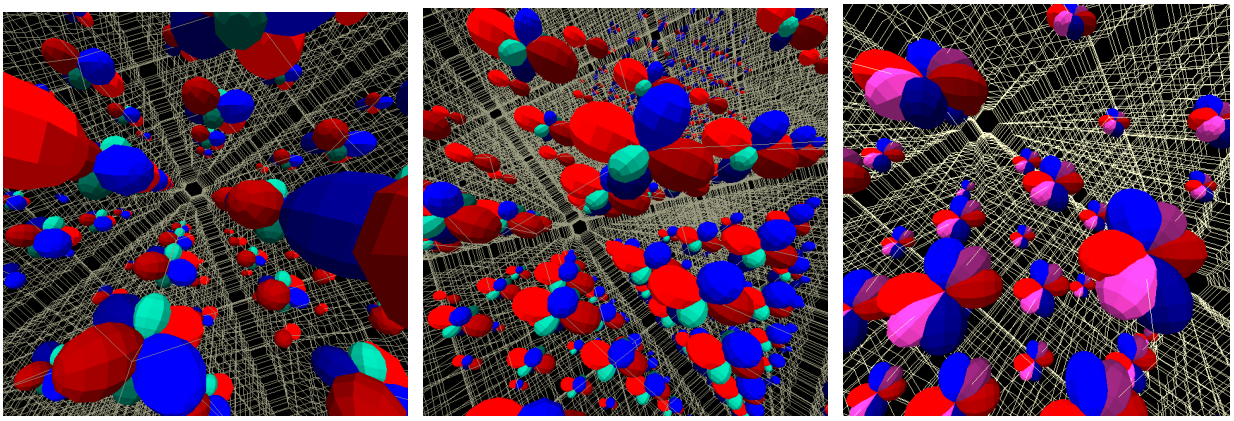
Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2005



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

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Abstract

This report summarizes the technical work of the Mathematical and Computational Sciences Division (MCSD) of NIST's Information Technology Laboratory. Part I provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II includes short articles describing selected recent technical accomplishments in more detail. Part III provides brief summaries of many of the research projects of the Division. Part IV provides listings of publications, technical talks, and other professional activities in which Division staff members have participated.

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Cover image. Visualizations of a quantum dot of gallium arsenide developed by Howard Hung of MCSD.

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

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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.

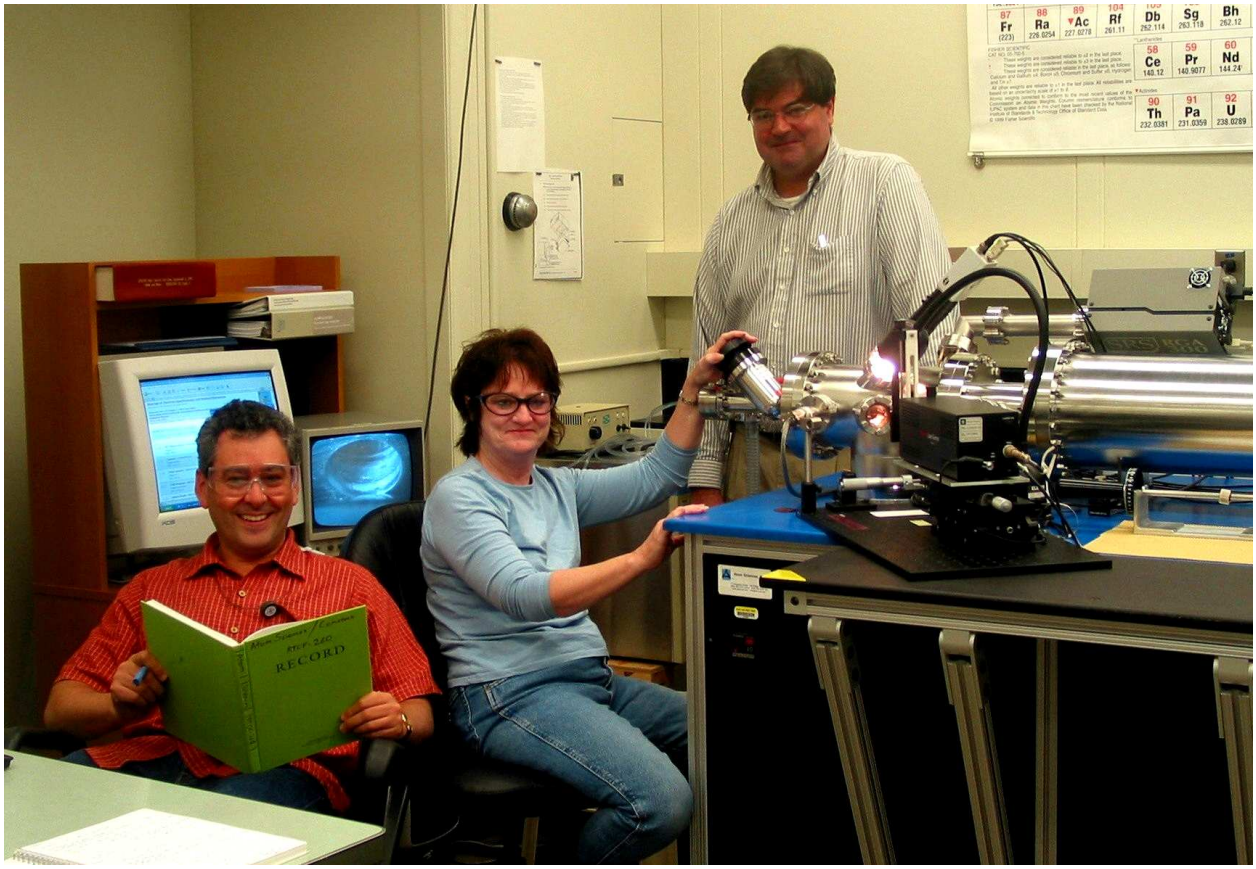
Goals: Develop effective methods for the solution to mathematical problems arising in metrological applications.

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 5^{th} 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.

Part II

Features

Architectures for Fault-tolerant Quantum Computing

In theory, quantum computers can efficiently simulate quantum physics, factor large numbers and estimate integrals, thus solving computational problems that are otherwise intractable. In practice, quantum computers must operate with noisy devices called "gates" that tend to destroy the fragile quantum states needed for computation. The goal of fault-tolerant quantum computing is to compute accurately even when gates have a high probability of error each time they are used. We are developing architectural concepts and error remediation strategies which will enable the development of practical quantum computing devices.

Emanuel Knill

Research in quantum computing is motivated by the great increase in computational power offered by quantum computers. There are a large and still growing number of experimental efforts whose ultimate goal is to demonstrate scalable quantum computing. Scalable quantum computing requires that arbitrarily large computations can be efficiently implemented with little error in the output.

One of the criteria necessary for scalable quantum computing is that the level of noise affecting the physical gates is sufficiently low. The type of noise affecting the gates in a given implementation is called the error model. A scheme for scalable quantum computing in the presence of noise is called a fault-tolerant architecture. In view of the low-noise criterion, studies of scalable quantum computing involve constructing fault-tolerant architectures and providing answers to questions such as the following:

> Q1: Is scalable quantum computing possible for error model E?
>
> Q2: Can fault-tolerant architecture A be used for scalable quantum computing with error model E?
>
> Q3: What resources are required to implement quantum computation C using fault-tolerant architecture A with error model E?

To obtain broadly applicable results, fault-tolerant architectures are constructed for generic error models. In such cases, the error model is parameterized by an error probability per gate (or simply error per gate, EPG), where the errors are unbiased and independent. The fundamental theorem of scalable quantum computing is the threshold theorem which answers question Q1 as follows:

> If the EPG is smaller than a threshold, then scalable quantum computing is possible.

Thresholds depend on additional assumptions on the error model and device capabilities. Estimated thresholds vary from below 10^{-6} to 3×10^{-3}, with 10^{-4} often quoted as the target EPG for experimental realizations of quantum computing.

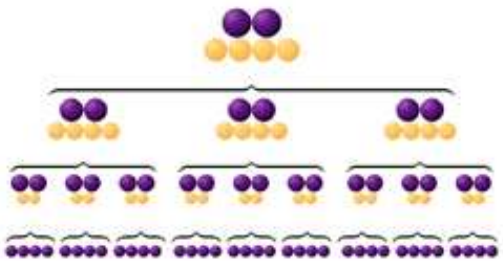


Figure 1. *The new NIST architecture for quantum computing relies on several levels of error checking to ensure the accuracy of quantum bits (qubits). The image above illustrates how qubits are grouped in blocks to form the levels. To implement the architecture with three levels, a series of operations is performed on 36 qubits (bottom row) each one representing a 1, a 0, or both at once. The operations on the nine sets of qubits produce two reliably accurate qubits (top row). The purple spheres represent qubits that are either used in error detection or in actual computations. The yellow spheres are qubits that are measured to detect or correct errors but are not used in final computations.*

Many experimental proposals for quantum computing claim to achieve EPGs below 10^{-4} in theory. However, in the few cases where experiments with two quantum bits (qubits) have been performed, the EPGs currently achieved are much higher, 3×10^{-2} or more in ion traps and liquid-state nuclear magnetic resonance (NMR) experiments, for example.

In our work we have provided evidence that scalable quantum computing is possible at EPGs above 3×10^{-2}. While this is encouraging, the fault-tolerant architecture that achieves this is extremely impractical because of large resource requirements. To reduce the resource requirements, lower EPGs are required.

We have developed a fault-tolerant architecture, called the C_4/C_6 architecture that is well suited to EPGs between 10^{-4} and 10^{-2}. We have analyzed the resource requirements for this architecture and compared it to the state of the art in scalable quantum computing.

The Architecture

Fault-tolerant architectures realize low-error qubits and gates by encoding them with error-correcting codes. A standard technique for amplifying error reduction is concatenation. Suppose we have a scheme that, starting with qubits and gates at one EPG, produces encoded qubits and gates that have a lower EPG.

Provided the error model for encoded gates is sufficiently well behaved, we can then apply the same scheme to the encoded qubits and gates to obtain a next level of encoded qubits and gates with much lower EPGs. Thus, a concatenated fault-tolerant architecture involves a hierarchy of repeatedly encoded qubits and gates. The hierarchy is described in terms of levels of encoding, with the physical qubits and gates being at level 0. The top level is used for implementing quantum computations and its qubits and gates are referred to as being logical. Typically, the EPGs decrease superexponentially with number of levels, provided that the physical EPG is below the threshold for the architecture in question.

The C_4/C_6 architecture differs from previous ones in five significant ways. First, we use the simplest possible error-detecting codes, thus avoiding the complexity of even the smallest error-correcting codes. Error correction is added naturally by concatenation. Second, error correction is performed in one step and combined with logical gates by means of error-correcting teleportation. This minimizes the number of gates contributing to errors before they are corrected. Third, the fault-tolerant architecture is based on a minimal set of operations with only one unitary gate, the controlled-NOT. Although this set does not suffice for universal quantum computing, it is possible to bootstrap other gates. Fourth, verification of the needed ancillary states (logical Bell states) largely avoids the traditional syndrome-based schemes. Instead, we use hierarchical teleportations. Fifth, the highest thresholds are obtained by introducing the model of postselected computing with its own thresholds, which may be higher than those for standard quantum computing. Our fault tolerant implementation of postselected computing has the property that it can be used to prepare states sufficient for (standard) scalable quantum computing.

The properties of the proposed architecture were determined with several months of calculations and simulations on large, conventional computer workstations. Although the new architecture has yet to be validated by mathematical proofs or tested in the laboratory, it provides some evidence that scalable quantum computation may be closer to our reach that previously believed.

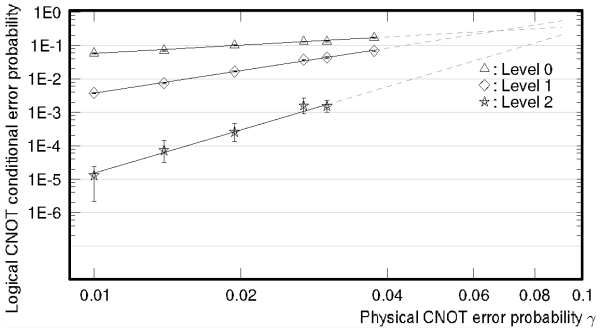


Figure 2. *Errors for a CNOT gate implementation at levels 0, 1 and 2. The errors are conditional on no faults having been detected. The error bars are 68% confidence intervals. As can be seen, errors decrease rapidly with increasing level at EPGs of 3% or below. Extrapolation suggests that this behavior persists for even larger EPGs. At high EPGs, the "no fault" condition happens rarely. Nevertheless it is possible to complete a quantum computation with polynomial overhead by using many trials to prepare relatively error-free states that can then be used to implement error-corrected logical gates with high success probabilities.*

Summary

We have given evidence that accurate quantum computing is possible with error probabilities above 3% per gate, which is significantly higher than what was previously thought possible. However, the resources required for computing at such high error probabilities are excessive. Fortunately, they decrease rapidly with decreasing error probabilities. If we had quantum resources comparable to the considerable resources available in today's digital computers, we could implement non-trivial quantum computations at error probabilities as high as 1% per gate.

References

E. Knill, Quantum Computing with Realistically Noisy Devices, *Nature* **434** (03 March 2005), pp. 39-44.

E. Knill, Scalable Quantum Computing in the Presence of Large Detected-Error Rates, *Physical Review A* **71** (2005), pp. 042322/1-7.

Quantum Logic Circuit Synthesis

Design automation is an important technique for finding efficient classical circuits. Given a Boolean function which the target circuit should implement, a synthesis program automatically determines a sequence of gates realizing this function. Quantum logic synthesis aims to build a similar toolset for quantum circuits, seeking the fewest number of one and two-qubit processes to achieve a target quantum computation. We have developed a technique of automatic quantum circuit synthesis for unstructured qubit evolutions improving a construction from the mid 1990s by a factor of more than one hundred. In addition, we have shown the new construction to be within a factor of two of optimal. For multi-level quantum logics (qudits) similar advances have led to the first circuits ever with optimal asymptotics.

Stephen S. Bullock

While classical computers manipulate bits which carry values of 0 or 1, quantum computers manipulate quantum bits (qubits) which are state vectors of two-level quantum systems. If the quantum computer is not exchanging energy with the outside environment, these qubit state vectors are rotated during the computation. Typical quantum algorithms call for implementing such a rotation, mathematically a unitary matrix, and then observing the qubits. Thus, while efficient Boolean circuits realize complicated functions on bits using a small number of logic gates, efficient quantum circuits break complicated unitary matrices into simple factors. These factors (quantum gates) typically correspond to manipulating one or two quantum bits.

The past two years have seen marked advances in the design of universal quantum logic circuits. Such circuits implement any possible unitary evolution by appropriately tuning their gate parameters. The new techniques are also overtly constructive. Unitary matrices implementing nontrivial quantum computations are large, e.g. requiring $2^n \times 2^n$ matrices for n qubits. The new quantum circuit synthesis algorithms rely on well-known matrix decomposition such as QR or the Cosine Sine Decomposition. For ten qubits, commercial software on a 2.5GHz PC requires a few seconds for these factorizations.

We illustrate basic quantum circuit design with an example. Each circuit in the figure below applies the same two-qubit computation, namely multiplying the *01* and *10* states by the complex number i while leaving *00* and *11* unchanged. Each qubit is represented by a single line or rail in the circuit. The boxes denoted *S* and *H* indicate single qubit operations, i.e. particular 2×2 unitary matrices. The gate spanning both qubits is a quantum controlled not, or CNOT. CNOT flips the target qubit (carrying the inverter) when the control qubit (black slug) carries *1*, so that these down-target CNOTs exchange *10* and *11*.

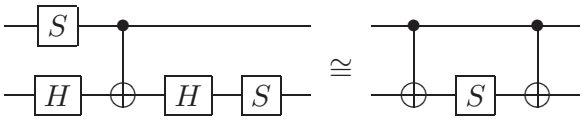


Figure 3. *Two quantum circuits for performing the same task.*

Although their target computation is the same, either diagram might be better suited to a given quantum computer implementation. For example, if CNOTs are costly while one-qubit gates are implemented more easily, then the circuit at left is preferable. Alternately, if one-qubit gates are expensive but CNOTs are cheap, then the circuit at right is preferable. In practice, CNOTs tend to be more expensive than one-qubit rotations, and three-qubit gates tend to be more difficult to implement than CNOTs. Further, while it is possible to build any unitary using exclusively one qubit gates and CNOT, simply employing one-qubit gates does not suffice. Thus, the following discussion of universal quantum circuits focuses on minimizing CNOT counts.

In fact, it is not obvious that CNOT and one-qubit gates suffice to build any unitary evolution. This was settled in 1995 in a landmark paper of Barenco, Bennett, Cleve, DiVincenzo, Margolus, and Shor. If n is the number of qubits on which the unitary operator acts, then these authors showed that $48n^3 4^n$ CNOTs suffice, in addition to many one-qubit gates. Shortly thereafter, Knill argued that some multiple $C4^n$ gates must be required for reasons of dimension. The result has a parallel in classical circuits. Namely, given a *random* bit-valued function on n bit strings, approximately $2^n/2$ strings will take on a value of 1. Thus, we expect $2^n/2$ gates are required to distinguish for which bit strings the circuit should return a nonzero value.

A Unitary-Universal *n* Qubit Circuit

In summer of 2004, we discovered a new unitary-universal n qubit quantum circuit requiring roughly $(1/2)4^n$ CNOTs, an improvement by a factor of two over the best known circuit at the time and a factor of $100n^3$ over the 1995 circuit. Moreover, work from the summer of 2003 had sharpened Knill's bound, actually valid for any two-qubit gate, to a specific bound of $(1/4)4^n$ CNOTs. Hence, the present circuit may never be improved by more than a factor of two.

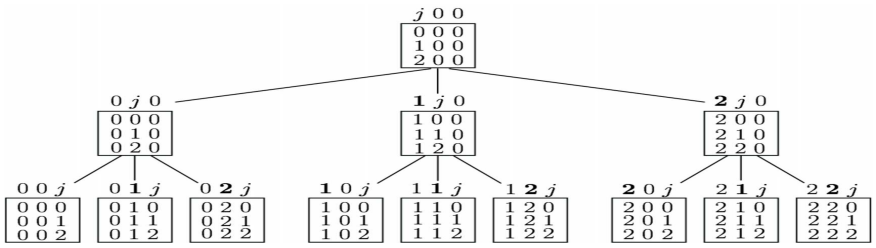


Figure 4. *Recursively generated tree for automated quantum circuit synthesis for three qutrits.*

The outline for deriving the circuit is as follows. The key step is to use the Cosine-Sine Decomposition (CSD) for matrices. The CSD splits any unitary matrix into three factors; the circuit elements outline in the box below represent the first and last. The slash in the circuit represents a multi-line carrying an arbitrary number of qubits, meaning U may be any unitary matrix on any number of qubits. Moreover, the circuit elements having the square box controls correspond to uniformly controlled rotations, a circuit block for which particularly CNOT-efficient circuits are known. Hence, the diagram employs the CSD to reduce construction of the n qubit U into four simpler n-1 qubit unitaries V_1, V_2, V_3, and V_4. This allows for a recursive construction which terminates with hand-optimized two-qubit circuits.

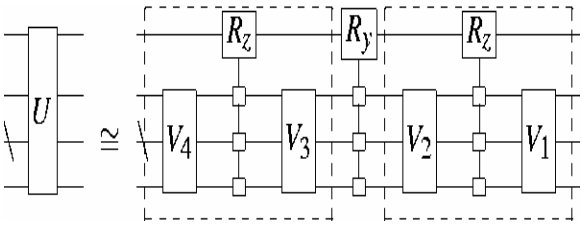


Figure 5. Basic quantum circuit synthesis decomposition.

Circuits for Quantum Multi-Level Logics

In addition, the efficiency of the circuit for quantum multi-level logics (qudits, d=level) has improved. One may think of a qudit by way of analogy: a qubit state is a quantum superposition of *0* and *1*, a qudit state is a quantum superposition of *0, 1, … d-1*. Knill's lower bound also stated that Cd^{n-2} two-qudit gates were required for any generic $d^n \times d^n$ unitary U. Yet the best known constructive procedure required Cn^2d^{2n} gates. In fall of 2004, we produced a new Cd^{2n} construction, closing this gap. The circuit exploits a variant of the QR matrix decomposition. The original asymptotically optimal qubit circuits, due to researchers at the University of Helsinki, also leaned on a QR technique and a Gray code cancellation. Rather than generalize the Gray code cancellation to base d numbers, the new circuit relies on a recursively generated tree. This tree describes which entries of the unitary matrix to construct with quantum gate elements at which time. A sample tree, for 3 qutrits (i.e., d=*3*, n=*3*) is shown above.

Lessons Learned

These specialized techniques for generic unitary matrices might help in optimizing other quantum circuits.

- Just as Boolean factorizations are important for classical circuit design, so too are matrix decompositions useful in quantum circuit design.
- It is possible to exploit parallels to classical logic synthesis. For example, one may view the side factors of the CSD as multiplexers, applying an n-1 qubit unitary matrix dependent on the most significant qubit.
- Novel aspects of quantum circuits must be explored thoroughly. For example, at the heart of the qudit circuit is a subcircuit capable of solving the hard problem of initializing a generic quantum memory state. In contrast, the classical problem of initialization trivially requires at most n bit flips.

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http://math.nist.gov/quantum/

Adaptive Finite Element Modeling of Two Confined and Interacting Atoms

High order finite element methods using adaptive refinement and multigrid techniques have been shown to be very efficient for solving partial differential equations on sequential computers. We have developed a code, PHAML, to extend these methods to parallel computers. We have applied this code to solve a two-dimensional Schrödinger equation in order to study the feasibility of a quantum computer based on extremely cold neutral alkali-metal atoms. Qubits are implemented as motional states of an atom trapped in a single well of an optical lattice. Quantum gates are constructed by bringing two atoms together in a single well leaving the interaction between them to cause entanglement. Quantifying the entanglement reduces to solving for selected eigenfunctions of a Schrödinger equation that contains a Laplacian, a trapping potential, and a short-range interaction potential.

William Mitchell

The idea of using the rules of quantum mechanics as a paradigm for computing has engendered a flurry of research over the last ten years. Strange quantum properties, such as entanglement, may yield a significant advantage, providing novel mechanisms for the solution of problems that are intractable on classical computers. Advances in diverse fields of physics have led to proposals for various alternate physical realizations of a quantum bit and related quantum gates, the quantum analog of one- and two-bit computer operations. We are interested in modeling a quantum gate with quantum bits that are based on ultra-cold atoms. Ultra-cold atoms can be confined by counter-propagating laser beams. The light creates a three-dimensional washboard potential or optical lattice. A single atom is held in each potential minimum or lattice site of the washboard. Two energy levels of an atom are associated with the "0" and "1" states of a quantum bit. By bringing two isolated atoms from separate sites together and having them interact, a two-quantum-bit operation can be realized.

First-principle modeling of the interactions of two atoms in a lattice site is numerically challenging, as length scales for the lattice and the mutual atom-atom interaction differ by orders of magnitude. Our work has applied advanced finite element techniques, including high order elements, adaptive grid refinement, multigrid solution methods, and parallel computing, to the solution of the Schrödinger equation that models this interaction.

For appropriately chosen laser intensities and geometries the lattice sites are approximately harmonic and cylindrically symmetric. This leads to a model for the relative motion of two atoms in a single site by a two-dimensional Schrödinger equation in cylindrical coordinates, i.e., an elliptic eigenvalue problem. The potential function in the Schrödinger equation consists of a short-ranged atom-atom interaction potential, modeled by a Lennard-Jones potential, and a trapping potential that describes the optical well.

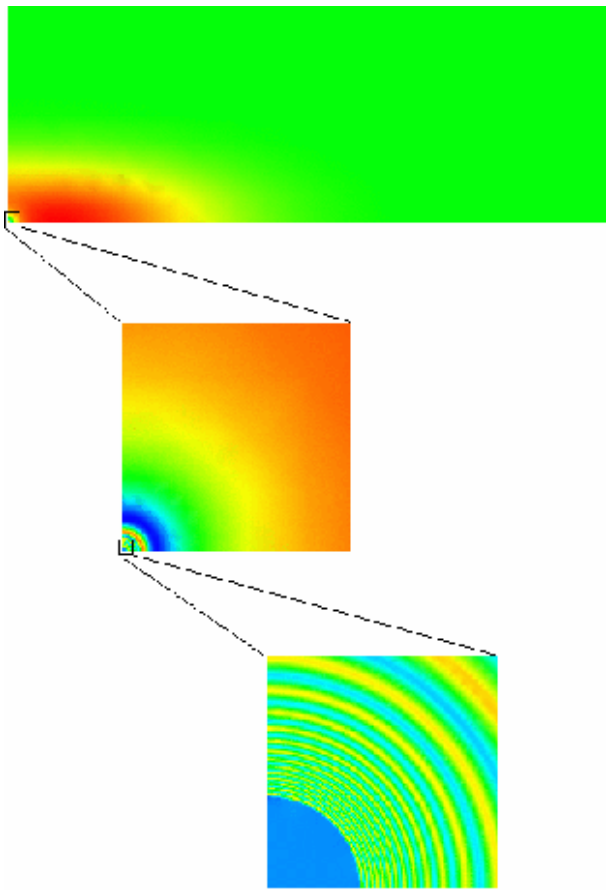

Figure 6. *Contour map of the computed wave function for the first trapping state of a model of interacting Cesium atoms. The large difference in scales between different parts of the wave function is illustrated by two levels of zooming.*

The interest lies in obtaining a small number of wave functions whose eigenvalues are closest to zero. These are called the trap states because they are eigenstates in which the eigenfunction extends from short to large atomic separations and in which the trapping potential plays an important role. Fig. 6 illustrates the nature of

the wave function for the first trapping state of a model of Cesium atoms.

The large difference between the scales of the wave due to the trapping potential, the large red wave in Fig. 6, and the waves due to the interaction potential, the small waves, which are evident through two levels of zooming the image, mandate the use of adaptive grid techniques. An adaptive grid technique begins with a very coarse grid, and then selectively refines elements by computing an error estimate for each element and refining those with large estimates. The process is repeated until a sufficiently accurate solution can be computed. The grid used for the solution shown in Fig. 6 consisted of approximately three million elements. The elements are extremely small in the area where the solution varies rapidly, and large in the outer regions where the solution varies slowly. Such an element distribution can lead to optimal utilization of resources during the solution process. If a uniform grid with elements the size of the smallest elements was used, for example, it would require on the order of 10^{17} elements, clearly showing the need for non-uniform grids for this problem.

Additional improvements in the solution have recently been made through the application of high order elements. Linear elements represent the solution as a piecewise smooth function that is linear over each triangle of the grid. High order elements use a higher degree polynomial on each triangle. Using a p^{th} degree polynomial, the error of the approximation decreases like h^{p+1} where h is the diameter of the element. Thus high order elements give an accurate solution with many fewer grid elements than in the linear case. For another Cesium model, a` solution with 3 accurate digits via linear elements required approximately 4.5 million degrees of freedom. The solution took 35 minutes on a 32-processor parallel computer. Using cubic elements, the same accuracy is obtained with 0.5 million degrees of freedom in 8 minutes on a laptop computer. However, we require much higher accuracy for realistic models. Using 5^{th} degree elements and resources comparable to the linear case, we have obtained solutions accurate to 8 digits.

Further improvements in the solution techniques will be made through our on-going research in the use of hp-adaptivity. In this approach, adaptive refinement is applied not only to the size of elements (h), but also to the polynomial degree over each element (p). The appeal of hp-adaptivity is that the error of the approximation can decrease exponentially in the number of degrees of freedom, whereas with fixed degree polynomials it can only decrease polynomially. Fig. 7 shows the exponential rate of convergence we have obtained for a model elliptic boundary value problem using hp-adaptivity. Polynomial convergence would appear as a straight line on this graph. The curvature of the line obtained by a least squares fit to the data illustrates that exponential convergence has been obtained. In our current research we are developing new error estimates that will allow us to apply hp-adaptive techniques to elliptic eigenvalue problems.

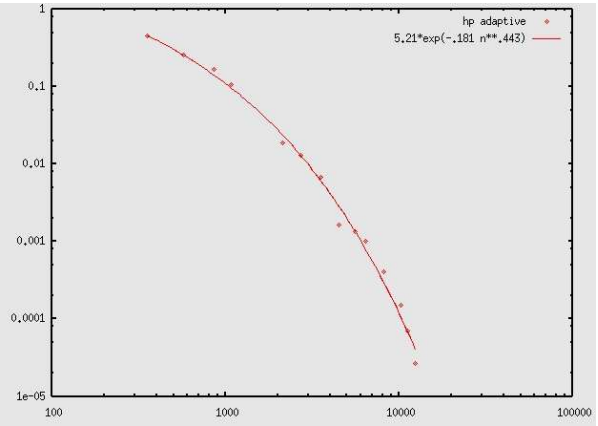

Figure 7. *Exponential convergence of the error vs. degrees of freedom for the hp-adaptive solution of an elliptic boundary value problem.*

With the recent addition of high order elements to our models, we are now beginning to perform numerical experiments on systems relevant to realistic atom traps. Currently we are investigation the effect of varying the scattering length of the interaction potential and eccentricity of the trapping potential on a model of Cesium atoms. 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.

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Participants

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Mathematical Modeling of Nanomagnetism

Measurement, understanding, and control of magnetic phenomena at the nanoscale each require the support of mathematical models of the physics involved, and software that correctly implements and makes predictions based on these models. The Object-Oriented MicroMagnetic Framework (OOMMF) project provides this capability in a public domain package of portable software components organized in an extensible framework. OOMMF software is widely used and cited in the physics and engineering literature. Current objectives are to continue to expand the features supported by components in the OOMMF framework, with focus on high priority items, such as thermal effects and spin transfer, motivated by their relevance to nanoscale sensor and spintronics work.

Michael J. Donahue and Donald G. Porter

Many existing and developing applications of nanotechnology make use of magnetic phenomena. Some of the most familiar and successful examples are information storage technologies such as magnetic recording media, GMR sensors for read heads, and magnetic RAM (MRAM) elements. Computational modeling continues to support advances such as the novel patterned magnetic recording media that promise to achieve recording densities of 1 Tb per square inch.

Applications of nanomagnetism modeling are widespread. For example, modeling was critical to the development of a fully magnetic logic gate and shift register accomplished at University of Durham and recognized by the Institute of Physics as one of the top ten stories in physics for 2002. Other efforts aim to develop logic devices that carry information in the form of the spin of a charge carrier, so called *spintronics* devices. In biotechnology, the use of paramagnetic beads to locate and position biological macromolecules is under study. In materials science, the probing capability of ferromagnetic resonance is used to characterize and measure material properties, where an understanding of nanomagnetodynamics is a key to interpreting experimental results. Other efforts in materials science are aimed at improved sensor designs capable of detecting magnetic fields that are both smaller in magnitude and more localized in space.

In each of these areas, the NIST Object-Oriented MicroMagnetic Framework (OOMMF) system is in use to enable nanoscale science and engineering. OOMMF is a portable public domain package organized in an extensible framework to enable computational simulation of magnetic systems.

One recent example of the use of OOMMF to support nanotechnology R&D is depicted in Fig. 8. An image of 2000 nm diameter ring of ferromagnetic material was produced by a magnetic force microscope (MFM). Such ring elements are proposed for both storage and sensor applications, where their utility is critically dependent on their precise behavior. The colors of the image represent the strength of stray magnetic field sensed at each location scanned above the ring. An MFM directly measures stray field; it does not directly measure the magnetization pattern found in the ring itself. A measured stray field does not uniquely determine what magnetization pattern produced the stray field. Also illustrated is a magnetization pattern computed by OOMMF software based on known parameters chosen to match the experimental work. The pattern of arrows represents the magnetization pattern predicted by the model, and it can be confirmed that the predicted pattern is consistent with the measured stray field. In complementary roles like this, modeling is able to indirectly deduce details of a nanoscale system that are not within the capability of direct measurement.

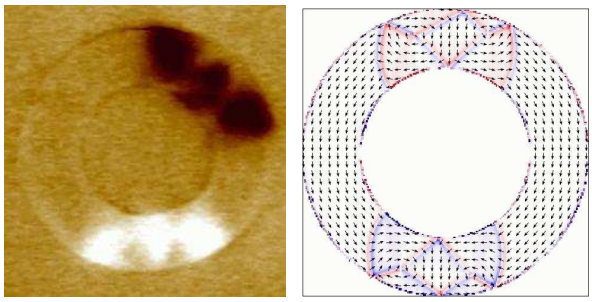

Figure 8. *Left: Image of 2000 nm diameter ring of ferromagnetic material produced by a magnetic force microscope. Right: Magnetization pattern computed by OOMMF based on known parameters chosen to match the experimental work.*

Many of the equations governing nanomagnetism were established long ago. The notable Landau-Lifshitz equation dates back to 1935, and William Fuller Brown established the fundamentals of *micromagnetic modeling* in articles and books published from the 1940s to 1970s. At that time, the applications of the theory were mostly limited to simple geometries that could be attacked analytically. It was not until the 1990s that widespread availability of significant inexpensive computing power made possible micromagnetic modeling for practical problems.

Unfortunately, the accurate solution of the relevant equations is more difficult than many physicists and

engineers realize. By the mid-1990s, many researchers and their students had produced their own simulation programs to support their work. While their publications were careful to list details of experiments and analyses, their home-grown software would typically only merit a high-level description. Usually the equations the software was meant to solve would be noted, but no reports of software testing were provided, and there was no opportunity to review its quality. The problems solved by these computer codes were typically precisely matched to a particular experiment, and it was rare that two independent teams would perform precisely the same computations to enable comparison.

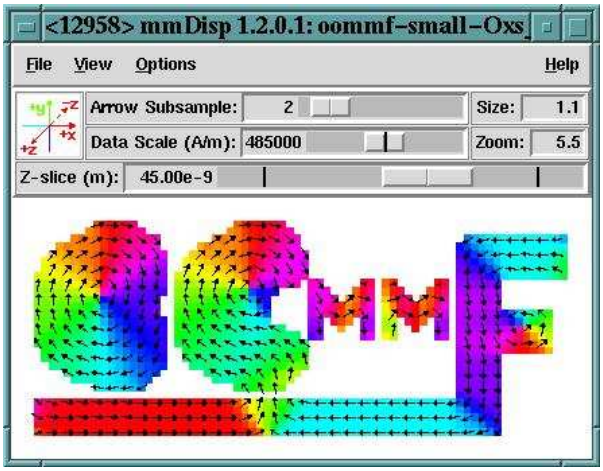

Figure 9. *Part of the graphical user interface for OOMMF.*

In 1996, NIST challenged this research community with a *standard problem*, inviting all those with magnetic modeling simulation software to attempt to compute some properties of a magnetization reversal similar to those routinely reported in the literature at the time, but all starting from the same assumptions. The results were alarming. The number of significantly different solutions almost matched the number of programs. Subsequent research has discovered flaws in both the programs and the problem. An important value of OOMMF is that it provides a transparent benchmark against which any research team developing their own magnetic modeling software can compare their results.

Those researchers for whom OOMMF provides all required modeling capabilities can, of course, also use OOMMF in place of developing their own software. In addition, OOMMF is structured as an extensible framework of software components, so those users who have needs beyond OOMMF's current capabilities can often extend it to meet their needs without the need to rewrite a new software package from scratch.

OOMMF has been remarkably successful in achieving its objectives. OOMMF has been downloaded more than 10,000 times. A growing number of peer-reviewed research publications cite use of OOMMF; more than 300 are listed on the OOMMF web site.

Current plans for OOMMF are to supply additional extension modules and to make improvements to the framework necessary to support the nanomagnetic simulations required in emerging research areas. For example, NIST research in the development of ultra-low field magnetic sensors requires reliable modeling of thermal effects, a component that OOMMF has until now not provided. There is also considerable interest in representing the effects of spin transfer in nanomagnetic systems. In each of these cases, research is active into determining the correct models.

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`http://math.nist.gov/oommf/`

Stability of Nanowires

Metallic or semiconductor nanowires are important components in many electronic technologies. At small length scales many materials exhibit unusual electrical, chemical, and thermal properties that are not observed in the bulk. Applications include novel electronic devices ranging from high efficiency lasers and detectors to exotic single electron transistors and cellular automata. The tendency of nanowires to fragment into nanospheres due to area-minimizing surface instabilities acts as a limit to the length of nanowires that can be used in nanodevices. This instability can also be used beneficially as a mechanism for the self-organization of chains of nanospheres from unstable nanowires. We have studied analytically the effect of surface tension anisotropy on this instability in order to help understand and control nanowire fragmentation. Our analysis predicts the wavelengths of the instability as a function of the degree of anisotropy of the surface energy of the nanowire.

Geoffrey McFadden

At the small length scales that characterize nanostructures, the importance of surface effects relative to volume effects becomes significant. Typical surface effects that can be important at the nanoscale include surface energy or capillarity, surface diffusion, surface adsorption, and surface stress and strain. In particular, the effects of capillarity must be taken into account in order to understand the tendency of nanowires to fragment when the rate of surface diffusion of atoms is high enough to allow shape changes to occur over practical time scales.

As shown by Plateau in his classical studies of capillary instabilities, a cylindrical interface with an isotropic surface free energy is unstable to volume-preserving axisymmetric perturbations whose wavelength exceeds the circumference of the cylinder. Such perturbations lower the total energy of the cylinder, leading to the breakup of the cylinder into a series of drops or bubbles. The stability of a liquid jet was subsequently studied by Lord Rayleigh, who argued that the length scale of the instability is determined by the perturbations having the fastest growth rate; the phenomenon has generally come to be known as the Rayleigh instability. The Rayleigh instability arises in a number of diverse applications, such as ink jet printing, two-phase flow, quantum wires, fiber spinning, liquid crystals, and polymer blends.

Because of the underlying crystal lattice, the surface energy of a liquid-solid or vapor-solid interface is generally anisotropic and depends on the orientation of the local normal vector at each point of the interface. The surface energy of a solid-solid interface between two crystals is also anisotropic in general, with the additional complication that the surface energy also depends on the direction cosines that characterize the relative orientations of the two crystals. Here we have considered a model of this type in which the surface energy depends only on the local normal vector.

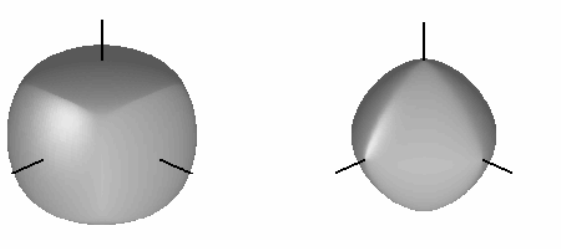

Figure 10. *Equilibrium shapes for materials with cubic anisotropy. These shapes are energy minimizing surfaces that are the anisotropic versions of soap bubbles (the isotropic case).*

An observation that partially motivates this work is the apparent stability of elongated nanowires that are grown in a bridge configuration or epitaxially on a heterogeneous substrate. The nanowires (alternatively called nanorods or quantum wires) are "one-dimensional" crystals with dimensions as small as one nanometer high, a few nanometers wide, and can be as long as a micron. There are long-standing studies on experimental techniques to grow nanowires, and the stability of these nanowires is beginning to come under study. Another motivation for the work is the recent observation that the Rayleigh instability of a nanowire can be used to produce self-organized chains of nanospheres with interesting electrical and opto-electronic properties. In either case it is desirable to develop models to predict the length scales of the instabilities in order to assess the geometry of the resulting structures.

Continuum modeling of nanowires provides some guidance as to their expected stability, though the strict applicability of continuum models is limited if the length scales approach atomic dimensions. There are a number of possible mechanisms that could stabilize a nanowire, including elastic interactions between the wire and the substrate, quantum electronic shell effects, and surface energy anisotropy. A useful model of the surface energy anisotropy for a cubic material is given by the expression $\gamma(n_x,n_y,n_z) = \gamma_0 [1 + 4 \varepsilon (n_x^4 + n_y^4 + n_z^4)]$. In the above figure we show examples of 3D equilibrium shapes co responding to this surface energy. The shapes are smooth for $-1/18 < \varepsilon < 1/12$. For $\varepsilon < 0$, the shapes resemble rounded cubes, with

[110] edges first forming at $\varepsilon = -1/18$. As ε decreases below $-1/18$, the edges extend toward the [111] directions, merging to form a corner for $\varepsilon = -5/68$. For $\varepsilon > 0$ the shapes are octahedral, with [100] corners first forming at $\varepsilon = 1/12$. These equilibrium shapes are most easily computed using the ξ-vector formalism of Hoffman and Cahn, which produces a closed-form expression for the equilibrium shape in terms of the surface energy. This is also useful in formulating the variational problem for the stability of a nanowire.

In collaboration with K. Gurski, George Washington University, and M. Miksis, Northwestern University, we have considered differentiable surface energies with anisotropies mild enough that the surface of the wire is smooth and does not exhibit any missing orientations. In order to examine the stability of the wire using a variational approach, we employ a general energy functional that describes the total surface energy of the system. This expression and the constraint of constant volume of the wire are perturbed about the two-dimensional equilibrium shape. The higher order terms in this perturbation expansion produce a condition for stability. For constant volume, if the perturbation increases the energy, the equilibrium state is stable, otherwise it is unstable.

Figure 11. *Capillary instability of a nanowire with an anisotropic surface energy with three-fold symmetry about the wire axis.*

For small levels of anisotropy, we evaluate the stability of an isolated nanowire approximately using asymptotics. For larger amplitudes of anisotropy, we compute solutions numerically. We find that surface tension anisotropy can either promote or suppress the Rayleigh instability, depending on the orientation of the nanowire and the magnitude and sign of the anisotropy. For general surface energies we derive an associated eigenproblem whose eigenvalues govern the stability of the wire. The eigenproblem is described by a pair of coupled second-order ordinary differential equations with periodic coefficients, which generally lack closed-form solutions. We have applied the analysis to a number of examples, including the above case of a cubic material. We have computed the stability of the wire to general perturbations when the axis of the wire is in a high symmetry orientation such as [001], [011], or [111].

In addition to determining the stability of an isolated wire, we have also examined how both the anisotropy of the surface energy of the wire and the interaction of the wire with a substrate affects the stability of the rod. The equilibrium configuration of a wire in contact with a substrate has an elegant description that can be obtained by again appealing to the Hoffman-Cahn ξ-vector formalism. This approach determines the contact angles in terms of the surface energies of the phases that meet at the contact line. Using general anisotropic surface energies we have then derived an associated eigenproblem that describes the stability of the system. The problem is described by a pair of coupled second-order ordinary differential equations with periodic boundary conditions along the axis of the rod and boundary conditions arising from the contact angles between the wire and substrate. We have considered the effects of the overall orientation of the crystal relative to the substrate and examined a range of contact angles. The substrate is assumed to be rigid with an isotropic surface energy.

We applied the analysis to a number of examples, including the case of a cubic material, and compute the stability of the wire to perturbations when the axis of the wire is aligned parallel to the high symmetry orientations [001], [011], and [111]. We assumed a weak anisotropic surface energy to eliminate missing orientations on the wire. The magnitude and the sign of the anisotropy determine the relative stability in comparison to the isotropic case. In general as the contact angle tends to 90 degrees the wire becomes more stable, which is analogous to the stability of a 3D planar film.

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Participants

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Improving Image Resolution in Nanotechnology

Current nanoscale electron microscopy images remain of relatively low quality. To address this issue we are developing improved mathematical tools for image analysis, and the use of such tools to provide measurable increases in resolution in state-of-the-art scanning electron microscopy. One very major difficulty lies in the large image sizes, often on the order of 1024×1024 pixels, or larger. This presents formidable computational challenges. Many new techniques are based on nonlinear partial differential equations, and typically require thousands of iterations, and several hours of CPU time, to achieve useful results. Real-time image processing algorithms are exceedingly rare and very highly sought after.

Alfred Carasso

A fundamental problem in scanning electron microscopy (SEM) is the fact that the shape of the electron beam that produced the image is seldom known to the microscopist. Therefore, image deblurring must proceed without knowledge of the actual point spread function that caused the blur. Such so-called *blind deconvolution* is fraught with difficulty, and little authoritative discussion of this subject is to be found in most image processing textbooks.

Nevertheless, in recent years, considerable progress was achieved at NIST in developing mathematical technologies that lead to real-time image processing algorithms. In addition, a unique new capability has been created, the so-called *APEX method*, that can achieve useful blind deconvolution of 1024×1024 SEM imagery in about 60 seconds on current workstations. Because of its manifold applications, this technology is the subject of intense and continuing research and development.

The APEX Method

The APEX method is an FFT-based direct blind deconvolution technique that can process complex high resolution imagery in seconds or minutes on current desktop platforms. The method is predicated on a restricted class of shift-invariant blurs that can be expressed as finite convolution products of two-dimensional radially symmetric Lévy stable probability density functions. This class generalizes Gaussian and Lorentzian densities but excludes defocus and motion blurs. Not all images can be enhanced with the APEX method. However, we have shown that the method can be usefully applied to a wide variety of real blurred images, including astronomical, Landsat, and aerial images, MRI and PET brain scans, and SEM images. APEX processing of these images enhances contrast and sharpens structural detail, leading to noticeable improvements in visual quality.

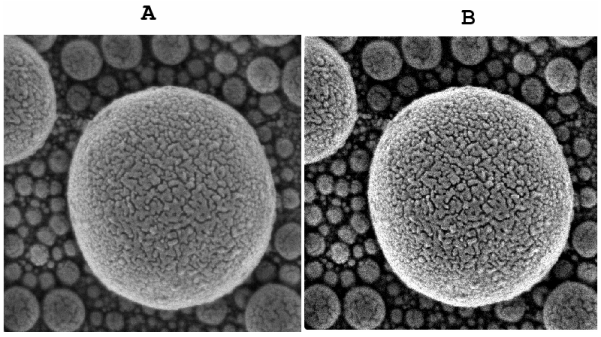

Figure 12. *APEX blind deconvolution of state of the art Scanning Electron Microscope imagery produces measurable increases in sharpness. (A) Original 1024x1024 Tin sample micrograph has Lipschitz exponent* $\alpha = 0.40$ *and TV norm = 13000. (B) Sharpened image has* $\alpha = 0.29$ *and TV norm = 34000.*

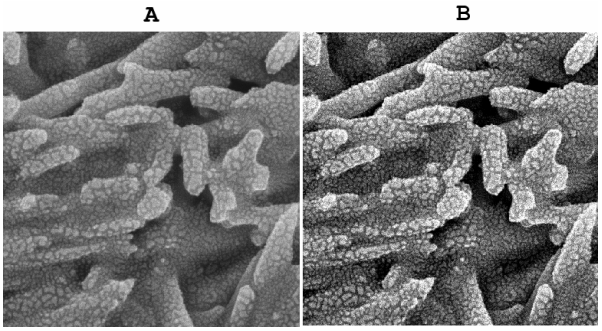

Figure 13. *APEX sharpening of SEM imagery. (A) Original 1024x1024 Magnetic Tape sample has* $\alpha = 0.35$ *and TV norm = 14000. (B) Sharpened image has* $\alpha = 0.26$ *and TV norm = 39000*

Application to SEM Imagery

Recently, a new Hitachi Scanning Electron Microscope was acquired by the NIST Nanoscale Metrology Group, capable of producing higher quality imagery than had previously been possible. A major challenge for our deconvolution algorithms was to demonstrate measurable increases in sharpening of such state of the art imagery. Two sharpness measures were used, the image Lipschitz exponent α, and the image discrete *total variation* or TV norm. Image sharpening increases the TV norm, due to the steepening of gradients, while it decreases the Lipschitz exponent as finer scale features become resolved. Examples of such sharpening are shown in Figs. 12 and 13. In Fig. 12A, the original *1024×1024* Tin sample micrograph has TV norm of 13000 and Lipschitz exponent $\alpha = 0.40$. The APEX-sharpened Fig. 12B has TV norm =

34000 with $\alpha = 0.29$. In Fig. 13A, the original *1024×1024* Magnetic Tape sample has TV norm = 14000 with $\alpha = 0.35$. The APEX-processed Fig. 13B has TV norm = 39000 with $\alpha = 0.26$. These very substantial sharpness increases are typical of those obtained in numerous other test images.

Measuring Image Smoothness

Most commonly occurring images $f(x,y)$ are not differentiable functions of the variables x and y. Rather, these images display edges, localized sharp features, and other fine-scale details or *texture*. Many digital image-processing tasks require prior specification of the correct mathematical function space in which the true image lies. If an image is incorrectly postulated to be too smooth, the processing algorithm may produce an overly smoothed version of the true image in which critical information has been lost.

During the last 10 years, a very considerable amount of image analysis research has been based on the assumption that most images belong to the space of functions of bounded variation. However, it has been subsequently discovered that such so-called total variation (TV) image processing sometimes results in unacceptable loss of fine-scale information. This phenomenon is now known as the *staircase effect*. In papers published in 2001, French researchers Gousseau, Morel, and Meyer, showed that most natural images are, in fact, not of bounded variation, and that TV image-processing techniques must inevitably smooth out texture.

Correct characterization of the lack of smoothness of images is a fundamental problem in image processing. It turns out that so-called *Lipschitz spaces* are the appropriate framework for accommodating non-smooth images. The L^P Lipschitz exponent α for the given image, where $0 < \alpha < 1$, measures the fine-scale content of that image, provided the image is relatively noise free. Heavily textured imagery has low values for α, while large values of α indicate that the image is relatively smooth. Estimating an image's Lipschitz exponent is a delicate problem. We have developed a new, computationally efficient, method for estimating α. It merely requires blurring the image by convolution with a specific singular integral kernel, and evaluating the discrete L^P norm of the difference between the blurred and original images. The rate at which this L^P norm tends to zero, as the kernel approaches the Dirac δ-function, is directly related to the Lipschitz exponent α. Since the required convolutions can be accomplished by FFTs, very minimal computational effort is thus needed to implement the resulting procedure. In addition, this approach has the advantage of allowing consideration of substantially wider Lipschitz spaces than is mathematically possible with existing procedures, thereby encompassing a much wider class of images.

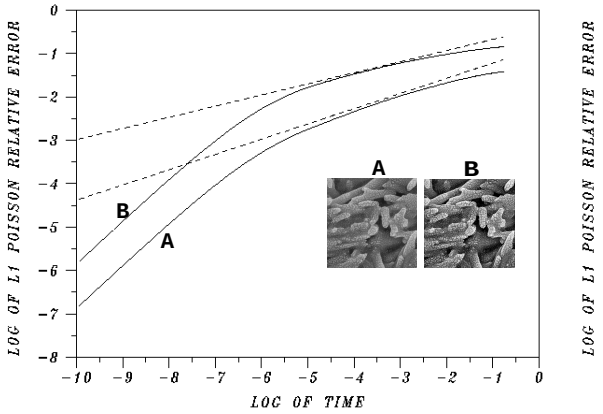

Figure 14. *The Lipschitz exponent α in an image can be obtained by plotting* $\log(\|U^t f - f\| / \|f\|)$ *versus* $\log t$ *as t tends to zero, where U^t is the Poisson kernel with width t. The slope of dashed line which asymptotes the solid trace for* $-6 < \log t < 0$ *is the Lipschitz exponent. Here, the original SEM image A has $\alpha = 0.35$. The APEX processed image B reveals more fine scale structure and has lower $\alpha = 0.26$. (See Fig. 13 for larger images of A and B.)*

Significant potential applications of this technology include the routine monitoring of image sharpness and imaging performance in electro-optical imaging systems, the performance evaluation of image reconstruction software, the detection of possibly abnormal fine-scale features in some medical imaging applications, and the monitoring of surface finish in industrial applications. In addition, specifying the correct Lipschitz space wherein an image lies can be used to solve the blind image deconvolution problem in a way that preserves texture, i.e., fine detail, in a recovered image. We recently have developed a new method, the Poisson Singular Integral (PSI) method, which yields an excellent approximation to optimal image filtering for a very wide class of images.

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Participants

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Creating Visual Models of Nanoworlds

The place where quantum and macro effects meet, the nanoworld is full of the unexpected. In such an environment, visual models of laboratory and computational experiments can be critical to comprehension. We are developing an immersive visual modeling system that enables scientists to easily view and interact with their data in multiple ways in real time.

Howard Hung, Steve Satterfield, James Sims, Adele Peskin, John Kelso, John Hagedorn, Terrence Griffin, and Judith Terrill

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Computational and laboratory experiments are generating increasing amounts of scientific data. Often, the complexity of the data makes it difficult to devise *a priori* methods for its analysis, or the data is from new landscapes, such as the nanoworld, where we have little experience. Moreover, there may be ancillary data, from databases for example, that would be helpful to have available. We are developing visual analysis capabilities in an immersive environment that allow scientists to interact with data objects in a three-dimensional landscape rather than simply viewing pictures of them. 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. With visual exploration, scientists can easily perceive complex relationships in their data, quickly ascertaining whether the results match expectations. Real time interaction adds to the potential for speeding the process of insight.

In a fast moving field like nanotechnology, it is important to be able to create and interact with new visual models quickly. Our visual environment is built for generality, flexibility and speed. Rather than a single monolithic program, it is a collection of tools designed to work together to create, display, and interact with visual models. We have created three main categories of tools: infrastructure software, representation software, and scene interaction software. We join programs together using Unix pipes and filters for creation and transformation. We construct Dynamically Shared Objects (DSO's) for functionality, and scenegraph objects for ease of placement.

DIVERSE

Our visual environment centers around a core infrastructure program called DIVERSE (Device Independent Visualization Environment – Reconfigurable, Scalable, Extensible). DIVERSE, which was developed by Virginia Tech with support and technical contributions by NIST, is an interface that facilitates the development of immersive computer graphics programs for use on a wide variety of graphics displays. DIVERSE provides a toolkit to load in previously compiled objects, called DSOs. DSOs can be used to describe the graphics display, input devices, navigation techniques or interaction styles for a given visualization. Using collections of DSOs, applications can be reconfigured without recompiling. The same DSO that defines how a wand controls an object can be used both in an immersive environment and on a laptop computer. With the ability to import the output of conventional visualization programs, and access to the increasing capabilities of commodity graphics cards, we have a very rich environment in which to express and communicate visual models.

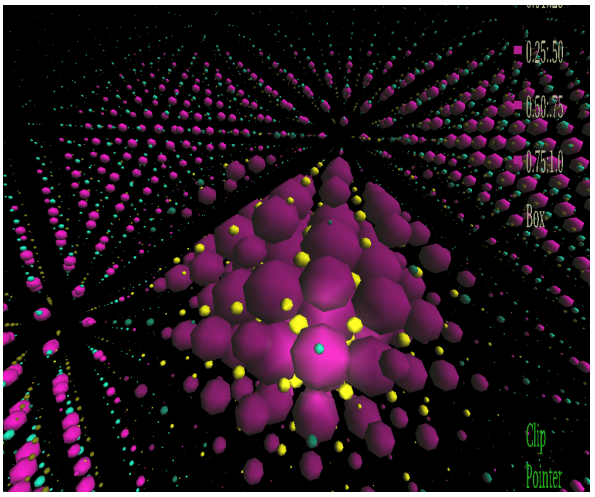

Figure 15. *Image of a quantum dot created from the output of a computer simulation of the optical properties of nanostructures. The spheres represent s-orbitals.*

Representation

Representation refers to the process of transforming raw data into a visual geometric format that can be viewed and manipulated. The key to quickly and easily visualizing scientific data in an immersive environment is the capability provided by the set of tools used to convert raw data to immersive data. We have created a variety of tools to make glyphs, color them, place them, and render them to a desired level of transparency and other properties. While our system is based on our own internal representation, we take

advantage of representations computed by other packages by providing tools to take the output of common packages and convert them into the format that places them in our environment.

Interaction

For efficient scientific exploration, it is important to have user interaction that is both easy to set up and easy to adapt to differing needs. Individual DSOs that add new functionality to our visualization software system are loaded at run-time, and their behavior is cumulative. Together, a set allows for a huge range of combinations data visualization modes. We have developed a wide range of DSOs that allow a user to interact with the objects to be viewed. This includes functionality to move objects around, select individual objects or sets, assign functionality to the selections, interact with outside software, bring data into the system, send data out of the system, and load or unload objects during visualization. They can also interactively select the level of detail in a scene. Individual DSOs can add simple capability to a scenegraph, such as adding a particular light source or an object to represent a pointer for the user to select objects. DSOs can also add tasks to the objects of a scenegraph. When selected, an object can be given the task of turning on or off another object or itself, or executing a command to interact with another DSO or an external program. Objects can change visibility, initiate new simulations, define clipping planes, and so on. DSOs provide a variety of ways to navigate through the environment, including changing the scale at will. They allow viewing of individual scenes as well as time sequences (i.e., movies). The output of an interaction can be saved as a simple image, as a movie, or the interaction itself can be saved as an experience that can be replayed at a later time.

Applications to the Nanoworld

We have successfully applied our visual analysis techniques and tools to the study of a variety of nanoscale phenomena. Among these are visual analyses of

- s-orbitals for the simulation of electronic and optical properties of complex nanostructures such as semiconductor nanocrystals and quantum dots (see Fig. 15),
- electric, magnetic, and energy field vectors from the simulation of optical scattering by metamagnetic materials (see Fig. 16),
- intermediate voltage electron microscope measurement approaches to attain three-dimensional chemical images at nanoscale-resolution, and
- dynamics of molecular interactions leading to the formation of smart gels.

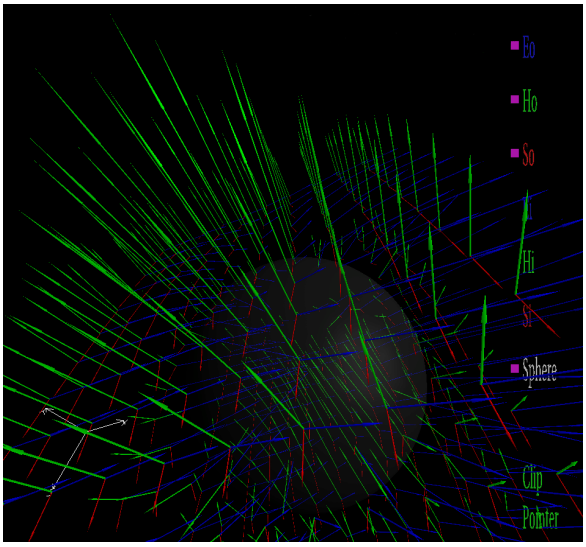

Figure 16. *Image of the electric, magnetic, and energy field vectors in a single time step in the simulation of resonant optical scattering by metamagnetic materials.*

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Participants

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`http://math.nist.gov/mcsd/savg/vis/`

Measurement Science in the Virtual World

We are developing tools for selection and measurement from within the immersive visualization environment. These visualizations and their accompanying analyses then yield quantitative results that extend the qualitative knowledge that is the typical product of visualization.

John Hagedorn, Adele Peskin, John Kelso, Steve Satterfield, and Judith Terrill

Laboratory experiments, computational experiments, measurement, analysis, and visualization are typically separate activities. This slows down the rate at which knowledge is gained. Combining them, where feasible, yields greater efficiency, and the resulting synergy can deepen understanding. We are working on combining measurement, real time immersive visualization, and analysis. Our immersive visualization environment is the main tool which enables this.

It is not always possible to perform desired measurements on laboratory data during the course of a physical experiment. For example, a reconstruction phase may be needed to get the data into a form where it can be measured. An example is tomographic reconstruction. The same is true for computational experiments. While measurements are typically gathered during runs, there are also many reasons why measurements may need to be taken during the analysis stage. Measurement from within the immersive environment provides unique capabilities in this regard. We are working to use these capabilities to enable such virtual measurements to be taken both during and after laboratory and computational experiments.

To bring measurement science into the virtual world we need the objects in the environment to be drawn and positioned with higher precision than is typical in applications of immersive virtual reality. To do this we first need the virtual space to be calibrated. Then we need to be able to select and measure properties of objects. Finally, we need to be able to operate on those measurements and relate them to both the immersive environment and the real world. We describe our approach to each of these in turn.

Calibration

The use of motion tracking devices is essential in immersive visualization systems. The location and orientation of the user's eyes must be continually tracked so that the system can render images of the virtual world, in stereo, in real-time. In addition, motion tracking is also commonly used to track hand-held devices (e.g., a wand) that operate as tools in the virtual world created within the immersive display.

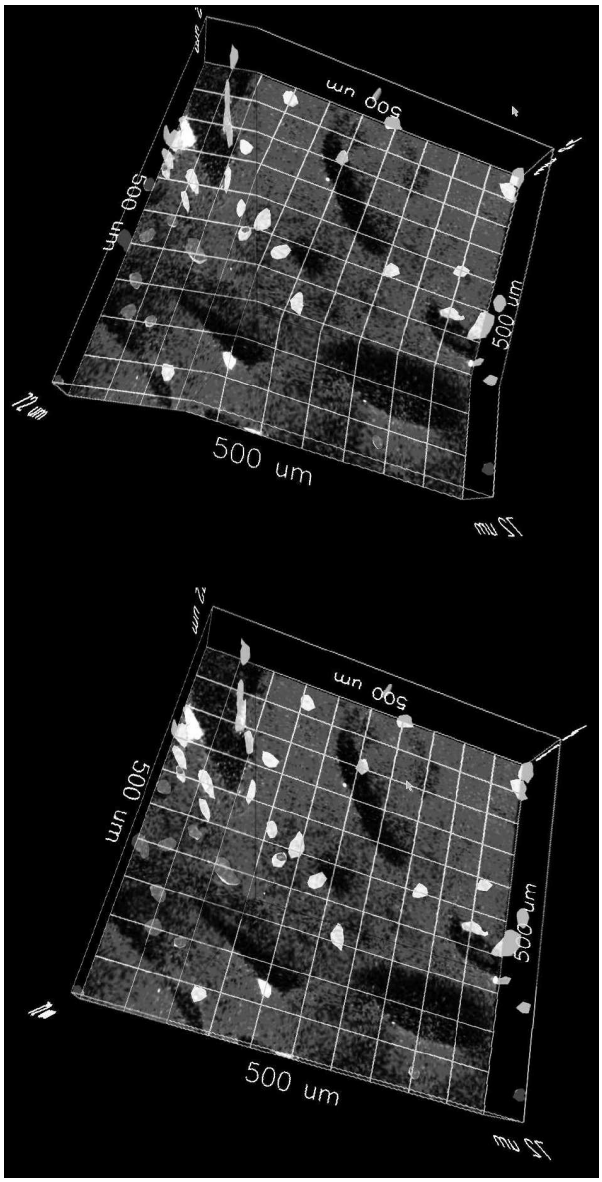

Figure 17. *The top image shows visual artifacts due to tracker error. The bottom image shows the same scene with tracker data corrected.*

Environmental factors such as the presence of metallic objects and electromagnetic fields generated by video monitors contribute substantially to errors in measurements reported by electromagnetic tracking devices. We have developed a method for calibrating and correcting location and orientation errors from electromagnetic motion tracking devices. This includes a new algorithm for interpolating rotation corrections at

scattered data points. This method, unlike previous methods, is rooted in the geometry of the space of rotations. Results have shown large improvements in the precision of both location and orientation measurements. The methods impose minimal computational burden.

Selection, Measurement, and Analysis

We have developed a capability for linear measurements in the immersive environment. Our objective is to build a software system within the environment that integrates the following tasks: (1) linear measurement, (2) analysis of the collected measurements, (3) display of the results, and (4) interactions with the data and analyses that will enable grouping of results. The goal of these tasks is to achieve greater understanding by generating quantitative results.

There are two main components to our implementation. The first is software that allows the user to manually make a series of linear measurements in the immersive environment. The second is a standardized 2D user interface displaying the measurement statistics and distribution in tabular and histogram form.

Our main objective in designing the user interface was to make the 3D measurement task direct and natural. The user makes a linear measurement simply by moving the hand-held wand to a point in the 3D virtual space, pressing a button on the device, then moving to a second point and pressing the button again. Visual feedback is given at each step of the process and the user is able to adjust each end point simply by grabbing it with the wand and repositioning it. The process is fast, simple, and intuitive. A user interface enables one to bring the measurements into an analysis and to display the results. In Fig. 18, the user has made measurements (shown in blue). The measurements have been brought out of the environment and a mean and standard deviation computed. They are also shown as a histogram in the upper right. Portions of the histogram can be selected and highlighted back in the immersive environment for a better understanding.

We have found that immersive visualization enables both qualitative and quantitative understanding of 3D structure that was not otherwise possible. These types of measurements made in the virtual environment would be very difficult to make with typical desktop visualization techniques. We are planning a variety of extensions to our selection and measurement capability for the future.

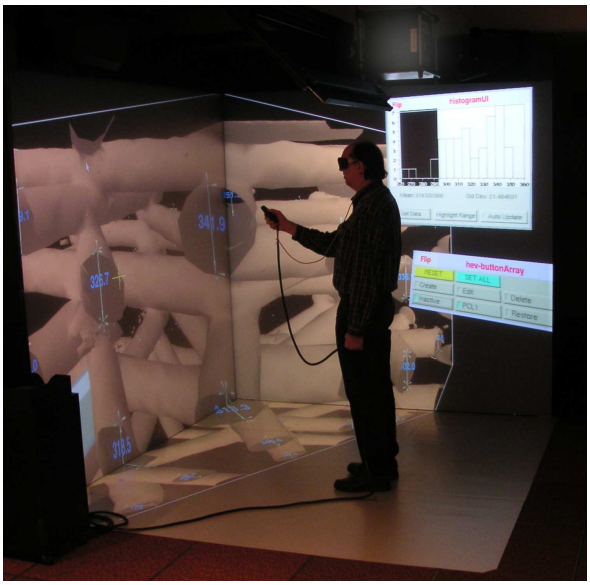

Figure 18. *A user in the NIST immersive visualization environment making measurements on a scaffold for tissue engineering. The measurements are shown in blue. The histogram of results is shown in the upper right.*

Current Applications

We are currently working on a variety of applications spanning several disciplines.

- Reference scaffold for Tissue Engineered materials
- Correlate microstructure with global properties of hydrating cement
- Particle identity and distribution at the nanoscale
- Stress and strain at the nanoscale

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Participants

J. Hagedorn, A. Peskin, J. Kelso, S. Satterfield, J. Terrill (MCSD); J. Dunkers, L. Henderson (MSEL)

Identifying Objects in LADAR Scanning Data

Laser scanning technology has developed into a major tool for geographic and geometric data acquisition. We are investigating the feasibility of using such technology for monitoring construction sites. A core problem in the analysis of such data is object recognition. Recently we demonstrated a technique for identifying particular objects, such as I-beams in noisy LADAR scanning data.

David Gilsinn

During the past decade, laser-scanning technology has developed into a major vehicle for wide-ranging applications such as cartography, bathymetry, urban planning, object detection, and dredge volume determination. One advantage of such scanning data is that it can provide information on spatial relationships that ordinary photography cannot. The NIST Building and Fire Research Lab (BFRL) is investigating the use of such technology to monitor progress of work on construction sites. Here laser scans taken from several vantage points are used to construct a surface model representing a particular scene. A library of 3D representations of construction site objects, obtained from CAD data sets, would also be used. The objects would be loaded into an associated simulation system that tracks both equipment and resources based on real-time data from the construction site obtained from laser scans.

Pick-and-place control of construction site objects is a major application. With automation and robotics entering on construction site scene, vision systems, such as LADAR (laser direction and ranging), will be incorporated for real time object identification, based on 3D library templates. Once objects, such as I-beams, are located, robotic crane grippers can be manipulated to acquire the I-beam. We are developing and testing algorithms for this particular task.

LADAR scans of I-beams of multiple lengths and angular poses relative to the scanning LADAR have been generated (see Fig. 19). A database of design specifications for potential I-beam candidates has been created. The LADAR scans generate a large number of points, ranging in the millions, which can be acquired seconds. These scans usually contain a large number of noisy data values arising from ground hits to phantom pixels caused by beam splitting at sharp edges.

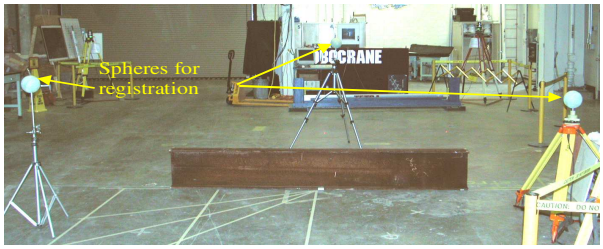

Figure 19. *Experimental configuration for scanning an I-beam by a LADAR placed at the camera location. The white lines on the floor are alignment marks for setting the I-beam at different angles relative to the LADAR. The spheres on the tripods are located for coordinate registration with a world coordinate system.*

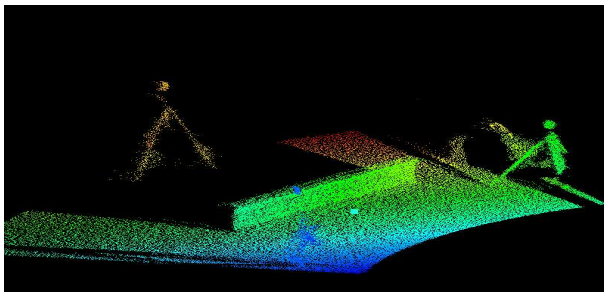

Figure 20. *The results of a scan of the I-beam in Fig. 19. The flat areas on either side of what appears to be the I-beam are floor hits. Notice the results of hits on the three tripods, one of which is seen as somewhat of a shadow in the lower middle of the scene. Also note the occlusion shadowing.*

Fig. 20 shows a typical LADAR scan. Whereas the photograph in Fig. 19 provides a clear image it does not provide coordinate information. Although each of the points in the figure are associated with an (*x, y, z*) coordinate relative to the LADAR, the identification of the nature of the objects scanned is quite difficult. The challenge is to use the database of design specifications, in this case of I-beams, to locate an object in the scanned image and to report its center-of-mass location and angular pose relative to the LADAR.

Three main tasks must be performed: segmenting the data points into groups corresponding to likely objects, identifying the segmented objects with the highest likelihood of being the object sought, and registering the object relative to a world coordinate system so that the LADAR scan can be related to a global coordinate system in which other objects are potentially located.

Segmentation Algorithms

Two algorithms have been developed. The first uses binning of the scanned points to reduce data volume. The bins are then examined to identify those that are likely to be phantom points or floor hits. Phantom points are coordinate points generated by the LADAR due to the internal process of averaging the returned beam signal. Due to the finite size of a LADAR beam,

a targeted point at the edge of an object can lead to a partial signal returns from both the object and a more distant one. The entire signal is averaged and a coordinate point returned somewhere between the two.

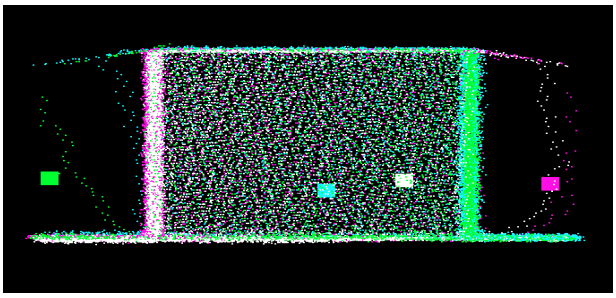

Figure 21. *Anomalies from scanning a box from different directions. Phantom points off of the top edges are seen as two lines beginning at the edges. Phantom points along the sides of the box are due to the averaging of LADAR hits along the sides of the box.*

In Fig. 21 a line of phantom points is seen emanating from the top edges of the test box. Phantom points due to hits along the edges are also visible. Bins that include phantom points and floor hits can be eliminated since they are likely to be sparsely populated. Object identification occurs when the bins are grouped into potential objects and bounding boxes are placed around them. These boxes are compared with bounding boxes defining I-beams in the database and the best fit is reported, along with the center-of-mass and pose of the bounding box. An example of the bounding box placed around the I-beam is shown in Fig. 22.

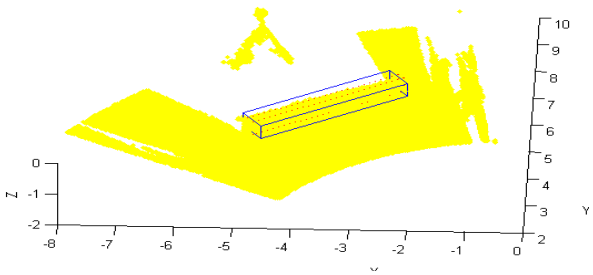

Figure 22. *Bounding box around the I-beam scanned in Fig 20.*

The second algorithm uses Triangulated Irregular Networks (TINs) to mesh the data. The density of the triangulated points is then visually examined to identify those triangle groups most likely to form objects. A TIN of the data in Fig. 20 is illustrated in Fig. 23. The bounding box procedure for object identification is then applied as before. Further work is needed with this algorithm to eliminate manual density inspection.

Evaluation

In order to determine the accuracy of the predicted pose of the I-beams, measurements at the four upper corner points of the I-beams were made using a laser-based Site Metrology System (SMS) developed by BFRL. These reference points were used to measure the performance of the algorithms in their ability to locate the points. The binning algorithm performed well in identifying length of the I-beam, the location of the center of the I-beam, and the angle relative to the LADAR scan direction until the I-beam's major axis was placed at 30 degrees and 0 degrees relative to the scan direction. Thus as the major axis of the I-beam became more aligned with the scan direction of the LADAR the algorithm had a harder time identifying the I-beam. The TIN algorithm performed better than the binning algorithm as the I-beam axis became aligned with the scan beam direction. However, as in the binning algorithm the TIN algorithm could not identify the I-beam when the major axis was aligned with the scan beam.

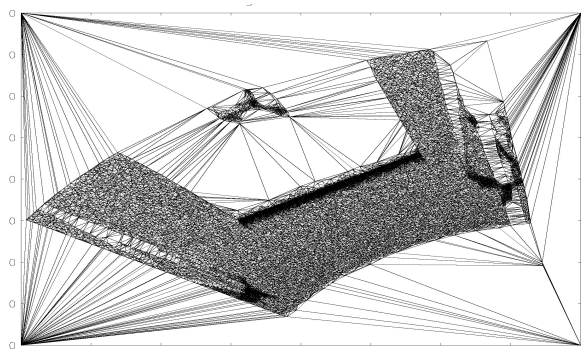

Figure 23. *TIN image of the data in Fig 20. The density of triangles can be used to locate the I-beam and reference sphere tripods.*

Future work will involve extending the bounding box concept to other shapes such as polygons, cylinders, etc. in order to develop a general comparison algorithm that covers most objects located at construction sites, such as vehicles, gas cylinders, etc.

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Participants

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Part III

Project Summaries

Mathematical Knowledge Management

Digital Library of Mathematical Functions

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30 authors under contract
25 validators under contract

http://dlmf.nist.gov/

Mathematical functions, from the elementary ones like the trigonometric functions to the multitude of special functions, are an integral part of all modern developments in theoretical and applied science. They are used to model natural phenomena in fields from quantum theory to astrophysics, formulate problems and solutions in engineering applications, and support numerical computations. To make effective use of mathematical functions, practitioners must have ready access to a reliable catalog of their properties.

Traditionally, in all fields of science, catalogs of relevant properties have existed in the form of massive published handbooks. These are still being produced and can be found on the desks of working scientists. Recently, however, the Web is showing great promise as a more advantageous method. A big potential advantage is that scientists can begin to integrate handbook data into documents and computer programs directly, bypassing any need for time-consuming and error-prone reentry of the data and providing for much richer interconnections between data (hypertext), possibilities for annotation, and so on. Another advantage is high-resolution graphics that users can rotate and view from any angle, giving them an unprecedented way of visualizing the complex behavior of mathematical special functions.

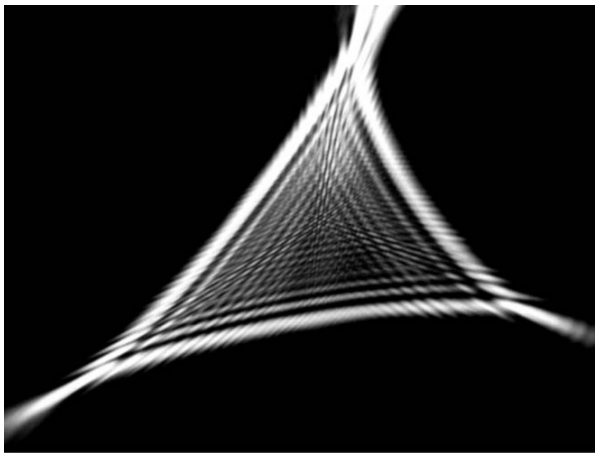

Figure 24. *A thin beam of light refracted by an irregularity in bathroom-window glass produces this image on a distant screen. The bright sharp-edged triangle is a caustic, that is, a line of focused light. The oscillating intensity of the interference fringes across the caustic is described by the Airy function. (Photo complements of Michael Berry, University of Bristol.)*

The Digital Library of Mathematical Functions has two main goals. First, we are reviewing the published literature on special functions, selecting the properties most relevant to current applications, and publishing an up-to-date handbook of the traditional sort. The most recent comprehensive handbook was published in 1964 by the National Bureau of Standards. Still in print and in widespread use, it is badly out-of-date with respect to recent mathematical research, current scientific applications of special functions, and computational methods. Second, we will disseminate the same information, with significant augmentations, from a Web site at NIST. The augmentations include live links to available online software and references, a math-aware search capability, a facility for downloading formulas into word processors and computer software systems, and interactive visualizations.

The project is large, and the contributors fall into several categories. The *editorial board* consists of 4

principal and 8 associate editors. They are responsible for the selection and presentation of the technical information in book and Web formats. Since the beginning of the project, the principal editors have met frequently to review progress and to make midcourse corrections when necessary. *Authors* consist of expert individuals selected for their published research achievements and their ability to write for the intended audience of scientists, engineers and mathematicians. Their contributions are being carefully edited and, in many cases, extensively revised by the principal editors to achieve uniformity of content and presentation across all 38 chapters. *Validators*, like the authors, consist of expert individuals selected for their research accomplishments. Their responsibility is to check the work of the authors and editors. This is a vital step to uphold the worldwide reputation of NIST as a reliable source of accurate, useful and timely scientific reference information. The *project staff* consists of highly qualified mathematicians and computer scientists whose responsibilities, broadly, are (i) construction of a mathematical database that encodes the entire technical content of the DLMF, (ii) application of advanced visualization methods and tools that enable users to display and manipulate complex functional surfaces, (iii) development of software tools to facilitate the production of the book and Web site, (iv) research into advanced techniques for the faithful translation of mathematical formulas and facts among different computer systems, and integration of software tool prototypes into the DLMF Web site, (v) research into the frontiers of technical search methodology to make possible effective queries involving fragments of technical mathematics, and integration of a math-aware search tool into the DLMF Web site. The *support staff* consists of individuals capable in the use of advanced mathematics document processors, symbolic and numerical computation packages, and bibliographic tools such as the ones provided by the American Mathematical Society.

The current status is that complete drafts of 37 chapters are in hand from the authors, and initial reports for 16 of these have been received from the validators. The 38th chapter is on hold and is unlikely to appear in the first edition because of editorial deficiencies. The prototype DLMF Web site, accessible only within NIST, contains 26 chapters. This prototype is about to be released for an external usability review. Substantial additional work remains to resolve cross-chapter references, refine the index, complete the final editing of the chapters, and arrange for a commercial publisher. The book and Web site are planned for release in 2006.

Outgrowths from the DLMF project will serve well as an effective basis for participation in future *mathematical knowledge management* activities related to mathematics and the Web. In fact, members of the project staff have already delivered invited and contributed talks at national and international conferences, and one of the principal editors is on the organizing committee for the 2006 international conference.

This work is supported in part by the National Science Foundation (NSF) and the NIST Systems Integration for Manufacturing Applications (SIMA) Program.

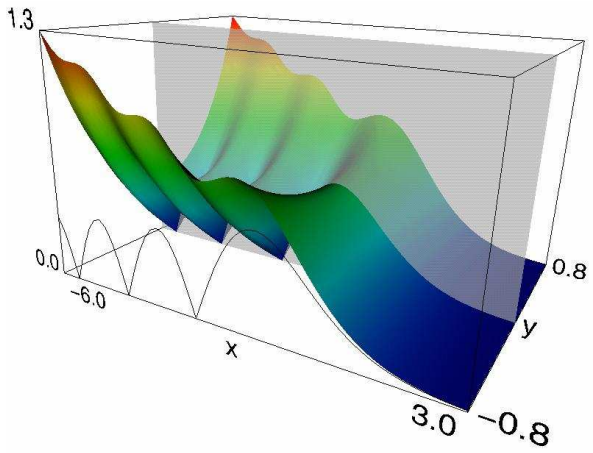

Figure 25. *The absolute value of the Airy function as a function of a complex variable. The interference fringes in Fig. 24 correspond to the oscillating behavior of the function when the variable is restricted to the negative real line.*

Representation and Exchange of Mathematical Data

Daniel Lozier
Bruce Miller
Abdou Youssef (George Washington University)
Jonathon Borwein (Dalhousie University)
Michael Kohlhase (International University Bremen)

The Web has had a tremendous impact in many areas of modern life. An example is the ability to search for very detailed information, such as a place to buy a part for a home appliance and instructions for installing it. A corresponding impact in science is the ability to locate and print published papers as well as ephemera such as unpublished manuscripts, working papers, and supporting data. In mathematics we can look forward to a future in which specific formulas, theorems, algorithms, numerical data sets, and graphical displays can be located quickly and easily, and in which effective tools exist for incorporating these artifacts

accurately and conveniently into papers and computer systems. However, many difficult issues need to be resolved before the full potential of this vision can be realized.

The vision is to provide a broad range of *mathematical knowledge* that is selected to meet the needs of scientists, engineers, educators, applied mathematicians, and others who use mathematics in their work. How should mathematical knowledge content be developed for maximum usability and impact? Some of the issues and needs regarding mathematical content are the following.

- Selection (e.g., math subfields)
- Authoring (writing for the Web)
- Representation (syntactic and semantic encodings)
- Identification (resource naming)
- Display (browser compatibilities)
- Servers (location, support)
- Search (math-aware search)
- Transforming (computer algebra)
- Exchange (without loss of mathematical meaning)
- Maintenance (revision management)

Mathematical Knowledge Management (MKM) is a growing international field of research at the interface between mathematics and computer science. MCSD is becoming a significant contributor due to its development of the Digital Library of Mathematical Functions. The DLMF project has gained recognition within the MKM community as the most ambitious content development effort anywhere in the world. The DLMF project team at NIST is facing all of the questions in the list above, and has developed partial answers to most of them. Progress was made in FY05 on the difficult questions involving mathematical semantics and search in mathematical knowledge databases. Employing the DLMF as a research laboratory, future work will center on developing more general techniques and tools for delivery of serious mathematics to advanced users.

This work is supported in part by the NIST Systems Integration for Manufacturing Applications (SIMA) Program.

Abdou Youssef (standing) and Bruce Miller are developing technologies and tools for the effective representation, exchange, and search of mathematical data on the Web.

Fundamental Mathematical Software Development and Testing

Sparse BLAS Standardization

Roldan Pozo
Iain Duff (Rutherford Appleton Labs)
Michael Heroux (Sandia National Laboratory)

http://math.nist.gov/spblas
http://www.netlib.org/blas/blast-forum

MCSD has played a leading role in the standardization effort for the Basic Linear Algebra Subprograms (BLAS) and continues to be a major contributor for the design and development of reference software and documentation. The BLAS are kernels for computational linear algebra comprising fundamental matrix/vector operations common to most scientific computing applications. By developing their applications in terms of standardized BLAS, computational scientists can achieve high levels of performance and portability. Computer manufacturers and software vendors enable this by providing high-performance implementations especially suited to a specific hardware platform.

The original BLAS, which were developed for dense vector and matrix operations from the late 1970s through the early 1990s, achieved this goal very well. More recently, the BLAS Technical Forum (an international consortium of industry, academia, and government institutions, including Intel, IBM, Sun, HP/Compaq/Digital, SGI/Cray, Lucent, Visual Numerics, and NAG) developed an updated set of BLAS standards which include several new extensions.

Among the most significant components of the updated BLAS standard is support for sparse matrix computations. R. Pozo of MCSD served as chair of the Sparse BLAS subcommittee during the standardization process. NIST was first to develop and release a public domain reference implementation for early versions of the standard, which were critical in shaping the final specification. After the standard was formally approved and the complete technical specification published, a special issue of the *ACM Transactions of the Mathematical Software* was devoted to the new BLAS standard, including a paper co-authored by R. Pozo and other subcommittee members providing an overview of the sparse matrix interface.

This year we released a new reference implementation of the standard, and a proposal for a simplified C++ interface. First, a new compact implementation of the Spare BLAS standard, coded in C++, was made available. The source code has been reduced to less than 2,500 lines, including support for all operations and data types: single precision, double precision, complex single precision, and complex double precision. (As a reference point, our first version of a Sparse BLAS library contained nearly half a million lines and required complicated Makefiles to generate and build the library.) Secondly, a new C++ interface and implementation has been developed that significantly simplifies the library even further. While the original standard described 79 functions and 23 matrix properties to contend with, the new simplified interface describes only 4 matrix types and 13 functions. This makes for a library that even simpler to integrate into scientific and numeric C++ applications.

SciMark, a Web-based Benchmark for Numerical Computing in Java

Roldan Pozo
Bruce Miller

http://math.nist.gov/scimark

The NIST SciMark benchmark continues to be one of the most widely used Java scientific benchmarks, and is now being considered by the SPEC Java subcommittee to be included in the new SPECjvm2006 benchmark. SciMark consists of computational kernels for FFTs, SOR, Monte Carlo integration, sparse matrix multiply, and dense LU factorization, representative set of computational styles commonly found in numerical applications. SciMark can be run interactively from Web browsers, or can be downloaded and compiled for stand-alone Java platforms. Full source code is provided, in both Java and C for comparison under different compilers and execution environments. The SciMark result is recorded in megaflops for the numerical kernels, as well as an aggregate score for the complete benchmark.

The current SciMark results database lists submissions from more than 3,000 submissions representing computational platforms from palm devices to high-end servers, and contains reports from nearly every operating system and virtual machine environment currently in use, including Solaris, FreeBSD, MacOS, Sun OS, IRIX, OSF1, Linux, OS/2, and Windows 95, 98, 2K, ME, NT, and XP.

SciMark and its kernel components have become a pseudo-standard in industry and academia. They were adopted by the Java Grande Benchmark Forum. Sun Microsystems used SciMark 2.0 to demonstrate the floating-point improvements to their Java Virtual Machine version 1.4.2.[1] Most recently, SciMark is being considered for inclusion in SPECjvm2006.

As of December 2005, the record for SciMark is more than 650 Mflops, with some of the kernel benchmarks (notably the LU factorization) running at nearly 1.2 Gflops on a single-processor PC.

TNT: Object Oriented Numerical Programming

Roldan Pozo

http://math.nist.gov/tnt/

NIST has a history of developing some of the most visible object-oriented linear algebra libraries, including Lapack++, Iterative Methods Library (IML++), Sparse Matrix Library (SparseLib++), Matrix/Vector Library (MV++), and most recently the Template Numerical Toolkit (TNT). This package has been downloaded by several thousand developers and is currently in use in several industrial and commercial applications. This year saw a major redesign and the introduction of two new components.

TNT incorporates many of the ideas we have explored with previous designs, and includes new techniques that were difficult to support before the availability of ANSI C++ compilers. The package includes support for both C and Fortran-style multidimensional arrays, vector, matrices, and application modules, such as linear algebra.

The design of TNT separates the interface specification from the actual implementation. This allows library developers to create specialized modules that take advantage of particular hardware platforms, utilize vendor-specific libraries, or implement different C++ strategies, such as expression templates, or instrumented versions for debugging sessions.

Recent developments in the latest design of TNT (version 3.0) provide support for both multi-dimensional arrays and integrate a new linear algebra module which includes fundamental algorithms (LU, Cholesky, SVD, QR, and eigenvalues), sparse matrix support (now with computational operations via the Sparse BLAS), and support for iterative methods in solving linear systems with dense or sparse matrices.

The TNT web site provides a basic implementation for testing and development, as well as links to other library packages that utilize the TNT interface. Full documentation and source code for all TNT components are available on-line.

[1] See http://java.sun.com/j2se/1.4.2/1.4.2_whitepaper.html.

A Metrology-Based Approach to Verification and Validation of Computer Models of High-Consequence Engineering Systems

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Daniel Lozier
Geoffrey McFadden
James Filliben (NIST ITL)
Hung-kung Liu (NIST ITL)
Emil Simiu (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)
Barry Bernstein (Illinois Institute of Technology)

As part of a 5-year joint competence project entitled "Complex System Failure Analysis: A Computational Science Based Approach," ITL staff formulated and began to address the following three questions on the computer simulation and analysis of complex structural system failures.

Question 1: Given a specific simulation of a complex structural system failure, how do we verify (in a mathematical and numerical sense) and validate (in an experimental sense) the simulation in order to assess its accuracy and uncertainty?

Question 2: Given a range of variability for each of a large number of known factors affecting

simulations of a complex structural system failure, what would be the ratio of times to failure calculated from a deterministic model vs. a stochastic one?

Question 3: If the answer to Question 2 is significantly large (say, between 1.5 and 3), and we accept the stochastic approach to the modeling of complex structural system failures, how do we design a suite of reference benchmarks such that the accuracy and uncertainty of such simulations can be rigorously evaluated?

To address Question 1 during FY05, we co-sponsored with the Defense Modeling and Simulation Office (DMSO) of the U. S. Department of Defense (DOD) a workshop entitled "V&V of Computer Models for Design and Performance Evaluation of High-consequence Engineering Systems" in November 2004. At this workshop, we described a five-step metrology-based approach to the verification (mathematics) and validation (experiments) of computer simulations. As part of this approach, we also discussed the need to formulate reference benchmarks in order to assess the accuracy and uncertainty of those simulations, and the need to solve the same problem using several different finite-element-method (FEM) software packages such as ABAQUS, ANSYS, LS-DYNA, MPAVE, SAFIR, etc.

To address Question 2, we began with a simple example of a 44-column grillage on fire and a comparative study of two models, one deterministic and the other stochastic, in order to calculate its time to failure under some idealized loading conditions. As described elsewhere in this report, we found the deterministic model over-estimates the time to failure from the stochastic model by almost a factor of two.

To address Question 3 we have outlined the design of a suite of reference benchmarks of different levels of complexity. Results of this investigation were reported in two papers:

- Fong, J. T., A B C of Statistics for Verification and Validation (V & V) of Simulations of High-Consequence Engineering Systems, *Proceedings of the 2005 ASME Pressure Vessels and Piping Conference*, July 17-21, 2005, Denver, Colorado, Paper No. PVP2005-71799.
- Fong, J. T., Filliben, J. J., deWit, R., Fields, R. J., Bernstein, B., and Marcal, P. V., Uncertainty in Finite Element Modeling and Failure Analysis: A Metrology-Based Approach, to appear in Feb. 2006 issue of ASME *Journal of Pressure Vessel Technology*.

This work has been supported in part by the NIST Director's Competence Program.

Mathematical Software Reference Databases

Ronald Boisvert
Joyce Conlon
Marjorie McClain
Bruce Miller
Roldan Pozo

http://gams.nist.gov/
http://math.nist.gov/MatrixMarket/
http://math.nist.gov/javanumerics/

MCSD continues to maintain a variety of public information services in support of mathematical software development and use. The Guide to Available mathematical Software (GAMS) is a problem-oriented cross-index and virtual repository of software components (e.g., Fortran subroutines and C procedures) for solving common mathematical problems. It indexes some 8,000 objects, providing access to documentation of commercial libraries in use at NIST as well as access to source of libraries developed at NIST or available through the *netlib* service of Oak Ridge National Labs and Bell Labs. We also maintain the Matrix Market, a repository of sparse matrices for use in testing algorithms and software for standard linear algebra problems. Finally, we maintain the JavaNumerics web page, a directory of research and development projects related to the use of Java for scientific computing.

The MCSD Web server continues to see high usage. During the last 12 months, the virtual server math.nist.gov satisfied more than six million requests for pages, or more than 16,000 per day. More than 875 Mbytes of data were shipped each day, and more than 55,000 distinct hosts were served. The virtual server gams.nist.gov, delivered 800,000 pages, or more than 2,200 per day. There have been nearly 100 million "hits" on MCSD Web servers since they went online as NIST's first web servers in 1994.

High Performance Computing

Computation of Atomic Properties with the Hy-CI Method

James Sims
Stanley Hagstrom (Indiana University)

http://math.nist.gov/mcsd/savg/parallel/atomic/

Impressive advances have been made in both experimental and theoretical studies of atomic structure. For atomic hydrogen and other equivalent two-body systems, exact analytical solutions to the nonrelativistic Schrödinger equation are known. It is now possible to calculate essentially exact nonrelativistic energies for helium (He) and other three-body (two-electron) systems as well. Even for properties other than the nonrelativistic energy, the precision of such calculations has been referred to as essentially exact for all practical purposes, i.e., the precision goes well beyond what can be achieved experimentally. These high-precision results have been produced using wave functions that include interelectronic coordinates, a trademark of the classic Hylleraas (Hy) calculations done in the 1920s.

The challenge for computational scientists is to extend the impressive accomplishments for He (the ability to compute, from first principles alone, any property of any two electron atom or its ion to arbitrary accuracy) to molecules and to atomic systems with three, four, and even more electrons. Where three electron atomic systems, i.e., lithium (Li) and other members of its isoelectronic series, have been treated essentially as accurately as He-like systems, demand on computer resources increases by 6,000 fold. Because of these computational difficulties, already in the four-electron case, i.e., beryllium (Be) and other members of its isoelectronic series, there are no calculations of the ground or excited states with an error of less than 10 microhartrees (0.00001 a.u.). This is where a technique developed by Sims and Hagstrom in a series of papers from 1971 to 1976 becomes important. They developed the Hy-CI method, which includes interelectronic coordinates in the wave function to mimic the high precision of Hy methods, but also includes configurational terms that are the trademark of the conventional Configuration-Interaction (CI) methods employed in calculating energies for many-electron atomic (and molecular) systems. Because of this, the Hy-CI method has been called a hybrid method. The use of configurations wherever possible leads to less difficult integrals than in a purely Hy method, and if one restricts the wave function to at most a single interelectronic coordinate to the first power, then the most difficult integrals are already dealt with at the four electron level and the calculation retains the precision of Hy techniques, but is greatly simplified.

In a paper published last year[2], Sims and Hagstrom discussed changes they have made to this methodology to most effectively use modern day computers to increase the size (number of terms) and resulting accuracy of the calculations. The availability of cheap CPUs which can be connected in parallel to significantly enhance both the processing speed and memory that can be brought to bear on the computational task, have brought computations that seemed hopeless only five years ago within reach, assuming the linear dependence problem can be obviated with extended precision. The goal is to extend techniques which are known to give the most accurate upper bounds to energy states to four and more electrons. The first step in this process was to efficiently evaluate the only difficult integral arising when using the Hy-CI technique in the case of the number of electrons greater than or equal to three, the three-electron triangle integral. They focused on recursive techniques at both double precision and quadruple precision while trying to minimize the use of higher precision arithmetic. Two papers describing this work are in progress: "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations II. Four-electron Integrals," and "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations III. Nuclear Attraction and Kinetic Energy Integrals". The latter resulted from a need a need to handle the more general case of non-spherically symmetric Slater-type orbitals (STOs).

Next they will tackle the difficult matrix assembly problem, and then to do a benchmark Be calculation. Progress to date has included finding a new Be radial limit (s orbital CI, no r_{ij}) that is better than any published result. Also, integrals are being calculated in blocks, each block independent of all others, so different blocks can be calculated on different processors.

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[2] J.S. Sims and S.A. Hagstrom, Math and Computational Science Issues in High-Precision Hy-CI Calculations I. Three-electron Integrals, *Journal of Physics B: At. Mol. Opt. Phys.* **37** (7) (2004), pp. 1519-1540.

In addition to virtual measurements of the properties of atoms, work is underway to extend high precision electronic energy calculations to diatomic molecules. They have completed a calculation on the ground state of the dihydrogen molecule which is the most accurate calculation ever done on a nontrivial molecular system. In a paper recently accepted by the *Journal of Chemical Physics*, they calculate hydrogen molecule Born-Oppenheimer (BO) energies for various internuclear distances in the range of 0.4 bohr to 6.0 bohr. All of their energies, including the BO ground state energy, are more accurate than any previously calculated. The calculations reported are similar to those described in the classic paper of Kolos and Roothaan, but go far beyond those as a reflection of the improved capability of modern computers, with results two orders of magnitude better than the error estimate of the best previous calculations.

In order to achieve this level of accuracy, they have been refining their QDE (quad-double with extended exponent) code to calculate on both the Linux cluster and our SGI to 32 digits accuracy. This code is based on Hida and David Bailey's C++ package but has the advantage of being Fortran 90, so no interface between C++ and Fortran is needed. This is the extended precision package needed for the final Be benchmark.

A parallel solver for the generalized eigenvalue problem proved essential for obtaining results over a range of internuclear distances R from 0.4 to 6.0 bohr. Sims and Hagstrom solve this secular equation using their own portable parallel inverse iteration solver. For an order N matrix, the generation of the matrices is of the order of N^2 while the solution of the secular equation is order of N^3. For a 4190 term wave function they achieved a factor of 30 speedup on 32 processors for the eigensolution step running on the NIST ITL/PL 147 processor cluster of Pentium, Athlon, and Intel processors running RedHat Linux. The parallelization proved extremely helpful not only for speeding the calculation up but also by spreading the total memory needed across the nodes of the cluster. The following paper describing the eigensolver is in progress: "Parallel Generalized Real Symmetric-Definite Eigenvalue Problem." The usual methods for this dense eigenproblem, as realized in for example the NAG and LAPACK libraries, fail for large dimensions. In addition, other methods used for large CI calculations fail in high-precision calculations which require Hy or Hy-CI, probably because of the large off-diagonal matrix elements in the (dense) matrices. For high precision, real*16 arithmetic is necessary for molecules and real*24 for atoms. Hence parallel packages like Scalapack, which is available only in real*8, can't be used as they stand, and are too big to contemplate conversion to real*16. For these reasons they developed their own portable, parallel eigensolver, GRSDEP, which will be useful in high-precision atomic or molecular calculations where large, dense matrices must be solved.

Computation of Nano-structures and Nano-optics

James Sims
John Hagedorn
Howard Hung
John Kelso
Steve Satterfield
Adele Peskin
Garnett Bryant (NIST PL)

http://math.nist.gov/mcsd/savg/parallel/nano/

Accurate atomic-scale quantum theory of nanostructures and nanosystems fabricated from nanostructures enables precision metrology of such systems and provides the predictive precision modeling tools needed for engineering applications including advanced semiconductor lasers and detectors, single photon sources and detectors, biosensors, quantum memory. Theory and modeling of nanoscale optics is essential for the realization of nanoscale resolution in near-field optical microscopy and for the development of nanotechnologies that utilize optics on the size-scale of the system, such as quantum dot arrays and quantum computers. We are working with the NIST Physics Lab to develop computationally efficient large scale simulations of such nanostructures. We are also working to develop immersive visualization techniques and tools to enable analysis of highly complex computational results of this type.

This year we completed a code enabling calculations on arrays of nanoparticles. The basic idea is to consider each nanoparticle as part of its own cluster, using the same input data as for a single nanoparticle, but, as the computation proceeds, information from neighboring atoms in each cluster is distributed to the appropriate processor in neighboring clusters, thereby "stitching together" the calculations on the clusters in the array. We have also done work on adding d basis orbitals to the parallel code. When these were added to the sequential code significant new features were observed. Further exploitation of this capability will require parallel computation.

These computations result in voluminous sets of output requiring sophisticated visualization techniques

to understand. This aspect of the work is discussed on page 59.

This work is being written up in a paper, "Advancing Scientific Discovery through Parallelization and Visualization III. Tightbinding calculations on quantum dots" with Howard Hung, William George, Steven Satterfield, Judith Terrill, Garnett Bryant, and Jose Diaz as co-authors.

Computational Modeling of the Flow of Concrete

William George
Julien Lancien
Nicos Martys (NIST BFRL)

http://math.nist.gov/mcsd/savg/parallel/dpd/

Understanding the flow properties of complex fluids like suspensions (e.g., colloids, ceramic slurries and concrete) is of technological importance and presents a significant theoretical challenge. The computational modeling of such systems is also a great challenge because it is difficult to track boundaries between different fluid/fluid and fluid/solid phases. We are utilizing a new computational method called dissipative particle dynamics (DPD), which has several advantages over traditional methods while naturally accommodating necessary boundary conditions. In DPD, the interparticle interactions are chosen to allow for much larger time steps so that physical behavior on time scales many orders of magnitude greater than that possible with molecular dynamics may be studied. Our algorithm (QDPD) is a modification of DPD, which uses a velocity Verlet method to update the positions of both free particles and the solid inclusion. In addition, the rigid body motion is determined from the quaternion-based scheme of Omelayan (hence the Q in QDPD).

We recently re-designed and reimplemented the QDPD (Quaternion based dissipative Particle Dynamics) application in Fortran 90. This allowed us to update the data structures used in the application to take advantage of advances in the Fortran language while maintaining most of the structure of the basic QDPD algorithm. Enhanced modularity, supported by the more advanced data structures, has resulted in a looser coupling between the computational aspects of the simulation and the required communications operations. This enables more freedom in optimizing each aspect of the parallel algorithm. A beta-level version of the new QDPD is now operational, and it will replace the previous version for production runs in 2006. To ensure portability, development and testing has utilized various machines such the ITL/PL Raritan cluster with the Portland Group Fortran compiler, Linux workstations with the GCC Fortran compiler gfortran, and SGI Fortran.

The following two presentations were made to describe this code.

W. George, J. Lancien, and J. Terrill, "MPMD Program Model for Scientific Computing," Scatter-Gather Session, SC05 International Conference for High Performance Computing, Networking, Storage, and Analysis, Seattle WA, Nov. 12-18, 2005.

J. Lancien, W. George, and N. Martys, "Quaternion based Dissipative Particle Dynamics," Virtual Cement and Concrete Testing Laboratory Consortium Meeting, NIST, Nov. 29-30, 2005.

Interoperable MPI

William George
John Hagedorn
Judith Terrill

http://impi.nist.gov

We are providing support to vendors of the Message Passing Interface (MPI) as they implement the Interoperable MPI (IMPI) protocols. In particular, we maintain the NIST IMPI conformance tester, manage the IMPI mailing list (interop@nist.gov), maintain the IMPI specification document and its errata, and in general promote the implementation of IMPI by the current MPI vendors.

This year we consulted with Andrew Lumsdaine and Jeff Squyres of the University of Indiana Open Systems Lab concerning the addition of IMPI to the new *OpenMPI* library which is being developed by Indiana University, the University of Tennessee, Los Alamos National Laboratory, the High Performance Computing Center, (Stuttgart), and Sandia National Laboratory at Livermore[3].

We also consulted with Dr. Yutaka Ishikawa, Professor of Computer Science at the University of Tokyo and Dr. Motohiko Matsuda of the Grid Technology Research Center of Japan's National Institute of Advanced Industrial Science and Technology (AIST). These researchers are involved in the development of GridMPI, a Grid-focused version

[3] See http://www.open-mpi.org/.

of MPI that currently uses IMPI[4]. In cooperation with the OpenMPI developers, they will also be adding full IMPI support to the OpenMPI library. Both AIST and the commercial MPI vendor Verari Systems, who acquired IMPI/MPI vendor MPI Software Technology, Inc., have explored possible extensions to IMPI to accommodate the dynamic process capabilities of MPI-2 and emerging cluster networking technologies.

The NIST IMPI tester has been under active use by several sites over the last 12 months, including AIST/GridMPI developers, PACX-MPI Meta-computing Library developers at the High Performance Computing Center of the University of Stuttgart, Germany, and others. This tester is used by developers of MPI libraries as they implement the IMPI protocols.

Screen Saver Science

William L. George
Justin Haaheim
Thomas Bugnazet

http://math.nist.gov/mcsd/savg/parallel/screen

The Screen Saver Science (SSS) project aims to develop a computing resource composed of a heterogeneous set of PCs, scientific workstations, and other available computers, that can be easily used by scientists to execute large highly distributed, compute-intensive applications. Each individual computer in this system makes itself available for participating in a computation only when it would otherwise be idle, such as when its screen saver is running. SSS is based on Jini, an open software architecture built on Java and intended for the development of robust network services.

There are several goals to this project. First, we hope to utilize the idle processing power of the many PCs, workstations, and cluster nodes we have available here at NIST to execute production scientific codes. The compute power of personal PCs and workstations continues to increase and they have become increasingly capable of executing large compute-intensive applications due to faster processors and larger main memories. Second, the SSS computing environment will allow us to develop and experiment with new highly parallel and distributed algorithms more suitable for emerging grid environments. Finally, the use of Java for scientific applications is of interest in general, and so the development of applications for SSS will give us the opportunity to explore this topic on actual production quality applications.

Up until recently, this type of project would have required a large investment in software development just to become minimally functional and so was not practical, especially for a small team of programmers. However, with the introduction of Jini, and more specifically the Jini based network service called Javaspaces, the most difficult parts of this project have now become trivial. Javaspaces is a portable, machine independent, shared memory system that expands upon the tuple-space concepts developed in the 1980s by David Gelernter of Yale University.

In this last year, we completed the restructuring of the SSS server and client processes to support pluggable authentication and authorization, encrypted communication, as well as method-level security constraints on all SSS threads. Full use of this security framework has not been enabled pending the availability of a suitable X509 certificate authority.

In addition, we developed a framework for supporting parameter study style computations. This framework has been designed to simplify the work needed by SSS applications programmers to adapt their parameter study or Monte Carlo style applications to work within SSS.

We are adapting SSS to run on idle compute nodes within the ITL/PL Linux cluster Raritan. This requires coordination with PBS, the job queuing system in use on Raritan, to identify idle compute nodes. Once installed, this will increase productive utilization of the Raritan cluster to close to 100%. Finally, we are collaborating with CSTL scientists to port the 3-dimensional chemical imaging application, EPQ, to SSS. This is a Monte Carlo application implemented in a mix of Java and Python that has been developed and run primarily in the MS Windows environment. Increased computational demands on this application, due to larger multidimensional simulations being attempted, have prompted the desire to move to a parallel/distributed algorithm.

[4] See http://www.gridmpi.org/gridmpi-0-6/

Virtual Measurement Laboratory

Creating Visual Models of Nanoworlds

Howard Hung
Steve Satterfield
James Sims
Adele Peskin
John Kelso
John Hagedorn
Terrence Griffin
Judith Terrill
Andrew Dienstfrey
Garnett Bryant (NIST PL)
Zahary Levine (NIST PL)
Carlos Gonzales (NIST CSTL)
Joy Dunkers (NIST MSEL)
Lori Henderson (NIST MSEL)
Ron Kriz (Virginia Tech)

See feature article, page 35.

Measurement Science in the Virtual World

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Adele Peskin
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Steve Satterfield
Judith Terrill
Andrew Dienstfrey
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Lori Henderson (NIST MSEL)

See feature article, page 37.

Tissue Engineering

John Hagedorn
John Kelso
Adele Peskin
Steven Satterfield
Judith Terrill
Joy Dunkers (NIST MSEL)
L. Henderson (NIST MSEL)
Marcus Cicerone (NIST MSEL)
Lyle Levine (NIST MSEL)

http://math.nist.gov/mcsd/savg/vis/tissue

Standard reference materials for the growth of tissue engineered products are needed for industry to develop the low cost manufacturing processes required for commercial success. This requires a quantitative understanding of the growth media for tissue engineered materials and their impact on cell growth. Applications include replacement tissues for skin, organs, and bone. We are working with MSEL scientists to use multi-modal imaging techniques to bring tissue engineering scaffolds into the virtual environment, where further measurement and analyses may be done.

MSEL scientists have gathered data on tissue scaffold materials using a variety of techniques, including optical coherence tomography (OCM) and confocal fluorescence (CFM) imaging. These provide multiple types of information on samples. Such methods have applications in a wide variety of areas, such as the characterization of biomaterials, the failure analysis of polymer composites, and the reliability of semiconductor devices. We have generated a variety of visualizations of OCM/CFM data from tissue scaffolds. Previously, CFM was used only for cell visualization. Recently we used CFM as well as OCM to image the scaffold, which had been stained.

We are also pursuing the use of the immersive visualization environment as a framework for more easily measuring distinguishing properties of scaffolds ("scaffold descriptors"), for support in developing consensus definitions of scaffold descriptors, for understanding automatic descriptor measurement methods, and for qualitatively evaluating and validating scaffold manufacturing techniques. This effort is being done in collaboration with researchers at the FDA, Mayo Clinic, University of Connecticut, Case Western Reserve University, American Society of Testing and Materials, and Macropore Biosurgery. Our

plan is to build a software system within the immersive environment to integrate the following tasks: measurement of scaffold characteristics, analysis of the collected measurements, display of the analysis, and interactions with the data and analyses that enable grouping of results. The goal is to enable interactions which will lead to greater understanding of the structural characteristics of the scaffold material.

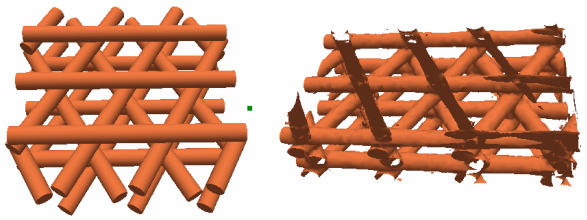


Figure 26. *Left: synthetically constructed scaffold based on the design specifications. Right: 3D reconstruction of a real scaffold made by solid freeform fabrication.*

To begin this effort, we have applied immersive visualization techniques to a straightforward manual linear measurement task to derive quantitative structural information from a digital 3D image of a tissue engineering scaffold. It was felt that this would enable interactive measurement of several important scaffold characteristics, one of which is pore size distribution and associated anisotropy. The specific scenario for this first implementation was as follows:

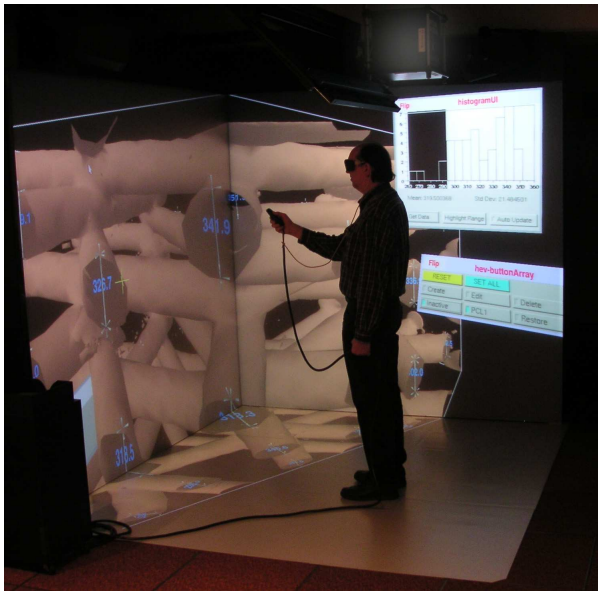
1. The user collects a set of linear measurements.
2. A simple statistical analysis is made.
3. The analysis, including the distribution of measurements, is presented to the user.
4. The user can interact with the measurement distribution in order to highlight measurements (back in the immersive environment) that fall within any selected range of values.

All of these tasks are performed in real-time.

Using this approach, a comparison was made of a synthetically constructed scaffold based on the design specifications and a 3D reconstruction of the scaffold made by solid freeform fabrication. See the figures above. This work will be extended to enable the measurement of pore size and orientation in tissue engineering scaffold structures. This involves the interactive creation of ellipsoids and the analysis of the characteristics of these ellipsoids. All of this work will be done within the immersive visualization environment. This work will be the subject of papers in both visualization and tissue engineering journals:

J. Hagedorn, S. Satterfield, J. Kelso, W. Austin, J. Terrill, and A. Peskin, "Correction of Location and Orientation Errors in Electromagnetic Motion Tracking," *Presence*, submitted.

J. Hagedorn, J. Dunkers, A. Peskin, J. Kelso, L. Henderson, and J. Terrill, "Quantitative, Interactive Measurement of Tissue Engineering Scaffold Structure in an Immersive Visualization Environment," *2006 IEEE International Symposium on Biomedical Imaging,* to appear.



William George performs an interactive measurement of scaffold diameters from within the immersive environment.

3D Chemical Imaging at the Nanoscale

William George
Steve Satterfield
John Hagedorn
John Kelso
Adele Peskin
Judith Terrill
Anthony Kearsley
Eric Steel (CSTL)
John Henry Scott (CSTL)
John Bonevich (MSEL)
Zachary Levine (PL)

http://math.nist.gov/mcsd/savg/vis/ChemImg/

A quantitative understanding of the distribution of chemical species in three dimensions including the internal structure, interfaces and surfaces of micro- and nanoscale systems is critical to the development of successful commercial products in nanotechnology. Current nanoscale chemical 3D measurement tools are in their infancy and must overcome critical measurement barriers to be practical. This project is developing intermediate voltage electron microscope measurement approaches to attain three-dimensional chemical images at nanoscale resolution. These approaches will be broadly applicable to nanoscale technologies from microelectronics to pharmaceuticals and subcellular biomedical applications.

MCSD collaborators are working on computational, visual analysis, and data management techniques and tools to enable the analysis of imagery to be generated by this project. Among the particular capabilities under development are the following.

- Techniques for the visualization of 3D data in an immersive environment
- Techniques for interactions with immersive visualizations
- Assistance with algorithms and codes
- Parallelization of simulation codes

We are porting the 3D chemical imaging application EPQ to SSS. This is a Monte Carlo application that is a simulation of scanning electron microscope, tracking the trajectories of electrons and determining the output of the detectors given a description of the target material. It is implemented in a mix of Java and Python, and has been developed and run primarily in the MS Windows environment. Increased computational demands on this application, due to larger multidimensional simulations being attempted, have necessitated the move to a parallel/distributed algorithm.

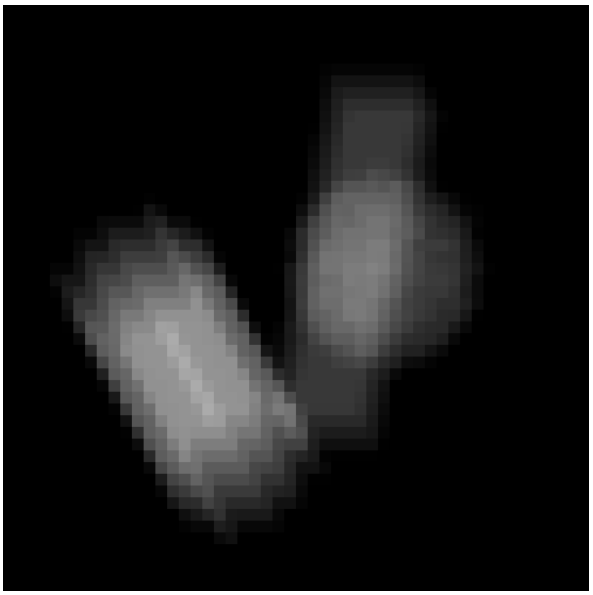


Figure 27. *This image demonstrates part of the functionality of the projection software. It simulates the projection of a volume containing a sphere, a cylinder, and a box onto a 2D sensor array at a specific orientation. Such an image would be generated experimentally as one of a tilt series that would then be used as part of a 3D reconstruction of the volume.*

We have developed several geometric algorithms to be used as part of a Bayesian reconstruction approach. These algorithms involve ray/voxel intersection testing and projection of voxels to two-dimensional pixel arrays.

Two papers are being written for submission to be submitted to *IEEE Transactions on Image Processing*: D. Malec, J. Hagedorn, and J. Soto, "Bayesian 3D Reconstruction of Chemical Composition from 2D Spectra," and Z. Levine, A. Kearsley, J. Hagedorn, "Bayesian Tomography for Projections with an Arbitrary Transmission Function with an Application in Electron Microscopy."

This work has been supported in part by the NIST Director's Competence Program.

Virtual Cement and Concrete Testing Laboratory

William George
Terence Griffin
John Hagedorn
Howard Hung
John Kelso
Julien Lancien
Adele Peskin
Steve Satterfield
James Sims
Judith Terrill
Clarissa Ferraris (NIST BFRL)
Edward Garboczi (NIST BFRL)
Nicos Martys (NIST BFRL)

The NIST Building and Fire Research Laboratory (BFRL) does experimental and computational research in cement and concrete. Recently, MCSD has been collaborating with BFRL in the parallelization of their codes and in creating visualizations of their data. In January 2001 the Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium was formed. MCSD assisted in this effort through presentations of our work with BFRL and demonstrations of visualizations in our immersive environment. The consortium consists of NIST and ten industrial members: Cemex Trademarks Worldwide, Ltd., Holcim (US) Inc., Degussa/MBT, National Ready Mixed Concrete Association, Association Technique l'Industrie des Liant Hydrauliques (ATILH), International Center for Aggregate Research (ICAR), W.R. Grace, Sika Technology AG, Verein Deutscher Zementwerke eV (VDZ), and Portland Cement Association. The overall goals of the consortium are to develop a virtual testing system to reduce the amount of physical concrete testing and to expedite the research and development process. This will result in substantial time and cost savings to the concrete construction industry as a whole.

MCSD continues to contribute to the VCCTL through collaborative projects involving parallelizing and running codes, creating visualizations, as well as presentations to the VCCTL current and prospective members.

This work has been supported in part by the Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium.

Visualization of Cement Hydration Models

http://math.nist.gov/mcsd/savg/vis/concrete/

We have developed visualizations of the outputs of the cellular automata cement hydration model CEMHYD3D. These data are a time sequence of 3D arrays that identify the material present at each element of the array at each time step. In the figures below the data represent 16 different materials. The features of interest range in size from about one hundred voxels to just a few voxels across. We have developed several tools for the visualization of such data, including the following:

- interactive selection of subsets of data,
- cube rendering of voxel elements,
- cross-sections through the volume of data, and
- coordination of various components into a coherent visualization.

These tools have been developed as reusable software modules that can be applied to a variety of types of volume data. See the figure below for an example.

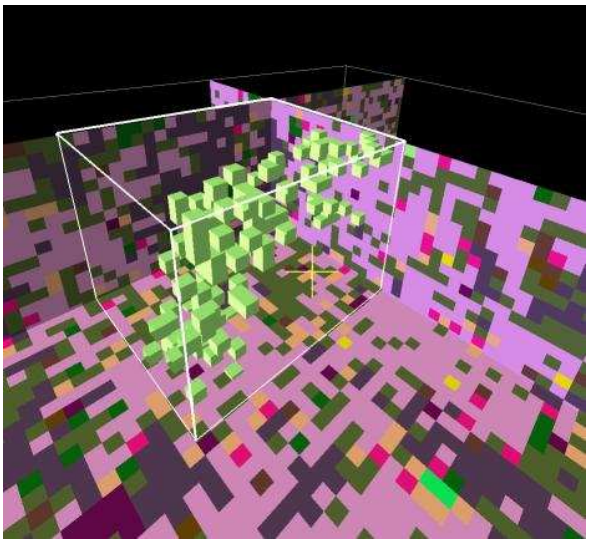


Figure 28. *A portion of the cement hydration data set output from CEMHYD3D. The user has interactively specified a region of interest (the small box) and the software is showing only the subset of the 3D data that is within that box, while simultaneously displaying orthogonal cross-sections based on the position of the region of interest box.*

This year BFRL developed a second cement hydration model, HydratiCA, to directly capture the chemistry, physics, and microstructure of hydration. Validation of this model was important to the VCCTL as it is an advance over the previous one. Visualization of the output of this model accelerated

the development of the model by quickly identifying bugs that would be difficult to find otherwise. The visualization was also an important part of the validation of the new model. It verified that nucleation was occurring at the correct locations in space. It verified that the formation of portlandite had the correct gradient. It clearly showed the uniformity of the dissolution of surfaces. It also showed that the kinetics had the correct sigmoid shape. These results were presented at the November 29-30, 2005 VCCTL meeting held at NIST.

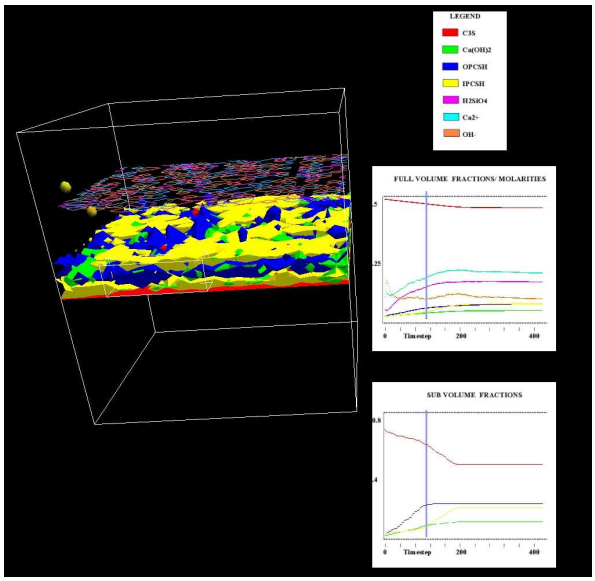


Figure 29. *Isosurfaces and isolines of selected phases of hydrating cement output from HydratiCA. The vertical line in the graphs on the right side shows the current state of the molarities for the volume.*

Visualization of Stress in Aggregate Flow

The high performance dissipative particle dynamics code for the modeling of aggregate flow developed jointly by MCSD and NIST BFRL (see page 51) is being used to study the motion of hard spheres under stress. Visualizations of the normal stress and shear stress computed by this model were requested by our VCCTL consortia partners, who were interested in understanding the spatial distribution of stresses in a suspension at the onset of a jamming transition. While it is known that are large stress fluctuations at the onset of jamming, it is not clear where the stresses occur. We developed a visualization that would depict the stresses between neighboring spheres in a suspension. It was found that, instead of the stresses being carried along a few "chains" which span the system, the stresses were, unexpectedly, homogeneously distributed at the onset of jamming. Such behavior, over long length scales, is indicative of a dynamical phase transition.

To produce the visualizations, the data was placed into groups based on the base-10 log of the stress between the spheres. The groups can be interactively turned on and off to better study the stress relationships. Additionally, two types of visualizations are now possible to represent both of the shear stress and normal stress values computed in the numerical simulation.

Movies of the simulations were shown at the May 10, 2005 VCCTL meeting that was held at Douai and Paris, France.

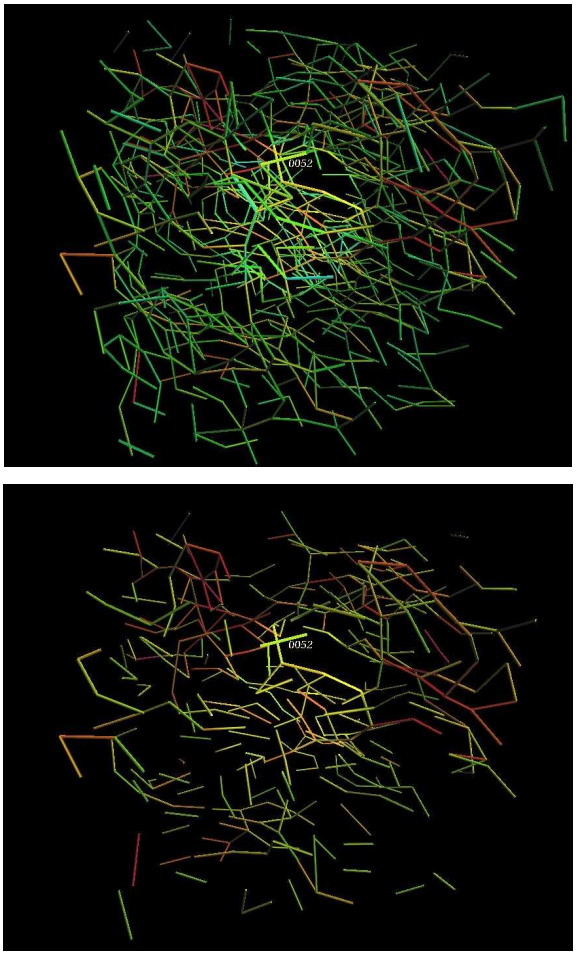


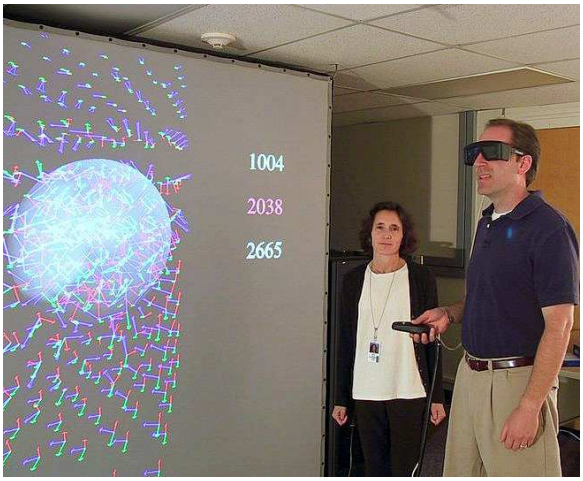
Figure 30. *The stress relationships between the spheres are represented as color coded sticks between the sphere positions shown in the top figure. The blue/green colors represent lower stress values while the yellow/red colors represent higher stress. Ranges of stress can be interactively selected. The bottom figure shows the same time step as the top figure with the lower stress values, LOG10 = 7, range removed from the scene.*

Visualization of Resonant Optical Scattering by Metamagnetic Materials

Adele Peskin
Andrew Dienstfry

http://math.nist.gov/mcsd/savg/vis/emfields/

New capabilities for fabricating materials at nanometer length scales have created the possibility of materials with new optical scattering properties. These materials are nanoscale dielectric and metallic scatterers, arranged in a periodic structure to harness resonant phenomena in their interaction with electric fields. Examples include photonic crystals, in which patterned dielectric structures are used as nanoscale optical waveguides. Multiple groups in the Electromagnetics Division (818) are studying meta-materials, whose surfaces reflect or transmit light at very controlled frequencies with high efficiency and selectivity. These structures present challenges for mathematical modeling. For a precise simulation of these fields, this project requires the full vectorial solution to Maxwell's Equations, capable of capturing both near and far fields, to bridge the coupling of resonances dictated by both the nanometer scale structures and the macroscopic scale structures. Convergence properties of resulting mathematical sums are extremely subtle and careful scalings are necessary.



Adele Peskin and Andrew Dienstfrey visualize electromagnetic fields in the MCSD/Boulder immersive visualization facility.

A huge amount of data comes out of these calculations. We are using immersive visualization to examine the complex dynamics of the electromagnetic fields. Field vectors are represented as geometric arrows in our three-dimensional immersive scene, and simulations of the periodic behavior of these vectors over time and frequency ranges give a complete picture of the outcome of these mathematical calculations.

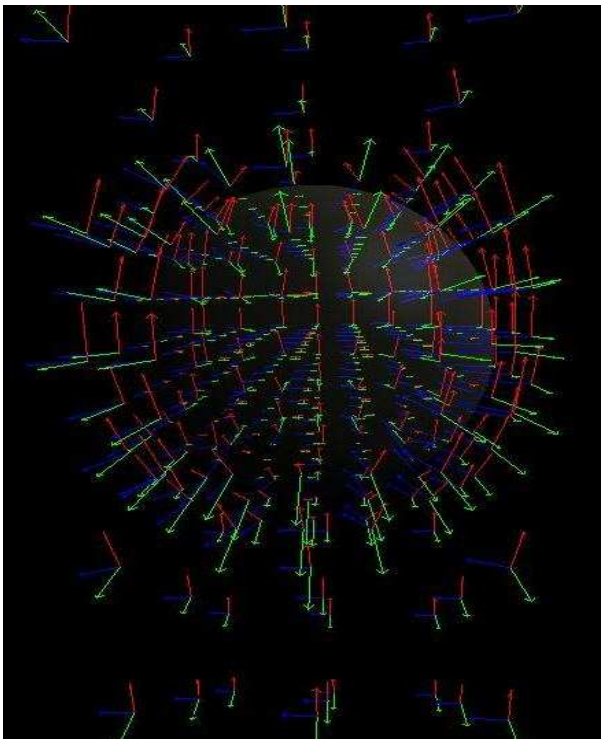


Figure 31. *A single time step in the simulation of this system at a frequency of 1004 hertz. The blue vectors represent the electric field, green vector the magnetic field, and red vectors the energy field.*

We used sets of data for the electric, magnetic, and energy field vectors in and around an array of a sheet of atoms in a nanostructure. These vectors vary in a time-periodic function, and vary over a wide frequency range. We visualized a single time step in the periodic cycle for 3 different frequencies, whose dynamics cover the widest frequency variations to set up the basic components of the visualization, how to display the field vector geometry, coloring, lighting, etc. Viewing the data in this environment gave a much broader overall view of the dynamics than previous two-dimensional visualization studies.

We also looked at the variation in electromagnetic field vectors over their periodic energy cycles. Simulations were set up for the same three frequencies. There was a trade off between viewing the low energy and high energy vectors at the same time, and between viewing large numbers of vectors without having too much information to cloud the picture. We used logarithmic scaling for the vector lengths. The phenomena, covering four orders

of magnitudes of vector length, were visually distinguishable using this method. The visualization was set up to display the periodic cycling of the electric, magnetic, and energy field vectors using this method.

We expanded the visualization model by looking at animations of the far field electric, magnetic, and energy vectors' periodic cycling at 3 specified frequencies. Previous studies had concentrated on near field vectors. We also looked at a frequency sweep: both near field and far field data at a particular point in time across a span of 100 frequencies.

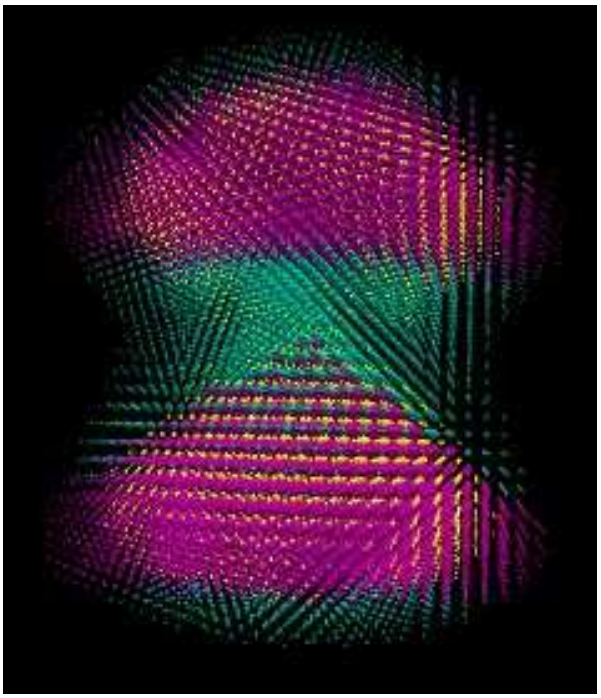


Figure 32. *Visualization of the S-orbitals of two individual quantum dots. The presence of significant S-orbitals between the dots indicates that tunneling is probable between the structures. While the structures are not connected physically, they are connected via quantum tunneling. They also created visualizations that show the orbitals and linear combinations of these orbitals as well as lines whose intersections show the locations of the atoms*

Visualization of Nano-structures and Nano-optics

James Sims
John Hagedorn
Howard Hung
John Kelso
Steve Satterfield
Adele Peskin
Garnett Bryant (NIST PL)

http://math.nist.gov/mcsd/savg/vis/nano/

We have developed computer codes for the visualization of the atomic structure. The codes are able to display the original lattice of the electrons and also display the core area of the computational results.. We created visualizations of double quantum dots which show the tunneling effect created by these two structures.

Additional visualizations were introduced to show contours and transparent surfaces in order to show charge densities in a coarser grain way as a lead-in tool for more complex visualizations. This visualization work was concentrated on giving a different representation for each region in a structure.

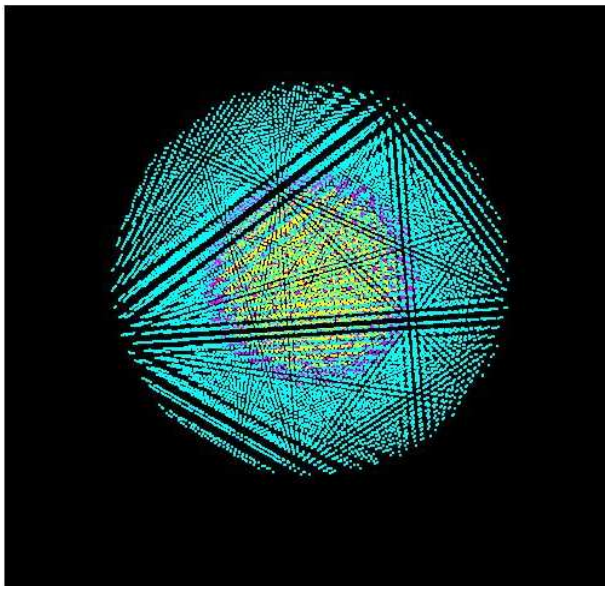


Figure 33. *Atomic lattice of a CdS/HgS/CdS core/well/clad nanohetero-structured nanocrystal (also known as a quantum do tquantum well). Atoms in the core are indicated by yellow, those in the HgS well by blue and the remaining atoms are in the clad.*

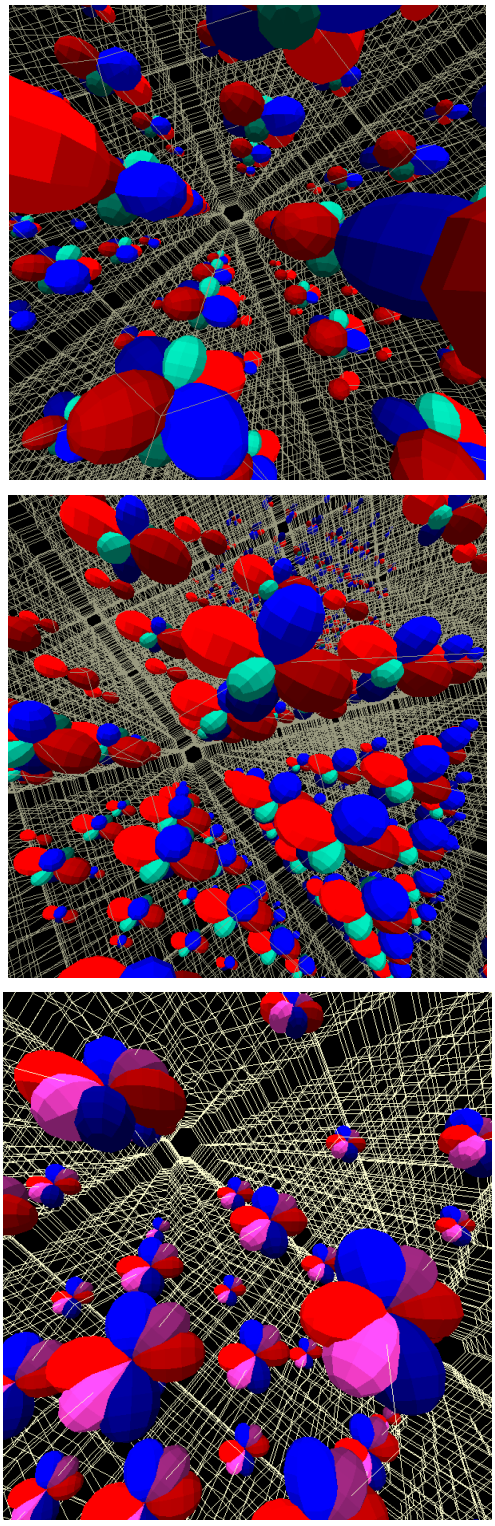


Figure 34. *Visualization of a quantum dot of GaAs. These three figures show the py orbital in dark blue, the px orbital in red, and a linear combination of px py pz. The line intersections indicate the nearest atom location.*

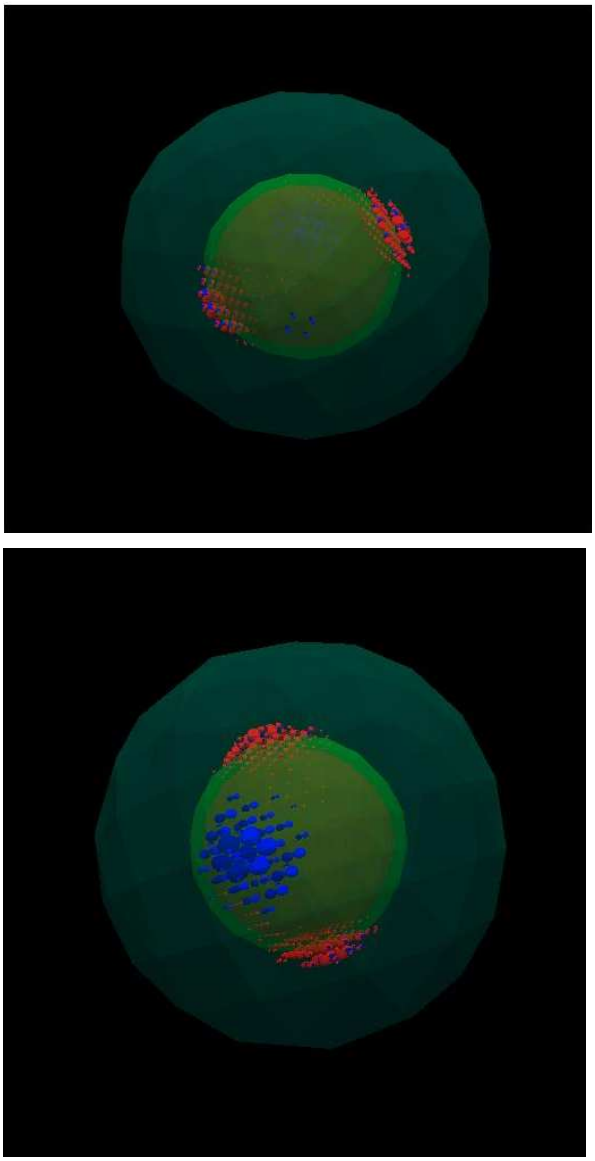


Figure 35. *Atomic scale charge density of a electronic state trapped in the well region of a CdS/HgS/CdS core/well/clad nanoheterostructured nanocrystal.*

Mathematical Modeling of Mechanical Systems and Processes

Stability of Nanowires

Geoffrey McFadden
Katherine Gurski (George Wasington University)
Michael Miksis (Northwestern University)

See feature article, page 31.

OOF: Finite Element Analysis of Material Microstructures

Stephen Langer
Andrew Reid (Drexel University)
Seung-Ill Haan (Univ. of Maryland Baltimore Co.)
Edwin Garcia (Pennsylvania State University)
Eric Ma (Montgomery Blair High School)
Edwin Fuller (NIST MSEL)
Craig Carter (MIT)

http://www.ctcms.nist.gov/oof

The OOF Project, a collaboration between MCSD, MSEL's Ceramics Division, the NIST 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. OOF is intended to be a general tool, applicable to a wide variety of microstructures in a wide variety of physical situations.

The OOF customer base is broad. As an indication of its breadth, during the past year technical support requests have been received from 11 US companies and laboratories[5], 12 US universities[6], and 13 foreign institutions[7].

During the past year the OOF team produced five beta releases of OOF2. OOF2 is a completely new version of the program, designed to be much more powerful and flexible than the original. OOF2 now solves two dimensional dielectric and piezoelectric problems, in addition to the linear elasticity and thermal conductivity problems that can be addressed by OOF1. New features introduced this year include the following.

- Piezoelectric physical properties: Piezoelectric materials couple strain and polarization, so that they change shape when a voltage is applied, or generate a voltage when an external force is applied. Adding piezoelectricity to OOF2 demonstrated that the extensibility built into its infrastructure actually works.
- Installation of a new graphics toolkit: The OOF2 GUI was originally built on the gtk+1.2 toolkit, which has become obsolete. Many beta testers had difficulty installing the old toolkit on their systems, so OOF2 was upgraded to gtk+2.6.
- Symmetric matrix testing: Finite element calculations ultimately boil down to the solution of a matrix equation. Matrix equations can be solved more efficiently if the matrix is known to be symmetric. Some, but not all, of the problems that OOF2 solves can generate symmetric matrices. The new feature automatically detects when a matrix can be symmetrized and does so if possible.
- A (long overdue) regression test suite.
- An experimental method of adapting a finite element mesh to the microstructural geometry by solving a pseudo-elasticity problem that moves mesh nodes towards material boundaries. This feature is still in development.

[5] U.S. companies and labs using OOF include: Balzers, CuraGen Corporation, Ford Research & Advanced Engineering, HoneyWell ES&S, Hughes Christenson Company Research & Development, Sandia National Laboratories, SC Solutions, Siemens, Solar Turbines (Caterpillar), Timken Research, United Technologies Research Center.

[6] U.S. universities using OOF include: Arizona State University, Carnegie Mellon University, North Carolina A&T University, North Carolina State University, RPI, University of Alabama at Birmingham, University of Connecticut, University of Illinois at Urbana-Champaign, University of Missouri-Rolla, University of Texas, University of Utah, University of Washington.

[7] Foreign institutions using OOF include: Aristotle University of Thessaloniki (Greece), Borealis GmbH (Denmark), Imperial College, London (UK), Industrial Research, Ltd (New Zealand), Karlstads Universitet (Sweden), Laboratoire des Mecanismes et Transferts en Geologie (France), MTU Aero Engines (Germany), National Institute for Space Research (Brazil), Universita di Bologna (Italy), University of Auckland (New Zealand), University of Goettingen (Germany), University of Limpopo (South Africa), University of Queensland (Australia).

In addition, an OOF2 users and reference manual was completed[8]. The reference section of the manual documents every OOF2 action and runs to about 900 pages, making a printed manual unwieldy; hence, the manual is available only on the web.

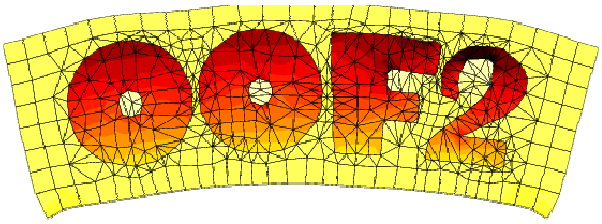


Figure 36. *Results of a calculation performed with OOF2. The lower corners of the sample are fixed in place and a temperature gradient has been applied from bottom to top. Thermal expansion of the letters has led to elastic deformation.*

Work began this year on the following future OOF2 features.

- Parallel computation. This is not absolutely require for OOF2, but will be necessary for a future three-dimensional version, OOF3D.
- Time-dependence and non-linearity: OOF1 and OOF2 2.0 only solve static linear problems. OOF2 2.1 will allow time dependent fields and boundary conditions, as well as non-linear equations, with the goal of solving plasticity problems.
- Subproblems: In many circumstances it's convenient to separate a problem into subproblems, and solve the subproblems sequentially. For example, a time-dependent chemical concentration field may couple to an elastic relaxation. If the time scale of the elastic relaxtion is very fast, it's possible to solve it quasi-statically at each time step of the chemical diffusion problem. In this case the subproblems concern different fields (elastic strain and concentration). It's also possible for subproblems to concern different parts of a microstructure: the interior of particles embedded in a matrix may be governed by different physics than the matrix.

OOF2 development has reached a transition period, after which the developers will spend less time on infrastructure and more time on applications. In the future we expect OOF2 (and later OOF3D) to be used and extended by researchers in industrial, academic, and government laboratories. NIST will continue to develop the code, but development will be mainly in collaboration with users, both at NIST and elsewhere.

[8] http://www.ctcms.nist.gov/~langer/oof2man/index.html

Materials Data and Metrology for Applications to Machining Processes, Frangible Ammunition, and Body Armor

Timothy Burns
Stephen Banovic (NIST MSEL)
Michael Kennedy (NIST MEL)
Lyle Levine (NIST MSEL)
Li Ma (NIST MSEL)
Steven Mates (NIST MSEL)
Richard Rhorer (NIST MEL)
Stephen Ridder (NIST MSEL)
Eric Whitenton (NIST MEL)
Howard Yoon (NIST PL)

The NIST Kolsky Bar Facility was originally designed and built to study the dynamic response of materials, mainly polycrystalline metallic alloys, under conditions of rapid temperature increase and compressive loading, in order to obtain improved constitutive stress-strain data for finite-element simulations of manufacturing operations involving high-speed machining. The Kolsky bar (also called the split-Hopkinson bar) compression test involves placing a thin, disk-shaped sample of the test material between two long, hardened steel rods, with the centerline of the sample disk aligned with the centerlines of the long bars. One of the steel rods is impacted by a shorter rod of the same material, sending a stress pulse into the sample. By design, the steel rods remain elastic in their response to the impact loading. The sample, on the other hand, deforms plastically at a rapid rate of strain, and instrumentation on each of the long steel rods can be used to determine the stress-strain response of the test material.

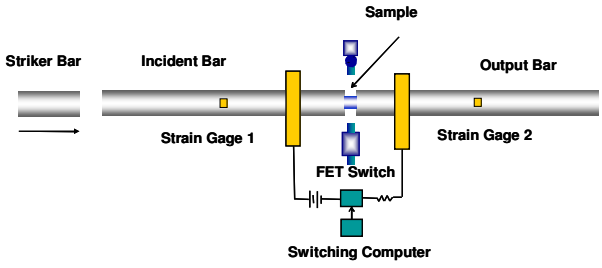


Figure 37. *Schematic drawing of the NIST pulse-heated Kolsky bar.*

While there are many Kolsky bars in laboratories at universities, U.S. Government DOD and DOE facilities, and defense contractors, the NIST Kolsky bar has the unique capability of pulse-heating a test specimen from room temperature to a significant percentage of its melting temperature in tens of

milliseconds, which mimics the rapid heating that occurs in thin cutting regions during a high-speed machining operation. The development of this capability was initially funded in large part by the NIST Intramural ATP Program, and new and/or improved instrumentation for this work continues to be supported by MEL, MSEL, PL, and ITL.

Timothy Burns (center) with Debasis Basak and Richard Rhorer (MEL) in the NIST Kolsky Bar Lab.

Now that the facility is operational, new applications have been found for its capabilities. During the present fiscal year, the pulse-heating capability of the facility was used in a study of the response of iron as part of an MSEL program in pipeline safety and integrity. In its room-temperature configuration, i.e., without pulse heating, the Kolsky bar was used to test ceramic specimens in support of an MSEL effort to initiate a program with the US Army Research Laboratory in Aberdeen, MD, on ceramic tank armor.

In a major effort during the past two fiscal years, the Kolsky Bar Team has received support from the National Institute of Justice (DOJ) through OLES, the NIST Office of Law Enforcement Research, to develop experimental methods and to perform studies of the dynamic response of frangible bullets. These bullets are manufactured from non-lead materials, usually by sintering. This involves the heating and compaction of a powder of several different constituents. The resulting mixture is then made into rounds by encasing it in brass or some other alloy. By first removing the brass casing, and then sectioning the bullets, cylindrical samples have been tested side-on in compression on the Kolsky bar, in what is known as the Brazil, or diametral test. Using a high-speed camera to determine the amount of compressive strain required to initiate fracture of a sample along its centerline, a good statistical estimate has been obtained during FY 2005 of the tensile strength of the bullet material.

In related work, modifications to the bar were designed this fiscal year for tension testing, and in collaboration with Wayne Chen of Purdue University, a small tension-testing bar has been used to study the mechanical behavior of soft body armor woven from fibers of the advanced polymeric materials PBO (Zylon) and Aramid (Kevlar). These tests will continue during the next fiscal year, and the results will be used by the US Department of Justice to determine what actions are required to ensure that soft body armor provides adequate protection to police officers in the field. Development of experimentally validated finite element models of bullet-vest interactions also continued, and will remain part of this ongoing program during the next fiscal year.

This work has been supported in part by the National Institute of Justice (DOJ) via the NIST Office of Law Enforcement Research.

Modeling and Simulation of High-Speed Machining Operations

Timothy Burns
Tony L. Schmitz (University of Florida)
D. Scott Duncan (University of Florida)

An area of manufacturing in which significant advances have occurred over the past few years is high-speed machining. New automated programmed machining centers provide material removal rates that vastly exceed what was possible even a decade ago. This has led manufacturers to rethink the design of various components. For example, an aircraft instrument panel that until recently consisted of an assembly of a number of sheet metal parts, connected by numerous fasteners where unwanted stress concentrations can occur, and which require an extensive inventory for parts storage, has been replaced by a monolithic aluminum part, manufactured on a high-speed machining center from a single block of aluminum using a number of different cutting tools, some with fairly long length to diameter ratios. The resulting panel is lighter, stronger, and quicker and cheaper to manufacture. Furthermore, the large bulk of material that is removed can simply be recycled.

One of the major limitations on the material removal rate in such a manufacturing process is the dynamics of the machining system, consisting of the spindle, tool holder, and cutting tool. If the cutting dynamics becomes unstable, so that tool chatter occurs, the surface finish becomes degraded, and the tool can

break, causing expensive delays in an assembly line for tool replacement. Research in the dynamics of machining has led to the use of stability lobe diagrams, which are curves of chip width vs. spindle speed, which separate the plane into zones of stable and unstable cutting. It turns out that the maximum material removal rate for a given spindle and holder can vary significantly with the length of the cutting tool, so that a given operation can be "tuned" by varying this length.

The methods that are used to obtain these stability diagrams require the frequency response of the tool point in the spindle-holder-tool system. This response, also called the tool-point receptance, can be obtained experimentally in each case by exciting the tool at its free end with an instrumented hammer, and then measuring tip response using an appropriate transducer, such as an accelerometer. With such data in hand, a stability lobe diagram can be developed for a given tool in a spindle-holder system, but each diagram depends upon tool length, so that extensive testing is required in order to optimize a given manufacturing operation. Furthermore, the required expertise and instrumentation to do this are not always available on the shop floor in a manufacturing facility.

Over the past several years, since Tony Schmitz came to NIST as an NRC postdoctoral fellow in MEL, a research program has been in progress, with the goal of developing methods for rapid prediction of the tool point response using a minimum number of measurements. The basic idea has been to use the well-established theory of Receptance Coupling Substructure Analysis (RCSA), in which the frequency response of a structure that is an assembly of two or more substructures is determined using the frequency responses of the substructures. For application to high-speed machining, the approach taken is to determine the response of a given spindle-holder system using experimental measurements, while the tool response is determined analytically by modeling it as a beam. The major difficulty in applying RCSA to the combined system is to develop a sufficiently accurate model of the joint that connects the cutting tool to the spindle-holder system.

Work during FY 2005 was concentrated on developing an improved joint model for coupling the two subsystems using RCSA. This effort will continue during the next fiscal year. In addition, gyroscopic effects on a rapidly spinning beam will be investigated for improved modeling of the cutting tool.

Phase-Field Modeling of Solidification under Stress

G.B. McFadden, MCSD
J. Slutsker (NIST MSEL)
J.A. Warren (NIST MSEL)
A. L.Roytburd (Univ. of Maryland College Park)
K. Thornton (University of Michigan)

For a number of years researchers in MSEL and ITL have collaborated on the modeling of phase transitions in materials by using a diffuse interface approximation to the surfaces that separate different thermodynamic phases in the bulk sample. These descriptions, sometimes called phase-field models, date back to work by van der Waals in the 19th century, and were later used by J. Cahn and coworkers in studies of spinodal decomposition and order-disorder transitions in condensed matter. Recent work at NIST includes the application of phase-field models to a variety of phase transitions, including the description of fluid-fluid interfaces, the effects of an electric field on interface properties during electrodeposition, and modeling stress effects during solid-state phase transitions.

Phase transitions involving either a crystalline or amorphous state in nano-volumes are basic mechanisms of modern phase-change recording. This process exploits an amorphous-to-crystalline phase change to record information onto electronic media such as DVDs. Due to the density difference between phases, transformations in confined volumes are accompanied by internal stresses. Thus, it is necessary to take into account the effect of internal stress during phase change recording. In this project we have modeled this "writing" process by considering phase transitions in a confined volume. The phase field model takes into account the simultaneous evolution of three fields: a phase field, a temperature field and a stress/strain field. A paper entitled "Phase-field modeling of solidification under stress," by J. Slutsker, K. Thornton, A.L. Roytburd, J.A. Warren and G.B. McFadden has been submitted for publication in *Acta Materialia*. This work considers the effects of stress on transformations between amorphous and crystalline phases in confined spherical nano-volumes, with applications to the phase-change recording processes.

This work has been supported in part by the National Science Foundation (NSF).

Modeling Fluid Flow and Materials Processing

G. McFadden
S. Coriell (NIST MSEL)
K. Gurski (George Washington University)
D. Cotrell (Lawrence Livermore National Laboratory)
W. Alley (Lawrence Livermore National Laboratory)
B. Alder (Lawrence Livermore National Laboratory)
M. Ali (King Saud University, Saudi Arabia)

G. McFadden, S. Coriell, and former NRC postdoctoral fellows K. Gurski and D. Cotrell are studying the stability of a two-layer fluid system subject to temperature-dependent capillarity. The classical treatment assumes that the two fluids are immiscible; in this work we compare that case to that in which the fluids are different thermodynamic phases of the same material. This problem is important in a number of applications, including supercritical steam turbines and the materials processing of monotectic systems. Of particular interest is the Marangoni effect in two-phase fluid systems, in which gradients in surface tension drive a flow along the interface. These flows are important even in low gravity, and this study was initiated to support experimental work by colleagues at the University of Alabama, Birmingham, on the formation of rod-like structures in monotectic systems being processed under microgravity conditions.

D. Cotrell and G. McFadden are considering the hydrodynamic stability of systems with boundary perturbations. These systems can model the effect of wall roughness on the transition to turbulence in hydrodynamics, which is a classical area being studied by Dr. Cotrell's colleagues at Lawrence Livermore National Laboratory. A paper entitled "Effect of an Axially-periodic Radius on the Linear Stability of Pipe Flow" is in internal review, and will be submitted to the *Journal of Fluid Mechanics*.

A paper entitled "Linear Stability of Cylindrical Couette Flow in the Convection Regime," by M.E. Ali (King Saud University, Saudi Arabia) and G.B. McFadden, has appeared in the *Physics of Fluids*. G. McFadden served on Dr. Ali's Ph.D. committee at the University of Colorado, and this paper is an outgrowth of a collaboration that involved the study of fluid flow in an annulus with differentially-rotating, heated sidewalls. That work, in turn, is related to a previous collaboration between MCSD and the MSEL Metallurgy Division on a analysis of experiments performed at the Rensselaer Polytechnical Institute that involved the stability of a cylindrical solid-liquid interface. In related work, D. Cotrell and G. McFadden studied the stability of Couette flow with an axial pressure gradient under the influence of viscous heating and other thermal effects; this work is appearing in the *Physics of Fluids*.

Modeling Nonequilibrium Boundary Condition at a Liquid-Liquid Interface

G. McFadden
D. Anderson (George Mason University)
M. Gurtin (Carnegie Mellon University)
E. Fried (Washington University)
P. Cermelli (University of Torino, Italy)

The motion of two fluid phases and the interface separating them has been a problem of scientific and industrial interest for centuries. Applications in which the understanding of the interface between two fluid phases is critical continue to emerge. As the complexity of these problems increases, particularly the complexity of the physics occurring at the interface, there is an increased need for robust methods for identifying the appropriate interfacial conditions to be applied in continuum models of the fluid--fluid interface. Equilibrium interfacial conditions for phase-transforming systems have been successfully derived based on variational arguments. However, these fail to extend to nonequilibrium settings where dissipative effects such as fluid viscosity are important.

In this work we address the problem of formulating nonequilibrium interfacial conditions for an interface between two fluids. The approach we adopt here is based on the formalism of configurational forces as developed by Gurtin et al. We specifically apply these ideas to fluid-fluid systems in which phase transitions may occur. Of particular interest are interfacial conditions such as the nonequilibrium version of the Gibbs--Thomson equation. The treatment based on configurational forces leads naturally to the inclusion of effects such as interfacial viscosity and interface kinetics. We have applied the model to the example of a liquid sphere growing into its supercooled vapor phase. We have found a novel solution that is the sum of similarity solutions, each of which is consistent with spherical growth with the square of the radius increasing linearly with time. Each of the similarity solutions satisfies a different ordinary differential equation with variable coefficients, and the solutions may be superimposed to satisfy the interfacial boundary conditions that are derived in the configurational force model. This work has been submitted to the *Journal of Fluid Mechanics*.

A Stochastic Approach to Modeling of Contact Dynamics of Silicon Cantilevers

Jeffrey Fong
James Filliben
Hung-kung Liu
Donna Hurley (NIST MSEL)
Douglas Smith (NIST MSEL)
Roland deWit (NIST MSEL)
R. Fields (NIST MSEL)
Jon R. Pratt (NIST MEL)
Barry Bernstein (Illinois Institute of Technology))
Richard S. Chadwick (NIH)

Beginning in April, 2005, researchers from ITL, MSEL, and MEL have been working together on an 18-month joint exploratory competence project to *initiate* the development of a stochastic approach to the nonlinear modeling of contact dynamics of silicon cantilevers and the *verification* (without validation) of the finite-element-method (FEM) simulations of those models at micro- and nanoscales for applications in atomic force microscopy (AFAM), nanoscale manufacturing, and biomedical nanomechanics. In particular, our goal is to better understand the process of tip wear and its influence on AFAM measurement of material properties. NIST researchers at its Boulder laboratories (Hurley, et al) have recently conducted experiments to determine the tip-sample contact stiffness and tip radius before and after AFAM measurements for several different cantilevers. They used two contact mechanics models to determine the radius theoretically, but the results varied indeterminately from those based on scanning electron microscope images.

In related work, Fong collaborated with R.S. Chadwick, a principal investigator at NIH Institute on Deafness and Other Communication Disorders (DOCD), in providing a new research opportunity in the National Academy of Sciences-National Research Council (NRC) joint NIH-NIST postdoctoral program. The title of the new opportunity is "Stochastic Modeling of Contact Mechanics of Cantilevers for Calibrating Cochlear Models of Human Inner Ear."

Fong also contributed a new NRC postdoctoral opportunity, entitled "Stochastic Modeling, Verification, Validation, and Calibration of Computer Simulations."

This work has been supported in part by the NIST Director's Competence Program.

Complex System Failure Analysis: A Computational Science Based Approach

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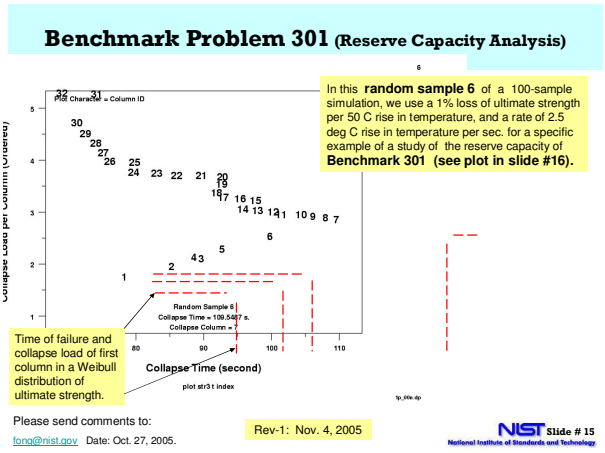
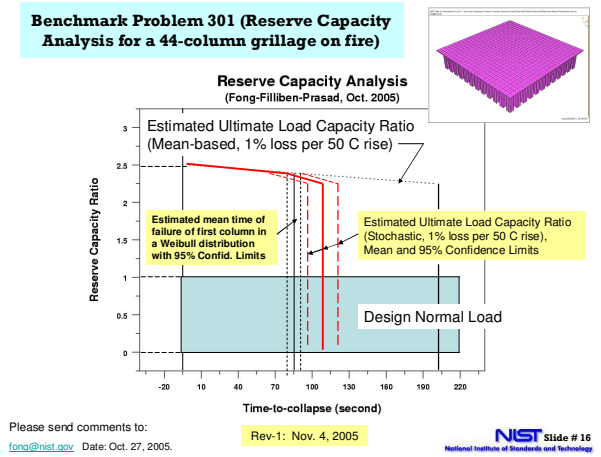
James Filliben
Hung-kung Liu.
Emil Simiu (NIST BFRL)
Dat Duthinh (NIST BFRL)
Therese McAllister (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)
Barry Bernstein (Illinois Institute of Technology)

Beginning in Feb. 2004, researchers from ITL, and BFRL have been working together on a 5-year joint competence project entitled "Complex System Failure Analysis: A Computational Science Based Approach." The objective of the project is to create the scientific basis for building failure investigation procedures that will allow NIST to accomplish its mission under the National Construction Safety Team Act (P.L. 107-231, Oct. 1, 2002), and is likely, over time, to be applicable for failure analysis and uncertainty determination of a broad range of complex physical, chemical, biological, and engineered systems of interest throughout NIST.

Since the physics of structural failure due to fire and other extreme loadings involves complex models and multi-physics simulations based on (a) an *incomplete* knowledge of the governing equations related to material properties and loads, (b) a *significant* variability in material properties, geometric dimensions, joint characteristics, and loading spectra throughout the time line from fire initiation, local damage and fire spread, regional damage and load redistribution, to critical global trigger and final collapse, and (c) a *lack* of a fixed geometric configuration for traditional simulation to take place due to an evolution of changing geometry as damage spreads from local to regional and global scales, we propose a *metrology-based* computational approach by first identifying a minimal number of computational tools suitable for this problem and then formulating an open-ended set of questions to attack the underlying physical nature of the problem.

The computational tools we propose to use are: (1) Finite Element Method (FEM)-based computational software packages, (2) Statistical software packages, (3) General purpose computational and system software packages.





The open-ended set of questions to be addressed begins with a comparative study of two models, one deterministic and the other stochastic, in order to calculate the time to collapse of a set of idealized structures under simple loadings (e.g., Reference Benchmark RB-301, the reserve capacity analysis of a 44-column grillage on fire where the deterministic model over-estimates the time to collapse from the stochastic model by almost a factor of two). The metrology-based approach utilizes specific results from the literature, namely, (1) standard reference benchmarks such as RB-301, (2) orthogonal fractional factorial design of numerical experiments as applied to FEM simulations, (3) ISO (1993) guides to the expression of uncertainty in experiments, (4) "best" least-square-fit of at least 4 grid-convergence FEM run results, and (5) a Bayesian approach to combining results from multiple methods.

This work has been supported in part by the NIST Director's Competence Program.

Modeling the Behavior of Cryocoolers

Abbie O'Gallagher
John Gary (MCSD retired)
Ray Radebaugh (NIST CSTL)

Cryocoolers are refrigerators that produce extremely cold temperatures. They have many applications ranging from military to medical. John Gary (now retired) and Abbie O'Gallagher of MCSD have been working with Ray Radebaugh of CSTL developing and improving a model called REGEN3.2 which is used in the design of cryocoolers. This model, besides being used by many researchers and designers throughout the community, has been used in house extensively by Ray Radebaugh.

In 2005, O'Gallagher and Radebaugh made almost 200 production runs using this model. These studies support Radebaugh's research into the design of very small cyrocoolers that must be run at very high frequencies. Such micro-cryocoolers are intended to be used in micro-electrical-mechanical systems (MEMS). This work resulted in the paper, "Regenerator Operation at Very High Frequencies for Micro-Cryocoolers," R. Radebaugh and A. O'Gallagher, *Advances in Cryogenic Engineering* **51** (2006). The paper was given at the Cryogenic Engineering Conference held in Keystone Colorado from August 29th through September 1st, 2005.

Recently, O'Gallagher has been doing computer experiments into the behavior of the REGEN3.2 model when the user specifies that the matrix is made up of layers of different materials. She and Gary continue to work on improving this model and its user interface.

Mathematical Modeling of Electromagnetic Systems

Mathematical Modeling of Nanomagnetism

Michael Donahue
Donald Porter
Robert McMichael (NIST MSEL)

See feature article, page 29.

High-Speed Waveform Metrology

Andrew Dienstfrey
Jack Wang (SED)
Tracy Clement (NIST EEEL)
Paul Hale (NIST EEEL)
Darryl Keenan (NIST EEEL)
Rich Mirin (NIST EEEL)
Dylan Williams (NIST EEEL)

New waveform metrology techniques are required to facilitate the research and development of future high-speed communications devices and applications including: fiber optic communications, high-speed micro-circuitry, ultra-wideband wireless communication, advanced radar systems, and remote sensing. For example, present fiber optic trunk-lines (the backbone of the internet) operate at data rates of 5 to 10 gigabits per second using time-division multiplexing (TDM). The limiting factor for this data rate is not the carrying-capacity of the optical fiber, but rather the components (electrical and electro-optic) which generate and receive the digital signals. Research on the next generation of TDM systems which are intended to operate at 40 gigabits per second and higher is ongoing. It is known that current measurement technologies are inadequate to characterize the frequency and time domain response functions of new high-speed sources, detectors, and instrumentation currently under development. To address this need, NIST began in 2004 a five-year competence project, "New Paradigms in High-Speed Waveform Metrology."

In the past fiscal year (2005) significant progress was made in characterizing the NIST-developed Electro-optic Sampling (EOS) system. The theoretical bandwidth of the EOS system is many orders of magnitude higher than any existing data waveform modulation scheme. In addition, EOS response characteristics are traceable to fundamental units. Thus, EOS technology will create the possibility for a traceability chain for optical and electrical waveform metrology that has not existed previously.

Further research was performed in using the EOS system to calibrate equivalent-time sampling oscilloscopes supplied by several manufacturers. The bandwidths of these oscilloscopes (50-100 GHz) are such that lumped-element, circuit-theory descriptions of components are insufficient. The necessary microwave techniques were detailed in a paper jointly authored by several members of the group, and which was submitted for publication in a special issue of the *IEEE Trans. in Microwave Theory and Techniques*.

A more robust paradigm for reporting uncertainties was explored. The idea is to propagate both variances and variance correlations through measurement devices and analyzes. This is expected to enhance uncertainty reporting on existing waveform parameter characteristics, as well as enable more detailed waveform descriptions which NIST can not currently report to customers for lack of a valid uncertainty analysis. A paper detailing the procedure was accepted for publication in TMTT.

Finally, a new algorithm was developed to investigate the recovery of the phase response of an equivalent-time sampling oscilloscope from its magnitude. In general, the class of linear response functions for which this is possible is called "minimum-phase". Broad criteria for a priori characterization of minimum-phase systems are lacking; thus empirical verification is required. There are a few technical difficulties in applying the necessary theory. These were overcome, and a procedure was implemented. Comparisons of the minimum-phase computations with direct measurement of the oscilloscope phase response verify the correctness of the algorithm, as well as indicate that the validity of the minimum-phase assumption over a large bandwidth. This analysis will prove essential for extending oscilloscope calibrations to the low end of the RF spectrum, and will serve to complement the high-frequency measurement capabilities of the EOS system. Details of this work have been described in another paper that will be submitted for publication in a peer-reviewed journal.

The coming fiscal year we hope to refine the results of 2005. Furthermore, we intend to advance the analysis procedures to include general deconvolution and regularization techniques. Based on the results of this first year of competence funding, NIST management has determined that the EOS platform will serve as the backbone for all future high-speed waveform metrology performed by NIST.

This work has been supported in part by the NIST Director's Competence Program.

Micromagnetic Modeling

Michael Donahue
Donald Porter
Robert McMichael (NIST MSEL)
Stephen Russek (NIST EEEL)

http://math.nist.gov/oommf/

Advances in magnetic devices such as recording heads, field sensors, magnetic nonvolatile memory (MRAM), and magnetic logic devices are dependent on an understanding of magnetization processes in magnetic materials at the nanometer level. Micromagnetics, a mathematical model used to simulate magnetic behavior, is needed to interpret measurements at this scale. MCSD is working with industrial and academic partners, as well as with colleagues in the NIST MSEL, PL, and EEEL, to improve the state-of-the-art in micromagnetic modeling.

M. Donahue and D. Porter in MCSD have developed a widely used public domain computer code for doing computational micromagnetics, the Object-Oriented Micromagnetic Modeling Framework (OOMMF). OOMMF serves as an open, well-documented environment in which algorithms can be evaluated on benchmark problems. 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 2005 alone, the software was downloaded more than 3000 times, and use of OOMMF was acknowledged in 79 peer-reviewed journal articles.

OOMMF is part of a larger activity, the Micromagnetic Modeling Activity Group (muMAG), formed in 1995 to address fundamental issues in micromagnetic modeling through two activities: the development of public domain reference software, and the definition and dissemination of standard problems for testing modeling software. MCSD staff members are involved in development of the standard problem suite as well. There are currently four standard problems in the suite, testing both static and dynamic magnetization properties. A fifth problem, dealing with modeling of thermal effects, is in development.

In large devices, random thermal effects tend to be self-canceling, but as device size decreases thermal effects grow in relevance. This is especially true in high sensitivity low field magnetic sensors, where performance is generally limited by thermal noise. A four-laboratory NIST Competence project (EEEL, MSEL, PL and ITL) to design a new generation of such sensors is in progress, and proper modeling of thermal effects within OOMMF is a key objective.

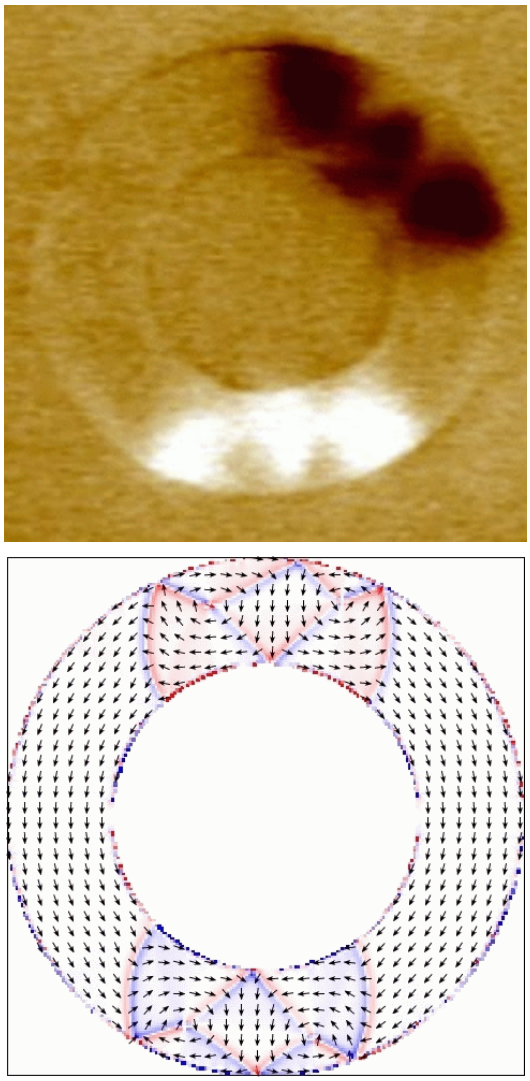


Figure 38. *Top: Image of 2000 nm diameter ring of ferromagnetic material produced by a magnetic force microscope. Bottom: Magnetization pattern computed by OOMMF based on known parameters chosen to match the experimental work.*

Another new feature being developed for OOMMF is the ability to model spin transport phenomena. There has been a surge of interest in spin transport, as judged by the number of presentations and articles related to the topic at conferences and in journals devoted to magnetism.

In addition to the continuing development of OOMMF, the project also does collaborative research using OOMMF. The MCSD micromagnetic project produced three journal papers and four conference presentations in the fiscal year 2005. Research included numerical techniques for eddy current calculation, modeling of a microfluidic magnetic trap platform used to position magnetic particles with nanometer precision, and model-based interpretation of MFM images of domain walls in ferromagnetic rings, confirming observations of multi-vortex domain wall states for the first time (see Fig. 38). A presentation about OOMMF was also made at the NIST/TEDCO Showcase in June, 2005.

This work has been supported in part by the NIST Director's Competence Program.

Time-Domain Algorithms for Computational Electromagnetics

Bradley Alpert
Leslie Greengard (New York University)
Thomas Hagstrom (University of New Mexico)

http://math.nist.gov/AlgoCEM

Acoustic and electromagnetic waves, including radiation and scattering phenomena, are increasingly modeled using time-domain computational methods, due to their flexibility in handling wide-band signals, material inhomogeneities, and nonlinearities. For many applications, particularly those arising at NIST, the accuracy of the computed models is essential. Existing methods, however, typically permit only limited control over accuracy; high accuracy generally cannot be achieved for reasonable computational cost.

Applications that require modeling of electromagnetic (and acoustic) wave propagation are extremely broad, ranging over device design, for antennas and waveguides, microcircuits and transducers, and low-observable aircraft; nondestructive testing, for turbines, jet engines, and railroad wheels; and imaging, in geophysics, medicine, and target identification. At NIST, applications include the modeling of antennas (including those on integrated circuits), waveguides (microwave, photonic, and at intermediate terahertz frequencies), transducers, and in nondestructive testing.

The objective of this project is to advance the state of the art in electromagnetic computations by eliminating three existing weaknesses with time-domain algorithms for computational electromagnetics to yield: (1) accurate nonreflecting boundary conditions (that reduce an infinite physical domain to a finite computational domain), (2) suitable geometric representation of scattering objects, and (3) high-order convergent, stable spatial and temporal discretizations for realistic scatterer geometries. The project is developing software to verify the accuracy of new algorithms and reporting these developments in publications and at professional conferences.

A problem that has been revisited during the past year is that of nonreflecting boundary conditions for the wave equation (and Maxwell's equations). Although earlier work of these researchers was successful in producing a procedure that is both spectrally accurate and highly efficient, its lack of flexibility in the shape of the boundary limits the variety of settings in which it has been adopted.

Alpert and his collaborators, in the period since the earlier work, have attempted to generalize the nonreflecting boundary procedures to rectangular domains. This year they became convinced that the highly nonlocal dependencies inherent in nonreflecting boundary conditions can be circumvented (or localized) by looking somewhat inside the domain. This hypothesis, arising in part by analytical work by Warchall, has prompted a renewed attempt to formulate an exact local nonreflecting boundary treatment. This work continues.

A paper on an inner product for scattering problems, "Half Space Representation of Acoustic Waves from Compact Sources," B. Alpert and Y. Chen, appeared in *Communications in Pure and Applied Mathematics* **58** (10) (2005), pp. 1358-1374.

The work has been recognized by researchers developing methods for computational electromagnetics (CEM) and has influenced work on these problems at Boeing and HRL (formerly Hughes Research Laboratories). It has also been cited widely, including by researchers at University of Colorado, University of Illinois, Michigan State University, Technion, University of Texas, and Yale University.

This work has been supported in part by the Defense Advanced Research Projects Agency (DARPA).

Quantum Dot Identification and Characterization

Bradley Alpert
Alexana Roshko (NIST EEEL)

We have d developed and implemented a procedure for the identification and size characterization of InGaAs quantum dots grown on a GaAs substrate. These nanoscale structures are grown by chemical vapor deposition (CVD) or molecular beam epitaxy (MBE) and are measured by atomic force microscopy (AFM) by Alexana Roshko and coworkers in the NIST Optoelectronics Division. Deposition of InGaAs on a substrate of GaAs results in formation of mounds, rather than layers, due to the mismatch of lattice cell dimensions for the two compounds. The electron containment characteristics of these nanoscale structures, or quantum dots (QDs), lead to unique electromagnetic properties that can be exploited in a variety of applications. The InGaAs mounds form at random positions and with random sizes, with population characteristics dependent on the precise growth environment which includes In, Ga, and As vapor pressures, temperature, and mixing.

In pursuing the goal of attaining a high-density, uniform size production of QDs, it is necessary to accurately characterize the size and distribution of dots formed throughout the wafer. At NIST a major component of this effort is the collection and processing of wafer height data as atomic force microscropy (AFM) images. An existing characterization method suffers certain errors and requires operator input, thereby limiting its effectiveness and interlaboratory reproducibility. This approach counts as QD local maxima exceeding a given height threshold, with the exclusion of other (presumed inseparable) local maxima within a square of given side length. The height threshold and square size, parameters input by the analyst, allow some tuning of this method to cope with images arising under different growth conditions. This flexibility is, however, a disadvantage for achieving comparability across laboratories. In addition, this approach suffers false negatives and false positives in identification when the underlying GaAs substrate contains its own hills and valleys (however gradual), when the QDs are highly variable in size, and when some QDs fall in the "shadow" of others nearby, due to their separation being smaller than the size of the AFM probe tip.

A new procedure, which is under evaluation to replace the earlier one, combines the computation of surface geometric properties, primarily curvature characteristics, with probabilistic analysis to significantly reduce false positives and false negatives in identification of QDs and to improve the accuracy of their shape determination. Tests are underway to determine whether the method can cope with various problems with the AFM data, such as inconsistent leveling of successive lines of the image and unexplained temporary height offsets, and whether parameters of the method can be chosen automatically based on image characteristics.

Terahertz Band Device Modeling

Bradley Alpert
Eyal Gerecht (NIST EEEL)

The terahertz electromagnetic frequency band (defined roughly as 0.3 to 10 THz), undeveloped until recently due to several signal generation, detection, and transmission hurdles including strong atmospheric attenuation, is increasingly recognized as a promising frontier for sensing for imaging and spectroscopy in biomedical and security applications. Energy transitions of important molecules in biology and astrophysics occur at terahertz frequencies. Terahertz radiation (T-rays) can penetrate clothing and, to some extent, can also penetrate biological materials, and because of its shorter wavelengths offers higher spatial resolution than do microwaves or millimeter waves.

Design and development of effective signal generators and detectors can be greatly accelerated by computational modeling. The terahertz band, which shares characteristics of microwave and optical frequencies, requires improved methods to accurately handle the disparity of component sizes in these devices. Present computational methods offer either full-wave modeling, for electrically small devices in which waves must be fully resolved, or geometric theory of diffraction, for electrically large devices that are smooth on the scale of many wavelengths.

We are developing methods to combine these two approaches, for modeling of quasi- optical detectors. This effort is in conjunction with terahertz imaging and spectroscopy work led by Eyal Gerecht of the NIST Electromagnetics Division. It may also support nanotechnology applications that require modeling of electromagnetic devices that span vastly different length scales. Commercial multiphysics modeling software (FEMLAB) with an electromagnetics module, recently acquired, will enable combination of finite element method computations, for the electrically small antenna-like part of the detector, with a custom diffraction method, for the lens-like part.

Physics Models for Transport in Compound Semiconductors

Howard Hung
Terrance Griffin
Herbert S. Bennett (NIST EEEL)
Alan Heckert

Physics models for carrier transport in semiconductors are essential inputs of computer programs that simulate the behavior of nano- and micro-electronic and optoelectronic devices. Such simulations increase understanding, reduce times-to market, and assist in making selections from among competing or alternative technologies. As devices shrink in size to nanometers, performing experimental measurements becomes more costly and time-consuming. This means that computer simulations will become more essential for advances in future nanotechnologies and for keeping the U.S. at the forefront of technological innovations.

Unlike many physics models that are based on using variations in parameters to fit experimental data, the NIST physics models developed in this project are based on quantum mechanical calculations with no fitting parameters to account for dopant ion effects and many-body physics effects. The calculations for interpreting Raman spectra include many body quantum effects and bandgap narrowing due to dopant ion carrier interactions. The many body quantum effects treat both electron-electron and electron-hole interactions. The results are unique because all other reported treatments for the electric susceptibility 1) do not treat these effects self-consistently; 2) are Taylor series expansions in either (Q / A) or (A/Q) , where Q is the magnitude of the normalized wave vector and A is the normalized frequency used in such measurement methods as Raman spectroscopy. These results will change the way researchers and process engineers interpret non-destructive measurements to extract the carrier concentrations and perhaps the carrier mobilities of GaAs wafers. The wafer carrier concentration is a key figure of merit associated with a go-no-go decision for determining whether a wafer meets specifications and should undergo further processing.

We are collaborating with EEEL to develop efficient computational methods for this problem, and to develop evocative three-dimensional displays of the results in our immersive environment. This year we studied the dependence of electron density on Fermi energy in compensated n-type gallium antimonide. Their results are consistent with the findings of experimental work reported in the literature concerning the relative distributions of electrons among the conduction subbands. Interpreting experiments for GaSb requires at least a three-band model and under some conditions may require a four-band model. Even though GaSb is intrinsically a direct semiconductor, their results show that electrons for n-type GaSb in the vicinity of the Fermi surface will have some characteristics that are similar to those for electrons in an indirect semiconductor. This work was described in the paper: “Dependence of Electron Density on Fermi Energy in Compensated N-type Gallium Antimonide,” H.S. Bennett, H. Hung, and A. Heckert, *Journal of Applied Physics* **98** (10) (November 15, 2005).

Quantum Information

Architectures for Fault-Tolerant Quantum Computing

Emanuel Knill

See feature article, page 23.

Quantum Circuit Synthesis

Stephen Bullock
Dianne O'Leary
Gavin Brennen (NIST PL)
V. Shende (University of Michigan)
Igor Markov (University of Michigan)

See feature article, page 25.

Adaptive Finite Element Modeling of Two Confined and Interacting Atoms

William Mitchell
Eite Tiesinga (NIST PL)

See feature article, page 27.

Realizing Quantum Information Processors

Emanuel Knill
Scott Glancy
Didi Leibfried (NIST PL)
Dave Wineland (NIST PL)

Quantum information processors will solve otherwise intractable problems such as factoring large numbers and quantum physics simulation, and will greatly improve the accuracy of Monte Carlo estimates. Current quantum information processors can manipulate no more than 8 quantum bits (qubits), which is sufficient for investigating quantum device behavior but not for exploiting the hoped-for computational advantages. The challenge is to obtain sufficiently capable quantum devices and to engineer appropriate architectures to build scalable quantum information processors. Quantum information is significantly more sensitive to errors than classical information. Thus one of the main problems is to obtain fault-tolerant architectures that can operate accurately at high error probabilities per device while making efficient use of available resources.

Our work involves (1) Characterizing and benchmarking quantum devices, particularly those based on ion traps and linear optics, and (2) Investigating fault-tolerant architectures with the goal of improving error tolerance and reducing resource requirements.

In the area of benchmarking, we continued collaborating with Dave Wineland's group in the Time and Frequency division, contributing to two important benchmarks. The first involved an implementation of the quantum Fourier transform, which is the subroutine that enables Shor's efficient factoring algorithm. This work appeared in *Science* **308** (2005), p. 997. The second consisted of preparing so-called cat states on up to six ion-qubits. Verified preparation of these highly entangled states is an excellent demonstration of quantum control. The paper describing this experiment is in *Nature* **438** (2005, p. 639. Still in progress is an experiment to characterize the computationally relevant error probabilities per gate for the current ion-trap system by executing long random pulse sequences. The goal is to accurately determine these error probabilities even though the measurements are themselves subject to error.

We also completed work on a particularly simple fault-tolerant architecture, using several new strategies to show by simulation that error probabilities per gate of several percent are tolerable. See the "feature" on this work elsewhere in this report, which was published in *Nature* **434** (2005), p. 39.

This work has been supported in part by the Defense Advanced Research Projects Agency (DARPA) and the NIST Director's Competence Program.

Optical Quantum Metrology and Quantum Computing

Emanuel Knill
Scott Glancy
Richard Mirin (NIST EEEL)
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Kevin Silverman (NIST EEEL)
Marty Stevens (NIST EEEL)
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Members of the MCSD are contributing to the development of an experimental research program in optical quantum metrology and quantum computing. This project will develop expertise in the preparation, manipulation, and measurement of exotic quantum states of light, such as entangled states of N photons and Schrödinger Cat states. The entanglement properties of these states can be exploited for high precision interferometry, quantum communication, and quantum computation. All of these technologies require the ability to control and measure very delicate and sensitive quantum states, and they will all benefit from this project. Furthermore, this project could have some short-term impact in medical imaging and nanotechnology. Quantum optical technology is potentially useful in medical imaging because of the improved depth resolution possible using entangled photons. Nanotechnology could benefit from methods for focusing light to better than the diffraction limit. This project will significantly expand NIST capabilities in quantum optical metrology, enabling us to expand our position as the global leader in measurement and enabling technology as applied to quantum optics.

Currently, NIST is the leading NMI in single photonics, with strong efforts in single photon sources, photon detectors, and quantum optics and information theory. Because this project was awarded funding in the FY2005 Competence Proposal competition, our experts in photon sources, detectors, and theory, have been able to combine their efforts into a single group. We have begun the design and construction of an optical homodyne system, which can be used to measure and reconstruct the quantum state of any single mode of light. This will serve as an essential element of many optics experiments. Our future plans include experiments to prepare and characterize squeezed light, Schroedinger cat states, entangled states of a few photons, and the demonstration of the violation of Bell's Inequalities. Many of these elements will be integrated in a versatile optics testbed capable of performing these and many other quantum optics tasks.

This work has been supported in part by the the NIST Director's Competence Program.

Mathematics of Metrology

Improving Image Resolution in Nanotechnology

Alfred Carasso
Andras Vladár (NIST MEL)

See feature article, page 33.

Identifying Objects in LADAR Scanning Data

David Gilsinn
Christoph Witzgall
Dianne O'Leary
Geraldine Cheok (NIST BFRL)
Alan Lytle (NIST BFRL)
William Stone (NIST BFRL)

See feature article, page 39.

Phase Modulation Measurements of Fluorescent Lifetimes

Fern Y. Hunt
Adolfas Gaigalas (NIST CSTL)

Fluorescent stains and dyes are used to visualize the structure and function of biological materials on the cellular and sub cellular level. Recently fluorescent probes have been used to visualize the activity of genes in an entire organism. Thus, fluorescent chemicals have and will continue to play a significant role in developing the knowledge needed for biomedical applications of research in genetics and molecular biology. Fluorescent photodegradation, the photo-chemical reactions that transform excited fluorophores to a non-fluorescent species, limits the effectiveness of these materials so the problem of understanding the relationship between fluorescent photodegradation and the wavelength of the excitatory light source is an important one.

A. Gaigalas of CSTL has explored this issue by performing phase modulation measurements with a lock-in amplifier. This powerful technique allows one to recover and amplify a weak signal even in the presence of significant noise and permits reliable measurements of small degradation rates. The apparatus is depicted in Fig. 39.

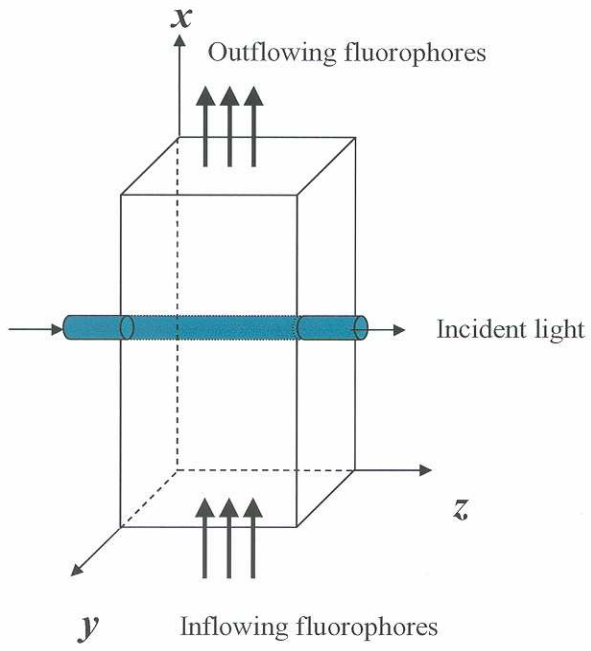

Figure 39. *Schematic of apparatus for performing phase modulation measurements with a lock-in amplifier*

A sample of fluid containing fluorescent particles (fluorophores) flows vertically in the x direction through a rectangular box and is stimulated by a laser light shining through the center. The fluid flow allows fresh populations of unabsorbed molecules to be exposed to the light over a period of time. The light beam initiates the reaction leading to fluorescence. When the intensity of the excitation light fluctuates periodically, the fluorescent emission is also periodic with the same frequency but it is shifted in phase. The emission is converted to an electrical signal and by suitable signal multiplication and filtering one can eliminate contaminating noise, which generally has a frequency different from the light. The phase is related to the fluorescence lifetime. Given the phase difference φ, Gaigalas obtained a formula for $\tan(\varphi)$ as a function of the wavelength of the incident light. It provided a good fit to the values obtained from the lock-in amplifier apparatus.

This year Hunt and Gaigalas developed a mathematical model describing the evolution of fluorophores as they flow through the apparatus. Using the fact that the excitation (and relaxation) rate was much larger than the photodegradation rate, the analysis allows us to focus on the fluorophores passing in front of the light beam, while we neglect the intial time period while they are far away. This leads us to consider a single differential equation instead of the pair of first order partial differential equations that constitute the model. Fig. 40 shows a representation of values of tan(φ) as a function of the laser frequency (in Hz) as calculated from our analysis. Fig. 41 shows the results of experiment. Qualitative agreement is good.

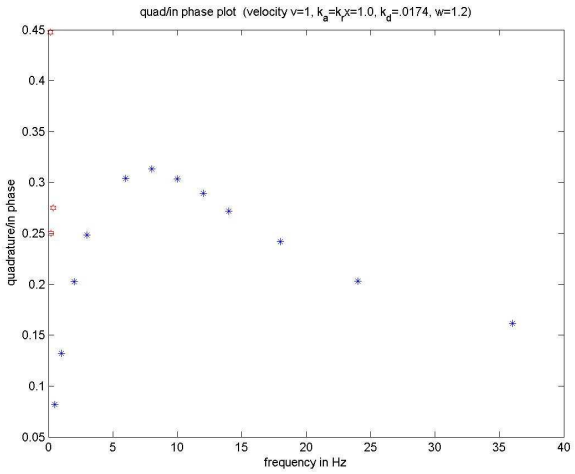

Figure 40. *Values of tan(φ) as a function of the laser frequency as computed from the model.*

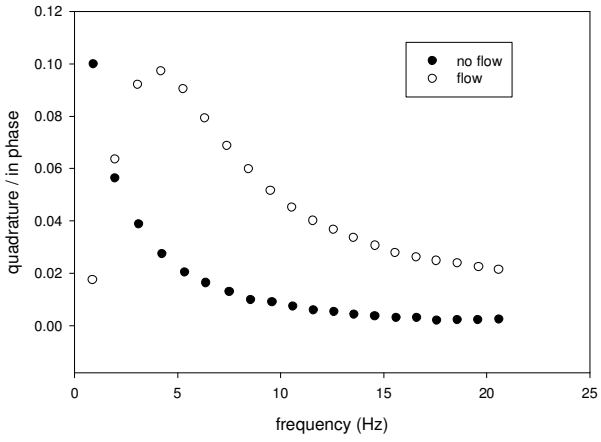

Figure 41. *Values of tan(φ) as a function of the laser frequency as measured by experiment.*

APEX Blind Deconvolution of Color Imagery

Alfred Carasso

Blind deconvolution of color imagery is a subject that is still very much in its infancy, but one in which there is growing interest in scientific and engineering applications. Major difficulties arise from the need to identify the distinct point spread functions associated with each color component. More serious difficulties arise from the possibility of *unbalanced* blind sharpening of individual color components. Conceivably, after a long and uncertain iterative process, the reconstituted color image may turn out to exhibit physically false colors, such as a green sky, or a purple sea. A fruitful mathematical framework wherein the blind color problem can be effectively tackled, has not yet been formulated.

One approach to color image processing traces its origin to high energy physics and string theory. Here, a color image is viewed as a *2D* manifold in *5D* space, namely, *{x, y, R(x,y), G(x,y), B(x,y)}*, where *R, G, B* are the red, green, and blue components of the color image *g(x,y)*. The so-called Polyakov functional is then defined on this manifold, and gradient descent minimization of this functional is implemented. This leads to the *Beltrami flow* equations, a coupled system of evolutionary nonlinear partial differential equations for the three time-dependent images *R(x,y,t), G(x,y,t), B(x,y,t)*. That system is then solved forward in time numerically, until a steady-state is reached. This formalism has been applied successfully to color image denoising. With considerable skill, such an approach might possibly be elaborated into a blind deconvolution procedure. However, the computational effort required to process large size imagery would be quite challenging.

A remarkable property of the APEX method previously developed here at NIST is the ease with which it can be applied to color imagery, and the plausibility of the ensuing results. The fact that deblurring is accomplished by marching backwards in time in a diffusion equation, (the SECB method, also developed at NIST), leads to significant control over the deconvolution process, enabling processing of *1024×1024* color imagery in quasi real-time.

The most natural way to use the APEX method is to first decompose the blurred color image into its three RGB components, apply the method to each component in turn, and then reconstitute the deblurred image. For each RGB component, visual monitoring of the backwards in time evolution as *t* tends to zero, is

accompanied by calculated diagnostic quantities such as the L^1 norm, which measures total radiant flux, and the total variation or *TV* norm, which measures image gradients. In well-behaved deconvolution, the total flux L^1 norm should be *conserved*, while the *TV* norm should increase monotonically as t tends to zero, and the image sharpens. Total flux conservation in each RGB component can be enforced by terminating deconvolution whenever the current L^1 norm exceeds the initial L^1 norm by more than a few percent. Such early termination is equivalent to readjusting the original trial optical transfer function. In this way, individual optical transfer functions are detected for each RGB component.

This methodology was systematically tested on numerous examples during FY 2005. Of particular concern was whether the strategy of enforcing L^1 norm conservation in each RGB component, was sufficient to maintain the balance of colors in the reconstructed image. This was found to be the case in all examples examined so far.

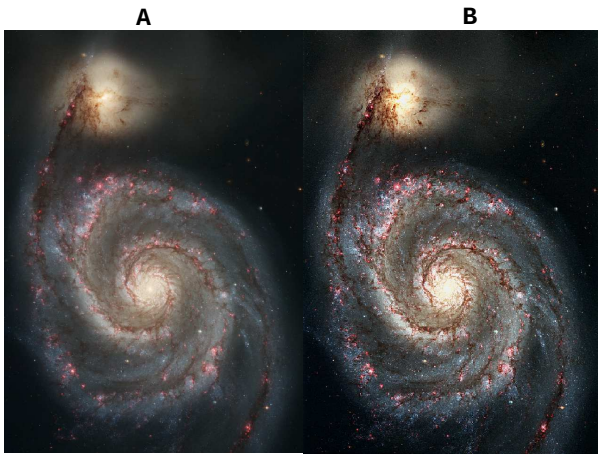

Figure 42. *(A) Hubble image of Whirlpool Galaxy M51. (B) The result of APEX sharpening.*

One particularly exciting field of application for APEX deconvolution is Hubble Space Telescope imagery. Some 750,000 one-of-a-kind images have already been acquired and archived, at a total cost exceeding six billion dollars. Credible digital enhancement of these images would add considerable value to this priceless collection. A paper discussing APEX processing of Hubble imagery has recently been submitted for publication, and two invited talks on this subject have already been given. A good example is shown in Fig. 42. Here, image (A) is the sharpest image ever taken of the Whirlpool Galaxy M51. That image was released by NASA on April 15, 2005 to mark the 15th anniversary of the Hubble Telescope. Image (B) is the result of APEX processing. There is clear visual evidence of sharpening, which can be quantitatively confirmed using various statistical measures.

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Simulation of Bioregulatory Networks Involved in Cell Cycle Control

G. B. McFadden
S. Kim (National Institutes of Health)
M. Aladjem (National Institutes of Health)
K. Kohn (National Institutes of Health)

G. McFadden is serving as co-advisor to S. Kim, a postdoctoral fellow in the Laboratory of Molecular Pharmacology in the National Cancer Institute at NIH and a guest researcher in MCSD at NIST; her NIH co-advisors are Mirit Aladjem and Kurt Kohn. Kim is developing models of bioregulatory networks that are involved in cell cycle control. The models consist of systems of nonlinear ordinary differential equations or delay differential equations that typically exhibit switching behavior, limit cycles, and other types of bifurcations.

Proper cell growth depends on a network of interacting molecules that monitors cellular metabolism and environmental signals. This network ensures that cells halt their growth in response to unfavorable conditions such as the absence of sufficient nutrients or the presence of potentially damaging agents. When cells escape these controls, the results are developmental abnormalities, genomic instability, and cancer. Although data about the individual molecules that regulate cell growth has increased substantially in recent years, our ability to make sense of this detailed information has not.

To understand how signals are transmitted through the network, we need to integrate molecular data in a clear, standardized, computer-readable format. NIH's Laboratory of Molecular Pharmacology has developed the Molecular Interaction Map (MIM) language, a tool

that encodes biological information in graphical form. The language allows simultaneous views of many interactions involving any given molecule, allowing MIMs to be used for analyzing bio-regulatory networks in the same way the circuit diagrams are useful for trouble-shooting electronic devices. Aladjem and Kohn have recently described electronic MIMs, which facilitate tracking of signaling pathways and allow easy access to annotations and data bases. The goal of this project is to elucidate the logic of signaling pathways from the multitude of molecular interactions depicted in the MIMs. Because of the complexity of information, this task is likely to be achieved by computer analyses.

The proposed project will combine the MIM tools with mathematical modeling to develop MIM-based computer simulations that will illustrate the processes by which cells govern DNA replication and cell cycle progression.

Computing Surface and Volume Estimates of 3-D Objects

Javier Bernal

A computer program has been implemented for computing surface and volume estimates of aggregates with a power crust algorithm. An aggregate is defined as an object in 3D space that has no holes and contains its center of mass in its interior. The power crust is a piecewise-linear approximation of the surface of a three-dimensional object that is computed from an approximation of the medial axis of the object. The medial axis is a skeletal shape associated with the object with the property that each point in the medial axis is the center of a maximal empty ball that meets the surface of the object only tangentially at two or more points. The approximation of the medial axis is computed by the program from a set of sample points on the surface of the object.

The main tools used by the program are the Voronoi diagram and the power diagram. At the end of the execution of the program a power diagram results whose cells have been labeled as being either inside or outside the object. The union of the cells labeled as being inside is then an approximation of the object. The fact that the object contains its center of mass in its interior is crucial during the labeling process.

Currently research is under way for developing a labeling algorithm that does not require that the 3D object contain its center of mass or some other known point in its interior.

Systems Identification and Parameter Estimation

Bert W. Rust

It is sometimes necessary to identify a system of ODEs describing dynamical relationships between a set of measured time series. A typical example involves the relationship between fossil fuel carbon dioxide emissions $P(t)$, atmospheric carbon dioxide concentrations $c(t)$, and global temperatures $T(t)$. Global warming will have impacts on the national economy. Insurance companies are interested in the problem, and NIST may have to consider it in setting new standards for insulation and other building materials.

Two refinements of the current model have been identified. The first adds a new term to the ODE relating $c(t)$ to $P(t)$ in order to model the effect of the Mt. Pinatubo eruption. The new $c(t)$ fit explains 99.97% of the variance in the measurements. High accuracy is important here because it is necessary to extrapolate the fit backward from 1959 to 1856.

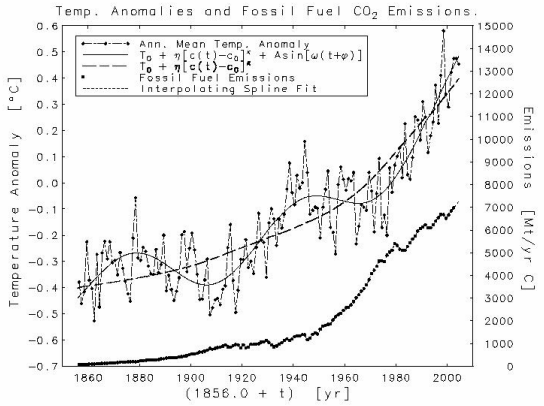

Figure 43. *The small diamonds are annual global average temperature anomalies. The solid curve is the fit of the new T(t) equation, and the long-dashed curve is the power law baseline for that fit. The small circles are annual global total fossil fuel emissions, measured in megatons of carbon, and the short-dashed curve is an interpolating spline used to calculate the c(t) used, in turn, to compute T(t).*

The second refinement replaces a linear relationship between $T(t)$ and $c(t)$ with a power law relation. The fit of the new equation is plotted in Fig.

43 together with a plot of *P(t)* for comparison with the temperature baseline.

The estimate for the new power law exponent was 0.667 +/- 0.067 which suggests the possibility of a Keplerian relationship between *T(t)* and *c(t),* i.e., temperature changes cubed are proportional to concentration changes squared. Other mathematical expressions can give similar baselines, but the current one posits a direct connection, through *c(t)*, between *P(t)* and *T(t).* It also demonstrates that global warming is accelerating, though at a slower rate than fossil fuel emissions.

Future work will concentrate on refining the ODE *for P(t)* and simultaneously fitting the solutions of all three equations to their respective time series.

Technology Transfer of Monte Carlo Strategies

Isabel Beichl
Francis Sullivan (IDA Center for Computing Sciences)

Monte Carlo methods are now ubiquitous in science and engineering for studying massive, complicated problems and data sets. Communicating new developments in Monte Carlo methods and applications to working scientists can have great impact. But it is sometimes difficult to reach a broad audience of scientists because people read the journals in their own discipline. To overcome this and to bring to light novel methods of recent years, we have edited a special issue of *Computing in Science and Engineering* (CiSE), devoted to new developments in Monte Carlo methods, to be published in the spring of 2006.

This special issue will include an article on ways to calculate mixing rates of the "classical" Monte Carlo Markov Chain method. The issue will also include articles on novel applications of the traditional Metropolis algorithm. We also highlight yet another Monte Carlo method, sequential importance sampling which is used for approximate counting and unbiased sampling of truncated data and which has been the subject of research efforts at NIST.

Early in 2001, CiSE published a special issue on "Top Ten Algorithms of the 20th Century. That issue, to which we were contributors, has had very large influence in the computational science community. It is still the most referenced issue of CiSE. We're hoping for similar success with the special issue on Monte Carlo methods.

Voting Systems

Peter Ketcham

The Help America Vote Act (HAVA) of 2002 gives NIST a key role in realizing nationwide improvements to voting systems. HAVA establishes the Technical Guidelines Development Committee (TGDC) in order to support the US Election Assistance Commission (EAC) in the development of voting system standards. The NIST Director serves as Chair of the TGDC. NIST research activities for the improvement of voting systems include:

- security of computers, networks, and data storage;
- methods to detect and prevent fraud;
- protection of voter privacy; and
- the role of human factors in the design of voting systems.

The NIST Voting Team produced an initial version of the Voluntary Voting System Guidelines (VVSG) and delivered the completed document to the TGDC for publication in May 2005. P. Ketcham of MCSD contributed to the VVSG in the areas of security testing as well as overall organization of the VVSG document. In support of the development of voting system standards, P. Ketcham managed the NIST Voting System Laboratory (VSL). The VSL contains voting equipment from a variety of vendors, including Election Systems & Software, Hart InterCivic, Populex Corporation, and Sequoia Voting Systems. In conjunction with several members of the NIST Voting Team, P. Ketcham organized a workshop, held October 7, 2005, entitled, "Developing an Analysis of Threats to Voting Systems." The workshop attracted attendees from state, county, and local governments around the country as well as members of the EAC. Ketcham also managed the workshop website and edited the workshop proceedings.

The NIST Voting Team is currently writing a more comprehensive version of the VVSG that will better serve the needs of voting system product developers, election officials, and testing laboratories.

Part IV

Activity Data

Publications

Appeared

Refereed Journals

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23. K. Irikura, R. Johnson, and R. Kacker, "Uncertainties in Scaling Factors for Ab-initio Vibrational Frequencies," *Journal of Physical Chemistry* **A** (109) (2005), pp. 8430-8437.
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25. R. Kacker and I. Olkin, "A Survey of Tables of Probability Distributions," *Journal of Research of the NIST* **110** (2005), pp. 67-77.
26. R. Kacker, R. Datla, and A. Parr, "Response to Comments on Statistical Analysis of CIPM Key Comparisons Based on the ISO Guide," *Metrologia* **42** (2005), pp. L13-L14.
27. E. Knill, "Quantum Computing with Realistically Noisy Devices," *Nature* **434** (2005), p. 39.
28. E. Knill, "Scalable Quantum Computing in the Presence of Large Detected-Error Rates," *Physical Review A* **71** (2005), pp. 042322/1-7.
29. E. Mirowski, J. Moreland, A. Zhang, S.E. Russek, and M.J. Donahue, "Manipulation and Sorting of Magnetic Particles by a Magnetic Force Microscope on a Microfluidic Magnetic Trap Platform," *Applied Physics Letters* **86** (2005), 243901.
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31. W.F. Mitchell, "Hamiltonian Paths through Two- and Three-Dimensional Grids," *Journal of Research of NIST* **110** (2005), pp. 127-136.
32. D.P. O'Leary and S.S. Bullock, "QR Factorizations Using a Restricted Set of Rotations," *Electronic Transactions on Numerical Analysis* **21** (2005), pp. 35-45.
33. T. Schaetz, M. D. Barrett, D. Leibfried, J. Britton, J. Chiaverini, W. M. Itano, J. D. Jost, E. Knill,, C. Langer, D. J. Wineland, "Enhanced Quantum State Detection Efficiency through Quantum Information Processing," *Physical Review Letters* **94** (2005), 010501.
34. R. Somma, G. Ortiz, H. Barnum, E. Knill, and L. Viola, "Nature and Measure of Entanglement in Quantum Phase Transitions," *Physical Review A* **70** (October 2004), 042311.
35. L. Viola and E. Knill, "Random Decoupling Schemes for Quantum Dynamical Control and Error Suppression," *Physical Review Letters* **94** (2005), 060502.
36. L. Yanik, E. Della Torre, M. J. Donahue, and E. Cardelli, "Micromagnetic Eddy Currents in Conducting Cylinders," *Journal of Applied Physics* **97** (2005), 10E308.

Other Invited Publications

1. R.F. Boisvert, R. Cools, and B. Einarsson, in "Assessment of Accuracy and Reliability," *Accuracy and Reliability in Scientific Software* (B. Einarsson, ed.), SIAM, Philadelphia (2005), pp. 13-32.
2. R.F. Boisvert and R. Pozo, "Java," in *Accuracy and Reliability in Scientific Software* (B. Einarsson, ed.), SIAM, Philadelphia (2005), pp. 160-169.
3. D. Donnelly and B. Rust, "The Fast Fourier Transform for Experimentalists, Part I: Concepts," *Computing in Science & Engineering* **7** (2) (March/April 2005), pp. 80-88.
4. D. Donnelly and B. Rust, "The Fast Fourier Transform for Experimentalists, Part II: Convolutions," *Computing in Science & Engineering* **7** (4) (July/August 2005), pp. 92-95.
5. D.P. O'Leary, "Blind Deconvolution: Errors, Errors Everywhere," *Computing in Science and Engineering*. Project: **7** (1) (Jan./Feb. 2005), pp. 56-59. Solution: **7** (2) (Mar./Apr. 2005), pp. 63-66.
6. D.P. O'Leary, "Blind Deconvolution: A Matter of Norm," *Computing in Science and Engineering*. Project: **7**, (2) (Mar./Apr. 2005), pp. 60-62. Solution: **7** (3) (May/June 2005), pp. 24-27.
7. D.P. O'Leary, "Finite Differences and Finite Elements: Getting to Know You," *Computing in Science and Engineering*. Project: **7** (3) (May/June 2005), pp. 20-23. Solution: **7** (4) (Jul./Aug. 2005).
8. D.P. O'Leary, "Eigenvalues: Valuable Principles," *Computing in Science and Engineering*. Project: **7** (4) (July/Aug. 2005), Solution: **7** (5), (Sept./Oct. 2005), pp. 67-70.

9. D.P. O'Leary, "Solving Sparse Linear Systems: Taking the Direct Approach," *Computing in Science and Engineering*. Project: **7** (5) (Sept./Oct. 2005), pp. 62-67, Solution: **7** (6) (Nov./Dec. 2005), pp. 77-80.

10. D.P. O'Leary, "Fast Solvers and Sylvester Equations: Both Sides Now," *Computing in Science and Engineering*. Project: **7** (6) (Nov./Dec. 2005), pp. 74-77, Solution: **8** (1) (Jan./Feb. 2006.

11. B. Rust and D. Donnelly, "The Fast Fourier Transform for Experimentalists, Part III: Classical Spectral Analysis," *Computing in Science & Engineering* **7** (5) (Sept./Oct. 2005), pp. 74-78.

12. B. Rust and D. Donnelly, "The Fast Fourier Transform for Experimentalists, Part IV: Autoregressive Spectral Analysis," *Computing in Science & Engineering* **7** (6) (Nov./Dec. 2005), pp. 85-90.

Conference Proceedings

1. M.D. Barrett, T. Schaetz, J. Chiaverini, D. Leibfried, J. Britton, W.M. Itano, J.D. Jost, E. Knill, C. Langer, R. Ozeri, and D.J. Wineland, "Quantum Information Processing with Trapped Ions," in *AIP Conference Proceedings* **770** (May 5, 2005), Issue 1, 350-358

2. T.J. Burns and T.L. Schmitz, "Receptance Coupling Study of the Dynamic Absorber Effect in Long-Overhang Tools," in *Proceedings of the 2004 ASME International Mechanical Engineering Congress and RD&D Expo*, Anaheim, CA, November 13-19, 2004, pp. 1-8.

3. T.J. Burns and T.L. Schmitz, "A Study of Linear Joint and Tool Models in Spindle-Holder-Tool Receptance Coupling," in *Proceedings of the Fifth ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control*, ASME 2005 International Design Engineering Technical Conferences, Long Beach, CA, September 24-28, 2005, DETC2005-85275 (CD).

4. L. Deshayes, L. Welsch, A. Donmez, R. Ivester, D. Gilsinn, R. Rhorer, E. Whitenton, and F. Potra, "Smart Machining Systems: Issues and Research Trends," in *Proceedings 12th CIRP Life Cycle Engineering*, Workshop, Grenoble, France (2005) (CD).

5. J.E. Devaney, S.G. Satterfield, J.G. Hagedorn, J.T. Kelso, A.P. Peskin, W.L. George, T.J. Griffin, H.K. Hung, R.D. Kriz, "Science at the Speed of Thought," *Ambient Intelligence for Scientific Discovery, Lecture Notes in Artificial Intelligence (LNAI)*, Y. Cai (Ed.), **3345** (February 2005), pp. 1-24.

6. J.T. Fong, "A B C of Engineering Statistics and a Reference Benchmark Approach to Verification and Validation (V & V) of Multi-Physics Simulations of High-Consequence Engineering Systems," in *Proceedings, Symposium on Applied Mechanics and Multi-Physics Simulations of High-Consequence Engineering Systems*, Stanford University, CA, April 18, 2005, pp. 169-216.

7. J.T. Fong, "A B C of Statistics for Verification and Validation (V & V) of Simulations of High-Consequence Engineering Systems," in *Proceedings of the. 2005 ASME Pressure Vessels and Piping Conference*, Denver, CO, July 17-21, 2005, paper no. PVP2005-71799.

8. D. E. Gilsinn, G. S. Cheok, and A. M. Lytle, "Pose of I-beams for Construction Site Automation," in *Proceedings of the 21st International Symposium on Automation and Robotics in Construction*, Jeju, Korea, September 21-25, 2004.

9. D. E. Gilsinn, "Discrete Fourier Series Approximation to Periodic Solutions of Autonomous Delay Differential Equations," in *Proceedings 5th ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control*, Long Beach, CA, Sept. 24-28, 2005.

10. D. E. Gilsinn, M. McClain, C. Witzgall, "Using Nonoscillatory Splines to Model Urban Environments," in *Proceedings of the SIAM Conference on Geometric Modeling and Computing: Seattle, 2003*, Ed. M. L. Lucian and M. Neamtu, Nashboro Press, Brentwood (2004), pp. 229-248.

11. B.W. Rust, "Separating Signal from Noise in Global Warming," *Computing Science and Statitstics* **35** (2005), pp. 263-277.

12. B. Saunders and Q. Wang, "Boundary/Contour Fitted Grid Generation for Effective Visualizations in a Digital Library of Mathematical Functions," in *Proceedings of the Ninth International Conference of Numerical Grid Generation in Computational Field Simulations*, pp. 61-71. Also, NISTIR 7228.

13. V.V. Shende, S.S. Bullock, I.L. Markov, A Practical Top-down Approach to Quantum Circuit Synthesis, Proc. *Asia and South Pacific*

Design Automation Conference, pp. 272-275, Shanghai, China, 2005, quant-ph/0406176.

14. X. Tang, L. Ma, A. Mink, A. Nakassis, B. Hershman, J. Bienfang, R.F. Boisvert, C. Clark and C. Williams, High Speed Fiber-Based Quantum Key Distribution using Polarization Encoding, in *Proceedings of SPIE* **5893**, Optics and Photonics Conference, San Diego, California, USA, July 31 - August 4, 2005.
15. Q. Wang and B. Saunders, "Web-Based 3D Visualization in a Digital Library of Mathematical Functions," in *Proceedings of the Web3D 2005 Symposium*, University of Wales, Bangor, UK, March 29-April 1, 2005, pp. 151-157.

Technical Reports

1. J. Bernal and C. Witzgall, "Integer Representation of Decimal Numbers for Exact Computations," *NISTIR 7144*.
2. H.-R. Fang and D.P. O'Leary, "Stable Factorizations of Symmetric Tridiagonal and Triadic Matrices," Computer Science Department Report CS-TR-4733, Institute for Advanced Computer Studies Report UMIACS-2005-41, University of Maryland, July 2005.
3. S.I. Haan, A. Reid, R.E. Garcia, and S. Langer, "The OOF2 Manual," (available on-line only, at http://www.ctcms.nist.gov/oof/oof2man/index.html).
4. F.Y. Hunt and A. O'Gallagher, "Sensitivity of Multiple Sequence Alignments to Perturbations in Cost Matrices, *NIST Technical Note 1472*.

Accepted

1. D.L. Cotrell and G.B. McFadden, "Linear Stability of Spiral Poiseuille Flow with a Radial Temperature Gradient: Centrifugal Buoyancy Effects," *Physics of Fluids.*
2. A. Dienstfrey, and J. Huang, "Integral Representations for Elliptic Functions," *Journal of Mathematical Analysis and Applications*.
3. D.M. Dunlavy, D.P. O'Leary, D. Klimov, and D. Thirumalai, "HOPE: A Homotopy Optimization Method for Protein Structure Predictio n," *Journal of Computational Biology*.
4. S.T. Erdogan, P.N. Quiroga, D.W. Fowler, H.A. Saleh, R.A. Livingston, E.J. Garboczi, P.M. Ketcham, J. G. Hagedorn, and S.G. Satterfield, "Three-dimensional Shape Analysis of Coarse Aggregates: Methodology and Preliminary Results on Several Different Coarse Aggregates," *Cement and Concrete Research*.
5. J.T. Fong, J.J. Filliben, R. deWit, R.J. Fields, B. Bernstein, and P.V. Marcal, "Uncertainty in Finite Element Modeling and Failure Analysis: A Metrology-based Approach," *ASME Trans. Journal of Pressure Vessel Technology*.
6. E.J. Garboczi, J.F. Douglas, and R.B. Bohn, "The Intrinsic Elastic Moduli of Rectangular Parallelepiped Inclusions Over a Modest Range of Shape and a Large Range of Property Contrast," *Mechanics of Materials*.
7. C. Holloway, M. Mohamed, E. Keuster, and A. Dienstfrey, "Reflection and Transmission Properties of a Metafilm with Application to a Controllable Surface Composed of Resonant Particles," *IEEE Transactions on Electromagnetic Compatibility*.
8. A. Kalsi and D.P. O'Leary, "Algorithms for Structured Total Least Squares Problems with Applications to Blind Image Deblurring," *Journal of Research of the National Institute of Standards and Technology*.
9. B.W. Rust, "Carbon Dioxide, Global Warming, and Michael Crichton's 'State of Fear'," *Computing Science and Statistics* **37**.
10. S.P. Schurr, A.L. Tits, and D.P. O'Leary, "Universal Duality in Conic Convex Optimization," *Mathematical Programming A*.
11. J. Sims and S.A. Hagstrom, "High Precision Variational Calculations for the Born-Oppenheimer Energies of the Ground State of the Hydrogen Molecule", *Journal of Chemical Physics*.
12. D. Williams, A. Lewandowski, T. Clement, C. Wang, P. Hale, J. Morgan, D. Keenan, and A. Dienstfrey, "Covariance-Based Uncertainty Analysis of the NIST Electro-optic Sampling System," *IEEE Transactions on Microwave Theory and Techniques*.
13. L. Yanik, E. Della Torre, and M.J. Donahue, "Micromagnetic Calculations of Eddy Currents with Time-Varying Fields," *Physica B*.

Submitted

1. D.M. Anderson, P. Cermilli, E. Fried, M.E. Gurtin, and G.B. McFadden, "Dynamical Sharp-

interface Conditions for Two-phase Viscous Heat-conducting Fluids," WERB.

2. D.M. Anderson, P. Cermilli, E. Fried, M.E. Gurtin, and G.B. McFadden, "Dynamical Sharp-interface Conditions for Two-phase Viscous Heat-conducting Fluids," *Journal of Fluid Mechanics.*
3. I. Beichl, S. Bullock, and D. Song, "A Quantum Algorithm Detecting Concentrated Maps," *NIST Journal of Research*.
4. I. Beichl and F. Sullivan, "The Other Monte Carlo Method," *IEEE Computing in Science and Engineering*.
5. I. Beichl, S. Bullock, and D. Song, "A Quantum Algorithm Detecting Concentrated Maps," *NIST Journal of Research*.
6. D.L. Cotrell and A.J. Kearsley, "Flow Control Through the Use of Topography," *Optimization and Engineering.*
7. D.L. Cotrell and G.B. McFadden, "Axial Flow Effects on the Linear Stability of Circular Couette Flow with Viscous Heating," *Physics of Fluids.*
8. R. Dersimonian and R. Kacker, "Quantification of Uncertainty in Meta-analysis," *Controlled Clinical Trials*.
9. J.P. Dunkers, J.G. Hagedorn, A. Peskin, J.T. Kelso, J.E. Terrill, and L. Henderson, "Interactive, Quantitative Analysis Of Scaffold Structure Using Immersive Visualization," *BIO2006: Summer Bioengineering Conference*.
10. J. T. Fong, "The Role of Engineering Statistics in a Reference Benchmark Approach to Verification and Validation of Multi-Physics Simulations of High-Consequence Engineering Systems," *Proc. of a Stanford Mechanics Symposium, Applied Mechanics and Multi-Physics Simulations of High-Consequence Engineering Systems*, Stanford University, CA, April 18, 2005.
11. S. Glancy and E. Knill, "Error Analysis For Encoding A Qubit In An Oscillator," *Physical Review A*.
12. D.E. Gilsinn and F.A. Potra, "Stability of Delay Differential Equations by Integral Equation Methods," *Journal of Integral Equations and Applications.*
13. K.F. Gurski, G.B. McFadden, and M.J. Miksis, "The Effect of Contact Lines on the Rayleigh Instability with Anisotropic Surface Energy," *SIAM Journal on Applied Mathematics*.
14. J. Hagedorn, S. Satterfield, J. Kelso, W. Austin, J. Terrill, and A. Peskin, "Correction of Location and Orientation Errors in Electromagnetic Motion Tracking," *Presence*.
15. J. Hagedorn, J. Dunkers, A. Peskin, J. Kelso, L. Henderson, J. Terrill, "Quantitative, Interactive Measurement of Tissue Engineering Scaffold Structure in an Immersive Visualization Environment", *IEEE Signal Processing Society International Conference on Image Processing*.
16. M.A. Hamstad and A. O'Gallagher, Effects of Noise on Lamb-Mode Acoustic Emission Arrival Times Determined by Wavelet Transform," *Journal of Acoustic Emission*.
17. R. Kacker, "Simpler Bayesian Alternative to the ISO Guide's Use of the Welch-Satterthwaite Formula," *Metrologia*.
18. Z. Levine, A. Kearsley, and J. Hagedorn, "Bayesian Tomography for Projections with an Arbitrary Transmission Function with an Application in Electron Microscopy", *IEEE Transactions on Image Processing*.
19. M. H. Park, Y. K. Hong, B. C. Choi, S. H. Gee, and M. J. Donahue, "Vortex Head-to-head Domain Walls and Its Formation Process in Onion-State-Stable Ring Elements," *Physical Review Letters.*
20. R. Radebaugh and A. O'Gallagher, "Regenerator Operation at Very High Frequencies for Micro-Cryocoolers," *Advances in Cryogenic Engineering*.
21. J. Slutsker, K. Thornton, A.L. Roytburd, J.A. Warren, G.B. McFadden, and P. Voorhees, "Phase-field Modeling of Solidification under Stress," WERB.
22. J. Slutsker, K. Thornton, A.L. Roytburd, J.A. Warren, and G.B. McFadden, "Phase-field Modeling of Solidification Under Stress," *Acta Materialia.*
23. X. Tang, L. Ma, A. Mink, A. Nakassis, B. Hershman, J. Bienfang, R.F. Boisvert, C. Clark and C. Williams, "High Speed Fiber-Based Quantum Key Distribution using Polarization Encoding," in *Proceedings of SPIE*, Optics and Photonics Conference, San Diego, CA, July 31 - August 4, 2005.

Presentations

Invited Talks

1. R. Boisvert, "A Handbook of Special Functions for the Digital Age," Symposium on Software Environments for Numerical Problems, University of Gent, Belgium, November 18, 2004.
2. S.S. Bullock, "Matrix Decompositions and Quantum Circuit Design," Laboratoire d'Informatique Thèorique et Quantique, University of Montreal, December 1, 2004.
3. T.J. Burns and T.L. Schmitz, "A Study of Linear Joint and Tool Models in Spindle-Holder-Tool Receptance Coupling," Fifth ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control, ASME 2005 International Design Engineering Technical Conferences, Long Beach, CA, September 24-28, 2005.
4. D.L. Cotrell, "Linear Stability of Spiral Poiseuille Flow and Comparison to Experiments," Arryx, Chicago, IL, January 13, 2005.
5. D.L. Cotrell, "Linear Stability of Isothermal and Non-isothermal Spiral Poiseuille Flow," Lawrence Livermore National Laboratory, Livermore, CA, January 24, 2005.
6. D.L. Cotrell, "Linear Stability of Isothermal and Non-isothermal Spiral Poiseuille Flow," NYU, Courant Institute of Mathematical Sciences, New York, NY, January 28, 2005.
7. J. Fong, "Verification and Validation of Computer Models," Southwest Research Institute, Oct. 11, 2004.
8. J. Fong, "A Metrology-based Uncertainty Analysis Approach to V & V of Computer Models of High-consequence Engineering Systems," Foundation '04: A Workshop for V&V in the 21st Century, Tempe, AZ, Oct. 13, 2004.
9. J. Fong, "Verification and Validation of Computer Models of High-consequence Engineering Systems," Lawrence Livermore National Laboratory, Livermore, CA, Oct. 18, 2004.
10. J. Fong, "Verification and Validation of Computer Models of High-Consequence Engineering Systems" NASA Ames Research Center, Moffett Field, CA, Feb. 2, 2005.
11. J. Fong, "A B C of Engineering Statistics and a Reference Benchmark Approach to Verification and Validation (V&V) of Multi-Physics Simulations of High-Consequence Engineering Systems," Stanford University Symposium on Applied Mechanics and Multi-Physics Simulations of High-Consequence Engineering Systems, Stanford, CA, April 18, 2005.
12. J. Fong, "Engineering Statistics for Verification and Validation (V&V) of Computer Simulations of High-Consequence Systems" at a joint colloquium of Departments of Mechanical Engineering and Mathematical Sciences, Clemson University, Clemson, SC, June 10, 2005.
13. J. Fong, "ABC of Statistics for Verification & Validation of Simulations of High Consequence Engineering Systems," ASME Pressure Vessels and Piping Conference, Denver, CO, July 21, 2005.
14. J. Fong, "A Reference-benchmark Approach to Verification and Validation (V&V) of Simulations of High-Consequence Engineering Systems," Battelle Columbus Laboratories, Columbus, OH, July 22, 2005.
15. J. Fong, "Stochastic Modeling of Complex Structural System Failures and a Metrology-based Approach to V&V of Computer Simulations," Departments of Engineering Science and Mechanics, Penn State University, State College, PA, September 23 2005.
16. F. Hunt, "Visualizing Frequency Patterns in DNA," Infinite Possibilities 2005 Conference, Spelman College, Atlanta, GA, April 1, 1005.
17. F. Hunt, "Visualizing Frequency Patterns in DNA," Sonya Kovalevsky Day, New College of Florida, Sarasota, FL, April 9, 2005.
18. F. Hunt, "A Markov Decision Approach to Bioinformatics," 13th INFORMS Applied Probability Conference, Ottawa Canada July 6, 2005.
19. F. Hunt, "Visualizing Frequency Patterns in DNA," Etta Falconer Lecture of the Mathematical Association of America and the Association for Women in Mathematics, MathFest, Albuquerque, New Mexico, August 5, 2005.
20. E. Knill, "Fault-tolerant Architecture for Very Noisy Gates," Fault-tolerant Quantum Computation Workshop, IBM, Yorktown Heights, NY, Aug. 29, 2005.

21. S. Langer, "OOF2: Object-Oriented Finite Element Analysis of Material Microstructures," Physics Department Colloquium, University of Illinois in Chicago, Chicago, IL, November 10, 2004.
22. S. Langer, "OOF2: Object-Oriented Finite Element Analysis of Material Microstructures," MCSD Seminar, January 11, 2005.
23. D.W. Lozier, "Measuring Error in Mathematical Computations and a Proposed Software Test Service for Special Functions," NIST Workshop on Verification and Validation of Computer Models for the Design and Performance Evaluation of High-Consequence Engineering Systems, November 8, 2004.
24. D.W. Lozier, "The DLMF Project: Lessons Learned and Future Directions," Special Functions: Asymptotic Analysis and Computation: A Conference in Honor of Nico Temme's 65th Birthday, University of Cantabria, Spain, July 5, 2005.
25. D.W. Lozier, "The DLMF Project: Lessons Learned and Future Directions," American Mathematical Society Eastern Section Meeting, Bard College, Annandale-on-Hudson, NY, October 8, 2005.
26. D.W. Lozier, "Math on the Web and the Digital Library of Mathematical Functions Project," Society for Industrial and Applied Mathematics Washington-Baltimore Section meeting, Baltimore, MD, November 9, 2005.
27. W.F. Mitchell, "Error Estimators for the hp Version of the Finite Element Method with Newest Node Bisection of Triangles," 8th U.S. National Congress on Computational Mechanics, Austin, TX, July 26, 2005.
28. D.P. O'Leary, "Numerical Linear Algebra in Image Deblurring," Third International School in Numerical Linear Algebra and Applications, Monopoli, Italy, September 11-17, 2005.
29. D.P. O'Leary, "Some Linear Algebra of Quantum Computing," Sandia National Laboratory, Livermore, CA, September 28, 2005.
30. D.P. O'Leary, "HOPE: A Homotopy Optimization Method for Protein Structure Prediction," University of Waterloo, October 21, 2005.
31. D.P. O'Leary, "Multi-Success," Convocation Address, University of Waterloo, October 22, 2005.
32. D. Porter, "Tools for Simulating Magnetic Phenomena at the Nanoscale," NIST/TEDCO Showcase, "Advancing the Frontiers of Bioscience and Nanotechnology," NIST, Gaithersburg, June 9, 2005.
33. B. Saunders, "Using Adaptive Mesh Generation to Capture Key Features of 3D Function Surfaces," Mathematical Association of America, Maryland, D.C., Virginia Section Meeting, Morgan State University, Baltimore, MD, November 6, 2004.
34. B. Saunders, "Dynamic 3D Visualizations of High Level Mathematical Functions," Elizabeth City State University, Elizabeth City, NC, February 22, 2005.

Conference Presentations

1. S.S. Bullock, D.P. O'Leary and G.K. Brennen, "Quantum Circuits for D-level Systems," DARPA Quantum Information Science and Technology PI Meeting, Scottsdale, AZ, November 18, 2004.
2. T. Burns, "Receptance Coupling Study of the Dynamic Absorber Effect in Long-Overhang Tools," International Mechanical Engineering Congress and R&D Expo, Anaheim, CA, November 15, 2004.
3. J. Devaney, S. Satterfield, J. Hagedorn, J. Kelso, A. Peskin, W. George, T. Griffin, and H. Hung, "Science at the Speed of Thought," Bowie State University, Bowie, MD, Oct. 29, 2004.
4. E. Della Torre, L. Yanik, M.J. Donahue, and E. Cardelli, "Micromagnetic Eddy Currents in Conducting Cylinders," Magnetism and Magnetic Materials 2004, Jacksonville, FL, November 7-11, 2004.
5. J. Devaney, "Automating Labeling with Machine Learning," Virtual Cement and Concrete Testing Laboratory Annual Meeting, NIST, Gaithersburg, MD, Nov. 15, 2004.
6. M.J. Donahue, F. da Silva, and D.P. Pappas, "Micromagnetic and Analytic Study of Small Zigzag Sensors," Magnetism and Magnetic Materials 2004, Jacksonville, FL, November 7-11, 2004.
7. M. Donahue, "Micromagnetic Calculations of Eddy Currents with Time-Varying Fields," 5th International Symposium on Hysteresis Modeling and Micromagnetics, Budapest, Hungary, May 30, 2005.

8. M. Donahue, "Vortex Head-to-Head Domain Walls and Their Formation in Onion-State Ring Elements," 5th International Symposium on Hysteresis Modeling and Micromagnetics, Budapest, Hungary, May 31, 2005.
9. W. George, J. Lancien, and J. Terrill, MPMD Program Model for Scientific Computing, SC05, Scatter Gather Session II, Seattle, WA, November 16, 2005.
10. D.E. Gilsinn, "Discrete Fourier Series Approximation to Periodic Solutions of Autonomous Delay Differential Equations," 5th ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control, Long Beach, CA, September 24-28, 2005.
11. S. Glancy, "Quantum Computation with Optical Coherent States," QIP2005: Eighth Workshop on Quantum Information Processing, MIT, Cambridge, MA, January 16, 2005.
12. S. Glancy, "Error Analysis For Encoding A Qubit In An Oscillator," Quantum Information, Computation and Logic: Exploring New Connections Perimeter Institute, Waterloo, Ontario, Canada, July 20, 2005.
13. A. Kearsley, "Automated Algorithms for Applied Spectral Analysis," NMIJ/BIPM Workshop on the Impact of Information Technology in Metrology, Tskuba, Japan, May 19, 2005.
14. J. Kelso, "Shell DIVERSE," ACM SIGGRAPH 2005 Conference, DIVERSE Birds of a Feather (BOF) session, Los Angeles, CA, August 4, 2005.
15. J. Kelso, "Shell DIVERSE," IEEE Visualization Conference, DIVERSE Birds of a Feather (BOF) session, Minneapolis, MN, October 27, 2005.
16. J. Lancien, "Quaternion Dissipative Particle Dynamics," Virtual Cement and Concrete Testing Laboratory Annual Meeting, NIST, November 8, 2005.
17. W.F. Mitchell, "Multigrid Methods for the hp Version of the Finite Element Method," 8th U.S. National Congress on Computational Mechanics, Austin, TX, July 25, 2005.
18. B. Rust, "Carbon Dioxide, Global Warming, and Michael Crichton's 'State of Fear'," Interface 2005 Conference, St. Louis, MO, June 10, 2005.
19. S. Satterfield, "Shell Script VR," ACM SIGGRAPH 2005 Conference, DIVERSE Birds of a Feather (BOF) session, Los Angeles, CA, August 4, 2005.
20. S. Satterfield, "Shell Script VR," IEEE Visualization Conference, DIVERSE Birds of a Feather (BOF) session, Minneapolis, MN, October 27, 2005.
21. B. Saunders, "Boundary/Contour Fitted Grid Generation for Effective Visualizations in a Digital Library of Mathematical Functions," Ninth International Conference of Numerical Grid Generation in Computational Field Simulations, San Jose, CA, June 11-18, 2005.
22. J. Sims, G. Bryant, and H. Hung, "Intrinsic Surface States in Semiconductor nanocrystals: HgS Quantum Dots," American Physical Society meeting, Los Angeles, CA, March 21-25, 2005.

Software Released

1. S. Bullock and D. P. O'Leary, MATLAB code for producing d-level quantum circuits, http://www.arxiv.org/abs/quant-ph/0410116.
2. D. Porter (contributors), Tcl/Tk 8.4.8 released November 22, 2004, Tcl/Tk 8.4.9 released December 7, 2004, and Tcl/Tk 8.5a2 released December 8, 2004, Tcl/Tk 8.4.10 and 8.5a3 released June 4, 2005.
3. D. Porter, trofs 0.4, December 21, 2004. http://math.nist.gov/~DPorter/tcltk/trofs/
4. J. Kelso, frameGrabber DSO, http://math.nist.gov/mcsd/savg/software/dsos/#id107212.
5. J. Kelso, frameTimeStamp DSO, http://math.nist.gov/mcsd/savg/software/dsos/#id105790.
6. S. Langer, OOF2 version 2.0.b3, 2.0b4, 2.0b5, 2.0b6, http://www.ctcms.nist.gov/oof/oof2.html.
7. A. Peskin, Image Filters, http://math.nist.gov/mcsd/savg/software/filters/
8. A. Peskin, light loader (lgt), http://math.nist.gov/mcsd/savg/software/loaders/#id100960.
9. R. Pozo, Template Numerical Toolkit (TNT), Version 1.2.4, Version 1.2.5, Version 1.2.6, Version 1.9, http://math.nist.gov/tnt/.
10. R. Pozo, Jama/C++ linear algebra package, Version 1.2.3.

11. R. Pozo, C++ reference implementation of the Sparse BLAS standard.
12. R. Pozo, Jama/TNT numerical linear algebra library, Version 1.2.6.
13. S. Satterfield and A. Peskin, Visualization Demos, http://math.nist.gov/mcsd/savg/demos/.

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. E. Vogel (EEEL), "Emerging Devices and Materials for Beyond CMOS," October 5, 2004.
2. S. Stein (CSTL), "How We Handle Mass Spectra," October 26, 2004.
3. A. Ray (Pennsylvania State University), "Anomaly Detection and Failure Mitigation in Complex Dynamical Systems," November 19, 2004.
4. R. Rehm (BFRL), "Mathematical Modeling of Community-Scale Fires," December 14, 2004.
5. S. Langer (MCSD), "OOF2: Object-Oriented Finite Element Analysis of Material Microstructures," January 11, 2005.
6. J. Warren (MSEL), "Modeling Polycrystalline Growth," January 25, 2005.
7. P. Marcal (MPAVE Corp.), "From Computer Aided Engineering Software to Information Driven Decision Making for High-Consequence Engineering Systems," February 8, 2005.
8. S. Gabriel (University of Maryland), "A Nash-Cournot Equilibrium Model for the North American Natural Gas Sector," February 16, 2005.
9. D. Wheeler (MSEL), "A Finite Volume PDE Solver Using Python (FiPy)," March 1, 2005.
10. M. Emelianenko (Pennsylvania State University), "A New Algorithm for the Automation of Phase Diagram Calculation," March 22, 2005.
11. M. De Graef (Carnegie Mellon University), "Beyond the Spherical Cow: A New Approach to Modeling Physical Quantities for Objects of Arbitary Shape," April 27, 2005.
12. L. Petrelli (Mount St. Mary's University), "PDEs from Monge-Kantorovich Mass Transporation Theory," May 11, 2005.
13. R. Szalai (Badapest University of Technology and Economics), "Bifurcations and Chaos in High-Speed Milling," June 1, 2005.
14. M. Mascagni (Florida State University), "Stochastic Methods in Electrostatics: Applications to Biological and Physical Science," June 16, 2005.
15. J. Lei (University of Texas at Arlington), "In-Parameter-Order: A Test Generation Strategy for Pairwise Testing," June 21, 2005.
16. G. Forney (BFRL), "Modeling and Visualizing Fire Without Getting Burned," June 29, 2005.
17. R. Lua (University of Minnesota), "Untangling Knots in Lattices and Proteins: A Computational Study," July 12, 2005.
18. R. van de Geijn (University of Texas at Austin), "Towards the Final Generation of Dense Linear Algebra Libraries," Aug. 25, 2005.
19. L. Melara (Colorado College), "A Homotopy Method in Regularization of Total Variation Denoising Problems," Aug. 30, 2005.
20. B. Rust (MCSD), "Carbon Dioxide, Global Warming, and Michael Crichton's State of Fear," Sept. 13, 2005.

Quantum Information Theory and Practice Seminar Series

1. Scott Glancy (MCSD), "Quantum Computation with Optical Coherent States", October 7, 2004
2. Trey Porto and Jamie Williams (PL), "Quantum Information Processing in Lattices", October 21, 2004
3. S. Bullock (MCSD) and G. Brennen (PL), "Quantum Circuits for d-level Systems", November 7, 2004.
4. Fred Strauch (PL), "Higher-order Hamiltonian Simulation and Local Reversibility", January 27, 2005.
5. Hilary Carteret (University of Montreal), "Noiseless Quantum Circuits for Measuring Entanglement", February 24, 2005.
6. Amitkumar Mahadevan (UMBC), "RCD Codes with Possible Quantum Applications", March 10, 2005.

7. Andreas Klappenecker (Texas A&M), "New Tales of the Mean King", March 24, 2005.
8. Lin Tian (PL), "Connecting the Worlds of Solid-state Quantum Devices and Quantum Optics," April 7, 2005.
9. Juha Vartianen (Helsinki University of Technology), "Unitary Transformations for Quantum Computing," April 21, 2005.
10. Howard Barnum (Los Alamos National Lab), "Quantum Query Complexity with Unitary Queries: Semidefinite Programming, Characterization, and Lower Bounds," May 5, 2005.
11. Ben Reichardt (University of California at Berkeley), "Specialized Quantum Error-correction Schemes," May 26, 2005.
12. Mark Byrd (Southern Illinois University), "Error Prevention using Leakage Elimination Operators," June 2, 2005.

Local Events Organized

1. I. Beichl, Co-organizer, SURF Symposium, August 9-12, 2005.
2. J. Fong, Organizer, Workshop on the Verification and Validation of Computer Models of High-consequence Engineering Systems, November 8-9, 2004.
3. D. Porter and A. Peskin, Planning Board Members, Metrology for the Magnetic Data Storage Industry Workshop, U.S. Measurement System Workshop Series.
4. J. Terrill, Planning Board Member, Antibody-based Metrology Workshop U.S. Measurement System Workshop Series.

External Events Organization

1. R. Boisvert, Co-chair of the Program Committee, Symposium on Scientific Computing and Mathematical Software in Emerging Sciences and Technology, Hong Kong, June 14-15, 2005.
2. R. Boisvert, Program Committee, International Symposium on Symbolic and Algebraic Computation, Beijing, China, July 2005.
3. R. Boisvert, Organizing Committee, IFIP Working Conference on Grid-based Problem Solving Environments: Implications for Development and Deployment of Numerical Software, Prescott, Arizona, July 17-21, 2006.
4. J. Fong Co-chair of the Organizing Committee, Symposium on Applied Mechanics and Multi-Physics Simulations of High-Consequence Engineering Systems, Stanford University, April 18, 2005.
5. J. Fong, Panel Session Chair, "Why do PVP engineers need statistics for decision making?" ASME Pressure Vessels and Piping (PVP) Conference, Denver, Colorado, July 21, 2005.
6. J. Kelso and S. Satterfield, Organizers, DIVERSE Birds of a Feather Session, ACM SIGGRAPH Conference, Los Angeles, CA, July 30 to August 5, 2005.
7. D.P. O'Leary, Organizing Committee, Householder Conferences (formerly the Gatlinburg series of conferences).
8. D.W. Lozier, Co-organizer, Minisymposium on Orthogonal Polynomials and Special Functions, SIAM Annual Meeting, Boston, MA, July 10-14, 2005.
9. D.W. Lozier, Prrogram Committee, Fifth International Conference on Mathematical Knowledge Management, Reading, England, August 10-12, 2006.
10. D. Porter, Session Chairman, "Micromagnetics II" 49th Conference on Magnetism and Magnetic Materials, Jacksonville, Florida, Nov. 8, 2004.
11. R. Pozo, Program Committee, Fifth International Conference on Engineering Computational Technology, Las Palmas de Gran Canaria, September 12-15, 2006.

Other Professional Activities

Internal

1. R. Boisvert and A. O'Gallagher, Members, ITL Diversity Committee.
2. R. Boisvert, Member, NIST People Council.
3. R. Boisvert, ITL Representative, NIST Nanotechnology Strategic Working Group.
4. R. Boisvert, ITL Representative, NIST Scientific Computing Steering Group.
5. A. O'Gallagher, Member, Boulder Exhibits Committee.
6. D. Porter, Member, ITL Awards Committee.

External

Editorial

1. B. Alpert, Associate Editor, *SIAM Journal on Scientific Computing*.
2. I. Beichl, Member, Editorial Board, *Computing in Science and Engineering*.
3. R. Boisvert, Associate Editor, *ACM Transactions on Mathematical Software*.
4. R. Boisvert, Editor of the Numerical Analysis, Mathematical Software, and Computational Engineering, Finance, and Science areas, Computing Research Repository (CoRR) preprint service, www.arXiv.org.
5. D. Gilsinn Special Issue Editor, *NIST Journal of Research*.
6. R. Kacker, Member, Editorial Board, *Total Quality Management and Business Excellence*.
7. R. Kacker, Member, Editorial Board, *Journal of Applied Statistics*.
8. D. Lozier, Associate Editor, *Mathematics of Computation*.
9. G. McFadden Associate Editor, *Journal of Crystal Growth*.
10. G. McFadden Associate Editor, *Interfaces and Free Boundaries*.
11. G. McFadden Associate Editor, *SIAM Journal on Applied Mathematics*.
12. W.F. Mitchell, Member, Editorial Board, *Applied Numerical Analysis and Computational Mathematics*.
13. D.P. O'Leary, Member, Editorial Board, *Computing in Science and Engineering*.

Boards and Committees

1. R. Bohn, Program Official, Dynamic Data Driven Application Systems Program, NOAA.
2. R. Boisvert, Chair, International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software).
3. R. Boisvert, Co-chair, ACM Publications Board.
4. R. Boisvert, Ex-officio Member, ACM Council.
5. R. Boisvert, Member, ACM Award Committee.
6. R. Boisvert, Member, Technical Review Committee, Institute for Defense Analysis Center for Computing Sciences.
7. F. Hunt, Member, Executive Committee, Association for Women in Mathematics.
8. F. Hunt, Member, Strategic Planning Task Force, Association for Women in Mathematics.
9. D.P. O'Leary, Member, External Advisory Board, Computer Science Department, George Washington University.
10. D.P. O'Leary, Member, SIAM-AMS-ASA-AWM-IMS-MAA-NCTM Joint Committee on Women.
11. D. Lozier, Vice Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
12. D. Porter, Member, Tcl Core Team.
13. B. Saunders, Member, Selection Committee, MAA/AWM Etta Z. Falconer Lecture.
14. B. Saunders, Member, Nominating Committee, MD-DC-VA section of the Mathematics Association of America (MAA).
15. J. Terrill, Member, NIST Representative, Federal High End Computing Implementation Task Force.
16. J. Terrill, Member, OpenFPGA Working Group.

Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including *ACM Transactions on Mathematical Software*, ASME, ASME 2005 International Design Engineering Technical Conferences, *Chemical Physics Letters*, *Computing in Science & Engineering,* Fifth ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control, *IEEE Sensors Journal, IEEE Transactions on Computer Aided Design, IMA Journal of Numerical Analysis, International Journal of Fatigue*, *International Journal of Human-Computer Studies, Journal of Physics D: Applied Physics, International Journal of Plasticity*, International Symposium on Symbolic and Algebraic Computation, *Inverse Problems*, *Journal of the American Society for Mass Spectrometry,* Journal of Applied Physics, *Journal of Computational Physics, Journal of Computational Statistics, Journal of Computational and Applied Mathematics*, *Journal of Magnetism and Magnetic Materials,*

Journal of Physics B: Atomic, Molecular & Optical Physics, Mathematics of Computation, Numerical Algorithms, Numerische Mathematik, *Physical Review A*, *Physical Review B, Physical Review E*, *Physical Review Letters, Proceedings of the 2004 ASME International Mechanical Engineering Congress and RD&D Expo*, *Proceedings 5th ASME International Conference on Multibody Sytems, Nonlinear Dynamics and Control*, SIAM book series, *SIAM Journal on Dynamical Systems, SIAM Journal on Optimization*, *SIAM Journal of Scientific Computing*, *SIAM Journal on Optimization*, *Total Quality Management and Business Excellence*,

2. Staff members review proposals for the following research programs: ATP, DoE, NSF.

External Contacts

MCSD staff members make contact with a wide variety of organizations in the course of their work. Examples of these follow.

Industrial Organizations

Applied Research Associates
Asian Technology Information Program
Aspeed Software
Charlotte NC Visualization Center
DirecWay
Engineering Software Research & Development, Inc.
Fujitsu
General Dynamics Advanced Information Systems
General Electric Research Lab
IBM
Instituto de Optica (Spain)
Institute for Solid State Electronics (Germany)
Invensys
Mayo Foundation
Novatek Inc.
Paulsson Geophysical Services, Inc.
Pfizer Labs
PicoChip Designs Ltd.
Polyphonic Human Media Interface
Raytheon
Rationelle Software-Entwicklung
Rose Biophysics
Science Information Systems Co., Ltd. (Japan)
Setterholm, Inc.
SGI
Siemens
SIXNET
Southern Appalachian Science & Technology Center
Synelec Visual Systems
Tektronix, Inc.
Transform Software & Services, Inc.
UGS Corp.
Unique Broadband Systems, Inc.
Xilinx, Inc.

Government/Non-profit Organizations

IDA Center for Computing Sciences
Center for Human Genetics
Department of Energy
Institute for Defense Analyses
Lawrence Livermore National Laboratory
L'Institut d'Informatique et Mathématiques Appliquées de Grenoble
NASA
National Center for Supercomputing Applications
National Institutes of Health
Naval Surface Warfare Center
NSA
Oak Ridge National Laboratory
Ohio Supercomputing Center
Office of Science and Technology Policy
Sandia National Laboratory
U.S. Army Armament Research
U.S. Army Research Lab
U.S. Water Conservation Lab

Academic Institutions

American University
Brown University
Carnegie Mellon University
Delft University of Technology (The Netherlands)
Duke University
Dutchess Community College
Emory University
Florida State University
Georgetown University
George Washington University
Hong Kong Baptist University (China)
Hong Kong University of Science & Technology (China)
Konstanz University
Indian Institute of Technology (India)
Indiana University
Jackson State University
Johns Hopkins University
Masaryk Univeristy (Czech Republic)
McGill University (Canada)
Observatory of Paris
Osaka University
Penn State University
Princeton University
Queen's University (Canada)
Rochester University

Savannah College
Seoul National University (South Korea)
Siena College
Swedish Institute of Computer Science (Sweden)
Technical University of Eindhoven (The Netherlands)
Texas A&M University
T.U. Kaiserslautren (Germany)
T.U. Linz (Germany)
University of Connecticut
University of Copenhagen (Denmark)
University of Erlangen-Nurenberg (Germany)
University of Hyderabad (India)
University of Maryland Baltimore County
University of Maryland College Park
University of Minnesota
University of Montreal (Canada)
University of Pennsylvania
University of Sherbrook (Canada)
University of Southern Mississippi
University of Texas at Austin
University of Texas at Arlington
University of Texas at San Antonio
University of Wisconsin Madison
Uppsala University (Sweden)

Part V

Appendices

Staff

MCSD consists of full time permanent staff located at NIST laboratories in Gaithersburg, MD and Boulder, CO. This is supplemented with a variety of faculty appointments, guest researchers, postdoctoral appointments, and student appointments. The following list reflects the status at the end of FY 2005.

Legend: F = Faculty Appointee, GR = Guest Researcher, PD = Postdoctoral Appointee, S = Student, PT= Part time

Division Staff

Ronald Boisvert, *Chief*
Robin Bickel, *Secretary*
Jeffrey Fong, PT
Roldan Pozo
Chris Schanzle

Mathematical Modeling Group

Geoffrey McFadden, *Leader*
Bradley Alpert (Boulder)
Timothy Burns
Alfred Carasso
Andrew Dienstfrey (Boulder)
Michael Donahue
Fern Hunt
Raghu Kacker
Anthony Kearsley
Peter Ketcham
Stephen Langer
Agnes O'Gallagher (Boulder)
Donald Porter

Mirit Aladjem, GR
Daniel Anderson, GR
Eric Baer, S
Richard Braun, F
Katharine Gurski, GR
Seung-Ill Haan, GR
Sohyoung Kim, GR
Dianne O'Leary, F
Florian Potra, F
Richard Yeh, GR

Mathematical Software Group

Daniel Lozier, *Leader*
Marjorie McClain
Bruce Miller
William Mitchell
Bert Rust
Bonita Saunders

Bruce Fabijonas, F
Leonard Maximon, GR
Frank Olver, GR
G.W. Stewart, F
Abdou Youssef, F

Optimization and Computational Geometry Group

Ronald Boisvert, *Acting Leader*
Isabel Beichl
Javier Bernal
David Gilsinn

Emanuel Knill (Boulder)

Theodore Einstein, GR
Saul Gass, F

Scott Glancy, PD
James Lawrence, F
Sita Ramamurti, GR
David Song, GR
Francis Sullivan, GR
Christoph Witzgall, GR

Scientific Applications and Visualization Group

Judith Terrill, *Leader*
Yolanda Parker, *Office Manager*
Robert Bohn
William George
Terence Griffin
John Hagedorn
Howard Hung
John Kelso
Adele Peskin (Boulder)
Steven Satterfield
James Sims

Julien Lancien, GR
Alexandre Thibau, S

Staff Leaving the Division During FY 2005

Joyce Conlon

David Cotrell, PD
Ioan Sucan, GR
Anocha Yimsiriwattana, GR

Brian Cordes, S
Justin Haaheim, S
Jarrett Inn, S
Javier Sanchez, S
Gaurav Thakur, S
Benjamin Zoeller, S

Acronyms

ACM	Association for Computing Machinery
AIP	American Institute of Physics
AMS	American Mathematical Society
ANSI	American National Standards Institute
APS	American Physical Society
ASME	American Society of Mechanical Engineers
ATP	NIST Advanced Technology Program
BFRL	NIST Building and Fire Research Laboratory
BLAS	Basic Linear Algebra Subprograms
CARB	NIST Center for Advanced Research in Biotechnology
CCS	IDA Center for Computing Sciences
CEM	computational electromagnetics
CFM	confocal fluorescence microscopy
CIO	Chief Information Officer
CSTL	NIST Chemical Science and Technology Laboratory
CWI	Centrum voor Wiskunde en Informatica (Amsterdam)
DARPA	Defense Advanced Research Projects Agency
DIVERSE	Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (visualization software)
DLMF	Digital Library of Mathematical Functions (MCSD project)
DOD	Department of Defense
DOE	Department of Energy
DPD	dissipative particle dynamics
DSO	distributed shared object
EEEL	NIST Electronics and Electrical Engineering Laboratory
FY	fiscal year
GAMS	Guide to Available Mathematical Software
GMR	giant magneto-resistance
IDA	Institute for Defense Analysis
ITL	NIST Information Technology Laboratory
IFIP	International Federation for Information Processing
IMA	Institute for Mathematics and Its Applications (Univ. of Minnesota)
JAMA	Java Matrix package
LADAR	Laser Distance and Ranging
MCSD	ITL Mathematical and Computational Sciences Division
MEL	NIST Manufacturing Engineering Laboratory
MIM	Molecular interaction map
MPI	Message Passing Interface
MRAM	magnetic random access memory
MSEL	NIST Materials Science and Engineering Laboratory
NBS	National Bureau of Standards (former name of NIST)
NIST	National Institute of Standards and Technology
NOAA	National Oceanographic and Atmospheric Administration
NSF	National Science Foundation

OCM	optical coherence tomography
OOF	Object-Oriented Finite Elements (software package)
OOMMF	Object-Oriented Micromagnetic Modeling Framework (software package)
PDE	partial differential equation
PHAML	Parallel Hierarchical Adaptive Multi Level (software)
PL	NIST Physics Laboratory
QDPD	quarternion-based dissipative particle dynamics
RAM	random access memory
RAVE	Reconfigurable Automatic Virtual Environment
SAVG	MCSD Scientific Applications and Visualization Group
SED	NIST/ITL Statistical Engineering Division
SEM	scanning electron microscope
SIAM	Society for Industrial and Applied Mathematics
SIGGRAPH	ACM Special Interest Group on Graphics
SPIE	The International Society for Optical Engineering
SSS	Screen Saver Science
SURF	Student Undergraduate Research Fellowship
SVD	singular value decomposition
TIN	triangulated irregular network
TNT	Template Numerical Toolkit
VCCTL	Virtual Cement and Concrete Testing Laboratory