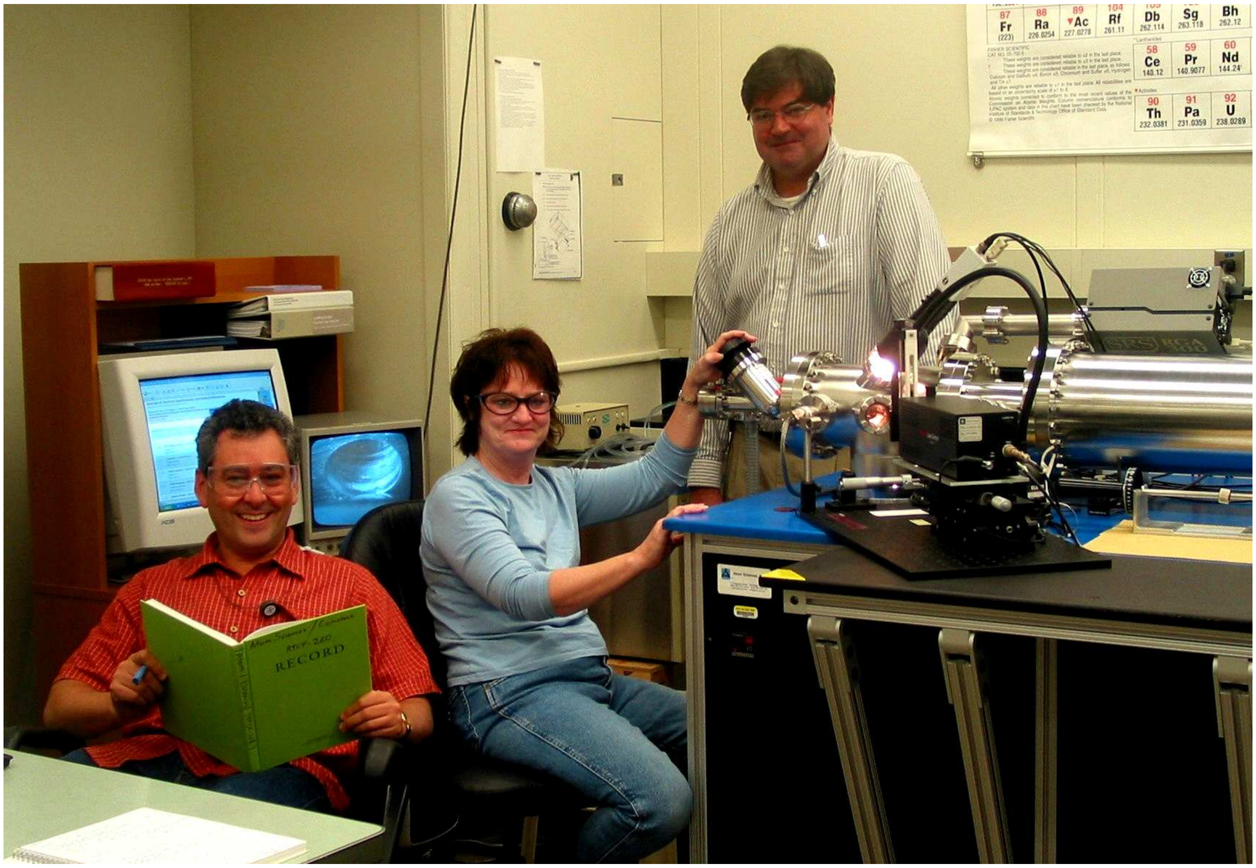
Mathematics of Metrology.

Goals: Develop effective methods for the solution to 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 techniques and tools enabling virtual measurement of chemical and material properties from first principles. Collaborate with NIST scientists to apply mathematical techniques to problems of measurement science. Galvanize interest within the applied and computational mathematics community for the study of problems occurring in measurement science.

Several crosscutting themes have emerged in the Division technical program. 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, models for studying the stability of nanowires, and parallel computing methods for models of optical properties of nanostructures.

Related to this is the growing Division portfolio related to ***quantum information***. Division staff members are collaborating closely with the NIST Physics Lab and Electronics and Electrical Engineering Lab to demonstrate the information processing capabilities of physical systems, including both ion traps and optical systems. We are developing architectural concepts for quantum information systems, including error control strategies promoting fault-tolerance. Finally, we are developing numerical methods enabling the solution of the Schrödinger equation for modeling the quantum states of neutral atoms for use as qubits.



Anthony J. Kearsley (left) is working with MSEL technician Kathleen M. Flynn and MSEL materials scientist William E. Wallace (right) to find optimal instrument parameters for using time-of-flight mass spectrometers. This will enable the development of an absolute molecular mass distribution polymer standard reference material. Kearsley has pioneered the use of robust mathematical optimization procedures to a variety of measurement science problems characterized by noisy data.

A third 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. For example, our OOF software for the finite element analysis of materials with complex microstructure enables analyses based on micrographs of real material samples, and hence is useful in manufacturing quality control applications. 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; we are working to develop such methodologies in collaboration with NIST scientists. Finally, we are also beginning the development of technologies to enable accurate interactive measurements during the analysis of data in immersive visualization environments. These tools have already seen application in the evaluation of prototype standard polymer scaffolds for the growth of human tissue.

Visualization techniques provide an important means for scientists to make sense of large volumes of scientific data, whether obtained for physical experimentation or computer simulation. Such ***data-intensive modeling and analysis*** is another recurring theme in our work. 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.

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.

A full-scale quantum computer could produce reliable results even if its components performed no better than today's best first-generation prototypes, according to a paper in the March 3 issue in the journal *Nature* by Manny Knill of MCSD. In that paper, entitled “Quantum Computing with Realistically Noisy Devices,” Knill proposes a fault-tolerant architecture based on hierarchies of qubits and quantum teleportation. Use of such architecture could lead to reliable computing even if individual logic operations (“gates”) made errors as often as 3 percent of the time -- performance levels already achieved in NIST Physics Laboratory experiments with ion traps, for example. The proposed architecture could tolerate error rates several hundred times higher than scientists previously thought necessary. As such, this work significantly lowers the bar for experimentalists striving to demonstrate feasibility of quantum computation in various physical systems. Knill’s work also shows that there is a tradeoff between resource requirements (i.e., overhead) and gate fidelity. At a 3 percent probability of error per gate (EPG) resource requirements are substantial, though at 1 percent EPG effective quantum computation seems feasible with resources comparable to the digital resources available in today's computers.

We are also working with the NIST Physics Lab to study the feasibility of a quantum computer based on extremely cold neutral alkali-metal atoms. In this system, qubits are implemented as motional states of an atom trapped in a single well of an optical lattice. Two-qubit quantum gates are constructed by bringing two adjacent atoms together in a single well leaving the interaction between them to produce the action of the desired gate. Quantifying the interaction in this system reduces to solving for selected eigenfunctions of a Schrödinger equation that contains a Laplacian, a trapping potential, and a short-range interaction potential. Solving for these eigenfunctions is computationally challenging due to the large variations in the functions over very small portions of the domain due to the trapping potential. For a typical problem of interest involving Cesium atoms, a uniform linear finite element grid would require at least 10^{17} elements to obtain three digits of accuracy, a computationally infeasible problem.

William Mitchell of MCSD has recently extended his parallel hierarchical-basis adaptive multigrid solver, PHAML, to solve problems of this type. Applying adaptivity and multigrid to the Cesium model required only 4.5 million degrees of freedom, and a solution was obtained in 35 minutes on a 32-processor computer cluster. This year Mitchell further extended PHAML to use high-order elements. Using cubic elements, the same accuracy is obtained with 0.5 million degrees of freedom in 8 minutes on a laptop computer. Nevertheless, much higher accuracy is required for realistic models. Using 5th degree elements and resources comparable to the linear case, Mitchell and his colleagues in the Physics Lab have obtained solutions accurate to 8 digits. We anticipate that the addition of hp-adaptivity will further reduce the solution time to the point where we can perform experiments with the multi-channel time-dependent equations that are required for realistic models of quantum gates.

Alfred Carasso achieved remarkable results this year in applying his deconvolution methods to the blind sharpening of color imagery. The need to identify the distinct point spread function associated with each color component (this is the "blind part") is quite challenging here. Avoiding *unbalanced* blind sharpening of individual color components is also necessary. Conceivably, after a long and uncertain iterative process, the reconstituted image may turn out to exhibit physically false colors, such as a green sky, or a purple sea. In Carasso's APEX method, deblurring is accomplished by marching backwards in time in a diffusion equation, (the SECB method, also developed at NIST), providing the opportunity significant control over the deconvolution process, enabling processing of 1024×1024 color imagery in near real-time. The strategy of applying the APEX method to each color component separately while enforcing L^1 norm conservation in each was found to be sufficient to maintain the balance of colors in the reconstructed image in all examples examined. Some particularly striking enhancements of recent Hubble space telescope imagery has been obtained, for example.

James Sims of MCSD, working with Stanley Hagstrom of Indiana University, has achieved record levels of accuracy in the development of computational methods for the virtual measurement of fundamental properties of molecules. Their recent result for the ground state of dihydrogen (H_2) represents the highest level of accuracy ever reached (10^{-12} hartree) in molecular quantum computations (except for trivial one-electron cases). Such quantum mechanical calculations have now yielded more accurate determinations of this fundamental property than can be measured experimentally. In an article recently accepted by the *Journal of Chemical Physics*, Sims and Hagstrom discuss how these best calculations to date were accomplished. Multiple precision computation and parallel computing were critical to obtaining these results. While most results were obtained using quadruple precision floating point arithmetic, critical portions of the computation subject to catastrophic cancellation required up to 160 decimal digits. The authors solved the secular equation using their own portable parallel inverse iteration eigensolver. Matrix construction was also parallelized to enable the needed memory to be spread across multiple processors and to eliminate additional communication steps. For a 4190 term wave function they achieved a speedup of 30 on 32 processors of the PL/ITL Linux cluster.

A team from the MCSD Scientific Applications and Visualization Group (John Hagedorn, Adele Peskin, John Kelso, Steve Satterfield, and Judith Terrill) are developing unique measurement capabilities for immersive visualization environments. In a first demonstration, they have developed tools allowing the user to interactively measure linear distances in a 3D scene, to manage sets of such measurements, and to perform interactive analyses from within the environment. Such capabilities may prove extremely useful for the exploration of 3D data obtained from physical measurement systems. For example, they are working with scientists from the NIST Materials Science and Engineering Laboratory to study 3D volumetric data obtained from a variety of techniques, including optical coherence tomography (OCM) and confocal fluorescence (CFM) imaging. In particular, they are evaluating manufactured polymer test scaffolds for the growth of human tissue. Here, interactive measurements are used to determine how close the manufactured scaffolds are to design specifications. One of the reasons that developing accurate measurements in the virtual environment is challenging is the potential errors induced by electromagnetic tracking devices used to identify position in the immersive environment. The SAVG team has developed a novel scheme for calibrating such tracking devices, and for correcting for such errors in real time.

Finally, the OOMMF software framework for micromagnetic modeling, developed by Michael Donahue and Donald Porter of MCSD, continues to make significant impact in the research community studying micro- and nanomagnetic phenomena and devices. During the past year alone, use of OOMMF has been acknowledged in 79 articles in peer-reviewed scientific journals, bringing the total number of articles citing OOMMF to more than 300.

Staff News

Joyce Conlon of MCSD retired from government service in 2005. She provided technical computing support to MCSD staff, served as MCSD Computer Security Officer, and participated in the Digital Library of Mathematical Functions project. Chris Schanzle, formerly of the NIST CIO Office joined MCSD in October 2005 to take over these duties.

Two NIST National Research Council Postdoctoral Fellows successfully completed their two-year terms during 2005. Stephen Bullock, a researcher in quantum information science, took a position at the Institute for Defense Analysis' Center for Computing Sciences. David Cotrell, who works in mathematical modeling in materials science, moved to the Lawrence Livermore National Laboratory.

Two temporary guest researchers spent time participating in MCSD research programs during 2005. Sita Ramamurti, a mathematician from Trinity University, spent her sabbatical at MCSD during the fall of 2005. She worked with Dr. David Gilsinn on research in dynamical systems. Ioan Sucan a graduate student recently graduated from the International University of Bremen, spent the summer at MCSD working with Bruce Miller on software for transforming Latex documents into content and presentation MathML.

Two MCSD staff members undertook details at other government agencies during the past year. Isabel Beichl was selected to participate in a sabbatical program within the Mathematics Research Group at the National Security Agency. She spent half of her time at the NSA this year to participate in this program. Robert Bohn of MCSD spent this year working with NOAA's High Performance Computing and Communications Office.

MCSD provided support for ten student staff members on summer appointments during FY 2005. 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.

MCSD Student Interns - 2005				
Name	**Institution**	**Program**	**Mentor**	**Project Title**
Eric Baer	Carnegie Mellon University	STEP	A. Kearsley	Computer programming.
Mei-Hsin Cheng	Northwest High School	Volunteer	A. Kearsley	Dataset Analysis for Sensing Devices
Brian Cordes	Worchester Polytechnic Institute	SURF	F. Hunt	Analyzing and Expanding a Mathematical Model of a Fluorometry Experiment
Justin Haaheim	Gustavus Adolphus College	SURF	W. George	A Framework for Parameter Study Applications in a Distributed Computing Environment
Jarrett Inn	Montgomery College	Entry Point!	J. Terrill	Compilation of MCSD reports for Division Web pages
Shamit Patel	River Hill High School	Volunteer	A. Kearsley	Dataset Analysis for Sensing Devices
Javier Sanchez	State University of New Jersey	SURF	A. Peskin	Immersive Visualization
Gaurav Thakur	University of Maryland	SURF	D. Lozier	Classical Theta Functions and Generalizations
Alexandre Thibau	Winston Churchill High School	Volunteer	J. Terrill	Convert FLYPHS Makers to conform to new format
Benjamin Zoller	University of Maryland	SURF	B. Miller	Developing an Online Sparse Matrix Repository for Testing and Comparing Linear Algebra Algorithms

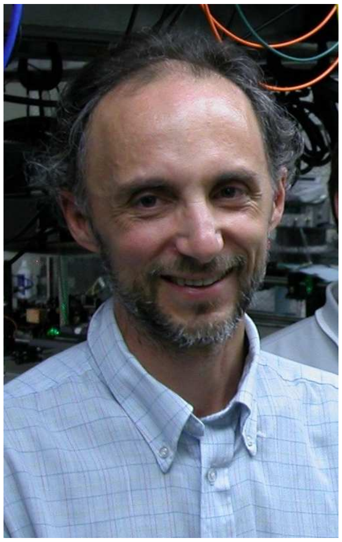
STEP: NIST Student Employment Program.

SURF: NIST Student Undergraduate Student Fellowship Program, an NSF-sponsored Research Experience for Undergraduates program.

Entry Point: American Association for the Advancement of Science (AAAS) program offering internship opportunities for students with disabilities.

Awards

MCSD staff garnered a variety of awards and recognitions during the past year. Emanuel (Manny) Knill, a mathematician in MCSD (Boulder) was recently 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 Manny's outstanding contributions to physics. In particular, Manny is 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 will be done in the March 2006 issue of APS News. Manny is MCSD's second APS Fellow. Dr. Geoffrey McFadden was elected in 2001.


Three of MCSD's 2005 award winners. Left: Dianne O'Leary received an honorary doctoral degree from the University of Waterloo. Center: Manny Knill was elected a Fellow of the American Physical Society. Right: Fern Hunt was a special recognition awardee at Science Spectrum Magazine's Emerald Honor Awards.

Fern Hunt received a Special Recognition Award at the annual Emerald Honors Ceremony held at the Baltimore Convention Center on September 17, 2005. The black-tie gala was the signature event of the week-long Minorities in Research Science conference sponsored by Science Spectrum magazine. Fern was recognized for a sustained record of fundamental contributions to probability and stochastic modeling, mathematical biology, computational geometry, nonlinear dynamics, computer graphics, and parallel computing, as well as for her efforts as a leading proponent at the national level for careers in mathematics among high school, undergraduate, and graduate students, especially for women and minorities.

Hunt was also selected to deliver the 2005 Etta Falconer Lecture. The plenary lecture was delivered at the Mathematical Association of America's yearly Mathfest conference held this year August 3-6 in Albuquerque. The lecture honors the memory of Dr. Etta Z. Falconer (1933-2002), former Associate Provost and Professor of Mathematics at Spellman College, who was a pioneer in promoting careers of minorities and women in mathematics. The lecture is sponsored by the Association for Women in Mathematics (AWM) in conjunction with the MAA. Fern's lecture was entitled "Techniques for Visualizing Frequency Patterns in DNA."

Dianne O'Leary, an MCSD faculty appointee from the University of Maryland College Park, received a Doctor of Mathematics, honoris causa, from the University of Waterloo for "outstanding contributions to research and education in the mathematical and computer sciences and leadership and promotion of women in the field." The degree was conferred at the University of Maryland's fall convocation which was held on October 22, 2005.

Timothy Burns of MCSD is a member of a team that has been selected to receive NIST's Allen Astin Measurement Science Award for 2004. The award is granted for outstanding achievement in the advancement of measurement science. The team was recognized for experimental and theoretical work enabling the development of constitutive models for materials at high-temperature, high-strain conditions. Joining Tim on stage at the December 1, 2004 NIST Award Ceremony was Brian Dutterer, Michael Kennedy, Richard Rhorer, and Eric Whitenton from MEL; Howard Yoon from Physics; and Richard Fields and Lyle Levine of MSEL.

Robert Bohn of MCSD, who is currently on detail to NOAA’s CIO Office, was selected as an awardee in NOAA's 2005 Administrator's Award program. Bob was honored as part of a group of 16 from the NOAA for “developing and issuing integrated requirements for a NOAA high performance computer system that realistically demonstrates the One-NOAA vision.”

Finally, MCSD guest researcher Christoph Witzgall was selected for designation as an ITL Scientist Emeritus. This honor for NIST alumni was recently approved by NIST to recognize outstanding retirees who continue to make important contributions to NIST programs. Chris was one of ITL’s first two retirees cited for this distinction.