

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

The first area and third areas accomplished primarily via collaborations with other technical units of NIST, supported by mathematical research in key areas. Projects in the second 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, as well as with the NIST Physics and Electronics and Electrical Engineering 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, fluid mechanics, electromagnetics, manufacturing engineering, construction engineering, wireless communications, bioinformatics, image analysis and computer graphics.

In addition to our direct collaborations and consulting, output of Division work includes publications in refereed journals and conference proceedings, technical reports, lectures, short

courses, 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 technical thrust areas, including their impetus, general goals, and expected long-term outcomes. The identification of these areas was part of a NIST-wide effort to identify and document its programs of work. 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, and hence there is added benefit.

**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
- ❑ Terrain modeling
- ❑ 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 (including computer software) will allow these benefits to accrue to the scientific community at large. Examples of the latter include (1) more widespread study of material science problems and the development of new technologies characterized by complex material microstructure, and (2) improvement in the accuracy and reliability of micromagnetic modeling software.

## 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 system, or the computation of a transform. Much mathematical research has focused on how to solve such problems efficiently. The most effective means of passing on 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
- ❑ 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.

## 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 effect such computations in a reasonable amount of time, one must often resort to parallel computers. The effective use of parallel 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 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.

**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.

- ❑ Parallelization of Feff x-ray absorption code
- ❑ Parallel computation of the ground state of atomic systems
- ❑ Parallel genetic programming
- ❑ Parallel computing and visualization of the flow of suspensions
- ❑ Modeling and visualization of dendritic growth
- ❑ 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 central 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.

## 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 more than 35 years the NBS *Handbook of Mathematical Functions* (AMS 55) has served this purpose. However, this book is now woefully out of date. Many new properties of these functions are known, many new scientific applications of them have come into use, 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. 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 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. The technology has only been demonstrated in laboratory settings, and a solid measurement and standards infrastructure is needed to move this into the technology development arena. Quantum computers have potential for speeding up previously intractable computations. ITL has been asked to support the work in the NIST Physics and Electronics and Electrical Engineering Laboratories to develop quantum processors and memory, concentrating on the critical areas of error correction, secure protocols, algorithm and tool development, programming, and information theory.

**Activities.** This project is an ITL-wide effort with participants in six Divisions. We are 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. We are 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 new 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, and the development and analysis of quantum algorithms.

**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

## **Technical Highlights**

### **Solidification Modeling**

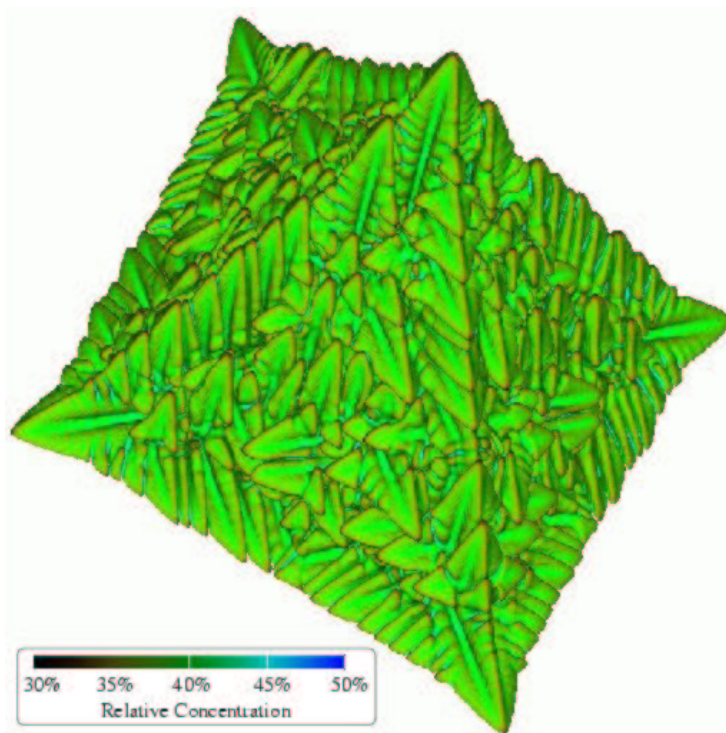
MCSD has participated in a long-term successful collaboration with the NIST Materials Science and Engineering Laboratory (MSEL) in the study of solidification and other types of phase transitions. The purpose of this work has been to develop an understanding of how materials processing techniques affect the physical properties of the resulting products. Mathematical models of such phenomena involve nonlinear free boundary problems in which the shape and dynamics of the interfaces that separate the material phases need to be determined in addition to the temperature and solute fields in both the solid and liquid phase. Traditional computational models carefully track the location of the solid-liquid interface in order to be able to apply the correct field equations and boundary conditions at each point in the domain. Tracking interfaces is extremely difficult, however, and these methods have not been able to operate in the most challenging regimes such as the formation of dendrites.

In the early 1990s an alternative approach, known as phase-field modeling was proposed. In phase-field models one does not track the solid-liquid interface directly. Instead, a new unknown is introduced, the "phase" or "order parameter", whose value is zero when the material is solid and one when it is liquid. Instead of applying interface conditions, one introduces a new equation, applied globally, that describes the evolution of the phase field. The new equations are nonlinear and difficult to solve numerically, and while the method seemed to reproduce physical-like behavior, its ability to model real materials was unclear. In a series of papers published with postdocs, guest researchers, colleagues in MSEL, and external researchers, Geoffrey McFadden of MCSD perfected the variational calculus used to derive the necessary field equations to describe solidification, and performed various asymptotic analyses. McFadden's leadership in the asymptotic analysis established concrete connections to traditional sharp interface models for solidification. Without this connection, the method would have remained an academic curiosity. These methods are now being applied to many problems in materials science where changes in topology occur, such as fracture. Today, a search of the term "phase field" will show the explosion of papers, demonstrating that these techniques are now revolutionizing phase transformation modeling.

MCSD staff members have continued to work closely with MSEL scientists to extend the applicability of phase field models to more complex cases, and to demonstrate their effectiveness in

modeling real materials. Recently, for example, G. McFadden has worked with J. Guyer, W. Boettinger, and J. Warren of MSEL to develop a phase-field model of electrodeposition, in which an electric field is used to control the plating of conducting electrolyte onto an electrode. This work extends previous modeling results for binary alloys by considering four-component systems, and including the electric field effects on the transport of solute. This work is in support of NIST experimental studies of electrodeposition in high-aspect-ratio trenches, where the goal is to fill the trench with deposited material before the trench pinches off, leaving behind a void.

One of the main attractions of phase-field models is that they are much more computationally attractive than traditional sharp-interface models. Computations in two dimensions are now routinely accomplished. Extending this to three dimensions presents scaling problems for both the computations and the subsequent rendering of the results for visualization. This is due to the  $O(n^4)$  execution time of the algorithm as well as the  $O(n^3)$  space requirements for the field parameters. Additionally, rendering the output of the three dimensional simulation also stresses the available software and hardware when the simulations extend over finite-difference grids of size  $1000 \times 1000 \times 1000$ . Working with J. Warren of MSEL, William George of MCS D has developed a parallel 3D dendritic growth simulator based on a finite difference methods applied phase-field models that runs efficiently on both distributed-memory and shared-memory machines. This simulator can also run efficiently on heterogeneous clusters of machines due to the dynamic load-balancing support provided by our MPI-based C-DParLib library. Striking visualizations of the resulting dendrites have also been produced (see below). A paper describing this effort recently appeared in the *Journal of Computational Physics*.



A simulated dendrite computed on a  $500 \times 500 \times 500$  finite difference grid with six-fold symmetry. The surface is colored according to the relative concentration of solute at the surface.



## Micromagnetic Modeling

The engineering of such IT storage technology as patterned magnetic recording media, and spintronic devices such as GMR sensors, magnetic RAM (MRAM), and magnetic logic devices, requires an understanding of magnetization patterns in magnetic materials at the nanometer level. Mathematical models are required to interpret measurements at this scale. MCS D is working with industrial and academic partners, as well as with colleagues in the NIST MSEL and EEEL, to improve the state-of-the-art in micromagnetic modeling.

One of our contributions is a public domain reference software package for micromagnetic modeling. The Object-Oriented MicroMagnetic Framework (OOMMF), which has been developed by Michael Donahue and Donald Porter, serves primarily as an open well-documented environment in which algorithms can be evaluated on benchmark problems. It also serves as a fully functional micromagnetic modeling system, handling both two and three-dimensional problems, and including sophisticated extensible input and output mechanisms. OOMMF has become an invaluable tool in the magnetics research community.

The extent of OOMMF's impact emerged clearly during 2002. This year, for example, the OOMMF code was downloaded more than 2000 times. Use of OOMMF was acknowledged in more than 20 papers published in peer-reviewed journals by authors external to NIST, including articles in *Science* and *Physical Review Letters*. One of these papers, in fact, was the basis of one of the "top 10 stories" of 2002 according to the Institute of Physics (see <http://physicsweb.org/article/news/6/12/14>). Number seven on this list was work of UK physicists who built a nanometer scale logic gate made entirely from metal that works at room temperature. In existing electronic circuits, semiconductor devices carry out logic operations. In such devices, the density of electron flow is limited, restricting how small these devices can be made. Metals have higher electron densities, so a metallic logic gate could be made smaller than a semiconductor one. Such devices would be ideal for mobile applications such as phones and smart cards because the data could be stored without a power source. As reported in *Science* in June 2002, the team from the University of Durham used OOMMF to determine the appropriate device widths for containing and controlling the magnetic domain walls. The controlled motion of the walls between magnetic domains is what enables fully magnetic logic operations.

The latest version OOMMF, released in October 2002, features extended methods for material properties specification, new solution methods, and a 170-page user's manual.

Michael Donahue and Donald Porter were honored with a NIST Bronze Medal in December 2002 for their work with the micromagnetics modeling community.

## Computation of Atomic Properties

MCS D computational scientist James Sims, in collaboration with Stanley Hagstrom of Indiana University, has computed the nonrelativistic energy for the ground 1S state of neutral helium to be -2.9037 2437 7034 1195 9829 99 a.u. This represents the highest accuracy computation of this quantity to date. Comparisons with other calculations and an energy extrapolation yield an estimated accuracy of one part in  $10^{-20}$ . Such high accuracy computations represent the state-of-the-art in virtual measurement for atomic systems. The computation was enabled by novel approaches utilizing high-precision parallel computing.

Exact analytical solutions to the Schrödinger equation, which determine physical properties of atomic systems, are known only for atomic hydrogen and other equivalent two-body systems. Thus, solutions must be determined numerically. In an article in the *International Journal of Quantum Chemistry*, Sims and Hagstrom discuss how this best calculation to date was accomplished. To obtain a result with this high a precision, very large basis sets must be used. In this case, variational expansions of the wave function with 4,648 terms were employed, leading to the need for

very large computations. Such large expansions also lead to problems of linear dependence, which can only be remedied by using higher precision arithmetic than is provided by standard computer hardware. For this computation, 192-bit precision (roughly 48 decimal places) was necessary, and special coding was required to simulate hardware with this precision. Parallel processing was also employed to speed the computation, as well as to provide access to enough memory to accommodate larger expansions. NIST's Scientific Computing Facility cluster of 16 PCs running Windows NT was utilized for the computation. Typical run times for a calculation of this size are about 8 hours on a single CPU, but only 30-40 minutes on the parallel cluster.

This work employs a very novel wave function, namely, one consisting of at most a single  $r^{12}$  raised to the first power combined with a conventional non-orthogonal configuration interaction (CI) basis. The researchers believe that this technique can be extended to multielectron systems. Work is in progress, for example, to see what precision can be obtained for atomic lithium, which is estimated to require a 6000-fold increase in CPU requirements to reach the same level of precision, making the use of parallel programming techniques even more critical.

## **Sparse BLAS Standardization**

MCSD is playing a leading role in the new standardization effort for the Basic Linear Algebra Subprograms (BLAS). The BLAS are kernels for computational linear algebra. If the interfaces to such kernels are standardized, computer manufacturers or software vendors can provide high-performance implementations especially suited to each given hardware platform. By developing their applications in terms of the BLAS, then, computational scientists can achieve high levels of both portability and performance for their applications. The original BLAS, which were developed from the late 1970s through the early 1990s achieved this goal very well. Recently, there has been renewed interest in extending this success to new areas. The BLAS Technical Forum (BLAST) was formed to coordinate this work. BLAST is an international consortium of industry, academia, and government institutions, including Intel, IBM, Sun, HP/Compaq/Digital, SGI/Cray, Lucent, Visual Numerics, and NAG. MCSD has been an active participant in this process. During the past year the Forum completed its work with the publication of a new BLAS standard (see <http://www.netlib.org/blas/blast-forum/>). The standard includes sections on extensions to the classic BLAS, a new set of extended precision BLAS, and BLAS for sparse matrix operations.

Roldan Pozo of MCSD served as chair of the Sparse BLAS subcommittee during the standardization process, and NIST was the first to develop and release a public domain reference implementation in ANSI C for early versions of the standard, which helped shape the final specification. The standard was formally approved and accepted in early 2002, with publication of the complete specification. In addition, a special issue of the *ACM Transactions of Mathematical Software* (TOMS) devoted to the new BLAS standard and implementations was published in June 2002. A paper devoted to the Sparse BLAS was included in the latter.

This year we are continuing our development of an ANSI C reference implementation for public release. In addition, we are beginning work on an alternate C++ binding to augment the official standard.

## **Special Functions in the Digital Age**

Eight MCSD and NIST PL staff members participated in a workshop on Special Functions in the Digital Age hosted by the Institute for Mathematics and Its Applications (IMA) at the University of Minnesota in Minneapolis from July 22 - August 2, 2002. The workshop was inspired by the MCSD Digital Library of Mathematical Functions (DLMF) project. About 80 researchers from 14 countries participated. According to the call for participation,

"The purpose of this program is to formulate, through concrete examples and experiences, the role and character of digital libraries in mathematics, and the mathematical and applied fields that would benefit from such a library. The first serious attempt to address these issues is the ongoing Digital Library of Mathematical Functions (DLMF) project at the National Institute of Standards and Technology (NIST). This workshop will take the DLMF project as a basis for assessing both the state of the art in special function theory, what aspects are of importance in applications, particularly to chemistry and physics, and the experiences gained in this project to formulate recommendations for how digital libraries of mathematics should be organized, utilized, and developed."

The DLMF is currently under development as an interactive Web-based information resource on the special functions of applied mathematics.

A major part of the workshop's program was devoted to the assessment of research progress and consideration of promising vistas for future research in (a) special functions, including combinatorial functions, orthogonal polynomials, the zeta function, elliptic functions, hypergeometric functions, statistical functions, Painlevé functions, Mathieu functions, Lamé functions, and spheroidal wave functions, (b) analysis tools, including asymptotics, algebraic and group-theoretic methods, computer algebra, numerical methods and software, and (c) applications in the physical sciences. Speakers surveyed what is of greatest importance in theory and applications, and what should be included in digital library projects. The remainder of the program was devoted to the development of digital libraries in the mathematical sciences, including the delivery of mathematics over the Internet. Among the distinguished group of speakers at the workshop were most of the authors of the DLMF's 40 chapters, as well as members of the DLMF editorial board.

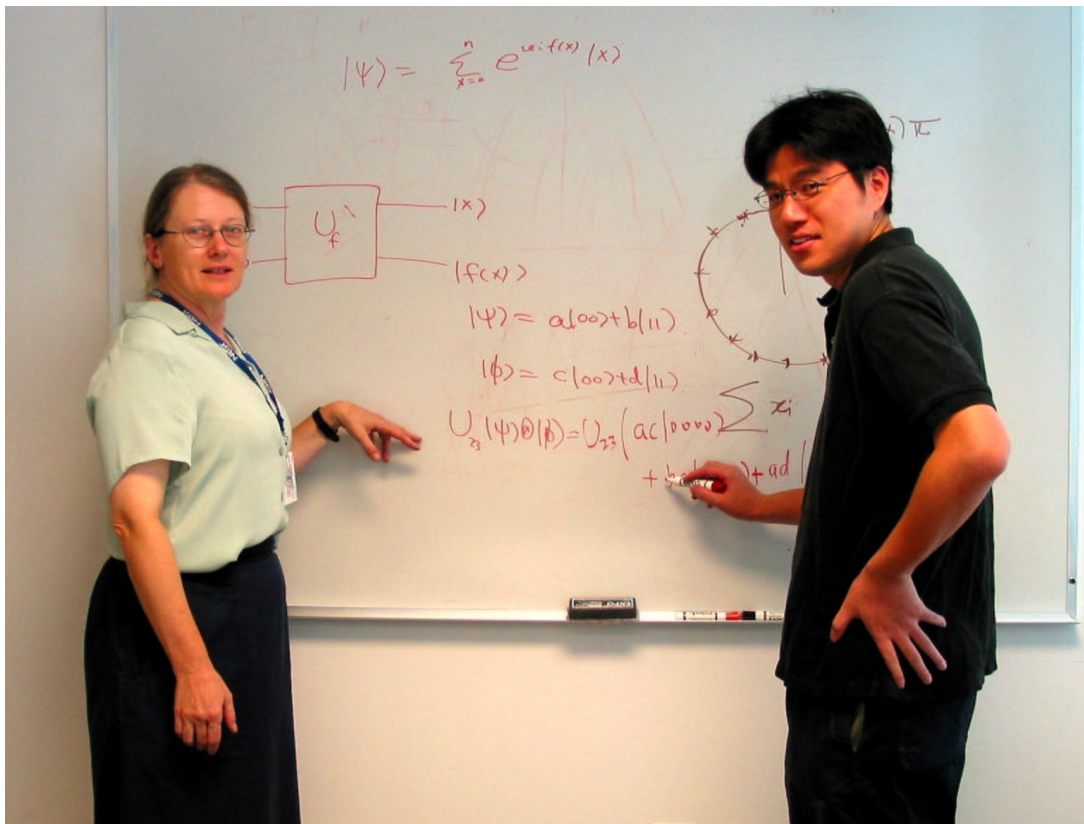
NIST participants (and the titles of their presentations) were as follows. From MCSD: Ronald Boisvert (Building the DLMF: Information Technology Issues), Daniel Lozier (Development of a New Handbook and Web Site of Properties of Special Functions), Bruce Miller (Representation, Display and Manipulation of Mathematics on the Web), Frank Olver, guest researcher from the University of Maryland (Error Bounds, Hyperasymptotics, and Uniform Asymptotics), Bonita Saunders (Interactive 3D Visualizations of High Level Functions in a Mathematical Digital Library), and Abdou Youssef, faculty appointee from George Washington University (Search Systems for Mathematical Equations). From PL: Charles Clark and William Reinhardt, faculty appointee from the University of Washington (New and old addition theorems and Landen identities for Jacobian elliptic functions: do these indeed give rise to "novel" solutions for non-linear PDEs?). Daniel Lozier and Frank Olver were on the workshop's organizing committee.

The workshop was the IMA's featured summer program for 2002. The IMA is an NSF-sponsored center established to increase the impact of mathematics by fostering research of a truly interdisciplinary nature. The IMA's work is carried out through a sequence of thematic programs ranging in length from two weeks to ten months, involving long-term, medium-term and short-term visitors, from academia, industry, and government.

## **Quantum Information Theory and Practice**

The use of the principles of quantum physics for the storage, transformation, and communication of information has the potential to revolutionize information technology. NIST has embarked upon an aggressive experimental program to test and demonstrate a variety of potential physical realizations of quantum memory and quantum processors (see <http://qubit.nist.gov/>). We have begun a new effort to complement and enhance this program, providing expertise to attack critical computer science and mathematics problems needed to transition such technology from laboratory experiments to realistic computing devices. In particular, we are developing algorithms and software tools to model quantum systems being engineered for computation in the NIST Physics Laboratory. We are also devising

architectural concepts, such as the layout of processors and memory, techniques of communication between components, and implementation of error correction schemes, for quantum computers that could be built from components under development at NIST. Integrated high-level designs of this type are critical to the practical realization of scalable quantum computers. Such studies will aid the experimental program with design decisions that affect the reliability and scalability of potential computation devices. We will also demonstrate the utility of such designs in the context of novel quantum algorithms, validating the practicality of a given architecture, and providing demonstrations of actual computations on prototype processors that are realized. This work will greatly accelerate the transition of quantum computation from laboratory experiment to practical realization.



Isabel Beichl and David Song discuss the performance of quantum algorithms.

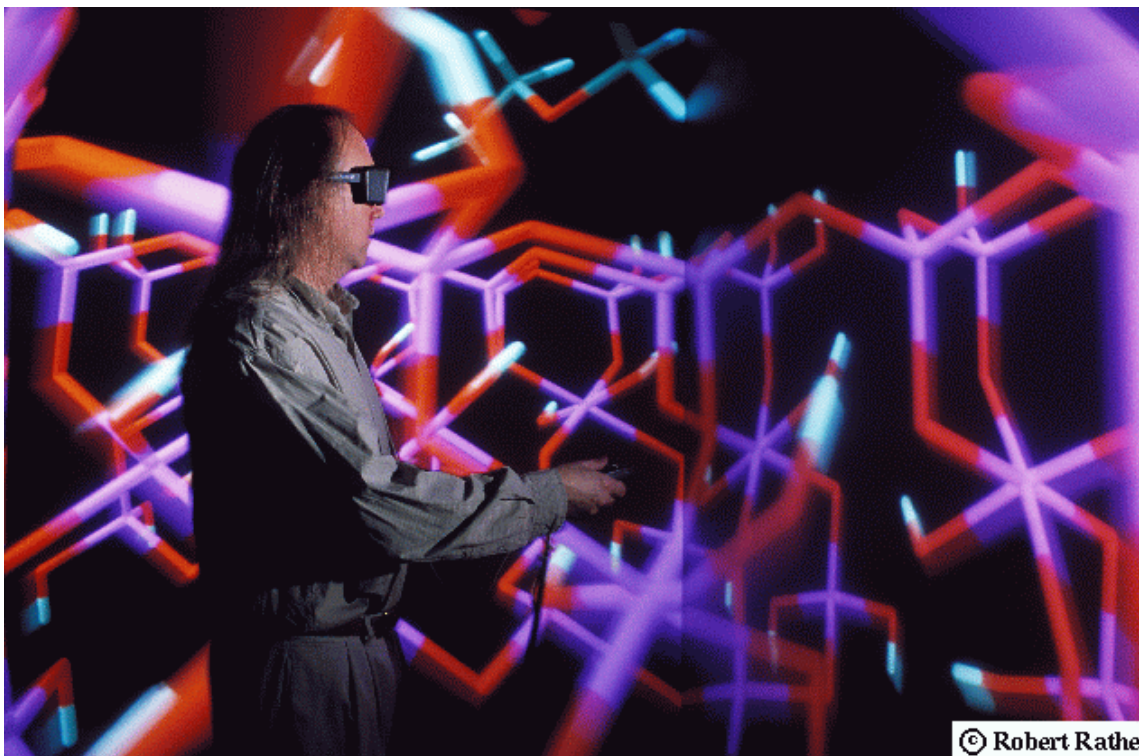
This past year, the NIST Director selected a proposal entitled “Quantum Information Theory and Practice” for 5-year funding under the NIST Competence Program. The proposal, which was championed by Ronald Boisvert and Carl Williams, supports the work of the MCSD quantum information project. The proposal was one of two competence projects selected for startup this year; the second, also in the area of quantum computing, was for the development of so-called SQUID-based quantum processors (i.e., “electrical atoms” constructed from superconducting Josephson junctions) within the NIST Electronics and Electrical Engineering Lab. We will be providing mathematical support to that project.

Our work on the competence project will concentrate on studies of architectures and algorithms compatible with experimental systems being developed within the NIST labs. Examples include recent work on a quantum bus architecture for lattice-based quantum computers. This is joint work of David Song of MCSD and Carl Williams and Gavin Brennen of the NIST Physics Lab. In a

lattice of qubits based on neutral atoms, two qubit gates can only be physically realized between adjacent qubits, calling scalability into question. We have shown how to use ancilla qubits to form a quantum bus in which two qubit gates are teleported. The fidelity of the proposed operations exceeds that of the more laborious swapping of quantum states to physically move qubits into position. A paper describing the quantum bus architecture has been submitted. David Song has subsequently begun a study of a theoretical implementation of Shor's factoring algorithm on such an architecture.

We have also begun various investigations of quantum algorithms. For example, Isabel Beichl and David Song, working with Francis Sullivan and Mike Robinson of the IDA Center for Computing Sciences, are developing a quantum algorithm for determining if a mapping from a finite set to itself is one-to-one. Classical algorithms require  $n$  steps, but the new algorithm is expected to require only  $n^{1/2}$ . The proposed method, which is related to Grover's search algorithm, uses phase symmetry, results about the  $p$ th roots of unity, and the density of prime numbers in the integers. A paper is being written.

Ronald Boisvert continues to co-ordinate the ITL-wide quantum information program, which includes the development of a testbed for quantum key exchange. That system will be demonstrated during FY2003.



Steve Satterfield visualizes the molecular structure of a smart gel in the MCSD immersive visualization facility. This project, which is a collaboration with the NIST Chemical Sciences and Engineering Lab and Kraft Foods, is studying systems with significant potential in both the food and pharmaceutical industries. Here, quantum chemical calculations as well as atomistic simulations are performed in order to understand the nature of the interactions between polyethylene oxide, PEO, and the clay laponite in water. Experimental evidence shows that at the appropriate concentration of PEO and laponite in water, the liquid mixture collapses to a gel after a mechanical disturbance such as a shake of the container. This gel goes back to the liquid phase after leaving the system at rest for a certain period of time.

## Immersive Visualization Environment

The MCSD Scientific Applications and Visualization Group has developed an immersive visualization environment that can be used to gain increased insight into large, complex data sets. Such data sets are becoming more commonplace at NIST, as high performance parallel computing is used to develop higher fidelity simulations, and combinatorial experimental techniques are used in the laboratory. Immersive visualization environments allow the scientist to interactively explore complex data by literally putting oneself inside the data.

Fully immersive computer graphics include one or more large rear projection screens to encompass peripheral vision, stereoscopic display for increased depth perception, as well as head tracking for realistic perspective based on the direction the user is viewing. The MCSD Immersive Visualization Laboratory is a RAVE (Reconfigurable Automatic Virtual Environment) from Fakespace Systems. The two-wall RAVE is configured as an immersive corner with two 8 ft. x 8 ft. (2.44m x 2.44m) screens flush to the floor and oriented 90 degrees to form a corner. The large corner configuration provides a very wide field of peripheral vision, with stereoscopic display and head tracking. The RAVE is driven by a Silicon Graphics Onyx 3400 parallel processor graphics super computer consisting of twelve 500MHz MIPS R14000 CPUs, 12GB memory and 3 Infinite Reality graphics pipes.

The primary software controlling the RAVE is an open source system from Virginia Tech called DIVERSE (Device Independent Virtual Environments-Reconfigurable, Scalable, Extensible). DIVERSE handles the details necessary to implement the immersive environment. SAVG has developed additional tools and techniques for quickly moving research data into the RAVE, often with little or no special-purpose graphics programming.

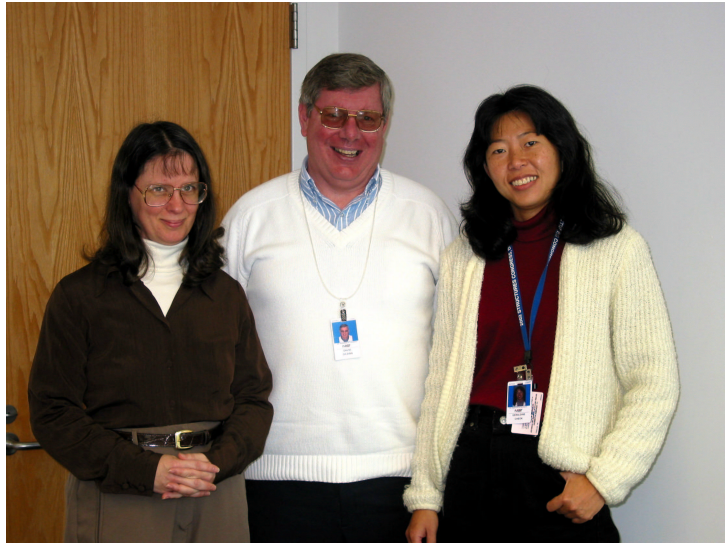
We are collaborating with a number of groups within NIST to apply immersive visualization to their science. These include the Virtual Cement and Concrete Testing Laboratory of the NIST Building and Fire Research Lab, and the Computational Chemistry Group of the Chemical Science and Technology Lab, who are modeling smart gels.

## Awards

**External.** Geoffrey McFadden, Leader of the MCSD Mathematical Modeling Group, was elected a *Fellow of the American Physical Society* (APS). McFadden was recognized “for fundamental insights into the effect of fluid flow on crystal growth and for an innovative approach to phase field methods in fluid mechanics.” McFadden's interest in the study of crystal growth began when he joined NIST in 1981. Since then he has published more than 100 papers with colleagues in MSEL, as well as with researchers at external institutions such as Carnegie Mellon University, Northwestern University, Rensselaer Polytechnic, and the University of Southampton. The APS's Division of Fluid Dynamics recommended the nomination. Fellowship in the APS is limited to no more than one-half of one percent of APS membership. Presentation of the award took place at the Annual Meeting of the Division of Fluid Dynamics held in San Diego, November 18-20, 2001.

David Gilsinn and Dianne O'Leary of NIST's Mathematical and Computational Sciences Division, along with Geraldine Cheok of NIST's Materials and Construction Research Division won the *Best Paper Award* for their contribution to the 19th Annual Symposium on Automation and Robotics in Construction (ISARC 2002). Their paper, entitled "Reconstructing Images of Bar Codes for Construction Site Object Recognition", was selected as top paper of the 88 manuscripts from 20 countries that accepted for presentation. The conference, which was sponsored by the International Association for Automation and Robotics in Construction, was held at NIST on September 23-25, 2002. In their paper, Gilsinn, O'Leary, and Cheok describe techniques for the automated recognition of bar codes from LADAR (laser distance and ranging) optics. In the process of sending and recovering optical signals from a scene, LADAR devices obtain three-dimensional data (distance,

angle, and intensity), which can be used to develop three-dimensional models. Although image reconstruction techniques are well known in association with traditional optical systems, this work represents one of the first to apply them in the context of 3D scanners. While current scanners generate beams that are much too coarse to get good reconstruction, with technology changes leading to finer resolution beams, effective reconstruction of objects may become feasible.



Left: Geoffrey McFadden, named a Fellow of the American Physical Society. Right: Dianne O’Leary, David Gilsinn, and Geraldine Cheok (BFRL) received the ISARC Best Paper Award for 2002.



NIST Bronze Medal winners. Left: Roldan Pozo and Ronald Boisvert, 2001 awardees. Right: Michael Donahue and Donald Porter, 2002 awardees.

**Internal.** In December 2001, Ronald Boisvert and Roldan Pozo of MCSD were awarded the NIST *Bronze Medal* “for leadership in technology transfer introducing significant improvements to the Java programming language and environment for scientific computing applications.” Referring to their work in co-organizing the Java Numerics Working Group, the citation continues, “Working in a highly politicized environment, the group was able to develop technical solutions admitting impressive improvements in Java performance, opening a new potential for highly portable network-based scientific applications”.

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”.

## Technology Transfer

MCSD staff members continue to be active in publishing the results of their research. This year 42 publications authored by Division staff appeared, 25 in refereed journals. Twenty-nine additional papers have been accepted and are awaiting publication. Another 22 are under review. MCSD staff members were invited to give 39 lectures in a variety of venues and contributed another 23 talks to conferences and workshops. Fifteen additional open technical presentations were given at NIST. The Division lecture series remained very active, with 39 talks presented (12 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 seven external events and four internal ones. Among these are the ACM Java Grande/ISCOPE Conference, the MathML International Conference, and the Conjugate Gradient Method’s 50<sup>th</sup> Birthday Celebration.

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 Fortran90 package utilizing MPI and OpenGL graphics. Several existing MCSD software packages saw new releases this year, including OOMMF (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. JAMA, the Java linear algebra package that we developed with the MathWorks registered 4,500 downloads, while TNT saw more than 9,000 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 in 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. Ronald 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. Donald Porter serves on the Tcl Core Team, which manages the development of the Tcl scripting language. Daniel 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), *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. Ronald Boisvert and Roldan Pozo chair the Numerics Working Group of the Java Grande Forum. Roldan Pozo chairs the Sparse Subcommittee of the BLAS Technical Forum. Michael Donahue and Donald Porter are members of the Steering Committee of muMag, the Micromagnetic Modeling Activity Group.

## **Administrative Highlights**

### **Staff News**

MCSD welcomed a variety of new staff members this year. David Song joined MCSD on a postdoctoral term appointment in October 2001. A Ph.D. in Physics from Oxford, Song works in the area of quantum information theory. At NIST he is concentrating on issues related to architectures and algorithms for quantum computers. In October 2002 he became a NIST NRC Postdoctoral Fellow. A second NRC Postdoctoral Fellow, Luis Melara, also joined MCSD in October 2002. Melara, a Ph.D. in Applied and Computational Mathematics from Rice, is working with Anthony Kearsley and Geoffrey McFadden to address problems in materials science using modern optimization techniques.

In October 2001, Yolanda Parker assumed the role of Office Manager for the MCSD Scientific Applications and Visualizations Group (SAVG), while in April 2002 Adele Peskin rejoined SAVG in Boulder to do collaborative research and tool development with an emphasis on scientific visualization. Jeffrey Fong, an MCSD retiree, rejoined the Division in February 2002 as a Guest Researcher. Fong, who specializes in the finite element analysis of structures, is undertaking collaborations with staff of the NIST MSEL and BFRL.

Finally, John Koontz and James Filla transferred to the ITL Information Services and Computing Division in June 2002. There they will provide support in the use of scientific application software by NIST staff.

MCSD provided support for 13 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.

<b>Name</b>	<b>Institution</b>	<b>Program</b>	<b>Mentor</b>	<b>Project Title</b>
April Andreas	Southern Methodist Univ.	SURF	I. Beichl	Develop new method for integer partitioning & produce software.
Eric Baer	Carnegie Mellon Univ.	Student	A. Kearsley	A method for predicting the behavior of Lagrange Multipliers in highly nonlinear problems
Brianna Blaser	Univ. of Washington	Student	B. Saunders	Development of graphics and visualizations for the DLMF Project
Harry Bullen	Montgomery Blair H.S.	Volunteer	S. Satterfield	Glyph Toolbox
Daniel Cardy	Univ. of Maryland	Student	F. Hunt	Bioinformatics research
Jessica Chang	Montgomery Blair H.S.	Volunteer	S. Satterfield	Glyph Toolbox
Kevin Chang	Montgomery Blair H.S.	Volunteer	S. Langer	OOF Project
Grace Chu	Montgomery College	Tech LEAP	B. Saunders	VRML graphics for the DLMF project.
Stuart Fletcher	Univ. of Maryland	SURF	D. Lozier	Foundations for web validation of mathematical software
Alex Harn	Montgomery Blair H.S.	Volunteer	S. Satterfield	Glyph Toolbox
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
Jacob Scott	Univ. of California at Berkeley	SURF	B. George	ScreenSaver Science: Distributed Computing in Java

## Looking Back: Historical Landmarks

### 50th Anniversary of Seminal NBS Publication Celebrated



Magnus Hestenes

The year 2002 marks the fiftieth anniversary of a numerical method for the solution of linear systems of equations which has been hailed as one of the top 10 algorithms of the twentieth century, spawning the work of an army of mathematical researchers, and enabling the solution of innumerable difficult problems in the sciences and engineering. The algorithm was the work of researchers from NBS and the Swiss Eidgenössische Technische Hochschule (ETH). This milestone was the subject of a recent symposium held at the ETH in Zurich, Switzerland, and co-sponsored by MCSD.

In December 1952 a paper entitled [Methods of Conjugate Gradients for Solving Linear Systems](#) by Magnus Hestenes and Eduard Stiefel was published in the Journal of Research of the NBS. The work described in this paper was done at the Institute for Numerical Analysis (INA), a part of NBS on the campus of UCLA. This institute was an incredibly fertile environment for the development of algorithms that might exploit the potential of the newly emerging automatic computing engines, especially algorithms for the solution of linear systems and matrix eigenvalue problems. Some of these algorithms are classified today under the term Krylov Subspace Iteration, and this paper described the first of

these methods to solve linear systems.

The impact of this work on scientific research has been enormous. More than 800 articles citing the original paper appeared during the period 1983-99, and many thousands more feature the term "conjugate gradients" in their title or abstract. In January 2000, *Computing in Science and Engineering*, a publication of the IEEE Computer Society and the American Institute of Physics, named Krylov Subspace Iteration as one of the Top 10 Algorithms of the Century, citing in particular the pioneering work of Hestenes, Stiefel, and NBS colleague Cornelius Lanczos. The paper of Hestenes and Stiefel was also celebrated in the NIST centennial publication *A Century of Excellence in Measurements, Standards, and Technology, A Chronicle of Selected NBS/NIST Publications, 1901-2000*. The description there provides additional information about Hestenes, Steifel, their collaboration at the INA, and subsequent developments ([HTML](#), [PDF](#)).

The 50th anniversary of the conjugate gradient was recently the subject of the Symposium on Iterative Solvers for Large Linear Systems held at ETH in Zurich. The Swiss Latsis Foundation and NIST co-sponsored the event, which took place on February 18-21, 2002. Sixteen invited speakers focused on current research in the conjugate gradient family of algorithms and on scientific computing applications that rely on them, including nuclear fusion computations, solution of the Ornstein-Zernike equations in chemistry, and groundwater pollution modeling. Dianne O'Leary, a faculty appointee in MCSD, presented an invited lecture entitled "Toward Understanding the Convergence of Krylov Subspace Methods". Ronald Boisvert of MCSD served as a member of the Program Committee.

# Methods of Conjugate Gradients for Solving Linear Systems<sup>1</sup>

Magnus R. Hestenes<sup>2</sup> and Eduard Stiefel<sup>3</sup>

An iterative algorithm is given for solving a system  $Ax=k$  of  $n$  linear equations in  $n$  unknowns. The solution is given in  $n$  steps. It is shown that this method is a special case of a very general method which also includes Gaussian elimination. These general algorithms are essentially algorithms for finding an  $n$ -dimensional ellipsoid. Connections are made with the theory of orthogonal polynomials and continued fractions.

## 1. Introduction

One of the major problems in machine computations is to find an effective method of solving a system of  $n$  simultaneous equations in  $n$  unknowns, particularly if  $n$  is large. There is, of course, no best method for all problems because the goodness of a method depends to some extent upon the particular system to be solved. In judging the goodness of a method for machine computations, one should bear in mind that criteria for a good machine method may be different from those for a hand method. By a hand method, we shall mean one in which a desk calculator may be used. By a machine method, we shall mean one in which sequence-controlled machines are used.

A machine method should have the following properties:

- (1) The method should be simple, composed of a repetition of elementary routines requiring a minimum of storage space.
- (2) The method should insure rapid convergence if the number of steps required for the solution is infinite. A method which—if no rounding-off errors occur—will yield the solution in a finite number of steps is to be preferred.
- (3) The procedure should be stable with respect to rounding-off errors. If needed, a subroutine should be available to insure this stability. It should be possible to diminish rounding-off errors by a repetition of the same routine, starting with the previous result as the new estimate of the solution.
- (4) Each step should give information about the solution and should yield a new and better estimate than the previous one.
- (5) As many of the original data as possible should be used during each step of the routine. Special properties of the given linear system—such as having many vanishing coefficients—should be preserved. (For example, in the Gauss elimination special properties of this type may be destroyed.)

In our opinion there are two methods that best fit these criteria, namely, (a) the Gauss elimination

method; (b) the conjugate gradient method presented in the present monograph.

There are many variations of the elimination method, just as there are many variations of the conjugate gradient method here presented. In the present paper it will be shown that both methods are special cases of a method that we call the method of conjugate directions. This enables one to compare the two methods from a theoretical point of view.

In our opinion, the conjugate gradient method is superior to the elimination method as a machine method. Our reasons can be stated as follows:

- (a) Like the Gauss elimination method, the method of conjugate gradients gives the solution in  $n$  steps if no rounding-off error occurs.
- (b) The conjugate gradient method is simpler to code and requires less storage space.
- (c) The given matrix is unaltered during the process, so that a maximum of the original data is used. The advantage of having many zeros in the matrix is preserved. The method is, therefore, especially suited to handle linear systems arising from difference equations approximating boundary value problems.
- (d) At each step an estimate of the solution is given, which is an improvement over the one given in the preceding step.
- (e) At any step one can start anew by a very simple device, keeping the estimate last obtained as the initial estimate.

In the present paper, the conjugate gradient routines are developed for the symmetric and non-symmetric cases. The principal results are described in section 3. For most of the theoretical considerations, we restrict ourselves to the positive definite symmetric case. No generality is lost thereby. We deal only with real matrices. The extension to complex matrices is simple.

The method of conjugate gradients was developed independently by E. Stiefel of the Institute of Applied Mathematics at Zurich and by M. R. Hestenes with the cooperation of J. B. Rosser, G. Forsythe, and L. Paige of the Institute for Numerical Analysis, National Bureau of Standards. The present account was prepared jointly by M. R. Hestenes and E. Stiefel during the latter's stay at the National Bureau of Standards. The first papers on this method were

<sup>1</sup> This work was performed on a National Bureau of Standards contract with the University of California at Los Angeles, and was sponsored (in part) by the Office of Naval Research, United States Navy.

<sup>2</sup> National Bureau of Standards and University of California at Los Angeles.  
<sup>3</sup> University of California at Los Angeles, and Eidgenössische Technische Hochschule, Zurich, Switzerland.

A highlight of the meeting was the emphasis on the history of the algorithms, with special lectures from some of the pioneers in the field. John Todd, Professor Emeritus of Mathematics at Caltech, who was Chief of the NBS Computation Laboratory from 1949-54, shared the story of how Eduard Stiefel came to the INA at the invitation of Olga Taussky (a consultant to NBS). Stiefel recognized some of his own results in Hestenes' technical report on conjugate gradients in the INA library, and made the decision to collaborate on the joint publication. Urs Hochstrasser, a student of Stiefel who also spent time at the INA, did some of the earliest computations with the conjugate gradient method. He recalled the excitement and interaction at NBS's INA. He later directed scientific policy for the Swiss government. Finally, Friedrich Bauer of the Technical University of Munich discussed the contributions of Stiefel and Heinz Rutishauser in Zurich.

The 130 attendees enjoyed a week learning some history and delineating new research directions in preconditioning, understanding stagnation, making the algorithms more generally applicable, and providing better information on the accuracy of the solutions.

### Three Former NIST Mathematicians Honored



John Todd (left), Olga Taussky-Todd (center), and Burton H. Colvin (right)

Three former NIST mathematicians were honored with the installation of their portraits in the NIST Gallery of Distinguished Scientists, Engineers and Administrators on the NIST campus in Gaithersburg, Maryland in ceremonies on September 5, 2002. The honorees were Burton H. Colvin, Olga Taussky-Todd, and John Todd.

Burt H. Colvin was recognized for his outstanding management of the applied mathematics program at NBS. Colvin was born in 1916 in West Warwick, RI, and studied mathematics at Brown University and at the University of Wisconsin, where he received a Ph.D. in 1943. He spent 21 years at Boeing, heading its the Mathematics and Information Sciences Research Laboratories from 1959-1972. He then came to NIST (then the National Bureau of Standards) to head its Applied Mathematics Division. In 1978 Colvin was named head of the NBS Center for Applied Mathematics, a position he held until 1986. During his tenure, Colvin raised the level of theoretical modeling at NBS by fostering collaborations between applied mathematicians and other NBS technical units. During his career, Colvin held many distinguished appointments, including President of the Society for Industrial and Applied Mathematics (1971-72), Chair of the Conference Board of Mathematical Sciences (1975-76), and Fellow of the American Association for the Advancement of Science. He was recipient of the Department of Commerce Silver (1978) and Gold (1981) medals for "consistently outstanding management of the applied mathematics program" at NBS, and he received a Presidential

Meritorious Rank Award in 1980. Colvin headed the NIST Office of Academic Affairs from 1986 until his retirement in 1991. He passed away on August 24, 2001 in Gaithersburg, MD.

John Todd was recognized for his research and leadership at NBS during the formative years of scientific computing. Born in Northern Ireland in 1911, Todd studied mathematics at Queen's University (Belfast) and at Cambridge. During World War Two he served in the Admiralty Department of Scientific Research and Experiment, where he was responsible for the Admiralty Computing Service. In 1947 Todd joined NBS, working closely with John Curtiss to establish the new National Applied Mathematics Laboratory (NAML, later known as the Applied Mathematics Division). NAML included the Institute for Numerical Analysis, which was housed at UCLA. In 1949, Todd became Chief of the NAML's Computation Laboratory in Washington. The Computation Laboratory co-developed (with the NBS Electronics Division) and operated the Standards Eastern Automatic Computer (SEAC). Dedicated in 1950, SEAC was the first operational stored-program electronic digital computers in the United States. Todd assembled a capable group of researchers, and both led and participated actively in research on mathematical methods for exploiting the new computational power that was at hand. He studied methods for evaluating mathematical functions, generating random numbers (for Monte Carlo calculations), conformal mappings, and computations with matrices. He worked on the construction of mathematical tables. During this period, NBS became the leading center for a newly emerging field of legitimate mathematical research: numerical analysis. In 1954, Todd became Chief of the Numerical Analysis Section of the Applied Mathematics Division, a position he held until 1957. While at NBS, Todd became increasingly aware of the need to train researchers in the emerging field of numerical analysis. In 1957 he decided to dedicate himself full-time to this endeavor by taking a position as Professor of Mathematics at the California Institute of Technology. Today John Todd is Emeritus Professor of Mathematics at CalTech, and in May 2001 a conference was held there to celebrate his 90th birthday.

Olga Taussky-Todd was recognized for her contributions to the NBS applied mathematics program in the areas of algebra, number theory, and matrix theory during her tenure there from 1947-57. Born in 1906, Olga Taussky was raised in Austria and received her doctorate in mathematics from the University of Vienna, later working with David Hilbert in Gottingen. In 1934 she moved to England, where she held several academic positions. She later applied her mathematical skills working for the British Ministry of Aircraft Production on such problems as the stability of aircraft designs. In 1938, while both were working at the University of London, Olga Taussky and John Todd married. Their collaboration, which lasted more than 57 years, was extraordinarily fruitful. In 1947, Taussky-Todd became a full-time consultant to the NBS NAML. Stimulated by the computer revolution, researchers such as Taussky-Todd began to establish matrix theory as a new field of study. Taussky-Todd's wide knowledge of mathematics and mathematicians is credited with playing an important part in the development of the NBS Institute for Numerical Analysis. Many researchers in linear algebra and applications were invited to NBS as staff or as visitors, making NBS the leading center for work in this area. Today, linear algebra and matrix theory are as a necessary tool for all scientists. Taussky-Todd also developed novel techniques for solving mathematical problems on the newly emerging computers. She left NBS in 1957 to join the faculty of the California Institute of Technology. There she was recognized by students and colleagues as one of Caltech's most gifted teachers and stimulating intellects. She was the first woman at CalTech to attain the academic rank of full professor. Selected by the L.A. Times in 1963 as "Woman of the Year", Taussky-Todd was hailed as one of the foremost mathematicians of her generation. She passed away in 1995 in Pasadena.

The NIST Gallery of Distinguished Scientists, Engineers and Administrators is located in the Administration Building on the NIST campus in Gaithersburg, MD. The gallery is sponsored by the NIST Alumni Association.