Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2006

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

January 2007

INFORMATION TECHNOLOGY LABORATORY

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Abstract

This report summarizes the technical work of the Mathematical and Computational Sciences Division (MCSD) of NIST's Information Technology Laboratory. Part I (Overview) provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II (Features) provides further details on nine particular projects with accomplishments of particular note this year. This is followed in Part III (Project Summaries) by brief summaries of all technical projects active during the past year. Part IV (Activity Data) provides listings of publications, technical talks, and other professional activities in which Division staff members have participated. The reporting period covered by this document is October 2005 through December 2006.

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Cover photo. Mathematician Howard Hung experiences a quantum dot in MCSD's immersive visualization environment. This photo appeared in the photo gallery of the online interactive edition of June 2006 issue of *National Geographic* associated with the feature article "Nano's Big Future." See http://www7.nationalgeographic.com/ngm/0606/feature4/gallery2.html. Photo by Mark Thiessen / National Geographic Image Collection.

Acknowledgement. We are grateful to Robin Bickel for collecting the information and organizing the first draft of this report.

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Part I

Overview

Introduction

There is now very widespread recognition of the critical role of applied mathematics and computation to both the advancement of science and engineering and to industrial innovation. Indeed, a recent report[1] of the President's Information Technology Advisory Committee (PITAC) states

> *"Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation."*

In a similar vein, a report[2] prepared on behalf of the National Science Foundation states

> *"Simulation-based engineering science … is a discipline indispensable to the nation's continued leadership in science and engineering. It is central to advances in biomedicine, nanomanufacturing, homeland security, microelectronics, energy and environmental sciences, advanced materials, and product development. There is ample evidence that developments in these new disciplines could significantly impact virtually every aspect of human experience."*

The importance to industry is also clear. According to the Council on Competitiveness[3], "high performance computing is not only a key tool to increasing competitiveness, it is also a tool that is essential to business survival."

The disciplines of applied mathematics, statistics, and computer science are the foundation for computational science and engineering. Research in mathematical and statistical analysis, numerical algorithms, software tools, high performance computing, and visualization provide the basis for mathematical modeling, computational simulation, and data analysis in all fields. In this regard, close cooperation between mathematicians, computer scientists, and application scientists are critical. As the PITAC report states, "the 21st century's most important problems … are predominantly multidisciplinary, multi-agency, multisector, and collaborative.**"** Indeed, much of the most innovative research is now occurring at the intersection of mathematics, computer science, and applications, e.g., in areas like nanotechnology, bioinformatics, and quantum information.

Information Technology at NIST. The mission of the National Institute of Standards and Technology (NIST) is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life. In particular, the NIST Measurement and Standards Laboratories conduct research that advances the nation's technology infrastructure and is needed by U.S. industry to continually improve products and services. The NIST Information Technology Laboratory (ITL) has the broad mission of supporting U.S. industry, government, and academia with measurements and standards that enable new computational methods for scientific inquiry, assure IT innovations for maintaining global leadership, and re-engineer complex societal systems and processes through insertion of advanced information technology. Through its efforts, ITL seeks to enhance productivity and public safety, facilitate trade, and improve the quality of life.

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[1] *Computational Science: Ensuring America's Competitiveness*, President's Information Technology Advisory Committee, June 2005.

[2] *Simulation-based Engineering Science: Revolutionizing Engineering Science Through Simulation*, Report of the National Science Foundation Blue-Ribbon Panel on Simulation-based Engineering Science, February 2006.

[3] *Study of US Industrial HPC Users*, Council on Competitiveness, 2004.

The other measurement science laboratories and research centers within NIST are also important customers of ITL. Indeed, NIST's measurement science research program has been transformed by the advent of computational science and engineering. Nearly every NIST project, both theoretical and experimental, typically now has critical computational components. In addition, an increasing number of NIST "products" are techniques, tools, and reference data to enable modeling, simulation, and data analysis in particular application domains.

To respond to the needs of its customers in industry, academia, government, and within NIST, ITL has developed a wide range of cross-cutting programs in areas such as information discovery, use, and sharing; complex systems; identity management; scientific discovery; and others. Applied mathematics and computational science plays an important role in these programs. This is clear from the four core competencies that ITL has identified as critical for it to carry out its work: (1) IT measurement and testing, (2) mathematical and statistical analysis for measurement science, (3) modeling and simulation for measurement science, and (4) IT standards development and deployment.

Mathematics and Computational Science at NIST. The Mathematical and Computational Sciences Division (MCSD) is one of six technical Divisions within ITL. MCSD provides leadership within NIST in the solution to challenging mathematical and computational problems. In particular, we seek to ensure that the best mathematical and computational methods are applied to the most critical problems arising from the NIST measurement science program. In addition, we also engaged in highly leveraged research and development efforts to improve the environment for computational science and engineering at large.

To accomplish these goals, MCSD staff members engage in the following types of activities: (a) peer-to-peer collaboration with NIST scientists and engineers in a wide variety of critical applications, (b) targeted outreach efforts with particular external communities to advance the state-of-the-art in their subfield, (c) development and dissemination of unique mathematical and computational tools, and (d) research in targeted areas of applied mathematics and computer science of high relevance to future NIST programs.

The technical work of the Division can be organized into eight general areas. We indicate overall goals and approach of each of these below. Of course, there is considerable overlap between these areas. Nevertheless, this breakdown provides a useful overview of Division thrusts.

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 and analysis.
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 modeling through the use of benchmarks (challenge prob-

lems) and reference software. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

Mathematical Modeling for Chemical and Biological Applications.
Goals: Enable effective mathematical and computational modeling for chemical and biological applications of critical importance to NIST programs. Improve the state-of-the-art in software for chemical and biological modeling and analysis.
Approach: Develop techniques and tools to enable accurate, reliable, and efficient modeling and simulation of chemical and biological systems. Collaborate with NIST scientists and engineers in the application of such techniques to critical NIST programs.

High Performance Computing.
Goals: Improve the quality and rate of scientific discovery through the effective 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.

High Performance Visualization.
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 high-end visualization. Collaborate with NIST scientists in the application of high performance visualization to high priority NIST projects.

Mathematics of Metrology.
Goals: Develop effective methods for the solution to critical 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 fundamental mathematical and computational techniques of widespread application. Galvanize interest within the applied and computational mathematics community for the study of problems occurring in measurement science.

Quantum Information Theory.
Goals: Develop fundamental understanding of potential of quantum mechanical systems for computation and communication.
Approach: Collaborate closely with the NIST Physics Lab and Electronics and Electrical Engineering Lab to demonstrate the information processing capabilities of quantum systems, including ion traps and optical systems. Develop architectural concepts for quantum information systems, including error control strategies promoting fault-tolerance. Develop techniques and tools enabling the analysis of behavior of quantum mechanical systems.

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 technical computing 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.

Crosscutting Themes. Several crosscutting themes indicative of current industrial trends have emerged in the Division technical program. In particular, 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, and parallel computing and visualization techniques for models of optical properties of nanostructures.

A second 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. One example is the integration of computer simulation with physical measurement. Our OOF software for the finite element analysis of materials with complex microstructure enables analyses based on micrographs of real material samples, a capability useful in manufacturing quality control applications. We are also developing technologies to enable accurate interactive measurements during the analysis of data from physical measurement in immersive visualization environments. These tools have already seen application in the evaluation of prototype standard polymer scaffolds for the growth of human tissue. Looking further into the future, 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, something that is rarely done today in any formal way. We are working to develop such methodologies in collaboration with NIST scientists.

Another recurring theme in our work is he need for the automated ***analysis of complex or large-scale scientific data*** sets, whether obtained from physical measurement or computer simulation. Often such data takes the form of images. In many cases the data is highly noisy. 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. Visualization techniques provide an important means for scientists to make sense of large volumes of scientific data; our immersive scientific visualization lab, along with its associated software tools and environment, provide unique capabilities in this regard.

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.

Imaging and visualization technology and tools were behind a number of the Division's major accomplishments for the year. In some cases this involved the development of new imaging technologies themselves. For example, we worked with scientists in the NIST Electronics and Electrical Engineering Laboratory (EEEL) to evaluate the potential of optical coherence tomography as a diagnostic tool for cancer. One of the distinguishing features of this imaging modality is that both the intensity and phase fields can be measured. In a paper published in *Optics Express*, the team showed that optical phase offers potentially new diagnostic information on biological scatterers of interest in cancer detection. Algorithms and software tools for electromagnetic modeling developed by Andrew Dienstfrey of MCSD enabled the theoretical verification of these results.

Techniques for the post processing of image data to compensate for unwanted effects of imaging systems has long been a need for NIST measurement science, and MCSD has led in the development of such techniques. One particularly effective technique is the APEX method for real-time blind deconvolution developed by Alfred Carasso. It is blind in that the point-spread function (PSF) causing the blur is not known a priori. The PSF is taken from a class of 2-D heavy-tailed probability density functions whose parameters are estimated from the image itself. Once the PSF is determined, the deconvolution proceeds by marching a diffusion equation backwards in time. With FFTs as its computational kernel, it is highly efficient, even for large images. The method has been shown to be effective on a wide range of imagery, including medical images and scanning electron microscope images. In a paper published in the October 2006 issue of *Optical Engineering*, Carasso describes an extension of the technique to color imagery, which he applies to enhance a wide range of Hubble Space Telescope and other astronomical data. The journal editors featured one of these enhanced images on the October issue's cover.

Highly useful scientific data can be extracted from images in many other ways. The OOF (Object Oriented Finite element) system enables the direct computational study of structure-property relationships in materials with complex microstructures through highly sophisticated image analysis. When running OOF, a user assigns material properties to the features in an image of a material's microstructure, and then performs virtual experiments on the material (to obtain stress-strain fields, for example). Unlike commonly available commercial finite element codes, OOF features both a powerful suite of tools for adapting a finite-element mesh to the microstructural geometry of an image, and a modular and extensible scheme for adding new or customized property data to the underlying model. This year a major new version of OOF was released. With a design that is highly modular and extensible, OOF2 enables a much wider range of applications than the original. A workshop for OOF users held at NIST in September 2006 to introduce the new system attracted some 40 researchers from around the world. OOF2 was developed by Stephen Langer and Andrew Reid of MCSD, in cooperation with the NIST Materials Science and Engineering Laboratory (MSEL).

Other measurement science applications are not necessarily as amenable to completely automated processing. In these cases a more hands-on approach is necessary. We are pioneering the use of immersive visualization for the interactive measurement and analysis of properties of physical systems which have been captured using three-dimensional imaging technologies. In doing so we are developing the tools needed to create a true virtual measurement laboratory. For

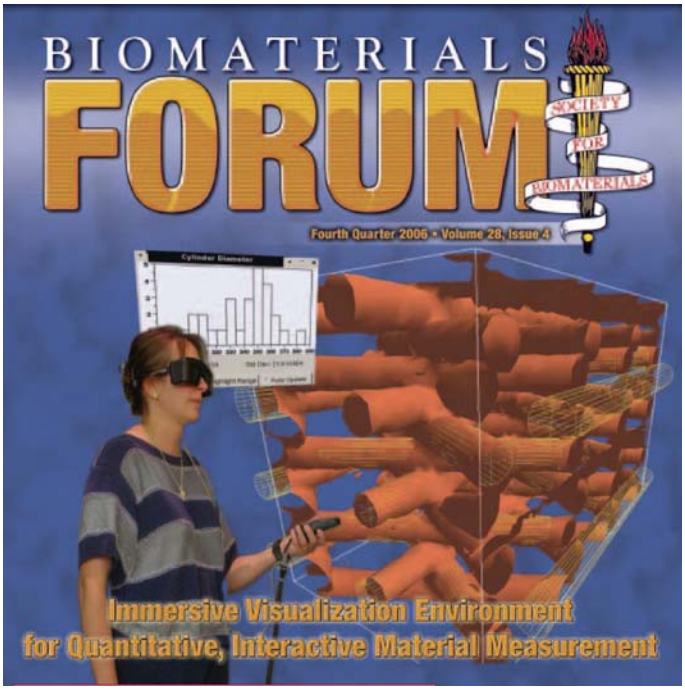


Figure 1. *MCSD work on quantitative interactive material measurement in an immersive visualization environment was featured on the cover of the 4th quarter 2006 issue of Biomaterials Forum. (This image used Courtesy of the Society for Biomaterials.)*

example, we have worked closely with MSEL scientists to characterize standard reference materials (e.g., polymer scaffolds) for the growth of tissue engineered products. To do so, three dimensional images that were generated with X-ray micro-computed tomography (μCT) were segmented and converted to a polygonal representation for the virtual environment. We then used interactive measurement and analysis tools we developed to compare an idealized "as designed" scaffold with an actual manufactured scaffold to determine differences in strut properties. This work was featured in a cover article in the fourth quarter 2006 edition of *Biomaterials Forum*.

Another type of virtual measurement is the prediction of physical properties of matter entirely through computation based on first principles. In a paper published this year in the *Journal of Chemical Physics*, James Sims of MCSD and Stanley Hagstrom of Indiana University announced a new high-precision milestone for the calculation of the disassociation energy of the hydrogen molecule (H_2). Accurate to 1 part in 100 billion, these are the most accurate energy values ever obtained for a molecule of that size, 100 times better than the best previous calculated value or the best experimental value. While very precise calculations have been done for systems of just three components such as helium (a nucleus and two electrons), Sims and Hagstrom are the first to reach this level of precision for H_2 with two nuclei and two electrons. The calculation requires solving an approximation of the Schrödinger equation using a series approximation. To make the problem computationally practical, Sims and Hagstrom merged two earlier algorithms for these calculations—one which has advantages in ease of calculation, and one which more rapidly achieves accurate results—into a hybrid with some of the advantages of both, known as the Hy-CI variational method. To enable the computation they developed specialized multi-precision arithmetic capabilities and a new parallel large-scale generalized matrix eigenvalue solver. The final calculations were run on a 147-processor parallel cluster at NIST over the course of a weekend—on a single processor it would have taken close to six months.

Large scale parallel computational methods developed by MCSD are also enabling the understanding of the properties of cement-based materials. William George and Judith Terrill of MCSD, along with Nicos Martys and Edward Garboczi of the NIST Building and Fire Research Laboratory were awarded 1,000,000 CPU hours on the 10,240-CPU Columbia supercomputer at NASA Ames Research Center for such work. The allocation was one of four awards of supercomputer time given out by NASA in a peer-reviewed competition for grand challenge computational science projects led by external researchers. The team is using NASA's supercomputer to study the flow, dispersion and merging of dense suspensions composed of rigid bodies having a wide range of size and shape under a variety of flow conditions. Access to the NASA machine

will allow modeling at a level and range impossible with existing computing facilities available at NIST. The new realism of these models will significantly improve the scientific basis for prediction and measurement of the flow properties of concrete.

Finally, we are working closely with the NIST Physics Laboratory to begin to develop a measurement science infrastructure to enable computation based upon quantum mechanical systems. While quantum computers have the potential for significantly speeding up many useful algorithms, building quantum computers is challenging. Currently available quantum devices can realize computations with only a few quantum bits (qubits) and steps. Atomic qubits in ion traps are currently considered one of the leading candidates for realizing large quantum computers. A team led by David Wineland at NIST (PL, Boulder) has arguably the most advanced laboratory in the world for studying such systems. Manny Knill of MCSD is providing the theoretical underpinnings to enable the team to determine the potential of this technology. This year the team implemented two benchmark quantum subroutines for up to six atomic qubits and analyzed the error of the implementations. The first benchmark involved creating "Schrödinger cat states" of four to six qubits. The second demonstrated an entanglement purification protocol that is expected to play a key role in large scale implementations of quantum computers and quantum communication protocols. Each of these landmark accomplishments were reported in papers published in *Nature*.

Technology Transfer and Professional Activities

The volume of technical output of MCSD remains high. During the last 18 months, Division staff members were (co-)authors of 50 articles appearing in peer-reviewed journals, including two published in *Nature*. 13 other invited articles and 14 papers in conference proceedings were published. Fourteen additional papers have been accepted and are awaiting publication, while 24 others have been submitted for review. Division staff members gave 28 invited technical talks and presented 19 others to conference and workshops.

MCSD continues to maintain an active Web site with a variety of information and services, including the Guide to Available Mathematical Software, the Matrix Market, and the SciMark Java benchmark. During calendar year 2006, the virtual server math.nist.gov satisfied nearly seven million requests for pages, or more than 19,000 per day. More than 1.7 Gbytes of data were shipped each day, and more than 539,000 distinct hosts were served. The virtual server gams.nist.gov, delivered 930,000 pages, or more than 2,500 per day. There have been nearly 115 million "hits" on MCSD Web servers since they went online as NIST's first web servers in 1994. Among our most popular software downloads for calendar year 2006 were: Template Numerical Toolkit (linear algebra using C++ templates): 15,310 downloads, Jama (linear algebra in Java): 13,656 downloads, and SparseLib++ (elementary sparse matrix manipulation in C++): 4,284 downloads.

Members of the Division are also active in professional circles. Nine staff members hold a total of 14 associate editorships of peer-reviewed journals. Three staff members served as guest editors organizing special journal issues. Staff members are also active in conference organization, two serving on organizing committees and four on program committees. Three staff members are organizing minisymposia for the upcoming International Congress on Industrial and Applied Mathematics (Zurich, 2007), four others organized sessions at meetings ranging from the SIAM Annual Meeting to SIGGRAPH.

Service within professional societies is also prevalent. Ronald Boisvert serves as Co-Chair of the Publications Board of the Association for Computing Machinery (ACM) and a member of the ACM Council, the association's board of directors. Fern Hunt serves on the Ex-

ecutive Committee of the Association for Women in Mathematics. Daniel Lozier serves as Vice-chair of the Society for Industrial and Applied Mathematics (SIAM) Activity Group on Orthogonal Polynomials and Special Functions. Staff members are also active in a variety of working groups. Ronald Boisvert serves as Chair of the International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software, Donald Porter is a member of the Tcl Core Team, and Bruce Miller is a member of W3C's Math Working Group. Judith Terrill represents NIST on the High End Computing Interagency Working Group of the Federal Networking and Information Technology Research and Development (NITRD) Program.

For further details, see Part IV (Activity Data) of this document.

MCSD Student Interns - 2006

Name	Institution	Program	Mentor	Project Title
Zachary Catlin	Purdue Univ.	SURF	S. Glancy	Characterization of quantum optical states.
Liuyuan Chen	Montgomery Blair High School	Student Volunteer	B. Rust	Wrote Fortran subroutines & made calculations with Fortran and Matlab
Michael Forbes	MIT	SURF	R. Kacker, D. Gilsinn	Combinatorial methods for software testing
Adam Lazrus	Charles E. Smith Upper School	Student Volunteer	J. Terrill	Distributed 3D Chemical Imaging: Porting a Serial Application to Screen Saver Science
Christine McKay	University of Maryland	SURF	W. George	A User Interface to a Distributed Computing Environment
David Warshawsky	Melvin J. Berman Hebrew Academy	Student Volunteer	J. Fong	Formulate simple framed structure design problem in 2D

SURF: NIST Student Undergraduate Student Fellowship Program.

Staff News

Howard Hung retired from NIST in July 2006 after more than 30 years of federal service. His long career featured many contributions to operations research, scientific computing, and visualization. He was most recently a member of the MCSD Scientific Applications and Visualization Group.

NIST/NRC Postdoctoral Associate Scott Glancy finished his two-year appointment in September 2006. He worked in the area of quantum information theory with Manny Knill in Boulder. Glancy was given a two-year extension on his appointment to continue this work. Christopher Schanzle, formerly of the NIST CIO Office joined MCSD in October 2005 to provide computer systems and programming support to Division staff. He serves as MCSD Computer Security Officer.

MCSD made two additional faculty appointments during FY 2006. These are made to full-time faculty members at local universities, who then typically spend about one day per week working in MCSD throughout the year. This year's new appointees were Daniel Anderson of George Mason University, an expert in mathematical modeling of fluid dynamics and materials phenomena, and Marc Olano of the University of Maryland Baltimore County, an expert in interactive 3D computer graphics.

Manny Knill of MCSD in Boulder was elevated to the status of NIST Fellow in September 2006. Designation as Fellow is the highest distinction given to NIST technical staff. There

is a limit of 30 Fellows NIST-wide. Geoffrey McFadden of MCSD is the only other NIST Fellow in ITL.

Two MCSD staff members completed details at other government agencies at the end of FY 2006. Isabel Beichl participated in a sabbatical program within the Mathematics Research Group at the National Security Agency. She spent half of her time at the NSA as part of this program. Robert Bohn of MCSD completed a two-year assignment with NOAA's High Performance Computing and Communications Office.

MCSD provided support for six student staff members on summer appointments during FY 2006. 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 are listed in the table above.

Figure 2. *Three of MCSD's 2006 award winners. Left: Bradley Alpert, winner of the 2005 Arthur Flemming Award. Center: Dianne O'Leary, Fellow of the Association for Computing Machinery. Right: Manny Knill, Fellow of the American Physical Society.*

Awards

MCSD staff garnered a variety of awards and recognitions during the past year. Bradley Alpert was named a winner of the 2005 Arthur Flemming Award. Established by the Downtown Jaycees in 1948, the Flemming Awards honor outstanding federal employees with at most 15 years of service. The program is administered by the George Washington University in conjunction with the Flemming Award Commission. Twelve separate awards are made each year in three categories: administration, science, and applied science and mathematics. Alpert was recognized in the latter category for a sustained record of fundamental contributions to scientific computing, including the development of fast algorithms enabling the solution to heretofore intractable problems of computational physics. He is also cited for his extensive collaborations with scientists and engineers to apply innovative techniques to the solution of diverse problems of scientific and technological interest. Finally, the award recognizes Alpert's work as a mentor and leading proponent of careers in mathematics for students at the high school, undergraduate, graduate, and post-graduate levels. The award was conferred in ceremonies in Washington, DC on June 13, 2006. Alpert is the fourth MCSD staff member to receive the Flemming Award. Pre-

vious MCSD awardees were Anthony Kearsley (2001), Fern Hunt (2000), and Geoffrey McFadden (1989).

Emanuel (Manny) Knill was 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 Knill's outstanding contributions to physics. In particular, Knill was 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 occurred in the March 2006 issue of APS News. Knill is MCSD's second APS Fellow. Geoffrey McFadden was elected in 2001. Knill was also given the designation of NIST Fellow in September 2006.

Dianne O'Leary, an MCSD faculty appointee from the University of Maryland College Park was named a Fellow of the Association for Computing Machinery (ACM). The ACM Fellows Program was established in 1993 to recognize and honor outstanding ACM members for their achievements in computer science and information technology and for their significant contributions to the mission of the ACM. Fellow status is limited to at most 1% of ACM members. O'Leary will be recognized at ACM's June 2007 award's ceremony in San Diego.

Ronald Boisvert and Dianne O'Leary were also honored as Distinguished Scientists by the ACM. They were included in a group of 49 professionals in ACM's inaugural class of distinguished members. The ACM Distinguished Membership Program recognizes members with at least 15 years of professional experience who have achieved a significant impact on the computing field.

Pete Stewart, an MCSD faculty appointee from the University of Maryland College Park was named a UMCP Distinguished University Professor. This formal title denotes an academic honor of highest distinction and is awarded to a limited number of the university's most accomplished professors.

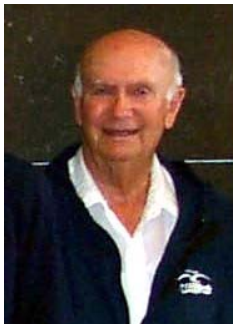
Finally, MCSD captured two of the four ITL Awards presented during 2006. Manny Knill was recognized with the ITL Best Journal Paper Award for "Quantum Computing with Realistically Noisy Devices," published as a feature article in *Nature*, volume 434, pages 39-44 (03 Mar 2005). MCSD's Scientific Visualization Team, comprised of Judith Terrill, Terrence Griffin, John Hagedorn, Howard Hung, John Kelso, Yolanda Parker, Adele Peskin, and Steven Satterfield, were honored with the ITL Outstanding Contribution Award for "outstanding service as ambassadors of ITL, providing numerous demonstrations of ITL's immersive scientific visualization capabilities which have led to widespread favorable recognition of NIST in the news media, as well as among stakeholders in Congress, industry, academia, and the general public".

Passings

Eleazer Bromberg. Dr. Eleazer Bromberg, 92, was a mathematician at NBS/NIST from 1979 until his retirement in 1999, after which he continued as a guest researcher in MCSD for several years. At NIST he served as technical advisor to several Lab Directors in the area of high performance scientific computing. This was Lazer's second career, however. After receiving his Ph.D. in applied mathematics from the Courant Institute of Mathematical Sciences at New York University in 1950, he served as head of the Mechanics Branch of the Office of Naval Research. In 1953 he returned to NYU, where he remained until 1979, serving in a variety of roles including Professor, Administrative Director of the AEC Computing Center (1953-58), Assistant Director of the Courant Institute (1959-66), Vice Chancellor for Academic Affairs (1970-73), and Deputy Chancellor (1973-75). He also held visiting positions at the Los Alamos Scientific Laboratory and the IDA Center for Computing Sciences. He passed away on March 27, 2006 in Philadelphia.

Howland Fowler. Dr. Howland Auchincloss Fowler, 76, came to NBS in 1957 as an NRC Associate and spent his next 37 years as an NBS physicist specializing in low-temperature physics and applied mathematics. He served as scientific advisor to the directors of several major NIST organizations. In 1991 he became Leader of the Scientific Visualization Group in the NIST Computing and Applied Mathematics Laboratory. He was (co-)author of more than 30 scientific papers. He retired in 1994 but continued as a guest researcher in MCSD until 2000. He passed away on September 3, 2006 in Bethesda, MD.

André Deprit. Former NIST Fellow Dr. André Deprit, 81, was a NBS/NIST mathematician from 1979 until his retirement in 1999; he continued as a guest researcher in MCSD until 2003. André received a D.Sci. degree in mathematics from the University of Louvain in 1957. He held a professorship at Louvain before coming to the US in 1964 to work at Boeing. He had appointments at NASA Goddard and the University of Cincinnati before joining NBS. André was a leading expert in the mathematics of celestial mechanics, and a pioneer in the use of symbolic computing to tackle problems in that field. The author of more than 150 technical articles, his work was very highly regarded in the fields of space flight mechanics and astrodynamics, resulting in numerous awards, including the James Craig Watson Medal from the US National Academy of Sciences (1972), the Dirk Brouwer Award from the American Astronomical Society (1984), and the Department of Commerce Gold medal (1986). He passed away on November 7, 2006 in Gaithersburg, MD.



Morris Newman. Dr. Morris Newman, 82, was a research mathematician at NBS from 1952-1977. He was awarded a DOC Gold medal in 1966 for his work on algorithms for solving exactly integral linear systems using congruence techniques. In 1968 he wrote the book *Matrix Representations of Groups* and in 1972 the book *Integral Matrices,* which became a classic. Recently he served as an Associate Editor of the NIST Digital Library of Mathematical Functions while an emeritus professor at University of California at Santa Barbara. He passed away on January 4, 2007 in Santa Barbara, CA.

Part II

Features

APEX Blind Deconvolution of Color Hubble Space Telescope Imagery and Other Astronomical Data

Over the last 50 years, signal recovery has become a fundamental and pervasive scientific activity. In research spanning length scales from the atomic to the cosmological, deconvolution now plays a critical role in extracting scientific content. In particular, because of its critical role in measurement science, the study of improved methods for deconvolution has been a long interest of MCSD. In recent years our attention has turned to the challenging problem of image deblurring, where we have developed a number of novel techniques. For example, NIST's APEX method is a technique for real-time blind deconvolution. It is blind in that the point-spread function (PSF) causing the blur is not known a priori. The PSF is taken from a class of 2-dimensional heavy-tailed probability density functions whose parameters are estimated from the image itself. Once the PSF is determined, the deconvolution proceeds by marching a diffusion equation backwards in time. The method relies on FFTs as its computational kernel, and hence is highly efficient, even for 1024x1024 images. The APEX method has been shown to be effective on a wide range of imagery, including medical images and scanning electron microscope images. Recently this method was extended to the sharpening of color imagery and to astronomical data.

Alfred Carasso

NIST's APEX blind deconvolution method, initially conceived from an abstract mathematical blueprint, has been found useful in sharpening a wide variety of images, including Hubble Space Telescope color imagery. This is discussed in a recent paper by A. S. Carasso in the October 2006 issue of *Optical Engineering*, the flagship research journal of the International Society of Optical Engineering (SPIE) [7]. The paper provides a detailed discussion of the application of the APEX method to astronomy, and includes visually striking enhancements of color Hubble imagery, as well as imagery from ground-based telescopes. One vivid example involving the Andromeda galaxy (Fig. 3) was selected as cover art by the journal Editors. Previous NIST work applying the APEX method to scanning electron microscopy (SEM) was published in the same journal some time ago [5]. Such microscopy work is ongoing, and remains of vital significance to NIST. Indeed, powerful new state-of-the-art SEM equipment has been acquired in support of NIST nanotechnology research. Considerable synergy is likely to be realized by comparing and contrasting the performance of the APEX method in such widely different contexts.

Figure 3. *Kitt Peak true-color Andromeda galaxy image. Top: original image. Bottom: after APEX processing.*

NASA's Hubble Telescope was launched in 1990, with an estimated total lifetime cost of around six billion dollars. Over 750,000 priceless images had been recorded and archived as of April 2005. These images have fundamentally increased our understanding of the universe, have enthralled the general public, and have significantly increased public awareness of scientific research.

Valuable additional information can quite likely be obtained from many of these images by the application

of appropriate sharpening methods. This is illustrated with the Tadpole galaxy example in Fig. 4. On the left is the original Hubble image taken in April 2002 using NASA's ultra sophisticated Advanced Camera for Surveys (ACS). Several clusters of young bright blue stars are visible in the Tadpole's spiral head and long tail. These and other foreground features are brought into sharper focus by applying the NIST-developed APEX sharpening procedure as shown on the right. However, of even greater interest, are the background features, which become much more evident in the APEX enhanced image. This background has been described by NASA as a "Whitman's Sampler" of galaxies, many of which are extremely far away, and represent "fossil samples of the universe's 13 billion year evolution."

Background. Deconvolution is the process of recovering a signal from measured data which has been subjected to a type of averaging process. For example, the fundamental 2-D deconvolution problem is to recover a signal f, such that

$$\int_{R^2} h(x-u, y-v) f(u,v)\, du\, dv = g(x,y)$$

where g is the recorded data (which may contain noise) and h represents the averaging process. The study of deconvolution requires tools from several branches of mathematics, including integral equations, calculus of variations, operator theory, probability theory, Fourier analysis, partial differential equations, numerical analysis, linear algebra, and wavelet theory. Not surprisingly, MCSD has long supported research in this area and is uniquely well-equipped for this task.

In prior years, our work focused on challenging 1-dimensional deconvolution problems of importance to the NIST measurement laboratories. These typically featured complex signals exhibiting non-differentiable singularities. Such behavior is associated with the arrival of propagating disturbances, and is of prime interest. One such situation occurs in acoustic emission studies, where experimental identification of elastic Green's functions is necessary. Another is the identification of dynamic Green's functions in complex structural networks, such as an orbiting space station. In each case, novel deconvolution techniques were devised by Carasso that could capture the singular Green's profile in the presence of noise [1, 2].

Much current scientific data is in the form of digital imagery. Whether the imaging instrument is an optical microscope, an electron microscope, a telescope, or any one of several medical imaging modalities, the resulting image is blurred due to distortions induced by the instrument, as well as by the medium through which the signal travels. In many cases, this distortion can be summarized and described by the imaging system's *point spread function* or PSF. Knowledge of the PSF, when this is available, enables sharpening of the blurred image through very careful numerical treatment of the recorded image. That task is highly non-trivial, as deconvolution is an unstable computational process that can severely amplify noise. Fundamental work in this area was done by Carasso, who invented the *slow evolution from the continuation boundary* (SECB) constraint to stabilize the inversion process [3]. Subsequently, further significant work focused on finding the right mathematical function space in which to pose the deblurring problem. Indeed, the commonly used space of functions of bounded variation has the notorious property of eliminating fine scale details in an image, and such loss of texture is wholly unacceptable in practice. A cure for this so-called *staircase effect* was urgently needed. In 2003, Carasso showed that most natural images are not of bounded variation, but rather belong to Lipschitz spaces of non-differentiable functions. Carasso then used the Poisson singular integral to create an effective deblurring method that can recover texture [6]. U.S. patents have been obtained, or are in process, for these inventions.

Blind Deconvolution. In many cases, the PSF describing the blur is unknown or incompletely known. Blind deconvolution seeks to deblur the image without knowing the PSF. This is an extremely challenging problem in which severe ill-conditioning is compounded with non-uniqueness of solutions. Most known approaches are iterative in nature and seek to simultaneously reconstruct both the PSF and the deblurred image. Such iterations are typically ill-behaved and may develop stagnation points or diverge altogether. When the process is stable, many thousands of iterations and several hours of computing are often necessary to resolve fine detail. Such procedures are not feasible for real-time processing of large size images of complex objects.

Published in 2001, NIST's APEX method represents a major breakthrough in blind deconvolution [4]. Like his previous work, Carasso's research in blind image deblurring has focused on developing reliable direct (non-iterative) methods, in which fast Fourier transform (FFT) algorithms are used to solve appropriately regularized versions of the ill-posed deblurring problem. The SECB and Poisson singular integral methods are direct FFT methods that assume the PSF is known. The blind APEX method is predicated on a preselected class of blurs in the form of 2-D radially symmetric, bell-shaped, heavy-tailed probability density functions, a class that generalizes Gaussian and Lorentzian distributions. By design, these blurs are chosen so as to have a crucial additional mathematical property, namely they must form a semigroup under convolution. An explicit mathematical formula for such blurs was worked out by the legendary French probabilist Paul Lévy in the 1930's in his celebrated work of the Central Limit Theorem. Use of that formula enables initial trial identification of the blur parameters by Fourier analysis

of the blurred image. Naturally, there is no assurance that this class of blurs is appropriate for a given image, and, in fact, not all images can be usefully enhanced with the APEX method. Nevertheless, APEX is effective on a surprisingly wide variety of images.

The semigroup property allows reformulation of the deconvolution problem into a mathematically equivalent problem of solving a generalized diffusion equation backwards in time, given the blurred noisy image as data at time *t=1*. Here, SECB regularization enables stable marching backwards towards the desired deblurred image at time *t=0*. Such *slow motion* deconvolution is a vital element of the APEX method. It allows for visual monitoring of the process, for the calculation of statistical diagnostics, and for the opportunity to curtail the process when noise amplification and/or ringing artifacts begin to appear. Such early termination is equivalent to interactive readjustment of the initially detected blur parameters. Because the entire computation is FFT-based, high resolution images, of size 1024x1024 pixels, can be handled in about 2-3 minutes on current desktop computers. Numerous trial deconvolutions using different parameters can thus be done. Such efficient exploration of parameter space is often a key to the successful solution of ill-posed inverse problems.

Astronomical color imagery. Blind deconvolution of astronomical images is a challenging problem of considerable interest. The applicability of the APEX method is not evident a-priori, and hinges on whether the assumed class of heavy-tailed blurs is appropriate for the various types of modern astronomical imaging devices. Color imagery presents a significant additional challenge, as each color component may have its own individual PSF, which must be identified separately. As is clear from Figs. 3 and 4, color is an important element in astronomical imagery. There is the real danger that the deconvolution process may upset the original balance of colors, and result in a deblurred image with physically false colors. Blind deblurring of color imagery is a subject that is still very much in its infancy.

A remarkable property of the APEX method is the ease with which it can be applied to color imagery, and the plausibility of the ensuing results [7]. This property stems directly from its ability to permit monitoring of the unfolding process in slow motion. In addition, quantities such as the image L_1 norm and the image gradient norm can be calculated at each discrete time level on the way to *t=0*. In well-behaved deconvolution, the L_1 norm of each color component should be conserved, while the gradient norm should increase monotonically. One can enforce L_1 norm conservation in each color component separately by terminating the deconvolution process for that component whenever the current L_1 norm exceeds its original value at *t=1* by more than a very few percent. This strategy of enforcing componentwise L_1 norm conservation has been found to maintain the balance of colors in all of the color examples to which the APEX method has been applied.

The example in Fig. 3 is one where the APEX-detected blue component PSF was much narrower than the red and green PSFs, indicating that the blue component image was perceived by APEX to be less blurred than the red and green. Such differential deblurring has clearly preserved the balance of colors.

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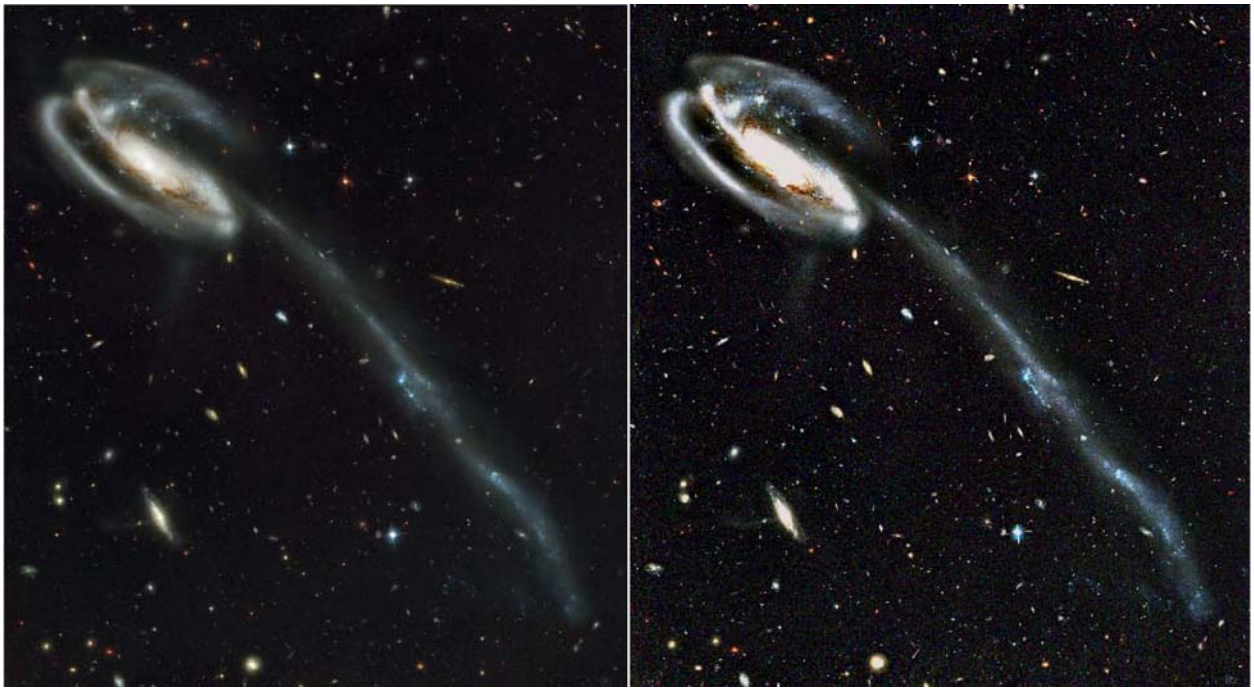

Figure 4. *APEX processing of Hubble TADPOLE galaxy. Enhancement of background is of considerable interest. Background said to contain a "Whitman sampler of galaxies stretching back to the beginning of time. Image obtained by NASA's most sophisticated Advanced Camera for Surveys (ACS).*

Optical Coherence Tomography for Biomedical Imaging

A wealth of biomedical imaging techniques are being developed for diagnosis and monitoring of a wide range of diseases. Well-known modalities include MRI, PET scans, and quantitative x-ray tomographic technologies (qCT). Recently, interest in optical coherence tomography (OCT) has grown as it has been demonstrated to give quantitative structural information pertaining to biological scatterers. One proposed application has been to use OCT as a diagnostic tool for cancer. NIST researchers are performing quantitative evaluations of this imaging modality. In doing so, a new channel for potentially useful diagnostic information has been identified.

Andrew Dienstfrey

Over a range of optical frequencies and scattering parameters, it has been shown that cell nuclei are the dominant contributors to back-scattered radiation. Thus, measurements can be inverted for nuclei features, for example the characteristic size. As many epithelial cell cancers (e.g., cervical, esophageal, colon, skin, oral) exhibit enlarged cell nuclei as a precancerous condition, it is hoped that a fiber-based OCT technique could serve as an early diagnostic tool for these disease models. Additional biomedical uses of OCT currently being investigated include: cellular substructure imaging, assessment of the efficacy of chemopreventative agents, and the measurement of characteristics of large-scale intracellular organization.

One of the novel characteristics of OCT is that both the intensity and phase of the fields of interest can be measured. This ability, although not unique to OCT, nevertheless distinguishes it from the majority of optical techniques which measure only the intensity (magnitude) of the optical field. Four OCT platforms were built by Shellee Dyer, Tasshi Dennis, and Paul Williams in NIST's Opto-electronics Division to investigate the quantitative potential of this technology.

For fixed polarization and point in space, the relationship between the incident and scattered fields may be viewed as a linear dynamical system. For such systems we have $E_s(f) = E_i(f)\, H(f)$ where f is the frequency of incident radiation, $E_{s,i}(f)$ are polarizations of scattered and incident fields, and $H(f)$ is the Fourier transform of the impulse response function. In some cases, measurements of $H(f)$ can be inverted for physical characteristics of the scatterers. As $H(f)$ is complex, its complete characterization requires the optical phases of $E_{s,i}(f)$. In addition to the complication of measuring optical phase, some investigators have assumed that this quantity carries no information not already encoded by the magnitude. Writing $H(f) = \rho(f)\exp(\mathrm{i}\,\phi(f))$, the mathematical statement is that $H(f)$ is minimum phase, in which case $\phi = K\ln(\rho)$, where K is a well-known singular integral operator. This minimum-phase assumption is common but, to our knowledge, has not been sufficiently explored until now.

A classical structure theorem from linear systems theory is a powerful aid in the analysis. The derivative of the phase with respect to frequency, $\phi'(f)$ is known as the relative group-delay (RGD). In terms of the RGD the theorem states that

$$\Delta'(f) \equiv \phi'(f) - \phi'_{mp}(f) = 2\pi\tau + \sum_n^N \frac{\gamma_n}{(f - f_n)^2 + \gamma_n^2}$$

In this equation τ denotes a time shift, and the summation terms come from "all-pass" or "Blaschke factors." Details aside, the conclusion is that the discrepancy between a minimum and non-minimum-phase response is not arbitrary but, rather, has a structure dictated by general theory.

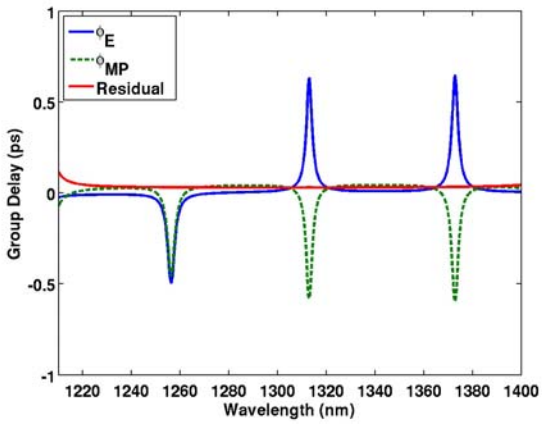

Figure 5. *True group delay and minimum phase group delay (blue solid and green dashed curves) are plotted as a function of wavelength for a single sphere (r=5 microns, n=1.41+0.003i). The true group delay resonances at λ=1.31μ and λ=1.375μ are inverted from those predicted by minimum phase analysis. Correcting the minimum phase for time shift and Blaschke factors as predicted by theory brings the two RGD in agreement. The residual after correction is shown in red.*

Two suites of software tools applicable to this problem have been developed within MCSD. The first computes full wave electromagnetic solutions to Maxwell's equations with multiple, fully general spherical scatterers in arbitrary position. The algorithm represents electromagnetic fields in terms of vector wave functions centered at sphere locations. Coupling between mutual spheres is achieved using appropriate translation operators. The second suite of tools performs the minimum

phase analysis. These codes compute the singular Kramers-Kronig operator K via product quadrature of a spline representation of sampled magnitude data. All algorithms were verified for accuracy and convergence by extensive numerical testing. Additionally, the spherical scattering code was validated by comparison with a single sphere code (Mie theory) developed previously by investigators in the NIST Physics Lab.

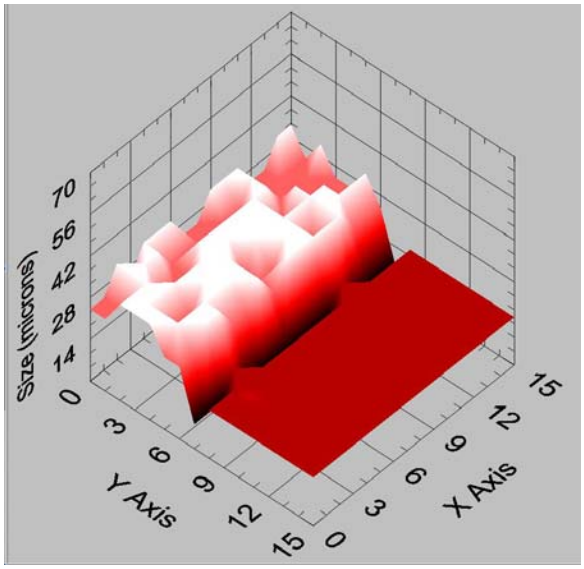

Figure 6. *Characteristic size of polystyrene spheres adhered to glass coverslip as determined by inversion of OCT measurements of back-scattered group delay. The ridge indicates the boundary between small and large spheres (r=14 and 28 micrometers). Spatial averages as a function position are indicated by the z-axis. The sphere positions and radii correspond well with measurement by microscopy.*

These codes were used to compute vector fields scattered by isolated spheres, along with the true complex response function, *H(f)*, as a function of frequency. The minimum phase response $\phi_{mp}(f) \equiv \left[K \ln\left(|H|\right)\right](f)$ was compared with the true phase response $\phi_E(f) \equiv \mathrm{Arg}(H(f))$. The group delays (derivatives) are plotted in Fig. 5. At the resonance near λ=1250nm, the true and minimum RGD agree. The two other resonances, however, are of opposite signs. According to theory, the RGD difference must be represented by a sum of a time-shift and Blaschke terms. A non-linear fit for τ and parameters $\{f_n, \gamma_n\}$ was performed. The minimum phase RGD augmented by the exponential and Blaschke terms determined by the non-linear analysis is subtracted from the true phase, and the difference (residual) is also shown in the figure. Clearly the differences between the minimum and true RGD are accounted for by the Blaschke terms as predicted by theory. This result demonstrates that back-scattering by a single dielectric sphere can exhibit both minimum and non-minimum-phase response. Although of an elementary character, to our knowledge this observation has not been made before. The conclusion is surprising as it contradicts heuristic notions of minimum-phase held by many in the optics and bioimaging communities.

Supported by these results, we find that optical phase offers potentially new diagnostic information independent of intensity. Additionally, for quantities that admit derivation by independent analysis of either phase or intensity, the error characteristics need not be the same. For example, many algorithms exist to invert intensity for scatterer size. Such procedures are prone to a systematic error in that the intensity of broadband light sources generally is not constant as functions of frequency. This modulation must be deconvolved from the experimental measurement so as to isolate the effect due to scattering. By contrast, phase analysis is invariant with respect to the intensity provided only that the intensity is non-zero. Thus phase-based analyzes are self-correcting with respect to this form of error. A microscope slide was coated with polystyrene spheres drawn from two populations. The manufacturer specified the average radii as r_1=15μ and r_2=26μ, both with 15% variance. The slide was imaged using the NIST spectroscopic OCT platform, and group delay measurements inverted for characteristic sphere size as a function of *xy*-location on the slide. The results are shown in Fig. 6. Quantitative comparisons of the radii computed by OCT compare well with independent measurements made via optical microscopy, as well as with the manufacturer's specifications.

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Measurement and Analysis of Tissue Engineering Scaffolds

Advances in tissue engineering are leading to the ability to grow cells for use in repairing or replacing skin, bones, and parts of bodily organs. In such applications, cells are seeded onto artificial structures, called scaffolds, where they undergo growth. Success of such procedures requires a quantitative understanding of the underlying growth media and its impact on cell growth. To this end, scientists in NIST's Materials Science and Engineering Laboratory (MSEL) have gathered data on tissue scaffold materials using a variety of imaging techniques. We are working with MSEL scientists to bring multi-modal imaging data on tissue engineering scaffolds into a virtual environment, where interactive measurement and analyses may be done. By developing techniques and tools to support applications of this type, we are extending the use of visualization from the qualitative to the quantitative.

John Hagedorn

One important consideration for the viability of tissue engineered products is the relationship between cell proliferation and the microstructure of the underlying scaffold material. Scientists in the NIST Materials Science and Engineering Laboratory have developed techniques for generating three-dimensional images of such scaffolds using X-ray micro-computed tomography (μCT). Such methods have diverse application in areas such as the failure analysis of polymer composites and the reliability of semiconductor devices. A recent application has been to the development and characterization of standard reference materials (SRMs) for the growth of tissue engineered products. SRMs of this type are needed for industry to develop low cost manufacturing processes required for commercial success.

We are pursuing the use of the immersive visualization environment (IVE) as a framework for more easily measuring distinguishing properties of scaffolds, for support in developing consensus definitions of scaffold descriptors, for understanding a variety of descriptor measurement methods, and for qualitatively evaluating and validating scaffold manufacturing techniques. The use of such real time immersive visualization (IV) techniques has been enabled by the continuing acceleration in speed and capability of commodity graphics processors. For this application, we have developed software that enables the measurement and analysis of tissue engineering scaffold materials from three-dimensional μCT data, which is segmented and converted to a polygonal representation for use in the IVE. In addition, we have developed software enabling a range of interactive measurements to be performed on such data in the virtual environment.

Figure 7. *An IVE user making scaffold measurements.*

For example, this software enables us to compare an idealized scaffold with a manufactured scaffold to determine differences in scaffold strut properties. Essential to this work is the use of immersive visualization which gives the researcher the ability to interact directly with data representations in ways that are not possible during data acquisition or with desktop systems. Structures are inspected and measurements made and analyzed during the immersive session. Using these measurements, researchers can assess the fidelity of actual scaffolds to the design model and evaluate the scaffold manufacturing processes.

While the initial processing of the image data was relatively straightforward, the analysis and measurement of geometric descriptors was more challenging. We built a software system within the IV environment that integrates the interactive measurement of scaffold characteristics, the analysis of the collected measurements, the display of the analysis, and the interactions with the data and analyses that enable grouping of results. To accomplish this, we implemented three types of measurement capabilities: measurement with lines, with cylinders, and with ellipsoids. The software enables the user to shape and place these objects interactively in the immersive environment. These forms are matched to the forms of fibers and pores in the data and serve as measuring devices. Analyses of the created geometry are presented to the user, and the user can interact with the data to derive additional information.

The initial measurement task that we undertook was the manual measurement of linear distances. It was felt that this step would enable the understanding of several important scaffold characteristics, one of which is strut diameter distribution and any associated anisotropy.

The specific scenario for this first implementation would be: (1) The user interactively collects a set of linear measurements. (2) A statistical analysis is made. (3) The analysis, including the distribution of measurements, is presented to the user. (4) The user interacts with the measurement distribution in order to highlight measurements that fall within any selected range of values. All of these tasks would be performed in real-time during the IV session.

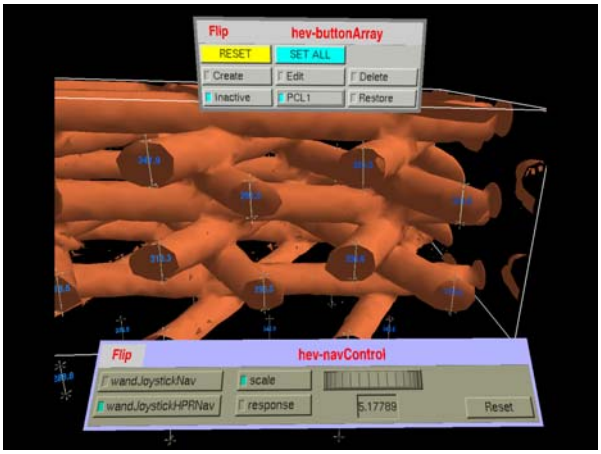

Figure 8. *Scaffold cross sections with diameter measurements.*

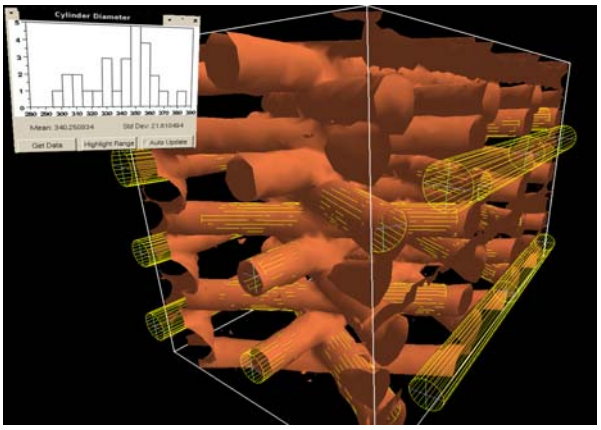

Figure 9. *Cylinder measurement and analysis tool.*

We performed measurements both on the "as-designed" scaffold model (generated synthetically from the design) and on the image of the actual manufactured scaffold material. The former are intended to validate the measurement method, while the latter are used to understand the scaffold structural characteristics and fabrication method. We derived descriptors such as gap width, spacing of fibers, angles between intersecting struts, etc., and compared the results to those from the as-designed scaffold. We found that the inter-junction strut diameter was about 19% smaller than the as-designed model. The at-junction strut diameter (or layer thickness) was about 33% smaller than the as-designed model. But the angular measurements correspond very closely to the design.

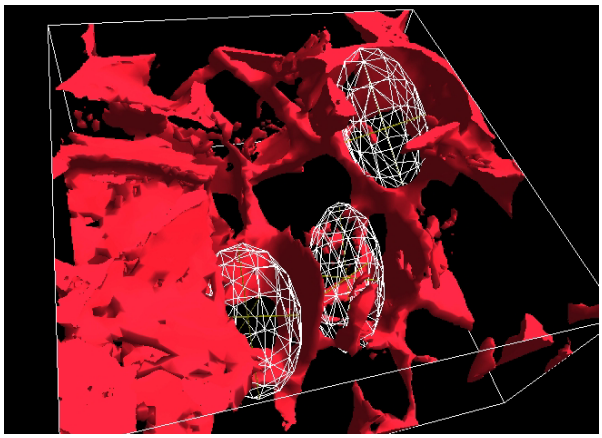

Figure 10. *Ellipsoid measurement tool used on a scaffold.*

We have found that IV enables both qualitative and quantitative understanding of 3D structure of tissue engineering scaffolds not otherwise possible. Measurements made within the virtual environment would have been very difficult to make with typical desktop visualization techniques.

The following IV measurement of descriptors should be implemented to enable further evaluation: layer planarity, strut diameter uniformity, strut circularity, and strut location. We also plan to use the immersive environment in conjunction with automatic measurement techniques that we are developing to aid in understanding the action of the automatic algorithms and as a way of validating those methods.

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

Visualization of Complex Function Data

Effective visualizations can help researchers obtain a more complete understanding of high level mathematical functions that arise in many applications. Thus, dynamic interactive 3D graphs of function surfaces will be a key component of the NIST Digital Library of Mathematical Functions, which is being developed to replace the classic NBS Handbook of Mathematical Functions (Abramowitz and Stegun, 1964). Designing software to plot complicated 3D surfaces can be a challenging task. The function data must be computed accurately, the plot must capture important surface features with little user input, and the plot should be accessible to users on a variety of platforms. Using techniques from numerical grid generation and various technologies, including the Virtual Reality Modeling Language, X3D, embedded 3D, and video capture, we have been able to address most of these issues to produce precise and informative visualizations.

Bonita V. Saunders

The NIST Digital Library of Mathematical Functions (DLMF) will include formulas, methods of computation, graphs, references, and links to software for more than 40 classes of high level mathematical functions. The web site will also feature interactive navigation, equation search, and dynamic interactive visualizations. A sample chapter on the gamma function is available at http://dlmf.nist.gov/Contents.

Precise 3D visualizations of complex functions enable exploration of attributes such as poles, zeros, and branch cuts. The development of such visualizations requires the accurate computation of function data and the determination of the best methods for rendering and disseminating the visualizations in an environment accessible to users on various platforms.

Function Evaluation. A key concern when constructing plots of complicated mathematical functions is accuracy, in both the data accuracy and the plot itself. To validate data accuracy we compute function values using at least two independent methods. This might involve the use of standard computer algebra packages, routines from commercial libraries and free repositories, or even personal Fortran and C codes from the chapter authors. While authors may provide initial versions of the plots, all functions are recomputed at NIST to insure the validity of the data.

Plot accuracy concerns the visual display of the data. Accurate visual representation of the function depends not only on the accuracy of the data, but also on the plotting tool or package. Commercial packages often have many built-in special functions, but their 3D plots are usually over a rectangular mesh, often leading to poor or misleading graphs. When function values lie outside the range of interest, many packages have trouble properly clipping the function surface. Furthermore, even when the plot looks satisfactory inside a package, it may be completely unacceptable when transformed for display on the web.

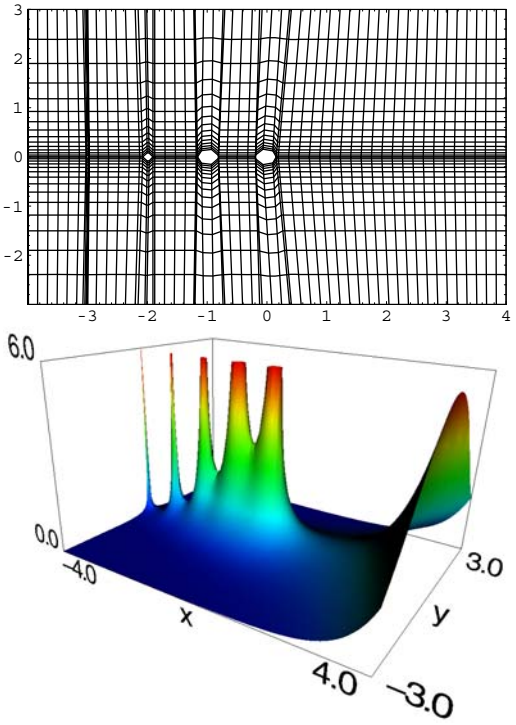

Figure 11. *Computational grid and modulus of the complex Gamma function Γ(x+iy).*

We have solved many of these problems using techniques of numerical grid generation, such as transfinite blending function interpolation and a modified tensor product spline generator, to design customized meshes fitted to selected contours of the function. By computing the function values over such a mesh, we can accurately represent key function features. See Fig. 11.

VRML/X3D. Once the function data is computed, it must be translated into a format that allows viewing on the web. We use Virtual Reality Modeling Language (VRML), a standard 3D format for which browsers and plugins for a variety of platforms are publicly available. While standard VRML controls such as rotate, zoom, and pan permit a user to examine a 3D display from an arbitrary direction and position, we have implemented additional capabilities such as dynamic cutting plane control, color map control, and scale control. For example, cutting plane control allows one to exam-

ine the intersection of a plane with a function surface as the plane moves through the surface in a direction parallel to the *x, y*, or *z* coordinate axis.

Many DLMF visualizations represent real or complex valued functions of the form $z=f(x,y)$. Users may choose a height-based color map, where height is $|z|$ if f is complex. For complex-valued functions one may also choose a mapping based on the phase of z. Two options for the phase based mapping are available: a continuous mapping of phase to color or a four-color mapping based on the quadrant of the phase angle. Fig. 12 illustrates the continuous spectrum mapping. Fig. 13 illustrates use of the scale control.

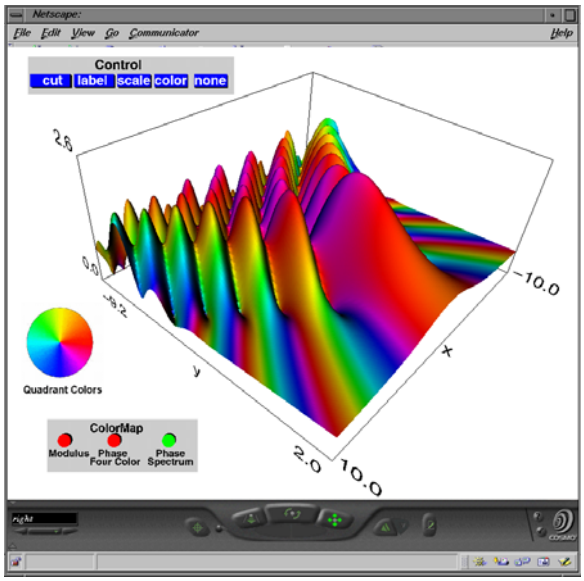

Figure 12. *Modulus of complex Pearcey integral function $\Psi_2(x,y)$ with continuous spectrum color map.*

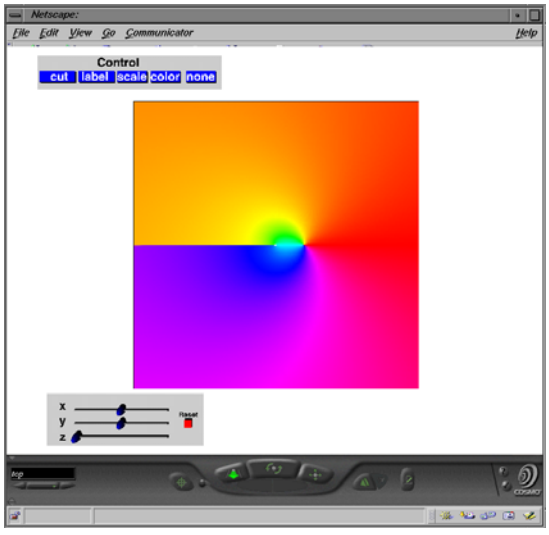

Figure 13. *Surface scaled down in z direction. Modulus of the complex log function is shown with phase based color map. Note the branch cut along the negative x axis.*

Alternative Technologies. In spite of the availability of VRML browsers, several things might preclude some users from gaining access to the DLMF visualizations. For example, a browser might not be available for their particular platform or configuration, or security concerns at their site may prevent the download of new software. To address such concerns, we have investigated several alternative technologies to render and disseminate the visualization of complex mathematical functions on the web: PDF document with embedded 3D graphics, animated movies using Apple QuickTime VR, and animated movies using video capture software. Based on user interaction capabilities and platform portability, it appears that embedded 3D graphics technology offers the most promise. We have used Adobe Acrobat 3D to create prototype interactive visualizations in PDF.

Over one hundred Web-based 3D visualizations for the NIST DLMF have been completed using VRML. Feedback from DLMF editors, authors, and other observers has been extremely positive. We continue to improve existing features and add new ones. One new feature being tested, for example, is a user capability to click anywhere on the function surface and obtain the coordinates. We also are seeking ways to improve the performance of the cutting planes, and working on adaptive grid techniques to decrease the size of some of our computational meshes.

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Participants

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High Precision Calculation of Fundamental Properties of Few-Electron Atomic and Molecular Systems

Computational scientists at MCSD and Indiana University have achieved record levels of accuracy in the development of computational methods for determining 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). H_2 has the distinction of being the first molecule whose dissociation energy was correctly predicted by quantum mechanical calculation (1968) before being measured reliably by experiment. Today we may be witnessing again a situation in which quantum mechanical calculations ("virtual measurement") yield more accurate determinations of this fundamental property than can be measured experimentally.

James Sims

NIST has long been involved in supplying critically-evaluated data on atomic and molecular properties such as the atomic properties of the elements contained in the Periodic Table and the vibrational and electronic energy level data for neutral and ionic molecules contained in the NIST Chemistry WebBook. Fundamental to this endeavor is the ability to predict, theoretically, a property more accurately than even the most accurate experiments. It is our goal to be able to accomplish this for few-electron atomic and molecular systems.

Impressive advances have been made in the study of atomic and molecular structure in both theory and experiment. 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 atomic helium (He) and other three-body systems as well. Even for properties other than the nonrelativistic energy, the precision of the calculation has been referred to as "essentially exact for all practical purposes" [1], i.e., the precision goes well beyond what can be achieved experimentally. Notwithstanding this theoretical advance, the scarcity of information (experimental and theoretical) on atomic energy levels is overwhelming, especially for highly ionized atoms. On the theoretical side, the availability of high precision results tails off as the state of ionization increases, not to mention higher angular momentum states. In addition, atomic anions have more diffuse electronic distributions, and therefore represent more challenging computational targets. On the diatomic molecular side, the presence of two fixed nuclei rather than one makes the integrals harder, hence exact analytical solutions to the molecular nonrelativistic Schrödinger equation are known (in the Born-Oppenheimer approximation) only for the one-electron H^+_2 ion and other equivalent one electron systems. The challenge for computational scientists is to extend the phenomenal accomplishments on atomic helium to three, four, and more electron atomic states and to molecular systems.

Dihydrogen, H_2, has the distinction of being the first molecule whose dissociation energy was correctly predicted by quantum mechanical calculation (1968) before this same quantity was measured reliably by experiment. Today we may be witnessing again a situation in which quantum mechanical calculations yield more accurate determinations of this fundamental property than can be measured experimentally. Very high precision approximations are now available for molecular hydrogen (a two-electron system) as a result of our calculated Born-Oppenheimer energies of $^1\Sigma_g^+$ states of H_2 using up to 7034 expansion terms in confocal elliptical coordinates with explicit inclusion of interelectronic distance coordinates up through r_{12}^7. We calculated Born-Oppenheimer (BO) energies for various internuclear distances in the range of 0.4 bohr to 6.0 bohr with an error of 1 in the 13th digit, for example, the nonrelativistic energy is -1.1744 7593 1399(1) hartree at the equilibrium R = 1.4011 bohr distance. The BO energies are what are used to provide the $X^1\Sigma_g^+$ potential energy curve which is critical to determining, theoretically, the dissociation energy D_0 of H_2, as can be seen from the figure.

Our results [2] are the most accurate energy values ever obtained for a molecule of that size; 100 times better than the best previous calculated value or the best experimental value, but the methods used are perhaps equally important. The calculation requires solving an approximation of the Schrödinger equation, one of the central equations of quantum mechanics. It can be approximated as the sum of an infinite number of terms, each additional term contributing a bit more to the accuracy of the result. For all but the simplest systems or a relative handful of terms, however, the calculation rapidly becomes impossibly complex. While very precise calculations have been done for systems of just three components such as helium (a nucleus and two electrons), we are the first to reach this level of precision for H_2 with two nuclei and two electrons.

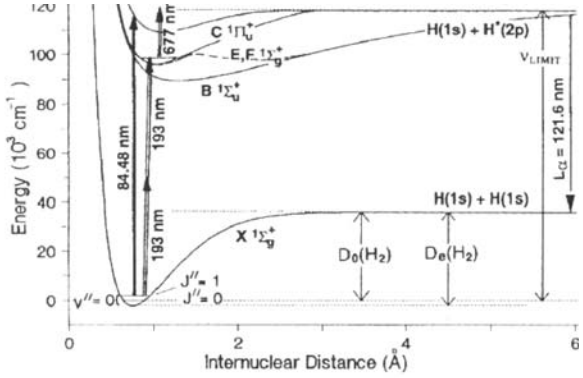

Figure 14. *Potential energy curves of H_2 showing transitions from the ground state to the $B^{\prime\prime}$ Σ_u state involved in photodissociation of H_2.*

To make the problem computationally practical, we merged two earlier algorithms for these calculations — one which has advantages in ease of calculation, and another which more rapidly achieves accurate results — into a hybrid with some of the advantages of both. We also developed improved computer code for a key computational bottleneck (high-precision solution of the large-scale generalized matrix eigenvalue problem) using parallel processing. Our final calculations were run on a 147-processor parallel cluster at NIST over the course of a weekend — on a single processor it would have taken close to six months.

Almost all results reported in our paper were obtained using quadruple precision (~30+ digits) floating point subroutines written in Fortran 90. In addition to quadruple precision, multiple precision floating point arithmetic was used for the Rüdenberg φ function, on which all integrals depend, and which is subject to catastrophic cancellations when computing differences in low precision. To address these problems we systematically increased the number of decimal digits used for only the φ part of the calculation up to a maximum of 160 decimal digits. In each case we obtained lower (i.e., more accurate) energies than previously reported results. The result for the ground state of H_2 represents, in fact, the highest level of accuracy ever reached (10^{-12} hartree) in molecular quantum computations (except for trivial one-electron cases) and is good enough to pin down the dissociation energy D_0 for H_2 to 0.001 wave number *if* one can separately calculate the adiabatic, relativistic, and radiative (QED) corrections accurately enough. This level of theoretical accuracy suggests that perhaps the experiment should be redone using 0.001 wave number as the target level of accuracy. That is, two orders of magnitude reduction in the current experimental uncertainties.

Now that high precision calculations are feasible for the two-electron molecular problem, we are shifting our focus back to the atomic problem. In going from He (two electrons) to Li (lithium, three electrons) to Be (beryllium, four electrons), the situation vis a vis high precision calculations degrades to the point that already at four electrons (Be) there are no calculations of the ground or excited states with an error of less than 10^{-6} a.u. To alleviate this problem, we are currently building the infrastructure for a calculation on the ground state energy level of the Be atom. This has involved removing several bottlenecks to highly accurate calculations using our method, including treatment of the three electron triangle integrals [3], treating the remaining three-electron kinetic energy and nuclear attraction integrals [4], and dealing with four-electron integrals [5]. The beryllium calculation will determine whether highly accurate calculations on atoms with $N \geq 4$ can become a reality.

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

Benchmarks for Quantum Computing with Ion Traps

Quantum computers have the potential for significantly speeding up many useful algorithms. However, building quantum computers is challenging. Currently available quantum devices can realize computations with only a few quantum bits (qubits) and steps. Atomic qubits in ion traps are currently considered one of the leading candidates for realizing large quantum computers. To determine the potential of current ion trap quantum computers, we implemented two benchmark quantum subroutines for up to six atomic qubits and analyzed the error of the implementations. The first benchmark involved creating "Schrödinger cat states" of four to six qubits. The second demonstrated an entanglement purification protocol that is expected to play a key role in large scale implementations of quantum computers and quantum communication protocols.

Emanuel H. Knill

The goal for experimental efforts in quantum computing is to obtain quantum devices that can be used as the basis for large quantum computers. Many different physical systems are being investigated for their utility in obtaining such devices. Examples include systems based on quantum dots, Josephson junctions, and ion traps. Although we are still a long way from realizing useful quantum computations, the physical system currently closest to the desired goal is based on ion traps.

In order to determine the suitability of a device for quantum computing and to compare it to other devices, it is useful to perform standard "benchmark" experiments. These can be used, for example, to characterize the error in the physical implementation of a quantum algorithm or to demonstrate a process or protocol useful for scaling up quantum computers. Well-known instances include quantum teleportation, quantum error correction, the quantum Fourier transform, entangled state preparations and entanglement purification. Each has been implemented for ion traps in the NIST Physics Lab; here, we focus on the last two, which allowed us to explore procedures involving up to six qubits.

Ion trap quantum computing. To build a quantum computer, it is necessary to supply qubits and the means for (a) preparing them in an initial state, (b) manipulating and coupling them, and (c) measuring their final state. In implementations featuring ion traps, the qubits are represented by the internal states of ions trapped along an axis by means of radiofrequency and static electric fields. For our benchmarking experiments, the ions are Beryllium, $^{9}Be^{+}$, cooled to their motional ground state by means of laser cooling, specifically Raman sideband cooling. The qubit states are given by two hyperfine levels that are manipulated by stimulated Raman transitions. Coupling between qubits is accomplished by use of common vibrational motions. Measurement is by detecting fluorescence: Only one of the two qubit states fluoresces when probed with appropriately tuned and polarized light. A picture of the electrodes used to trap the ions is shown in Fig. 15. The trap features multiple trapping zones and allows for moving, separating and recombining ions. These features are crucial for scaling up the ion trap system for building large quantum computers, and they enabled the implementation of the purification protocol.

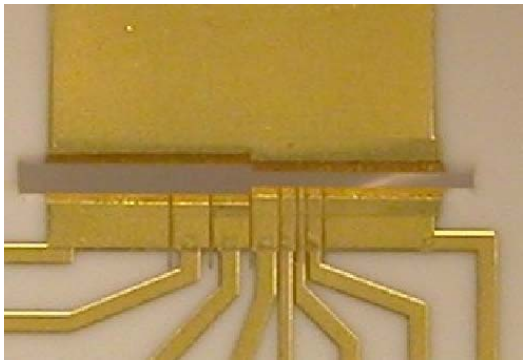

Figure 15. *The multizone ion trap used in our experiments. The ions are trapped in the slot midway between the gold electrodes.*

Schrödinger cat states. Schrödinger cat states are equal superpositions of a pair of highly distinguishable configurations. They are named for Schrödinger's (in)famous thought experiment involving a cat in an isolated deadly contraption, which according to quantum theory exists in a superposition of being dead and being alive until "observed". Because of the distinguishability of the two configurations in a cat state, one expects an equal probability of finding the system in one of the two configurations rather than a superposition. Superpositions are distinguished from probability distributions by the possibility of interference. Because of the fragility of these effects, their demonstration is a good test of the ability to control and couple the qubits.

A single ion qubit's state space is spanned by configurations or states that can be labeled |up> and |down>, distinguishable by their spin and energy. However, because in the absence of light they are largely decoupled from the environment, they are not considered highly distinguishable on their own. To create cat states, we use up to six ion qubits. The six qubits have two states $|up_6\rangle$ and $|down_6\rangle$, where in state $|up_6\rangle$ ($|down_6\rangle$) all qubits are in state |up> (|down>, respectively). This pair of states is in a sense maximally distinguishable for six qubits and their equal superposition is a cat state of six qubits.

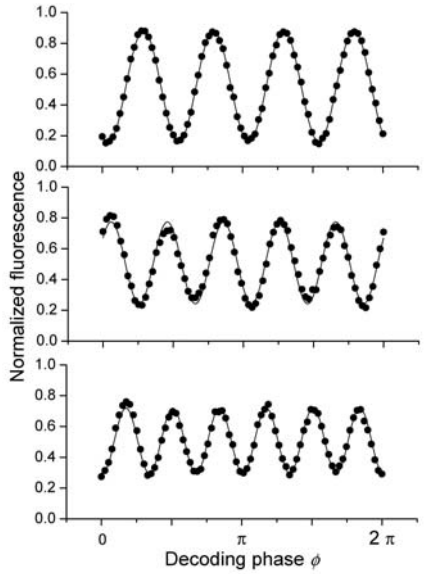

Figure 16. *Cat state coherences. The quality of the prepared states is determined by the contrast, i.e., the amplitude of the fringes in an interference experiment. These are shown for cat states of four, five and six ion qubits (top to bottom). The reduction in amplitude is due to the increasing fragility of the states as more qubits are involved.*

To determine how well we can create ion qubit cat states, we performed interference experiments that are sensitive only to the coherence in the superpositions. See Fig. 16. The amount of interference (the "contrast") can be used to determine the fidelity with which we prepared the cat states. The fidelities decreased from 0.76 for four qubits to 0.51 for six, which is state-of-the-art for accuracy of control of this many qubits. An additional property of the cat states is that they have entanglement that cannot be attributed to a proper subset of the qubits, that is, they are globally entangled. The data shows that such entanglement was present.

Purification. One of the most useful resources in quantum computation and communication are pairs of qubits in maximally entangled states. Equivalent to cat states for two qubits, these can be used for teleporting quantum states over long distances without transporting qubits, and for implementing computations involving remote qubits. Because in typical applications the two qubits of an entangled pair are far apart, it is difficult to prepare the state with low error. Entanglement purification is a procedure to reduce the error without further use of quantum communication. It requires the use of local quantum gates and a measurement to compare two pairs of entangled but noisy qubits. If the comparison is "good", one pair of less noisy qubits is obtained. Entanglement purification will likely play an important role in any large scale quantum computer.

Implementing entanglement purification using the ion trap required four ion qubits. For initial state preparation and the crucial qubit comparison gates, we realized specially designed four qubit gates. To measure the ions, we separated them into two sets of two, measured the first two at once to determine whether the comparison was good, and then used tomographic state analysis to see how good the entangled state on the remaining two ions was. The purified entangled pair was compared to the unpurified pairs to see whether we were able to improve the entanglement. Because of the complexity of the experiments, errors introduced by the purification procedure prevented an ideal improvement, though it was nevertheless significant (Fig. 17).

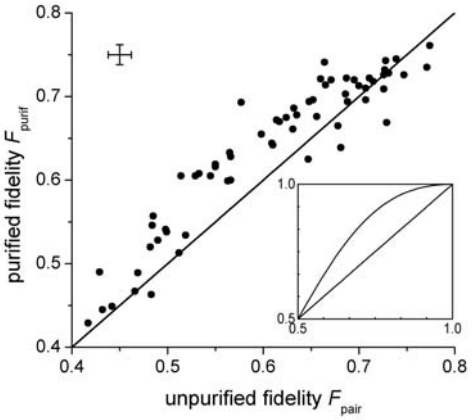

Figure 17. *Purified fidelity as a function of unpurified fidelity. The dots in the figure represent individual experiments. Each involved applying a known error to the initially prepared entangled pairs of qubits. The fidelity of the unpurified (purified) pairs determines the x-axis (y-axis, respectively) position. The diagonal line is the line where the purified and unpurified fidelities are the same. There is a range of errors for which an improvement in fidelity is obtained. For comparison, the curved solid line in the inset shows the theoretical purified fidelity as a function of the unpurified fidelity assuming all gates and measurements are ideal.*

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OOF: Object-Oriented Finite Elements

Rapid increases in computer power have created an opportunity for investigators to use computational methods to tackle both larger and more complex problems than had been possible previously. However, this will occur only if we can create tools which take advantage of this computational power, while at the same time encapsulating the sophisticated numerical methods which handle the complexity. In the field of materials science, the direct computational study of structure-property relationships in complex microstructures is enabled by OOF, the Object-Oriented Finite Element system. A collaboration between MCSD and the NIST Materials Science and Engineering Laboratory, this new tool provides finite-element computational capabilities in a modular, extensible framework designed to speak the language of materials scientists. Version 2.0 of OOF was released to the public in September 2006.

Stephen Langer

The Object-Oriented Finite Element (OOF) project produces software that enables the direct computational study of structure-property relationships in materials with complex microstructures. When running OOF [1], a user assigns material properties to the features in an image of a material's microstructure, and then performs virtual experiments on the material. Unlike commonly available commercial finite element codes, OOF features both a powerful suite of tools for adapting a finite-element mesh to the microstructural geometry of an image, and a modular and extensible scheme for adding new or customized property data to the underlying model. Property data can also be specified independently of a particular problem, and shared between problems and between researchers.

The archetypal OOF user is a materials scientist with deep knowledge of the materials under study, but possibly little or no knowledge of the more technical aspects of computational modeling. Such an investigator is interested in examining multiple interactions between regions of a spatially complex microstructure, but is not an expert in modeling techniques, finite element basis functions, sparse matrix solvers, etc. The OOF program provides, on the one hand, a powerful tool set for managing the parts of the problem where the investigator is knowledgeable (e.g., constitutive rules, microstructural geometry) and, on the other hand, push-button access to sophisticated numerical tools which implement the model. As software, OOF occupies a niche unlikely to be served by commercial software, and benefits substantially from the breadth of expertise and institutional memory present at NIST. The development team combines expertise in physics, materials science, and software engineering.

Inputs to an OOF analysis are one or more images representing the microstructure, and the physical properties of the components of the microstructure. The images can be micrographs obtained experimentally or the output of a simulation. The user segments each image into homogeneous regions, assigning to each appropriate material properties. Using the adaptation tools, a finite element mesh is constructed which matches the geometry of the microstructure. Boundary conditions are applied, representing loads in a virtual experiment, the equations are solved, and the resulting configuration of fields and fluxes is measured.

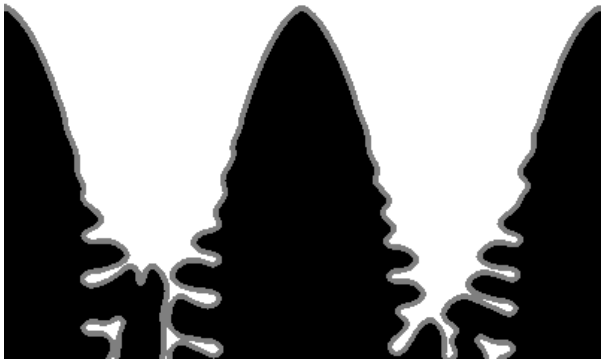

Figure 18. *A microstructure from a simulation of dendritic growth. The three colors correspond to regions with different chemical compositions. (Courtesy of J. Warren, NIST MSEL.)*

This very general scheme not only allows for a direct simulation where real-world properties and microstructure are known, but also allows OOF to function as a design tool. If properties are known, it's possible to use OOF to "search" among candidate microstructures for optimal behavior. If, on the other hand, the microstructure is known but the properties are not, a parametric study can be done to determine optimal parameters, either to reproduce observed behavior or to achieve desired behavior. The relative rapidity and cheapness of the OOF analysis enables many more design iterations than could be achieved by direct experimentation.

Earlier versions of the OOF software have already shown the value of this approach. Version 1.0, originally released in 1998, has been modified and extended many times since. In 1999, it earned a "Technology of the Year" award from *Industry Week* magazine. However, OOF1 failed to realize one of the major goals of the project, i.e., to create a software platform that users could easily extend by adding their own physical models. The original version of OOF1 solved only linear

elasticity problems. A second version was created at NIST to solve problems with coupled elasticity and thermal diffusion, and an MIT student created versions that incorporated piezoelectricity and chemical diffusion. These were used to study ceramic thermal barrier coatings on turbine blades [2], Li-ion batteries [3], and polycrystalline piezoelectric transducers [4], among other things [5, 6]. In the process it became clear that OOF1 was too difficult to extend, and that maintaining a zoo of different versions was not practical.

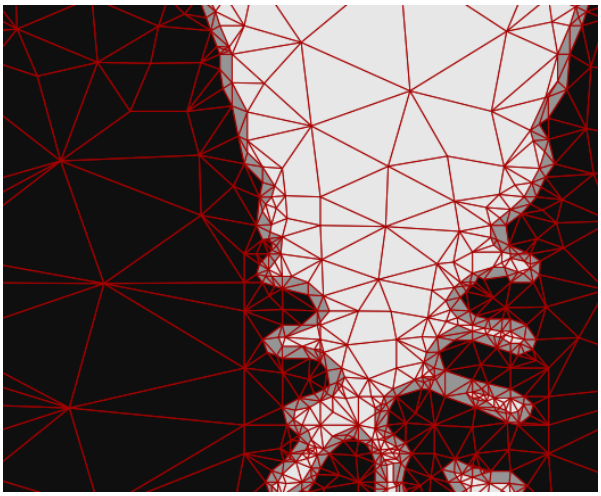

Figure 19. *A portion of the microstructure, meshed with OOF2.*

OOF2 was initially released in early September 2006. It is a complete rewrite of the program designed to overcome the shortcomings of OOF1. The features of all the different versions of OOF1 coexist amicably within the OOF2 framework. Unlike OOF1's fixed material types, OOF2's materials are created by assembling a collection of diverse properties (e.g., elastic modulus, piezoelectic modulus, heat capacity, orientation) at run time. New property definitions can be created and loaded in a modular fashion. In addition to more powerful and flexible ways of defining material properties, OOF2 allows more kinds of finite elements. While OOF1 only supported linear triangles, OOF2 contains linear and quadratic triangles and quadrilaterals, and new types can be added easily. OOF2 also contains improvements in mesh creation, boundary conditions, and solvers. OOF2 is threaded, meaning that it can perform more than one operation at a time, which vastly improves the user experience.

At the OOF workshop held at NIST in August 2006, some 40 OOF users shared their experiences with OOF1, and were introduced to OOF2. Users came from five US industries, three US government laboratories, and 18 universities, representing a broad cross-section of instructional, research, and commercial interests.

Current and future developments will enhance OOF2 in a number of ways. The development team is currently adapting the software to run in parallel on a cluster, and is also extending its range to include periodic boundary conditions, plasticity and other nonlinear properties, time dependence, and partitioning of problems into multiple subproblems. Parallelization will enable the software to handle large data sets, and is a prerequisite for a planned extension to a fully three dimensional computational domain. Further expansion beyond these broad capabilities will be driven by user requirements.

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

Modeling Fluid Flow in Materials Processing

Materials processing techniques often involve the initial preparation of a sample of material in one thermodynamic state, such as the material's liquid phase at a high temperature, and carefully allowing the sample to transform into a desired final state, say the sample's solid phase at lower temperatures. During this process an interface separates the material that remains in the initial state from the material that has reached its final state. The shape of this interface has a critical effect on the quality of the resulting material. In many applications a planar interface is optimal, which leads to the formation of homogeneous samples. Such samples will typically have desirable mechanical or electronic properties. In contrast, nonplanar interfaces can lead to unfavorable inhomogeneities that can degrade the performance of the material. It is often found that while a planar interface is possible in theory, in practice it may become unstable under the combined effects of convection and heat transfer. Determining the stability of the interface is therefore critical in order to understand and control materials processing in many applications.

Here we consider the processing a sample from one liquid phase to another, such as in the condensation of a liquid from its gas phase. In this case we need to consider the stability of a fluid-fluid interface subject to a temperature gradient perpendicular to the interface. For a phase-transforming system this results in the generalization of a classical hydrodynamic stability problem for fluids that are subject to the effects of buoyancy and surface tension gradients. In such systems, for large enough temperature gradients, a planar fluid-fluid interface can undergo bifurcations to nonplanar geometries with associated changes in the state of convection and heat flow throughout the sample.

Geoffrey B. McFadden

The study of the stability of a fluid-fluid interface is important in a number of scientific and technological applications. In this project we consider two fluid layers separated by a horizontal planar interface subject to a vertical temperature gradient. The effects of various driving forces on the stability of the system can be taken into account, including buoyancy (known as Rayleigh-Benard convection), the effects of bulk density differences (known as Rayleigh-Taylor instabilities), and the effects of surface tension gradients along the interface (known as Marangoni instabilities). If the two layers represent different phases of the same material the stability results for a two-phase bilayer system are quantitatively and even qualitatively different than for those of an immiscible system. For the two-phase system we find particularly interesting stability results at low wavenumbers, where we discover a new mode that is sensitive to the differences in material properties, specifically the enthalpy and entropy difference between the two phases.

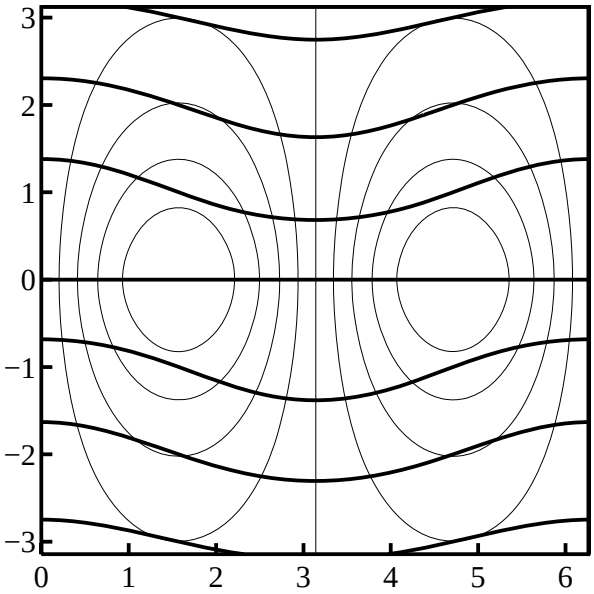

Figure 20. *Streamfunction contours (light lines) and temperature contours (dark lines) for flow in the two-layer system. The interface corresponds to the streamline at y = 0.*

To estimate the relative importance of these types of instabilities for a two-phase system, we consider a bilayer geometry in which a horizontal fluid-fluid interface separates two semi-infinite layers of a single-component fluid. This problem is still sufficiently complex that we generally resort to a numerical determination of the linear stability of the system, including the possibility of temporally oscillatory modes with significant interfacial deformations. The governing equations contain a large number of dimensionless parameters, including a Rayleigh number, Marangoni number, Bond number (ratio of the forces of buoyancy and surface tension) and Crispation number (a measure of interface deformation), and ratios of material properties of the two phases.

In particular, we have performed linear stability calculations for horizontal fluid bilayers that can undergo a phase transformation, taking into account both buoyancy effects and thermocapillary effects. We compare the familiar case of the stability of two immiscible fluids in a bilayer geometry (the "inert" case) with the less-studied case in which the two fluids represent different phases of a single-component material. The two cases differ in their respective interfacial boundary

conditions We find that, as in the inert case, the two-phase system can be linearly unstable to either heating from above or below. Instability in the two-phase case persists to small wavenumbers in the case of heating from below.

To help understand the mechanisms driving the instability on heating from below, we performed both long-wavelength and short-wavelength analyses of the two-phase system. The short-wavelength analysis shows that the instability is driven by a coupling between the flow normal to the interface and the latent heat release at the interface. The coupling is illustrated in the contours of the temperature and streamfunction for the two-phase system case; see Fig. 20. Here the fluid flow is normal to the interface, and the downflow in the center tends to compress the distance between isotherms near the interface in the upper phase, while expanding the distance between them in the lower phase. The opposite is true for the regions with upflow at the interface. The resulting net change in the temperature fluxes at the interface is balanced by the evolution of latent heat at the interface, which in turn is driven by the vertical velocity at the interface. When the system is heated from below as shown, these effects reinforce each other to drive the instability. When the system is heated from above, the effects are in opposing directions and no instability is possible

The mechanism for the large wavelength instability is more complicated; see Fig. 21. The detailed nature of the instability depends on the Crispation and Bond numbers. We find that a two-phase system that is heated from below is subject to a type of morphological instability that is similar in origin to other, more familiar, instabilities that occur in materials processing applications. Multiphase systems are typically subject to instability if one or more of the phases is in a thermodynamic state of metastability; specifically, if there are regions of space where the actual phase of the system is not the phase of lowest free energy under the given conditions. Examples include *superheating* (a solid above its melting point), *supercooling* (a liquid below its melting point), *supersaturating* (a solution beyond its solubility limit), or compressing a gaseous component beyond its vapor pressure. A crystal of binary alloy growing from its melt is subject to instability if the liquid ahead of the interface is c*onstitutionally supercooled*. In this case, the driving force for instability is the release of free energy accompanying the phase transformation from a higher energy phase to a lower energy phase. The resulting instability generally displays a wavelength that is determined by a balance between surface energy (stabilizing) and the difference in bulk free energy between the phases (destabilizing).

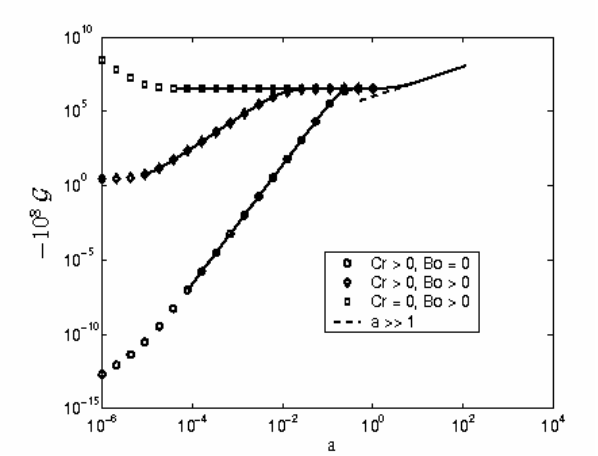

Figure 21. *Marginal stability curves for a two-phase water-steam system heated from below .The vertical axis represents critical values of the dimensionless temperature difference across the layers, and the horizontal axis is the lateral wavenumber of the instability.*

Three cases are shown in Fig. 21. The upper curve results from setting the Crispation number to zero while the lower curve corresponds to setting the Bond number to zero. Both the Crispation number and Bond number are present for the middle curve. The solid curves correspond to numerical results. The symbols on the curves correspond to analytical results from a small-wavenumber approximation. The results illustrate the sensitivity of the system to the effects of the Bond number and Crispation number.

This work is currently being extended to the important case of multicomponent materials.

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Participants

G. B. McFadden (MCSD); S. Coriell (MSEL); K. Gurski (George Washington University); D. Cotrell (Lawrence Livermore National Laboratory)

An Accurate Model for Measuring Fluorophore Photodegredation Dynamics

Fluorescent dyes, stains and probes play a prominent role in the measurement and detection of scientific phenomena on a small scale. Difficult problems in material science, chemistry, and nanotechnology can be investigated, for example, by using fluorescent techniques to enable the observation of the dynamics of single molecules. In biomedical and biotechnology applications fluorescent materials are used to obtain qualitative and quantitative information about processes on the cellular and sub-cellular level. However, the sensitivity and accuracy of such techniques is severely limited by natural fluorescent signal decay. This process, called photodegredation, is the sequence of photochemical reactions that transform excited fluorescent particles (fluorophores) to a non-fluorescent species. A thorough understanding of fluorophore photodegradation dynamics is necessary to enable the effective use of this measurement technique. In this work, we develop a mathematical model of photodegradation dynamics that justifies the use of a particular functional form to fit fluorescent signal measurements in the frequency domain.

Fern Y. Hunt

Photodegradation is due to a combination of processes that occur on multiple time scales, which makes the experimental interpretation of the time-dependent dynamics difficult. Recently scientists in the Biochemical Sciences Division of the NIST Chemical Sciences and Technology Laboratory (CSTL) developed a frequency domain based method for measuring photodegradation using an apparatus known as a lock-in amplifier [1]; see in Fig. 22. A sample of fluid containing fluorophores flows vertically in the x direction through a flow cell and is stimulated by laser light shining through the center. The fluid motion allows fresh populations of unperturbed molecules to be exposed to the light and minimizes the effects of uncontrollable convective and diffusive mass transport. When the intensity of the light fluctuates periodically the fluorescent emission is 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 reduce noise and extract a weak signal. The experiment is repeated for a number of excitation frequencies, thus allowing the estimation of the fluorescent photodegradation rate from the parameters of an impedance curve that is fitted to the measurements.

Specifically, the link between the measured phase shift and the photodegradation rate is a formula for the total fluorescence in the apparatus as a function of time. The formula comes from a mathematical model of the underlying process, allowing the fluorescence to be written in terms of physical parameters [2]. Here, the light is assumed to be distributed uniformly throughout the flow cell. In this case, the total fluorescence at any time can be written in terms of the averaged fluorophore concentration. If the impedance curve (showing the ratio of the imaginary and real parts of the Fourier transform of the fluorescence as a function of laser light frequency ω) is fit to the functional form

$$\frac{p_1 \omega}{p_2 + \omega^2}, \qquad (1)$$

the parameters p_1, p_2 can then be expressed in terms of the photodegradation rate and other physical parameters thanks to the tractability of the expression for the total fluorescence.

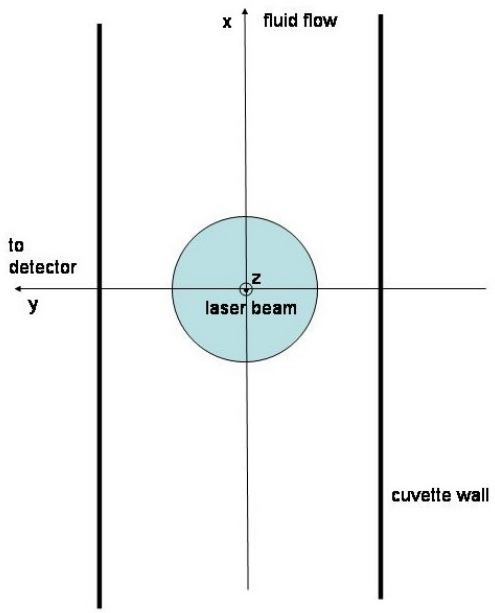

Figure 22. *Schematic diagram of a lock-in amplifier for measuring fluorophore photodegradation.*

In collaboration with CSTL scientists, we have examined the more physically realistic case of a laser beam that has a Gaussian power distribution. Here the photochemical reaction rates, which depend on power, will also depend on the location in the beam. Therefore the time evolution of the total fluorescence has to take into account the fluorescent response in a non-uniformly illuminated region.

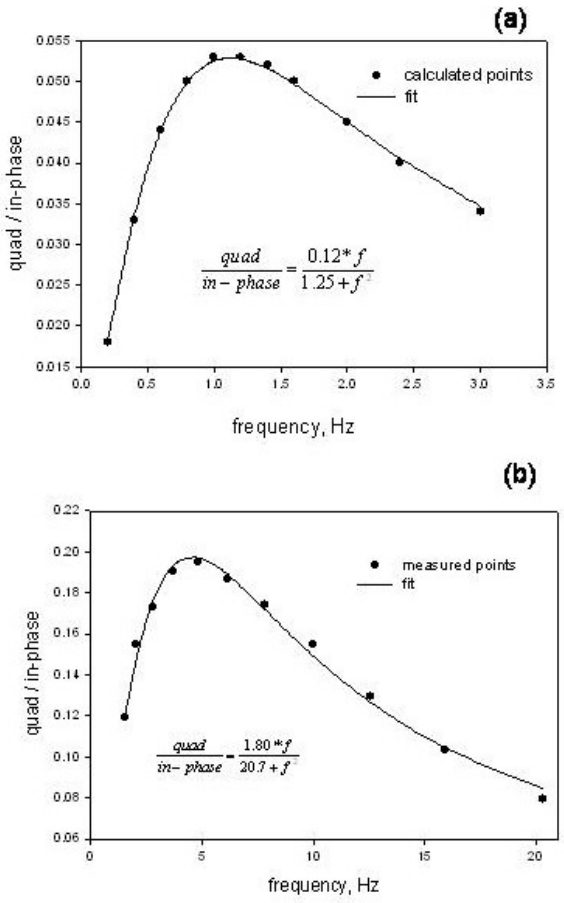

Figure 23. *Impendence data for (a) the model and (b) physical measurement. Data points are fit to the same functional form in each case, yielding the shown curves.*

Starting with a (rather simplified) model of the kinetics associated with excitation, relaxation and photodegradation, we analyzed a pair of coupled partial differential equations that describe the changes in fluorophore populations due to the kinetics and the convective fluid flow. The boundary conditions for this problem take into account the continuous entry of fluid into the apparatus from its base. Using singular perturbation techniques, we obtain a reduction in the mathematical complexity of the model by taking advantage of disparate time scales (photodegradation is much slower than any other process in the model). We then derive a single partial differential equation for the total fluorophore population (to leading order in a perturbation parameter). When the amplitude of the periodic component of the light is relatively small, spatial averaging can be performed to yield an ordinary differential equation that is accurate up to a small error. The measured fluorescence can be modeled approximately in terms of the spatially averaged fluorophore population. These two equations, then, constitute an experimentally accessible model for the fluorescence that can be used to estimate the photodegradation rate in a manner analogous to [2].

Fig. 23(a) shows the impedance curve generated by the solution of the model equations, while Fig. 23(b) shows the curve obtained by measurements with the lock-in amplifier. While they demonstrate only qualitative agreement, both sets of data are fit well with the functional form of Eq. 1.

Our analysis is comprehensive. The steps used to derive the model are mathematically justified and the order of magnitude of the errors in the perturbation approximation is estimated. In addition to being applicable to either the uniform, Gaussian, or Gaussian-like light distribution, we believe our analysis would apply to the more complicated kinetic model that provides a more detailed description of the photodegradation process. Two technical papers describing this work are in process [3, 4]. Using analytical techniques in [4], we can obtain information about the relationships between the fit parameters and the physical constants of the experiment. This will allow us to obtain quantitative agreement in the impedance curves.

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Participants

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Numerical Optimization of Complex Instrumentation

A novel approach has been created for the selection of optimal instrument parameters that yield a mass spectrum which best replicates the molecular mass distribution of a synthetic polymer. The application of implicit filtering algorithms was shown to be a viable method to find the best instrument settings while simultaneously minimizing the total number of experiments that need to be performed. This includes considerations of when to halt the iterative optimization process at a point when statistically significant gains can no longer be expected. This work represents part of an effort to develop an absolute molecular mass distribution polymer Standard Reference Material by matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry.

Anthony J. Kearsley
William E. Wallace

Typical analytical instrumentation optimization is performed by the analyst by simply applying the "factory settings" or by "optimizing by eye". This is because an exhaustive search of the parameter space for modern instrumentation with many adjustable parameters is prohibitively time consuming. Nevertheless, a variety of mathematical methods exist that can allow the experimentalist to optimize instrument settings without performing an exhaustive search. Broadly classified, these methods are all forms of numerical optimization. When the topology of the search space is very complex, for example when it has great sensitivity to one or more parameters (as mass spectrometers often do) the methods used are part of the field of nonlinear programming. They are nonlinear because some (or all) of the instrument parameters do not have a linear relationship between parameter value and measurement response. An example is laser intensity in matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry and its effect on signal to noise ratio, where a relatively sharp threshold is observed experimentally.

Stochastic numerical optimization methods are important in mass spectrometry because all mass spectra have random noise. This noise varies as the instrument parameters are adjusted, and the noise will often change across the spectrum. Measurement noise presents a significant challenge to any optimization method, especially for cases where signal to noise is not the measurand to be optimized. Nevertheless, numerical optimization methods offer experimentalists a way to tune the instrument parameters to achieve the desired goal without having to search all possible parameter combinations. To measure the absolute molecular mass distribution of a synthetic polymer, it would be ideal to locate a region in parameter space where the instrument response function was uniform across the entire mass range. Finding the instrument response function is necessary to calibrate the intensity axis of the mass spectrum, that is, to go from mass spectrum to molecular mass distribution. If the instrument response function is uniform then the relative peak areas in the mass spectrum correspond directly to the relative abundances of individual n mers in the sample. A uniform instrument response function would be a line of zero slope. If not uniform, the instrument response function could slowly vary across the mass range, preferably linearly with mass. The optimal conditions are those that give the simplest (or flattest) instrument response function, that is, the one with the smallest derivative.

To measure the instrument response function, a gravimetric mixture was made of three low polydispersity polystyrenes that were very close in average molecular mass. The optimal instrument settings are those that provided the closest match between the total integrated peak intensity of each of the three polymers with the known gravimetric ratios. Note that there is no guarantee (or even assumption) that the optimal instrument settings that give the flattest instrument response function will also yield optimal signal to noise ratios. In fact, there is no reason to believe that a search for the instrument settings that optimize the response function will not lead into a region where the mass spectra becomes so noisy as to make peak integration impossible. Thus, to find the optimal instrument settings we used stochastic gradient approximation methods. These methods have proven to be extremely robust in cases where the measured data is very noisy.

Optimization is performed by defining an objective function $J(x)$ where x is a vector consisting of the instrument parameters. In our case, the objective function is the sum of the squared differences between the amount of each polymer in a mixture created gravimetrically and the amount of each polymer in the mixture found by mass spectrometry. When this function is zero, the gravimeter concentrations match the concentrations found by mass spectrometry and the instrument is optimized. The function $J(x)$ is a noisy function with respect to the parameter vector x due to the inherent statistical noise in the mass spectra. This complicates the task of numerically locating the minimum of $J(x)$. The fact that each evaluation of $J(x)$ requires an experiment, and subsequent interpretation of experimental results, means that there is a high cost for each function evaluation. This further complicates any nu-

merical procedure that seeks to minimize *J(x)*. Finally, there are values of the vector *x* (for example, out of range instrument parameter settings) for which *J(x)* cannot be evaluated.

One method for minimizing noisy functions that seeks to approximate the gradient of the objective function is called implicit filtering. Broadly speaking this method uses a very coarse grained step-length to build a finite difference approximation to the gradient of *J(x)*. This gradient is then used to generate descent directions for a minimization process. As iterates draw closer to the solution, and the objective function decreases, the finite difference step-length is decreased until it approaches a number small enough to suggest convergence to a minimum.

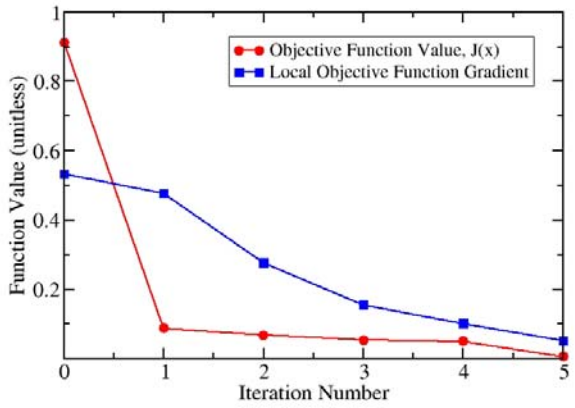

Figure 24. *The objective function J(x) and its local gradient value as a function of iteration step*

Fig. 24 shows the objective function *J(x)* and its local gradient value as a function of iteration step. There is an initial steep drop in the objective function flowed by gradual movement to the optimal parameter settings. The gradient of the objective function also decreases steadily. These monotonic responses indicate that the optimization routine is stable. At the optimum value the objective function is so small that it cannot be reduced further due to the inherent noise in the measurement. Likewise, the step size indicated for each parameter at this point is so small as to be below the precision of the instrument's settings.

Fig. 25 shows the individual instrument parameter values as a function of iteration number. The values oscillate about their final values as the optimization proceeds. The laser intensity undergoes the greatest excursions decreasing in the first two iterations, returning to its initial value in the third iteration, and then increasing in the fourth iteration before settling into its final value. The four other parameters make an excursion in the direction of their final values in the first iteration, return to their initial value in the second iteration, and find the equilibrium values by the third iteration. This zigzag pattern is characteristic of the nonlinearity of the system. The nonlinearity arises from the fact that the instrument parameters are coupled, that is, varying one requires all others to vary in response if *J(x)* is to move closer to its optimal value. Thus, the vector x_{i+1} has a tendency to be normal to the vector x_i. The laser intensity varies the most and seems to be the dominant variable. It seeks its stable value before the other parameters can settle down.

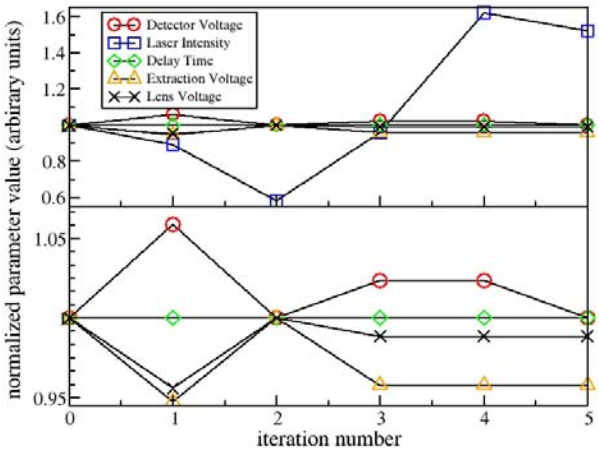

Figure 25. *Individual instrument parameter values as a function of iteration number*

Summary. A specialized noise-adapted filtering method has been applied to the problem of finding the optimal instrument parameters for a MALDI-TOF mass spectrometer. Finding the optimal instrument parameters was a critical step in creating an absolute molecular mass distribution polymer Standard Reference Material. The task of tuning the instrument's five main parameters could not be approached by exhaustive search methods given the amount of effort needed to take and to reduce the data in a statistically meaningful way at each set of instrument parameters. Additionally, this method produces an estimate of the sensitivity of each optimal parameter estimate not available to traditional exhaustive search methods. Each of the subtasks in the process could be automated to create an integrated closed-loop optimization scheme.

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Participants

A. J. Kearsley (MCSD), K. M. Flynn, C. M. Guttman, W. E. Wallace (MSEL).

Part III

Project Summaries

Mathematical Modeling of Mechanical Systems and Processes

OOF: Object-Oriented Finite Elements

Stephen Langer
Andrew Reid
Seung-Ill Haan (UMBC)
Rhonald Lua (Penn State University)
Valerie Coffman (Cornell University)
R. Edwin Garcia (Purdue University)

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

See feature article, page 37.

Modeling Fluid Flow in Materials Processing

Geoffrey B. McFadden
Sam Coriell (NIST MSEL)
Katherine Gurski (George Washington University)
David Cotrell (Lawrence Livermore National Labs)

See feature article, page 39.

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

Timothy Burns
Steven Mates (NIST MSEL)
Richard Rhorer (NIST MEL)
Eric Whitenton (NIST MEL)

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. The goal was 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.

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, and ITL.

With support from the National Institute of Justice (DOJ) through OLES, the NIST Office of Law Enforcement Standards, the NIST Kolsky bar has also been used in its room-temperature configuration to develop experimental methods and to perform studies on the dynamic response of frangible bullets. During the present fiscal year, temperature uncertainty due to uncertainty in the emissivity of the deforming sample was addressed by adding a thermocouple temperature measurement capability. In addition, a method was developed for correcting the sample stress-strain curve for the effect of the heat and electric current conducting graphite foil that is placed between the sample and the inner ends of the high-strength steel rods.

A new direction in research that was initiated this year has involved an attempt to relate the microstructure of medium carbon steel to the measured stress-strain response of the material under pulse-heated loading conditions. The basic idea here is that some thermally-activated changes in the material's microstructure have insufficient time to run to completion under the rapid heating conditions that are present in high-speed machining operations, with the result that higher cutting forces are required for these processes. More tests were also performed on frangible bullets for the NIST Office of Law Enforcement Standards program, but the amount of effort was limited due to reduced funding for the work.

This work is supported in part by the National Institute of Justice (DOJ) through the NIST Office of Law Enforcement Standards (OLES).

Modeling Time Delay Effects for Machine Tool Chatter Control

David E. Gilsinn
Sita Ramamurti (Trinity University)

Surface quality is critical in many machining operations such as the manufacture of antenna dishes and optical devices. In such applications surface measurements are routinely performed in the micrometer range. Understanding how various machine tool parameters and operating conditions relate to surface features at such length scales remains quite challenging. Mathematical modeling of the dynamics of machine tool systems plays a crucial role in this regard.

Machining systems consist of the spindle, tool holder, and cutting tool. The dynamics of such systems can involve multiple delay affects. For example, in turning operations the progress of the cutter across the surface is relatively slow compared to the spindle speed so that any slight imperfections in a previous cut can affect the current cut. Depending on the nature of the imperfections the result can be chatter, which is a vibration of the tool against the material surface. That is, it is a periodic oscillation affect. Chatter can arise as the result of a bifurcation in which model parameters are set so that certain critical parameter settings are passed and the nature of the dynamics changes abruptly. This can lead to poor surface quality. In milling operations the cutting tool has multiple cutters. There are models of milling operations that involve coupled dynamic systems with multiple delay affects. The aim of this project is to understand the nature of oscillatory solutions of these coupled dynamical systems and at what point critical bifurcations occur so that machinists can set the cutting parameters in order to avoid the onset of chatter.

Chatter can occur as the result of nonlinearities in the dynamics models. The current work on this project is concentrated in two areas. In the first, work involves determining conditions under which approximate periodic solutions for models with delay actually approximate true periodic solutions. Progress along this line has been published by Gilsinn and Potra [1], and Gilsinn [2]. These results, however, only address the problem in the case of a single nonlinear system with one delay. In the second area of concentration, work is focused on understanding the nature of periodic solutions that arise when the models involve coupled nonlinear systems. Various classes of solutions can arise. Both of the systems can have constant solutions, one can have a periodic solution while the other a constant solution, and finally there can be coupled periodic solutions. The coupled periodic solutions can generate a surface of solutions called an invariant torus. The stability of these surfaces is related to the stability of the system model. There are a number of approaches to the problem of approximating this invariant torus. One that appears to be efficient and successful was developed by Sita Ramamurti, who used multivariate splines to model the tori and then solved for the coefficients so that the multivariate splines satisfied a partial differential equation related to the coupled systems that defined the invariant torus.

Work during FY07 will involve the study, first of all, of conditions for periodic solutions for a single system with two delays. The work on coupled systems will be extended comparing the current multivariate spline algorithm to other algorithms in the literature. The objective is to determine the most efficient approach to computing invariant tori before introducing time delays into the coupled systems. Introducing time delays raises the complexity of the computational algorithms for approximate solutions. Therefore it is important that we work on systems with known periodic behavior. Any algorithms developed must work on those. That is why we have worked with variations of the classic Van der Pol oscillator. Before working with the complex milling models in the literature we must be confident that we can reproduce known results.

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Numerical Modeling of Deformation and Diffusion

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J. A. Warren (NIST MSEL)
S. R. Coriell (NIST MSEL)
C. Campbell (NIST MSEL)
J. Guyer (NIST MSEL)
J. A. Dantzig (Univ. of Illinois at Urbana-Champaign)
R. F. Sekerka (Carnegie Mellon University)

The recent interest in the design and operation of nanoscale systems has prompted increased attention to problems of stress and diffusion in thin layers and other small-scale geometries. The underlying process represents a complicated modeling problem in which the diffusion process is affected by the deformation due to plastic and elastic forces in the sample, and, conversely, the deformation field is affected by interdiffusion that may induce strain due to differences in the molar volumes of the various constituents. This inherent coupling makes an understanding of the process challenging, and progress is often possible only

through a combination of modeling, analysis, and computations.

The Kirkendall effect is a well-known consequence of a disparity in the intrinsic diffusion coefficients of the components in alloy diffusion couples. The effect has three manifestations: a shift of inert markers parallel to the diffusion direction (deformation with pure axial displacement), lateral shape changes (displacements with a component orthogonal to the diffusion direction), and the formation of voids. We have developed a model that includes a description of the uniaxial Kirkendall effect, capturing the deformation parallel to the diffusion direction, and at the same time obtaining the concomitant lateral deformation [1].

A solution to the coupled equations describing diffusion and deformation can be obtained using Fourier analysis for the case under consideration. We obtain limiting behavior for thin and thick cylinders and slabs, and compute numerical results of the model for the lateral shape change which compare favorably with experimental measurements of the deformation observed in gold-silver alloys. In collaboration with J. Dantzig (Univ. of Illinois) this work has been extended to include the effects of difference in partial molar volume, and the resulting model was solved using a commercial finite element package to predict strongly coupled effects of diffusion and deformation [2].

In multiphase binary diffusion couples that maintain planar interfaces between phases, both experimental evidence and theoretical analysis has revealed interfacial discontinuities in the Kirkendall velocity, as well as multiple Kirkendall planes. Under the usual assumptions of the diffusion model for the Kirkendall effect, the magnitude of the velocity discontinuity is proportional to the difference of the differences of the intrinsic diffusion coefficients for each phase. Questions arise about the implications of the discontinuity in the context of the deformation and stress state in the diffusion couple. To clarify these points, we are examining the moving interface problem using both diffuse and sharp interface approaches. The diffuse interface approach predicts a Kirkendall velocity field that is continuous but suffers a large change across the diffuse interface. The net motion of the material is studied by tracking the trajectories of inert markers distributed throughout the sample and defining independent diffusion fluxes (intrinsic fluxes) with respect to these markers. In Fig. 26 we illustrate marker motion for a two-phase, one-dimensional diffusion couple with nonlinear intrinsic diffusivities. The figure shows examples of multiple Kirkendall planes, as well as discontinuous Kirkendall velocities at the phase boundary.

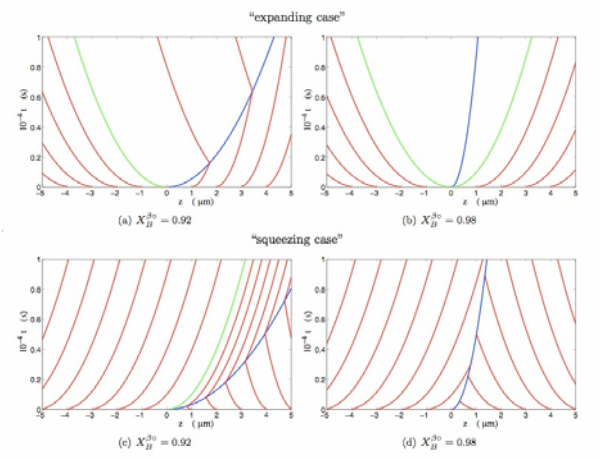

Figure 26. *Trajectories of Kirkendall markers on the original interface (green) and at other initial positions (red). The blue trajectory is the position of the two-phase boundary.*

References

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Modeling of Contact Dynamics of Silicon Cantilevers

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This research began in April, 2005 when ITL and MSEL were awarded a 2-year joint exploratory competence project by the NIST Director's Office. The objective was to *initiate* the development of a stochastic

approach to the nonlinear modeling of contact dynamics of silicon cantilevers and *verification* (without validation) of the finite element method (FEM) simulations at micro- and nano-scale for applications in atomic force microscopy (AFM), nanoscale manufacturing technology, and biomedical nano-mechanics.

During the first seven months of the project (Apr. – Sept. 2005), ITL proposed a plan to develop new computational algorithms based on finite element method for micro- and nano-scale applications in order to better understand the process of tip wear and its influence on AFM measurement of material properties as observed by NIST researchers in their recent experiments to determine the tip-sample contact stiffness and tip radius before and after AFM measurements for several different cantilevers.

ITL collaborated with MEL, MSEL, and numerous non-NIST researchers to carry out this plan. During FY06, ITL developed a computational algorithm for the determination of the resonance frequencies of a single-crystal silicon cantilever with a built-in sensitivity and uncertainty analysis tool associated with a fractional factorial orthogonal experimental design.

The methodology developed in FY06 at the conclusion of the funding of this exploratory project will be applied, subject to availability of new funds, to three additional stochastic models that simulate the dynamic behavior of a typical AFM cantilever with a hemispheric or prismoidal tip, namely, (1) forced vibrations of the cantilever when its tip is in contact with a rigid half-space, (2) forced vibrations of the cantilever when its tip is in contact with an elastic half-space, and (3) forced vibrations of the cantilever when its tip is in contact with an elastic layer on a rigid substrate.

This work is supported by the NIST Innovations in Measurement Science Program.

Characterization of Microdomain Lattice Defects in Block Copolymer Thin Films

Javier Bernal
Jack Douglas (NIST Polymers Division)

An image analysis algorithm is being implemented for the characterization of microdomain lattice defects in block copolymer thin films. The algorithm is based on the idea of the Voronoi diagram of 2-D dynamic data, i.e., the Voronoi diagram of moving points in the plane. Here the moving points are the centroids of individual microdomains and the object is to visualize defect structures from their Voronoi diagram over time. As the points move, topological events occur at certain critical instants in time that cause a change in the Voronoi diagram of the points. Accordingly, maintaining the Voronoi diagram over time in an efficient manner is crucial.

Complex System Failure Analysis

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This research began in February 2004 when ITL and BFRL were awarded a 5-year joint Innovations in Measurement Science project. The objective was to create the scientific basis for building failure investigation procedures that (a) will allow NIST to accomplish its mission under the National Construction Safety Team Act (P.L. 107-231, Oct. 1, 2002), and (b) will be 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 and beyond.

During the first eight months of the project (Feb. – Sep. 2004), ITL proposed to develop three specific computational tools designed for analysis of complex building failures:

- Tool-1 (Sensitivity Analysis): Design of experiment-based sensitivity analysis of a class of structure-impact-fire collages models.
- Tool-2 (Verification): Stochastic finite element analysis and benchmark-based verification of simulations of structure-failure models.
- Tool-3 (Progressive Collapse): Stochastic global progressive collapse models and material-property-based time-to-collapse models with uncertainty estimates.

ITL collaborated with MSEL, BFRL, and numerous non-NIST researchers to carry out this plan. During

FY05, Tool-1 was developed and applied to an ongoing NIST investigative project related to the study of the collapse of the World Trade Center. During FY06, Tool-2 and -3 were developed and applied to a simplified progressive collapse model of a 44-column single-floor steel grillage on fire with two stochastic variables, namely, the ultimate strength of the structural-grade material and the surface temperature of the steel when a structure is on fire.

Plans for FY07-08 are to further develop Tool-2 and -3 and apply them to more complex structures involving two additional stochastic variables, the reduced stiffness of the joints due to aging, and the fracture toughness of the structural-grade material.

This work is supported by the NIST Innovations in Measurement Science Program.

View of the NIST campus in Gaithersburg, Maryland.

Mathematical Modeling of Electromagnetic Systems

Optical Coherence Tomography for Biomedical Imaging

Andrew Dienstfrey
S. Dyer (NIST EEEL)
T. Dennis (NIST MSEL)
Paul Williams (NIST MSEL)

See feature article, page 27.

Micromagnetic Modeling

Michael Donahue
Donald Porter
Robert McMichael (NIST MSEL)
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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.

Michael Donahue and Donald 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 2006 alone, the software was downloaded more than 2,700 times, and use of OOMMF was acknowledged in 85 peer-reviewed journal articles.

OOMMF is part of a larger activity, the Micromagnetic Modeling Activity Group (μMAG), formed 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. Additional standard problems dealing with issues such as thermal effects and the effect of representation errors when boundaries do not align with the computation grid are 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. An Innovations in Measurement Science 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.

Progress on computational issues has been a recent focus. Techniques to minimize or control errors introduced when the spatial resolution of the computation grid does not exactly represent the boundaries of the simulated material are in development. Also being pursued are code revisions to exploit the concurrency opportunities made possible by the increasing availability of multi-core hardware platforms. Another focus area is the modeling of spin momentum transfer to magnetic domain walls arising from electric current flow. This spintronic effect is expected to play an important role in the near-term development of magnetic memory and logic devices.

The project also does collaborative research using OOMMF. The MCSD micromagnetic project produced three journal papers, one book chapter, and two conference presentations in FY 2006.

This work is supported in part by the NIST Innovations in Measurement Science Program.

Time-Domain Algorithms for Computational Electromagnetics

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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.

During the past year Alpert and Dienstfrey have collaborated to attack the problem of fast eigenfunction transforms that arises in some time-domain electromagnetics computations (as well as elsewhere). In particular, representations of functions as expansions of eigenfunctions from Sturm-Liouville differential equations, which enable efficient application of certain naturally-occurring operators, must themselves be obtained typically by transforming from pointwise function values. Recent progress in fast algorithms for these transformations, from many researchers and resulting in methods analogous to the fast Fourier transform (FFT) to compute the discrete Fourier transform, has not yet achieved the efficiency to enable widespread acceptance of these new methods. Many of the methods rely on a divide-and-conquer approach that requires repeated interpolation of functions having a prescribed form and it is this operation that consumes the majority of the computation time in a transformation. Alpert and Dienstfrey have discovered, from an identity satisfied by the Green's function of a Sturm-Liouville equation, a new fast algorithm for these interpolations. This algorithm is expected to outperform significantly the fastest existing method for interpolation, which is based on the fast multipole method.

Although these eigenfunction expansions are more specialized than Fourier expansions, they are essential for efficient computation in certain special settings, which include spherical or elliptical geometry, plane-polar representations, bandlimited signals, and a number of more unusual problems. The recent work is expected to result in faster transforms, as well as fast applications of certain related operators, that arise in these problems.

Earlier work of this project 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).

Modeling of Optical Spectra

Peter Ketcham
Eric Shirley (NIST PL)

Among the materials exploited by optical technology are crystalline materials with useful properties in the ultraviolet spectral range. These materials are incorporated into ultraviolet optical systems and optoelectronic devices that have relevance to photolithography, in particular, and the semiconductor manufacturing industry in general. However, these materials are not fully understood, and significant experimental uncertainties exist in their ultraviolet optical properties. In conjunction with the NIST Physics Lab, MCSD is performing first-principles calculations of the optical properties of these materials. Advanced theoretical models of the optical properties are based upon the absorption of a photon and the production of an electron-hole pair. Simpler models, which do not take electronic excitations into account, may fail to give quantitatively accurate results. The inclusion of electron-hole interactions in the theoretical model involves extensive computations which in turn demand high-performance computing systems.

This year, P. Ketcham began a collaboration with E. Shirley to implement these theoretical models on multicore, multiprocessor, large-memory, high-performance computing systems. Both message-passing and multithreaded approaches to a parallel implementation were investigated. In the near term, efforts will center on the development of parallel codes and the refinement of the underlying mathematical models. Long-term goals may include the implementation of theoretical models addressing strongly correlated systems and multiple electronic excitations.

Mathematical Modeling for Chemical and Biological Applications

An Accurate Model for Measuring Fluorophore Photodegredation Dynamics

Fern Hunt
A. K. Gaigalas (NIST CSTL)
L. Wang (NIST CSTL)

See feature article, page 41.

Optical Coherence Tomography for Biomedical Imaging

Andrew Dienstfrey
S. Dyer (NIST EEEL)
T. Dennis (NIST MSEL)
Paul Williams (NIST MSEL)

See feature article, page 27.

Simulation of Bioregulatory Networks Involved in Cell Cycle Control

Geoffrey McFadden
S. Kim (National Institutes of Health)
Mirit Aladjem (National Institutes of Health)
Kurt Kohn (National Institutes of Health)

G. McFadden of MCSD is a co-advisor to S. Kim, a postdoctoral fellow in the Laboratory of Molecular Pharmacology in the National Cancer Institute at NIH; her NIH co-advisors are Mirit Aladjem and Kurt Kohn. The team 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.

Much current work focuses on a protein known as p53, a tumor suppressor that causes cell cycle arrest or programmed cell death in response to stress signals such as DNA damage. A loss of p53 function, either by mutations or by deregulation, often leads to cancer. Too much p53 protein results in premature aging and cell death. Thus, regulating the appropriate levels of p53 is essential for cell survival, and the p53 protein is indeed subject to a tight regulation. Two related proteins, Mdm2 and Mdmx, are known regulators of p53: Mdm2 can facilitate degradation of p53 whereas the mechanism of the regulatory interaction of Mdmx with p53 is not clear. It is also not obvious how those three molecules will operate together under various conditions. To address those questions, a mathematical model is being developed to investigate the interactions of these three partner molecules by numerical simulations.

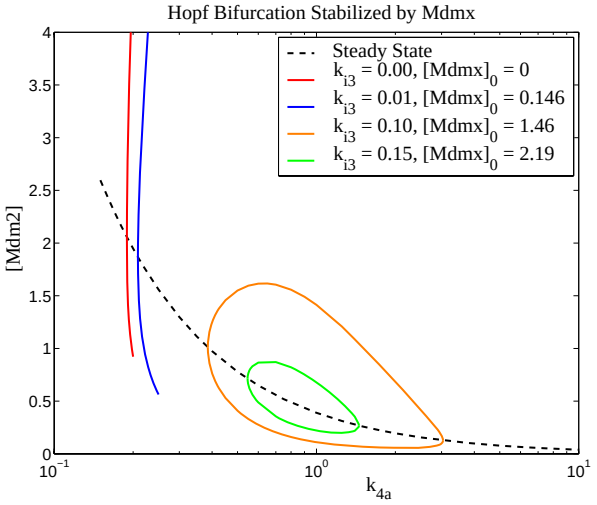

Figure 27. *Bifurcation diagram showing the concentration of Mdm2 in the system as a function of the kinetic parameter k4a.*

An interesting feature of this system is the experimental observation of time-periodic behavior of the measured amounts of p53 and Mdm2 in the system under certain conditions. In Fig. 27 we show a bifurcation diagram based on our model illustrating the effect of Mdmx on the long time stability of the system. In this plot we show results as two model parameters, k_{4a} and k_{i3}, are varied. The parameter k_{4a} governs the kinetics of the interaction of p53 with Mdm2, and the parameter k_{i3} governs the production rate of Mdmx. The dashed curve shows the steady state value of Mdmx as a function of the parameter k_{4a}. For $k_{i3} = 0$ there is no Mdmx in the system. The steady state is initially stable for small values of k_{4a}, but loses stability at a Hopf bifurcation point at a critical value of $k_{4a} = 0.19$, and is thereafter unstable. A limit cycle is observed for $k_{4a} > 0.19$, and the maximum and minimum values of Mdm2

over a cycle of the oscillation are shown as the red curve. The amplitude of the oscillations grows sharply with increasing k_{4a}. As k_{i3} increases, the presence of Mdmx stabilizes the system, with eventual elimination of the Hopf bifurcation for $k_{i3} > 0.2$. These results show the stabilizing effect that Mdmx has on the system at long times: for large enough amounts of Mdmx in the system the entire branch of steady state solutions is found to be linearly stable.

This modeling work is intended to guide experimental investigation of the role of Mdmx in the cell cycle that will be performed by Kim at the NIH.

Virtual Measurements in Quantum Chemistry

Raghu Kacker
Karl Irikura (NIST CSTL)
Russell Johnson (NIST CSTL)

By a virtual measurement we mean a prediction along with uncertainty for the value of a measurand determined from a computational model as an alternative to a physical measurement. An important application is quantum chemistry, where carefully determined uncertainties from simulations have not been reported. As the technology improves, the need and importance of reliable uncertainties is being recognized. This project is focused on developing methods for quantifying the uncertainty associated with a virtual measurement in quantum chemistry. The benefits accrue to research and development of chemical processes, materials development, and drug discovery.

Our first paper published in *Metrologia* [1] describes the generic approach and illustrates it with quantification of uncertainties associated with atomization enthalpies. A second substantive paper published in the *Journal of Physical Chemistry* [2] describes the uncertainties in scaling factors for *ab initio* vibrational frequencies. This paper includes a large table that displays scaling factors and their associated uncertainties for eight theoretical methods and five basis sets. Each of forty scaling factors and uncertainties are based on over 3,000 independent vibrational frequencies from the Computational Chemistry Comparison and Benchmark Database. Values of scaling factors from the literature are given when available. This is the first table to quantify such uncertainties. Also, this is the largest such table ever assembled, and this is the most extensive such study.

A third study, now in progress, is on zero-point energies. Here, benchmark experimental measurements are not available. Our collaborators are calculating required data for bi-atomic and poly-atomic molecules from available information. We will then use our approach to quantify uncertainties associated with virtual measurements of zero-point energies.

References

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[2] K. K. Irikura, R. D. Johnson III, and R. N. Kacker, Uncertainties in Scaling Factors for ab Initio Vibrational Frequencies, *Journal of Physical Chemistry A* **109**(37) (2005), pp. 8430-8437.

Systems Identification and Parameter Estimation for Environmental Applications

Bert W. Rust

Identifying a system of ordinary differential equations describing dynamical relationships between measured time series is a challenging problem. An important example involves the relationship between fossil fuel carbon dioxide emissions *P(t)*, atmospheric carbon dioxide concentrations *c(t)*, and global temperatures *T(t)*.

A new refinement of the current model has been enabled by appending ice core measurements to the *c(t)* time series in order to extend it back to the beginning of the measured *T(t)* record. The new relationship between the two variables is illustrated in Fig. 28.

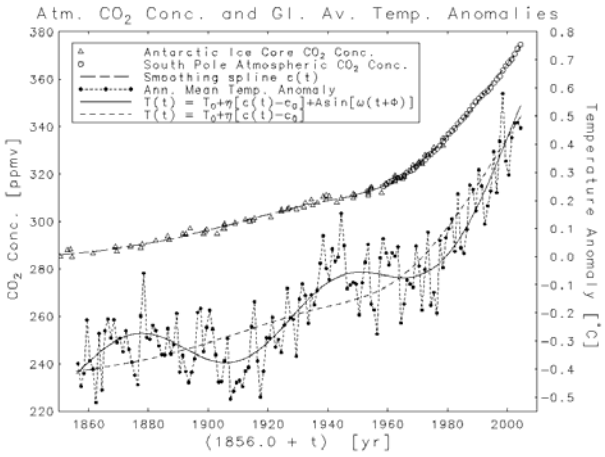

Figure 28. *Atmospheric CO_2 concentration and global average temperature anomalies.*

In the top curve, the circles are measured atmospheric concentrations, the triangles are concentrations derived from ice cores, and the long-dashed curve is a smoothing spline fit. In the lower plot, the solid dots are measured annual global average temperature anomalies, and the solid curve is the fit of the new *T(t)* equa-

tion which is given in the legend. The values of *c(t)* used to make this fit were taken from the smoothing spline fit in the upper plot. The short-dashed curve is the baseline for the *T(t)* fit. It now appears that a linear relation between the two can completely explain the baseline for the warming. The plotted baseline also shows that the warming is accelerating.

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

Improvement in Modeling Cryocoolers

Abbie O'Gallagher
John Gary (MCSD retired)
Yonghua Huang (NIST CSTL)

The Regen3.2 package has been an important tool for modeling cryocooler behavior. This package was originally written by John Gary of MCSD and continues to be highly valuable to researchers in the field.

Recently, O'Gallagher and Gary have been working to expand and improve it in several ways. In particular, another formulation of the problem, previously undocumented and only available in-house as RG4mm, will be bundled with Regen3.2 to create a larger package which will be called Regen3.3. It will be possible to use either method through one user interface. The new method is based on a conservation law formulation. It gives superior results in some cases, especially for those in which the matrix of material inside the regenerator is made up of layers of different materials. In addition, thanks to guest researcher Yonghua Huang, the user will now be able to choose to specify that the gas which is flowing inside the matrix is helium-3, rather than the standard helium-4.

Mathematics of Metrology

Numerical Optimization of Complex Instrumentation

Anthony J. Kearsley
William E. Wallace

See feature article, page 43.

APEX Blind Deconvolution of Color Hubble Space Telescope Imagery and Other Astronomical Data

Alfred S. Carasso

See feature article, page 23.

Nonlinear Image Analysis and the Mumford-Shah Functional

Alfred S. Carasso

Image segmentation entails separation of an image into its constituent parts. One approach is to partition an image based on abrupt changes in gray levels. This requires locating sharp edges in the image. Given an image *w(x,y)*, the Mumford-Shah approach seeks to find a simpler approximating image *u(x,y)* consisting of piecewise constant or piecewise smooth regions. This simpler image *u(x,y)* is to be obtained by minimizing the Mumford-Shah cost functional. However, this minimization problem is highly unusual and is not directly solvable. It requires finding two unknowns of a quite different kind, the best approximation *u(x,y)*, and the corresponding discontinuity or edge set *K*. Highly sophisticated approaches to this problem were devised in the 1990's by the Italian mathematicians De Giorgi, Ambrosio and Tortorelli, using the notions of *Gamma convergence and elliptic regularization*. In that theory, the edge set *K* is replaced by an auxiliary function *v(x,y)*, defined to equal zero on *K* and unity outside of the set *K*. Minimizing the Mumford-Shah cost functional now requires solving a linear elliptic Helmholtz partial differential equation for the auxiliary edgemap *v(x,y)*. The coefficients in this Helmholtz equation are specific functions of the gradients in the original image *w(x,y)*. These gradients are only defined at the mesh points of the original image grid. In addition, the Helmholtz equation contains certain unknown regularization and convergence parameters, which must be correctly set *a priori* to obtain meaningful results. Unfortunately, the theory offers little useful guidance on how to set these parameters.

A. Carasso has successfully implemented the above approach by coding a Helmholtz solver on rectangles with Neumann boundary conditions, and where the variable coefficients are defined only at mesh points. Finite difference ADI methods were used. Considerable effort was then expended in researching and understanding how to appropriately set the regularization parameters in the Mumford cost functional. Most reasonable parameter choices produced badly obscured noisy images, as opposed to the desired clean edge maps. It turned out that Carasso's initial parameter choices were off by several orders of magnitude, but there was no way to know that *a priori*. The sensitivity of the results to one particular parameter, ε, is illustrated in Fig. 29. Image (A) is a given sharp image of the aircraft carrier USS Eisenhower. Image (B) is the computed edgemap using what appeared to be a reasonably small value of ε, $\varepsilon = 1\times10^{-9}$.

This produced an obscured map with smeared edges that are not useful. Choosing a significantly smaller value, $\varepsilon = 5\times10^{-14}$, produced image (C) where the edges are now very faint and almost invisible, and where there is no trace of the sea. The successfully obtained edgemap using the "correct" parameter choice $\varepsilon = 1\times10^{-12}$, is shown in image (D). Clearly, Mumford-Shah methodology requires practical experience on a wide variety of images in order to arrive at correct parameter values.

One significant application of the Mumford-Shah theory is image deblurring. Important results have been reported by Israeli and French researchers on using Mumford edgemaps as prior regularizing information. Such an approach merits long-term study, as it can apparently produce high quality restorations even at high levels of image noise. Mumford-Shah deblurring requires solving a difficult variable coefficient integro-differential elliptic problem, one where the differential operator is not positive definite, but is supplemented by a positive definite Fredholm integral operator. Conjugate gradient and other iterative techniques are being applied to this problem, and numerous experiments are being performed on noisy imagery to evaluate the effectiveness of this proposed technique.

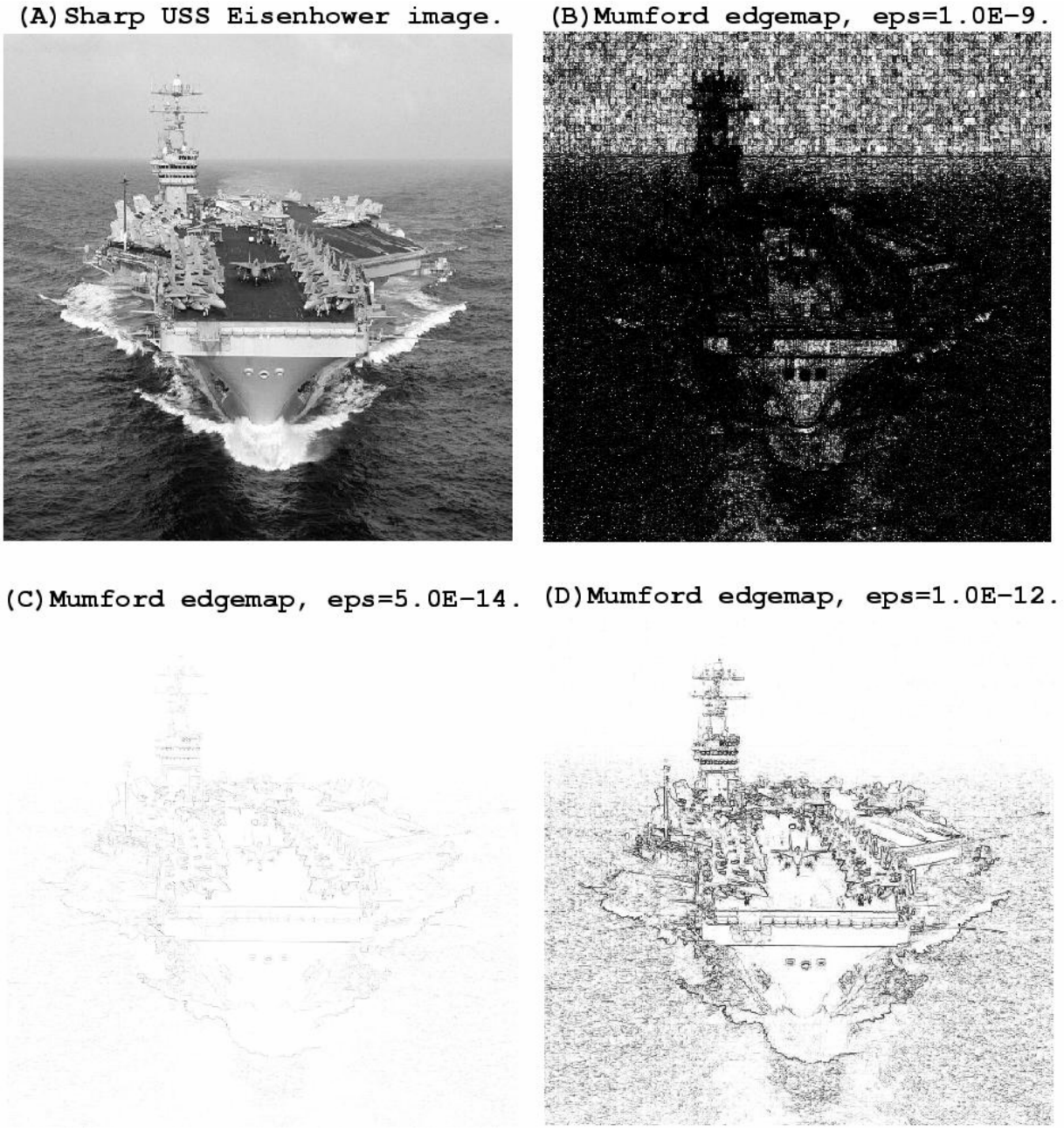

Figure 29. *Correct choice of regularization parameter ε is crucial for obtaining useful Mumford-Shah edge map. (A) Sharp image. (B) Computed edgemap with ε too large smears edges and obscures result. (C) Too small a value for ε makes edgemap almost invisible. (D) Correct value* $\varepsilon = 1 \times 10^{-12}$ *was found after many trials.*

Sparse Representations in High Dimensional Geometry

Bradley Alpert
Yu Chen (New York University)

Can one (a) reliably construct an N-pixel image from $N^{1/4}$ measurements, or (b) transmit a message despite jamming by a clever adversary who manages to corrupt almost 1/3 of the bits?

For several years computational experiments and practice have supported the use of the L_1 norm for fitting models to measurements in certain applications. In the past two years, theory has begun to catch up to practice, to remove some of the mystery of these computations, and to open up many new applications. Emmanuel Candes, David Donoho, Anna Gilbert, Ron DeVore, their collaborators, and a growing list of other researchers have provided both algorithms and theorems to suggest a new approach to information acquisition and processing, one in which extremely underdetermined problems can be solved well by finding sparse, or sparsest, solutions.

A class of problems that arises often in medical practice is the construction of images from tomography or magnetic resonance measurements. When one requires a quantitative characterization of the object being measured, however, as is typical at NIST, existing filtering and approximation methods may not be adequate. In addition to systematic modeling of noise in the measurement process, it is necessary to develop representation spaces for scatterers that enable images to be constructed as sparse representations having fewer unknowns than the number of measured parameters. The representations should not sacrifice detail resolved by the measurements.

The recent mathematical advances mentioned above suggest that these image construction problems, in which sparse representations must be drawn from very high dimensional spaces, can be solved using methods that follow from, or are suggested by, the optimization methods used by the newly characterized procedures. This project is exploring whether the ability to systematically find sparse representations from possibly noisy data enables recovery of accurate representations of scatterers, even when their properties may be discontinuous in space. The initial approach involves applying the sparse recovery methods, and experimenting with others, to Fourier data generated from numerical models of scatterers. The deficiencies of the resulting recoveries are characterized and point to ways that the representation space should be altered and the recovery procedures extended.

Applications in Security

Isabel Beichl

A two year detail at NSA was recently completed as part of the NSA Mathematical Sabbatical Program. Methods initially developed at NIST were refined and enhanced to apply to real problems relevant to national security. Details cannot be supplied here but, in general terms, new techniques were invented by importing ideas from statistical physics to computational graph theory. Several large programs were written to apply the methods to important problems. Results were reported in three classified papers. In addition, two talks were given, one to the mathematics research group at NSA and one to the research staff if the IDA Center for Computing Sciences. We are now planning to apply this expertise in other areas.

This work was supported by the National Security Agency.

Automated Combinatorial Testing for Software (ACTS)

Raghu Kacker
Jim Lawrence
Michael Forbes
Rick Kuhn (NIST ITL)
Ramaswamy Chandramouli (NIST ITL)
Vadim Okun (NIST ITL)
Paul Black (NIST ITL)
Jeff Offutt (NIST ITL)
Yu (Jeff) Lei (University of Texas - Arlington)
Renee Bryce (University of Nevada - Las Vegas)

We consider testing of software whose inputs can be described by a sequence of parameters, each with a fixed set of values. A test of such software is specified by selecting a particular combination of values for the parameters. Testing all possible combinations is impractical even for modest software. Thus, researchers seek testing methodologies which ensure "good" coverage of parameter space using a more modest number of tests. One such approach is known as *combinatorial testing*. A subset of all combinations of test inputs which includes each t-way combination of parameter values at least once is called a covering array of strength t. Most of the existing work on methods and tools focuses on 2-way (pair wise) testing. However, a study of actual faults conducted by NIST has shown that while 2-way testing can detect a large fraction of faults, it may not be adequate. About 95 % of faults in that study involved 4-way or lower order interactions; further, almost all faults could be detected by 6-way

combinatorial testing in the types of software that were investigated. Thus high *t*-way combinatorial testing may in practice be equivalent to exhaustive testing.

This ITL inter-divisional project has the following objectives. (1) Develop efficient and scalable algorithms and tools to generate covering arrays for multi-way combinatorial testing for software. The number of parameters may vary over large ranges and they may have different values (heterogeneous configurations) and involve various constraints. (2) Integrate concepts from algebraic combinatorial methods and computational methods. (3) Investigate integration of combinatorial testing and automated test generation tools (such as model checking) to develop automated combinatorial testing tools. (4) Demonstrate successful application of the tool in specific areas. The benefit is to advance the technology of combinatorial software testing.

We have developed a prototype tool, called Fire-Eye, which generates covering arrays for multi-way combinatorial testing and non-homogeneous arbitrary configurations based on a deterministic algorithm, called IPOG (in parameter order, general). Large input configurations remain a challenge because the space and time required for searching candidate *t*-way combinations increase exponentially. We have developed an algorithm to reduce the space and time required for high degree of combinatorial coverage. We have developed another prototype tool, called Paint-Ball, implementing a randomized version of the greedy algorithm, at each stage searching from all possible *t*-way combinations that are not yet covered. After sufficiently large number of the *t*- way combinations have been covered, the remaining combinations are covered by tests that are appended deterministically.

We have developed a paper that serves as a proof-of-concept for integrating combinatorial testing with model checking to provide automated specification based testing. Michael Forbes (summer student from MIT) developed and demonstrated an improvement of the IPO algorithm (IPOv2) for 3-way coverage. We have developed a combinatorial testing strategy for reachability testing of concurrent programs. A paper has been submitted for publication.

We intend to release the two tools (Fire-Eye and Paint Ball) for public use in the spring of 2007. We also intend to have papers on the underlying algorithms published in conference proceedings. During the summer of 2007, we will further investigate Michael Forbes' improvement. We are actively seeking applications of combinatorial testing for we believe that specific applications should direct our efforts.

Quantum Information

Benchmarks for Quantum Computing with Ion Traps

Emanuel H. Knill
Dietrich Leibfried (NIST PL)
David Wineland (NIST PL)

See feature article, page 35.

Quantum Computing Theory

Scott Glancy
Emanuel Knill
Howard Barnum (LANL)
Rolando Somma (LANL)
Geraldo Ortiz (University of Indiana)

The implementation of quantum computers is based on a substantial body of theoretical work showing the utility of quantum algorithms and providing techniques for protecting quantum devices from inevitable noise. Our contributions to quantum computing theory include work on better understanding the limitations as well as the power of quantum computers, a powerful strategy for obtaining pure entangled states as a computational resource, and better methods for measuring observables in quantum physics simulations on quantum computers.

To study the limitations of quantum computers, we considered a model of computing where the computational steps are limited to evolutions under a space of Hamiltonians forming a known semisimple Lie algebra. We found that under these circumstances, all the results of a computation can be efficiently simulated using classical computers. Because the states reachable in this model of computing are characterized as generalized unentangled states, this supports the thesis that generalized entanglement is required for exploiting the full power of quantum computers. This work relates to well-known results concerning the limitations of so-called Clifford gates and linear optics for fermions. Further work is needed to unify these results and further illuminate the reasons why quantum computers appear to be more powerful than classical computers.

An important problem for quantum computers and quantum communication is to ensure that initial states are as desired with little noise. Typically, the available states are too noisy. To remove the noise, researchers have proposed the use of purification protocols whereby one can produce a less noisy state from a number of noisy copies of the state of interest. Such protocols were known for purifying the class of states known as Calderbank-Shor-Steane (CSS) states. We showed that there are simple protocols that can purify any stabilizer state, which are more general than the CSS states.

One of the most promising applications of quantum computers is to the simulation of quantum physics. In most such simulations, the desired answer is the expectation of an observable. The simplest way to determine such an expectation with a given accuracy $1/n$ is to run the simulation $1/n^2$ times, make a von Neumann measurement of the observable each time, and take the average of the answers. For sufficiently well understood observables, it was known that the resources needed could be reduced from $1/n^2$ to $1/n$ by taking advantage of quantum mechanical effects. We showed that essentially the same improvement is possible for any observable under mild assumptions.

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[2] S. Glancy and E. Knill, "Entanglement Purification of Any Stabilizer State," *Physical Review A* **74**, 2006, 032319/1-11.
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This work is supported in part by the Defense Advanced Research Projects Agency (DARPA) and the NIST Innovations in Measurement Science Program.

Optical Quantum Metrology and Quantum Computing

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Emanuel Knill
Tracy Clement (NIST EEEL)
Alan Migdall (NIST PL)
Richard Mirin (NIST EEEL)
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Marty Stevens (NIST EEEL)

Members of the MCSD are contributing to the development of an experimental research program in optical quantum metrology and quantum computing. This project is developing 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. 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.

In the last year we designed and built an optical homodyne system, which we can use to measure and reconstruct the quantum state of any single mode of light. Our homodyne system operates with an efficiency equal to the best known comparable systems, and we continue to make improvements. Members of the MCSD designed software which is used to reconstruct a quantum state from thousands of individual homodyne measurements. This system will serve as an essential element of many future optics experiments. The theoretical analysis of the state reconstruction procedure is still in progress.

Our plans include experiments to prepare and characterize squeezed light, Schrödinger 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.

References

[1] J. Rehacek, Z. Hradil, E. Knill, and A. I. Lvovsky, "Diluted Maximum-Likelihood Algorithm for Quantum Tomography," quant-ph/0611244, 2006.

This work is supported in part by the NIST Innovations in Measurement Science Program.

High Performance Computing

High Precision Calculation of Fundamental Properties of Few-Electron Atomic and Molecular Systems

James Sims
Stanley Hagstrom (University of Indiana)

See feature article, page 33.

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 modeling tools needed for engineering applications such as advanced semiconductor lasers and detectors, single photon sources and detectors, biosensors, and 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 nanoscale, 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.

We have completed a code for calculations on arrays of nanoparticles. The basic idea is to consider each nanoparticle as part of its own cluster of nodes, using the same input data, but as the computation proceeds, information from neighboring atoms in each cluster of nodes has to be distributed to the appropriate processor in neighboring clusters of nodes, thereby "stitching" the calculations on the clusters of nodes in the array together. A significant new feature of this code is the ability to use not just an sp3s* basis, but also an sp3d5s* basis in the parallel runs.

We have done many runs with the new code. This series of calculations could not have been done with the sequential code, because of both the parallelization and the new stitching capability. We are writing this up in the paper, "Advancing Scientific Discovery through Parallelization and Visualization III. Tight-binding Calculations on Quantum Dots". A related paper was presented at the March APS meeting:

> J. Sims, G. W. Bryant, and H. Hung, "Excitons in Negative Band-Gap Nanocrystals," American Physical Society March Meeting, Baltimore, MD, March 2006.

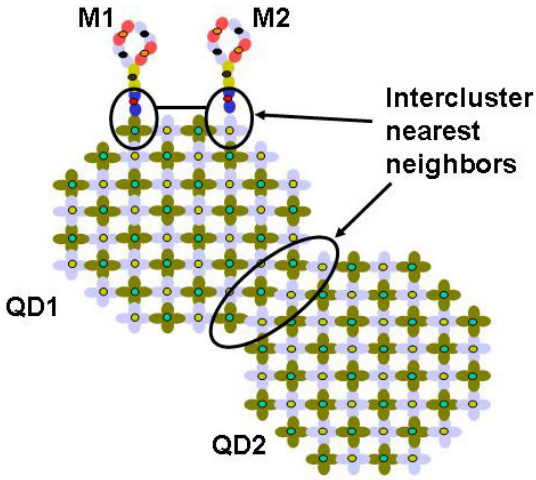

Figure 30. *Illustration of intercluster nearest neighbors in a nanosystem with four subsystems: two quantum dots (QD1 and QD2) and two conjugating molecules (M1 and M2).*

Computational Modeling of the Flow of Concrete

William George
Julien Lancien
Christine McKay
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 but presents a significant theoretical challenge. The computational modeling of such systems is challenging because of the difficulty in tracking 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 large 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 inclusions. In addition, the rigid body motion is determined from the quaternion-based scheme of Omelayan (hence the Q in QDPD). Parallelization of the algorithm is important in order to adequately model size distributions, and to have enough resolution to avoid finite size effects.

This year we were awarded one million CPU-hours on the NASA Supercomputer, Columbia. This machine is a 10,240-CPU system based on SGIs NUMAflex architecture. The system is comprised of 20 SGI Altix 3700 superclusters, each with 512 Intel Itanium 2 processors (rated at 1.5 GHz). Each supercluster features 1 terabyte of memory with global shared memory access, for a total of 20 terabytes of memory system-wide. Columbia was put into production in June 2004. A press release on the award can be found at http://www.nasa.gov/home/hqnews/2006/mar/HQ_06086_super_computer_time.html

The NASA allocation is one of four awards of supercomputer time given out in a peer-reviewed competition for grand challenge computational science projects led by external researchers. The successful NIST proposal was submitted by William George (team lead) and Judith Terrill of MCSD, along with Nicos Martys and Edward Garboczi of BFRL. Entitled "Modeling the Rheological Properties of Suspensions: Application to Cement Based Materials," the proposal stems from a long-term MCSD/BFRL collaboration on high performance computer modeling of cement and concrete systems. The team will use NASA's supercomputer to study the flow, dispersion and merging of dense suspensions composed of rigid bodies having a wide range of size and shape under a variety of flow conditions. Access to the NASA machine will allow modeling at a level and range impossible with existing computing facilities available at NIST. Current modeling of suspensions at NIST facilities has been limited to a few thousand particles and a factor of five to ten in particle size range. Utilization of NASA's Columbia system will provide the capability to simulate suspensions an order of magnitude larger in the number of inclusions and size range. The new realism of these models will significantly improve the scientific basis for prediction and measurement of the flow properties of concrete.

We ported the QDPD application to the NASA Columbia system and have run timing and scalability tests on this code. Results of these tests, using up to 256 processors, identified scalability issues. We developed a new parallel algorithm that scales linearly, up to approximately 500 processors on large computations, in order to remedy these issues.

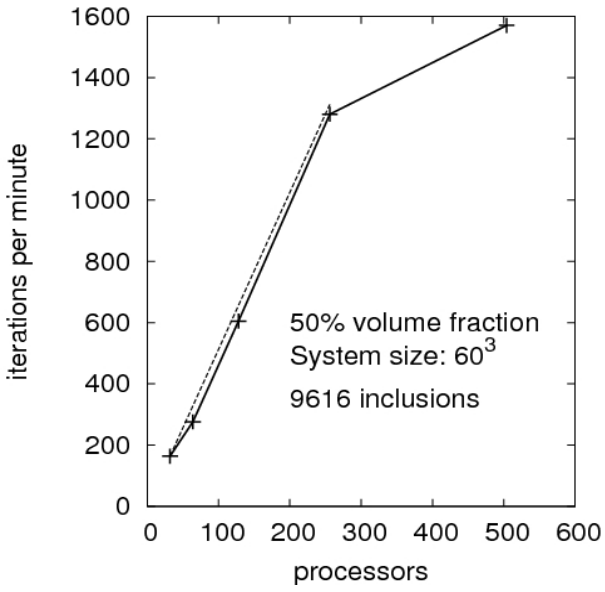

Figure 31. *Scaling of new parallel algorithm on Columbia system. Above ~300 processors, the algorithm could handle a larger system size.*

We have processed a large number of production runs of QDPD on the NASA Columbia machine. Most runs now use 500 processors or more. At this time all of the "finite size effect" runs have been completed and we have begun the study of systems with poly-sized inclusions. More than 240,000 CPUs hours of compute time has been used to date. We have completed the following simulations using a size of 60x60x60 and 648,000 fluid particles, with mono-sized spherical inclusions, and all combinations of: volume fractions: 20%, 30%, 40%, 45%, and 50%, and dimensionless shearing velocities: 0.1, 1, 3, 10, 30, 100.

Our investigation of finite size effects is meant to determine the resolution needed for scientifically meaningful results, as illustrated in Figs. 32 and 33. In both cases the volume fraction and the shear rates were the same. The smaller system was 30 cubed and the bigger was 60 cubed. Clusters form because of an attractive Van der Waals force between the spheres. But in the first figure, the lower resolution leads to a confinement effect and the system separates into two groups. In the second figure, the resolution is adequate to allow the Van der Waals force to form natural clusters.

Over 300 GB of output has been generated and transferred from NASA's NAS facility in Mountain View California to local storage at NIST. We are developing new techniques for managing and visualizing this data. Previous runs consisting of 10s to 100s of inclusions have been visualized, however the current

runs contain up to 10,000 inclusions. New techniques are needed due to the order of magnitude increase in size of the output from these computations.

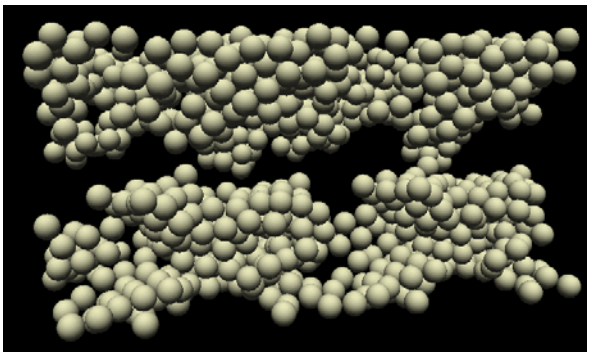

Figure 32. *Separation of particles into two clusters in above image is a confinement effect due to small system size*

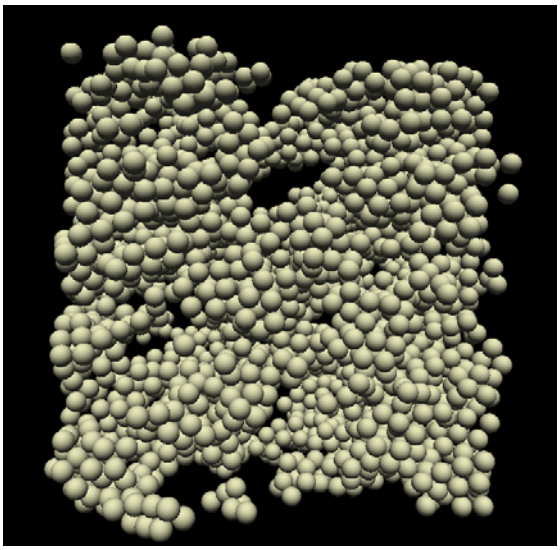

Figure 33. *The above image shows same system when the resolution is increased. The resolution is adequate to allow the natural clusters to form.*

Some I/O performance improvements have been made to QDPD to reduce the amount of output generated by each computation. I/O has been improved with some trade-offs being made which favor post-processing of the output as needed rather than managing this during the computation. These I/O improvements are still under test.

Testing has begun on QDPD runs which use general shaped aggregates with locally computed surface normals and curvatures. The last study we will perform on the NASA computers will be on systems with realistically shaped aggregates in a range of sizes. These studies should be completed by Spring 2007.

We released the new parallel QDPD code, implemented entirely in Fortran 90, to the Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium along with the user guide, "Users Guide to QDPD". This first release uses spheres as the aggregate with analytical calculations of surface normals and curvatures.

Presentations

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[2] J. Lancien, W. George, and N. Martys, "Quaternion Based Dissipative Particle Dynamics," VCCTL Consortium meeting, Nov 29-30, 2005, NIST.

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

Screen Saver Science

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Justin Haaheim
Thomas Bugnazet
Christine McKay

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 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 straightforward. 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.

Over the past year we have developed a system of scripts to manage SSS workers on the compute nodes of the ITL/PL Linux cluster Raritan, thus enabling us to utilize every free cycle. We have also enhanced SSS is several basic ways. The user interface, specifically for submission of SSS computations to the Raritan cluster, and the retrieval of results has been simplified. The SSS infrastructure has been improved to simplify its building, packaging, and distribution, and to better support application development by multiple researchers

In collaboration with CSTL researchers J-H. Scott and N. Richie, we have completed the port of their application, which simulates the operation of a Scanning Electron Microscope, from its original form as a serial computation in Python and Java, to a parallel distributed application in pure Java. This application is now ready to run in the SSS environment. Test runs of a 3D Chemical Imaging application, previously modified into a distributed computation, have begun on 32 processors of the Raritan cluster.

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.

We worked with Andrew Lumsdaine and Jeff Squyres, of the University of Indiana Open Systems Lab, concerning the addition of IMPI support to the new MPI library "Open MPI". This is a collaborative project to provide an open, state of the art, MPI library. Members of the OpenMPI project include Cicso Systems, Myricon Inc, Sun Microsystems, Voltaire, the Advanced Computing Laboratory of Los Alamos National Laboratory, Univ. of Houston Dept. of Computer Science, High Performance Computing Center Stuttgart (HLRS) at the University of Stuttgart, Innovative Computing Laboratory in the Department of Computer Science at the University of Tennessee, Mellanox Technologies, the Open Systems Laboratory of the Pervasive Technologies Lab at Indiana University, and the Scalable Computing Research and Development at Sandia National Labs (http://www.openmpi.org/).

We 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 of MPI that currently uses IMPI (see http://www.gridmpi.org/gridmpi-0-6/). In cooperation with the OpenMPI developers, they have agreed to implement and contribute full IMPI support for the OpenMPI library. As a result, Drs. Ishikawa and Matsuda attended an OpenMPI developer's workshop in April 2006, sponsored by Cisco Systems, to help finalize the addition of IMPI to the OpenMPI library distribution. Small changes were proposed to the OpenMPI library to better support the IMPI protocols as implemented by Drs. Ishikawa and Matsuda. After these changes were made to OpenMPI, the testing of IMPI support within OpenMPI revealed minor additions to the OpenMPI library are needed to complete the IMPI support within OpenMPI. These are in progress.

We worked with Carsten Clauss, of RWTH Aachen University, Germany, on the use of the IMPI conformance tester. Dr. Clauss is active in a project supporting heterogeneous coupled clusters using an MPI implementation called MetaMPICH.

Both AIST and Verari Systems, who acquired IMPI/MPI vendor MPI Software Technology, Inc., are interested in exploring possible extensions to IMPI to accommodate the dynamic process capabilities of MPI-2 and the changing cluster networking technologies

The NIST IMPI tester has been under active use by several sites over the last 12 months. This tester is used by developers of MPI libraries as they implement the IMPI protocols.

High Performance Visualization

Measurement and Analysis of Tissue Engineering Scaffolds

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

See feature article, page 29.

Virtual Measurement and Analysis Laboratory

Terrence Griffin
John Hagedorn
John Kelso
Adele Peskin
Steve Satterfield
Judith Terrill

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. In some cases, the data is from new landscapes, such as the nano-world, where we have little experience. Moreover, there may be ancillary data, from databases for example, to which concurrent access would be helpful. We are developing visual analysis capabilities in an immersive environment that allow NIST scientists to interact with, measure, and analyze their data in real time. With such visual exploration, scientists can easily perceive complex relationships in their data, quickly ascertaining whether the results match expectations. This system functions as a unique scientific instrument.

This year we have completed the move to the SGI Prism. We have nearly completed the rewrite of our DIVERSE software so that it uses the open source software OpenSceneGraph instead of SGI's OpenGL Performer. This has given us increased capability as well as access to the source code to enable extension and performance tuning.

Measurement Science in the Virtual World

Adele Peskin
John Hagedorn
Judith Terrill
James Filliben (NIST ITL)
Karen Kafadar (NIST ITL)

In this project, we seek to quantify errors introduced during the construction of renderable objects from scientific data, especially errors resulting from rendering such objects in the immersive environment.

We have begun by developing programs that measure rendering errors of points, lines, and 3D triangles. Statistics have been gathered to quantify the amount of error and to determine what factors influence rendering error. We have created a set of cases to study error in isolines as a function of mesh size, the source of the data, and the objects the data are describing.

An earlier paper on calibration of immersive virtual environments was accepted by the journal *Presence*.

In related work, we have developed line, cylinder, and ellipsoid interactive measurement tools, and developed analysis tools for the data gathered.

See Fig. 34 for an example of the cylinder measurement and analysis tool.

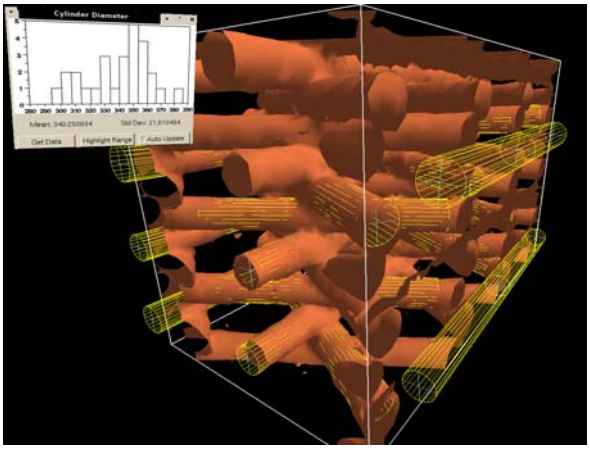

Figure 34. *Cylinder measurement and analysis tool used on rendered objects derived from measured data taken from a tissue engineering scaffold.*

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. MCSD has an ongoing collaboration with them to develop highly efficient parallel implementations of their modeling codes and in creating visualizations of their data. This work is done in the context of the Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium which we helped form in 2001. The NIST-led consortium consists of eight industrial members: BASF Admixtures (MBT), Ready Mixed Concrete (RMC) Foundation, Association Technique l'Industrie des Liant Hydrauliques (ATILH), National Stone Sand and Gravel Association (NSSGA), W.R. Grace, Sika Technology AG, Verein Deutscher Zementwerke eV (VDZ), and the 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 overall research and development process. It is expected that this will result in substantial time and cost savings to the concrete construction industry as a whole. MCSD continues as an active participant in the VCCTL.

Visualization of Concrete Aggregate Flow. In support of the VCCTL, X-ray tomography has been used to create a database of individual aggregate samples spanning about four decades in size. Examples include cement particles, sand, and rocks. These realistic aggregate shapes can then be incorporated into codes used to model the rheological properties of cement-based materials. We are developing techniques to represent and display simulated flows of such aggregates on the desktop and in an immersive visualization environment. Raw data from the X-ray tomography of each aggregate is transformed to yield two separate representations, one appropriate for the simulation, and the other appropriate for the visualization. See Figs. 35 and 36. While the representation for visualization references the same aggregate, it also has the ability to support differing levels of realism; see Fig.37.

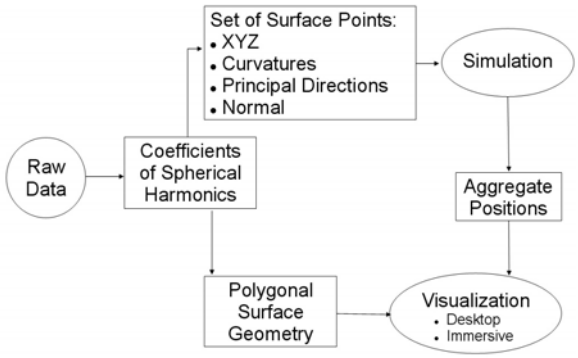

Figure 35. *The raw data from the X-ray tomography of each aggregate is processed into one data set that is input into the simulation, and another data set that is used in the visualization.*

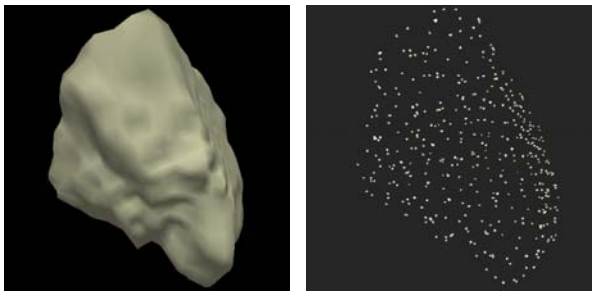

Figure 36. *On the left is the polygonal representation used in the visualization; on the right is the point representation used in the simulation.*

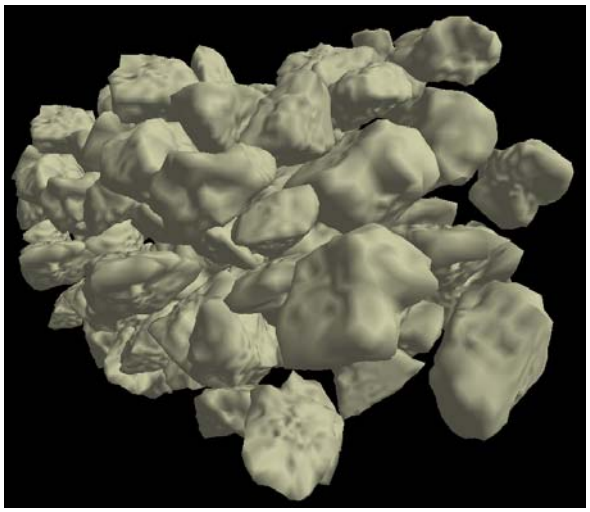

Figure 37. *Snapshot from a computer simulation of a sheared suspension of cement particles. The cement particles shapes were obtained via X-Ray microtomography and are approximately 10-50 micrometers in size. These simulations play an important role in understanding how particle shape influences the rheological properties of suspensions.*

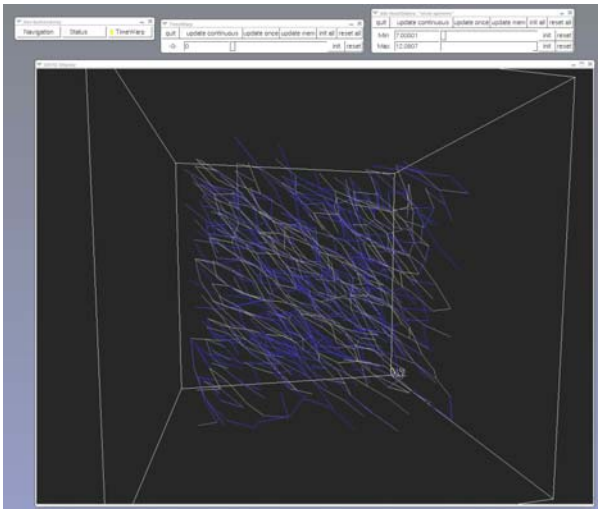

Figure 38. *A snapshot of the sfvis tool.*

Visualization of Stress in Aggregate Flow. A high performance dissipative particle dynamics code for the modeling of aggregate flow developed jointly by MCSD and BFRL 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 there 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 among neighboring spheres in a suspension. This capability has already proven quite useful. For example, as a result of viewing our visualizations, it became clear 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.

Recently, our dynamic hard sphere stress visualization software was completely re-written to utilize the open scene graph software tree, and renamed Suspension Flow Visualization (sfvis). sfvis allows the interactive exploration of simulation output. The preliminary version implements spheres color coded to stress values. A slider allows the displayed spheres to be culled, matching the desired range for stress values. Exploration can utilize color coded spheres that represent the total stress values at each point, or color coded line segments that represent stress values between each point. A slider allows control of the animation speed. See Fig. 38.

To produce the visualizations, the data is 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 the shear stress and normal stress values computed in the simulation.

The new software is very efficient. In one test case, use of the new software reduced the application load time from 7 minutes to 30 seconds. sfvis will ultimately be utilized to visualize the large-scale data sets generated by the BFRL/MCSD QDPD code utilizing the time we were awarded on the NASA Columbia supercomputer.

A demo exploring the flow of suspensions withsfvis was presented at the Nov 29-30, 2006 VCCTL meeting that was held at NIST Gaithersburg.

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

Visualization of a Coal Mine

Terence Griffin
Adam Lazrus
Judith Terrill
Chiara Ferrarais (NIST BFRL)

Using data supplied by Joseph Francis Giacinto and Leonard Geruus Rafalko (ERM) in conjunction with Paul Anthony Petzrick (Maryland Department of Natural Resources), we created visualizations of an abandoned coal mine under consideration for remediation.

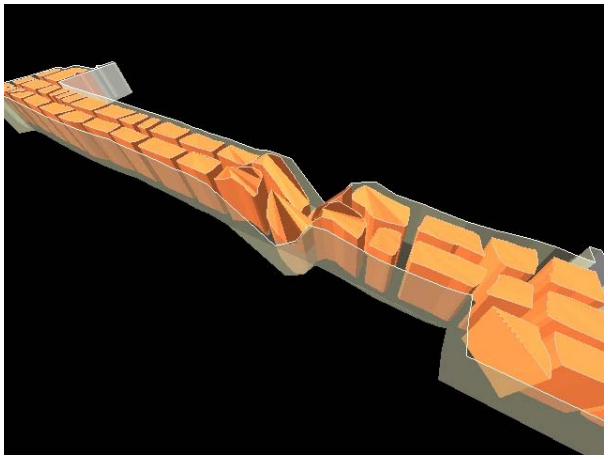

Figure 39. *3D Visualization of a coal mine. Sunken area in middle is clearly visible.*

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 atomic structure obtained from theoretical models and computational simulations of the optical properties of nano-scale atomic systems developed in collaboration with colleagues in the NIST Physics Lab. The visualization codes are able to display the original lattice of the electrons as well as the core area of the computational results. Using this code, we have 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 coarse-grained charge densities as a step toward more complex visualizations. This visualization work required the use of a different representation for each region in a structure. See Figs. 40 and 41. A paper on this work was presented at the March meeting of the American Physical Society (APS):

> J. Sims, G. W. Bryant, and H. Hung, "Excitons in Negative Band-Gap Nanocrystals," APS March Meeting, Baltimore, MD, March 2006.

Howard Hung's immersive visualization of a quantum dot appeared in the online supplement of the June 2006 issue of *National Geographic* magazine[4]. See the cover of this report.

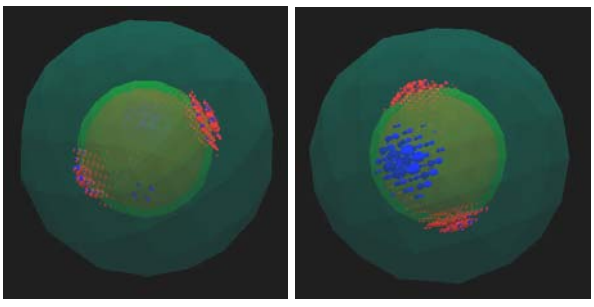

Figure 40. *Two different views of atomic state density of an electronic state trapped in the well region of a nanohetereostructured nanocrystal.*

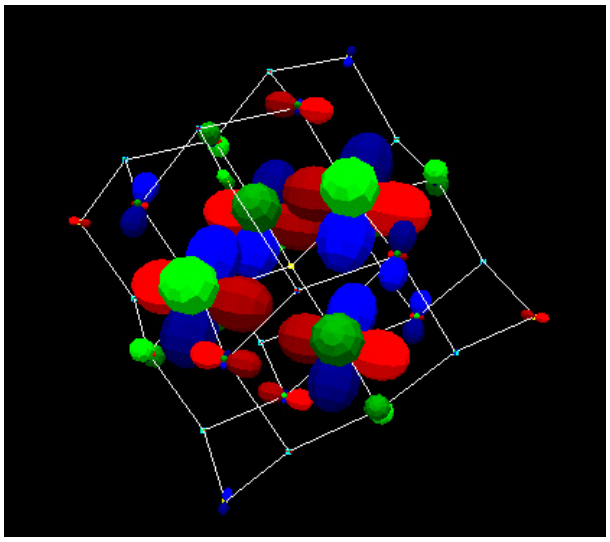

Figure 41. *Image of p orbitals. The white lines in the figure are the nearest neighbors of each atom.*

Feature Detection

Adele Peskin
Judith Terrill

To enable visualization of measured three-dimensional data it is necessary to convert the data into a form suitable for a graphics system. The new representation may, in fact, offer advantages for purposes other than pure visualization. Recently we have begun to explore the extraction of information on 3D features from polygonal surfaces used in visualization systems. Such polygonal surfaces do not have connectivity information themselves, but the associated adjacency lists can, in fact, be used for feature detection. To enable this work, we have developed filters to compute connectivity graphs of polygonal surfaces represented in our savg file format.

To explore the feature detection capabilities of such representations, we implemented software to find the curve-skeletons of images of 3D objects. The software, stores the voxels from image files in an octree, and then defines a 3D field across each voxel based on its distance from surface edges. The curves grow from critical points in the field. See Figs. 42 and 43. Similar software was used to create streamlines in electric and magnetic field data, which was originally visualized only as a set of vectors. The divergence of each field was calculated numerically, and then points of maximum divergence were used as seed points of the streamlines. See Fig. 44.

[4] http://www7.nationalgeographic.com/ngm/0606/feature4/ gallery2.html

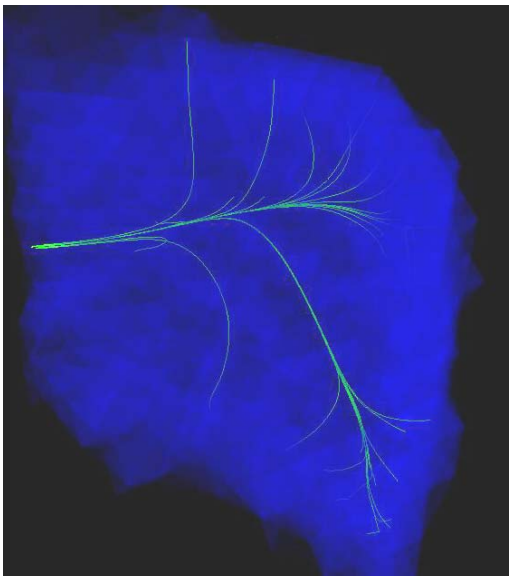

Figure 42. *Curve-skeleton from an image file of a rock.*

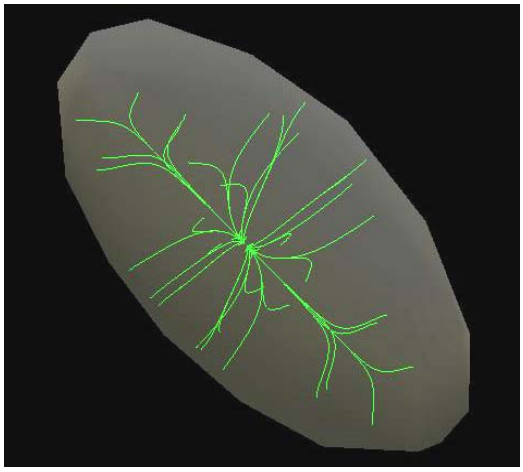

Figure 43. *Curve-skeleton made from the divergence field on an ellipsoid.*

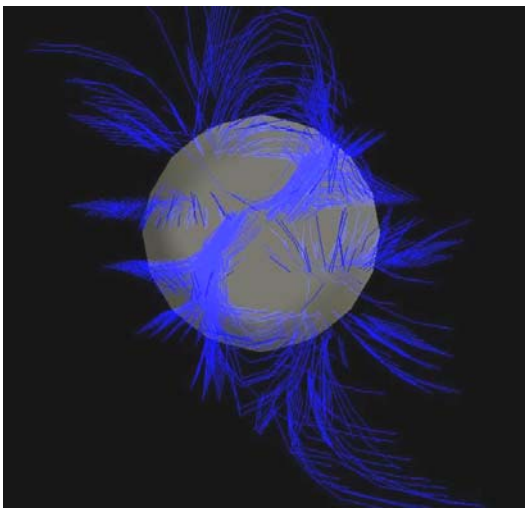

Figure 44. *Streamlines of the electric field around an array of atoms in a nanostructure.*

3D Chemical Imaging at the Nanoscale

William George
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John Hagedorn
John Kelso
Adele Peskin
Judith Terrill
Anthony Kearsley
Eric Steel (NIST CSTL)
John Henry Scott (NIST CSTL)
John Bonevich (NIST MSEL)
Zachary Levine (NIST 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 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: techniques for the visualization of 3D data in an immersive environment, techniques for interactions with immersive visualizations, algorithms and analysis, and parallelization of simulation codes

We recently completed a port of the 3D chemical imaging application EPQ to our parallel distributed software environment, SSS. EPQ is a Monte Carlo application that is a simulation of a scanning electron microscope, tracking the trajectories of electrons and determining the output of the detectors given a description of the target material. It was implemented in a mix of Java and Python, and was 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. Test runs of this application have begun on 32 processors of the ITL/PL Raritan cluster.

We completed a Fortran program to compute the alignment of fiducial marks with an unknown rota-

tion axis. The alignment is a critical phase of microtomography. In contrast to medical imaging, where it is possible to hold the samples and detectors fixed on the scale of the pixel (about 100 um), generally this is impossible in microtomography where the pixels are typically 1 nm for electron microscopy or 10 nm for x-ray microscopy. In practice, every image is subject to an arbitrary translation which must be removed by an analysis of the scene. Solutions to the alignment problem generally either include or exclude fiducials. Here, we use fiducial marks. In addition, we assume rigid-body motion of all the fiducials. We also assume that the fiducial marks may be distinguished from one another in each image and identified with a single three-dimensional object. Typically in tomography where a single-axis tilt series is acquired, the experimentalist reports the tilt angle as a single value. In the present work, the tilt axis may be in almost any direction; only the case of the tilt axis aligned with the beam direction is excluded.

One paper was written on this work:

Z. Levine, A. Kearsley, and J. Hagedorn, “Bayesian Tomography for Projections with an Arbitrary Transmission Function with an Application to Electron Tomography,” accepted by *Journal of Research of NIST*.

This work has been supported in part by the NIST Innovations in Measurement Science Program.

Fundamental Mathematical Software Development and Testing

OOF: Object-Oriented Finite Elements

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Rhonald Lua (Penn State University)
Valerie Coffman (Cornell University)
R. Edwin Garcia (Purdue University)

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

See feature article, page 37.

Parallel Adaptive Refinement and Multigrid Finite Element Methods

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Eite Tiesinga (NIST PL)
Pascal Naidon (NIST PL)

http://math.nist.gov/phaml

Finite element methods using adaptive refinement and multigrid techniques have been shown to be very efficient for solving partial differential equations on sequential computers. Adaptive refinement reduces the number of grid points by concentrating the grid in the areas where the action is, and multigrid methods solve the resulting linear systems in an optimal number of operations. W. Mitchell has been developing a code, PHAML, to apply these methods on parallel computers. The expertise and software developed in this project are useful for many NIST laboratory programs, including material design, semiconductor device simulation, and the quantum physics of matter.

This year the effort was focused on two areas: preparing PHAML for its first non-beta release, and application of PHAML to solve Schrödinger's Equation for eigenvalues and eigenstates relevant to optical traps for neutral atoms, in collaboration with E. Tiesinga of the Quantum Processes group of NIST's Atomic Physics division. Understanding the interactions of adjacent atoms corresponding to qubits of a quantum gate involves computing multiple eigenvalues in the middle of the spectrum, with eigenstates that have sharp gradients, which is a very challenging computation. The major accomplishments for FY 2006 are the following:

- Added support for curved domains in PHAML.
- Wrote a comprehensive suite of test problems for PHAML.
- Wrote an extensive User's Guide for PHAML.
- Several other minor improvements to PHAML were made. Four minor releases of the code occurred as the code evolved.
- Performed numerical experiments with the trapped interacting atoms model to see how the eigenvalues are affected by varying the scattering length of the atoms and the aspect ratio of the trap.
- Computed solutions of Schrödinger's Equation in the stadium domain.
- Computed solutions of a 2-channel Feshbach model.
- P. Naidon used PHAML to numerically confirm his theories concerning collisions of trapped atoms.

Future work will continue to enhance PHAML with additional capabilities and robustness, improve the hp-adaptive method to work automatically with more general problems, parallelize the high order multigrid method, study error estimators for eigenvalue problems, improve the robustness of the Schroedinger application code, perform further physics experiments using the code, and extend the application to a multichannel model with time-dependent systems of equations.

References

[1] W.F. Mitchell, "The Addition of hp-Adaptivity to a Parallel Adaptive Finite Element Program," Twelfth SIAM Conference on Parallel Processing for Scientific Computing, February 2006.

[2] W.F. Mitchell, "PHAML: A Parallel hp-Adaptive Multigrid Program for 2D Elliptic Problems," Fifth International Conference on Scientific Computing and Applications, May 2006.

[3] W.F. Mitchell, "A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids," *Journal of Parallel Distributed Computing*, to appear.

[4] P. Naidon, E. Tiesinga, W.F. Mitchell and P.S. Julienne, "Effective-range Description of a Bose Gas Under Strong Confinement," *New Journal of Physics*, submitted.

[5] W.F. Mitchell, "PHAML User's Guide," NISTIR 7374, 2006.

Sparse BLAS Standardization

Roldan Pozo
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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. Subsequently, 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.

We subsequently have developed several C and C++ implementations of the standard. This year we completed and relesed a second-generation simplified C++ interface which serves to further reduce the software complexity overhead by shrinking the number of lines in the specification and corresponding code. While our previous implementations of the Sparse BLAS managed to fit all of the functionality and operations into 2,500 lines of C++ code, the latest proposal introduces an even smaller interface that captures the core operations of the Level 1, 2, and 3 kernels in less than 150 lines. (As a reference point, our preliminary version of a Sparse BLAS library in 1996 contained nearly half a million lines and required complicated Makefiles to generate and build the library.) This new condensed interface uses ANSI C++ templates and virtual abstract classes to ensure that derived Matrix classes adhere to the function signatures, yet it remains type independent, thus allowing for further extensions, such as interval classes or extended precision arithmetic.

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 Fast Fourier Transforms (FFTs), Sucessive Over-Relaxation (SOR), Monte Carlo integration, sparse matrix multiply, and dense LU factorization, representating a 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 contains entries from more than 3,500 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.[5] Currently, SciMark inclusion in SPECjvm2006 is under development.

As of January 2007, the highest score being reported for SciMark is 1,043. This corresponds to the average Mflop performance of the five kernels, with some kernels such as LU factorization reporting over 2.0 Gflops on dual core processor PCs.

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

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 thousands of developers (more than 15,000 downloads in calendar 2006, for example) 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 3.2) provide support for both multidimensional arrays and integrate linear algebra modules which include fundamental algorithms (LU, Cholesky, SVD, QR, and eigenvalues), sparse matrix support, and support for iterative methods in solving linear systems with dense or sparse matrices. In particular, a new interface proposal for iterative methods has been presented and new implementations are under development to integrate TNT with other software libraries.

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.

A Metrological Approach to the Verification & Validation of Computer Models of High Consequence Engineering Systems

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Hung-Kung Liu
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)
Borchin Chang (Drexel University)
Jack Zhou (Drexel University)
Barry Bernstein (Illinois Institute of Technology)
Willem Roux (Livermore Software Technology)
Nielen Stander (Livermore Software Technology)
Glenn B. Sinclair (Louisiana State University)
Tomasz Wierzbicki (MIT)
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Cary Tuckfield (Savannah River Nat. Lab, DOE)
Ala Tabiei (University of Cincinnati)
John Bowles (University of South Carolina)
Yuh J. Chao (University of South Carolina)
Bill Ranson (University of South Carolina)
Don Edwards (University of South Carolina)
Robert Rainsberger (XYZ Scientific Applications)

This research grew out of two competence projects entitled "Complex System Failure Analysis: A Computational Science Based Approach (FY04-08)" and "Modeling of Contact Dynamics of Silicon Cantilevers for Applications in Atomic Force Microscopy, Nanoscale Manufacturing Technology, and Biomedical Nano-mechanics (FY05-06)." A summary of each of those two projects appears elsewhere in this report.

An outstanding issue in those two competence projects and in emerging technologies such as nanotechnology and biotechnology, is the reliability of the underlying scientific and engineering (S&E) software. Such software enables the modeling and simulation needed to develop new instrumentation, to gain understanding of fundamental principles that enable development of new technologies and products, and to design safety-critical engineering systems. S&E software systems have grown in size and complexity, today often involving millions of lines of code. Those complex codes, developed over many years by large teams, deliver simulations of reality over a wide range of spatial and temporal scales. Since S&E software codes are never released with a global "guarantee" of correctness, the users must devote considerable resources to plan and conduct *ad-hoc* numerical experiments before using the software with confidence. The process of determining whether S&E software correctly produces the solution to an abstract mathematical model is

termed *verification*. Determining whether the computer model serves as a sufficiently good proxy for the physical system under study is called *validation*.

Verification of S&E software is difficult primarily because, unlike physical experiments for which metrology (e.g., NIST SRMs) serves as the basis for correctness, there is no "metric" for the user to gauge the effectiveness of numerical experiments. In FY05 and 06, ITL collaborated with MSEL and numerous non-NIST researchers and succeeded in developing a new approach to code verification by extending the so-called combined variance estimate method in round-robin and key-comparison metrological experiments to computer-generated simulations.

Subject to the availability of new funds, a number of applications of this metrological approach to code verification are being planned for a variety of engineering models ranging from nano-indentation to fracture toughness of reactor vessels.

Mathematical Knowledge Management

Visualization of Complex Function Data

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Qiming Wang (NIST ITL)
Sandy Ressler (NIST ITL)
Daniel Lozier
Frank W. J. Olver

http://dlmf.nist.gov/

See feature article, page 31.

Representation and Exchange of Mathematical Data

Bruce Miller
Daniel Lozier
Abdou Youssef
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.

- Authoring for multiple media.
- Conversion of legacy documents.
- Representation for both syntax and semantics.
- Classification and identification of mathematical resources.
- Display and accessibility of formulas.
- Math-aware search.

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 FY 2006 on authoring and conversion of LaTeX documents to web formats, and on difficult questions involving mathematical representation. 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.

Related to this work, Bruce Miller and Abdou Youssef were invited participants in the Hot Topic Workshop on The Evolution of Mathematical Communication in the Age of Digital Libraries held at the Institute for Mathematics and Its Applications, University of Minnesota, on December 8-9, 2006. Daniel Lozier served on the Program Committee of the Fifth International Conference on Mathematical Knowledge Management held in Reading, UK, on August 10-12, 2006. Youssef presented a talk there also. Finally, Bruce Miller has been an active participant in the W3C Math Working Group.

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

Math Search Techniques and Systems

Abdou Youssef
Bruce Miller

The vast reach of the Internet and emerging XML-based technologies have prompted efforts worldwide to create and codify digital libraries of mathematical, scientific, and engineering contents, for the purpose of processing and disseminating technical knowledge at an unprecedented scale. Notable examples include the Digital Library of Mathematical Functions (DLMF) project at NIST, and the W3C XML-based mathematical markup language standard, MathML.

To benefit from such digital libraries, users should be able to search those libraries conveniently and effectively. Toward that end, several important objectives must be met: Users should be able to search not only for text, but also for formulas, equations, expressions, and other mathematical constructs. Due to the heavy usage of symbolic and abstract notations in math and science, the search should be based not only on explicitly occurring terms, but also on metadata that describe the contents and the structures and relationships therein. For users to identify relevant search results quickly, the hits should be rank-ordered using relevance criteria appropriate to (1) the special nature of mathematical information, and (2) the needs and skill sets of specialized users. To further assist users to select relevant hits, each hit must be accompanied with a brief yet representative and query-relevant summary of the target document.

This project is involved in developing search techniques and systems that meet those objectives. Early on in the project, effective techniques were developed that fulfilled the first objective. In 2006, the project focused on the incorporation, utilization and refinement of math metadata for more powerful, more useful search. Metadata sets were created for various mathematical entities, making use of the available literature and standard terminology and nomenclatures used in the mathematical and scientific communities. Search technology was developed in the project for integrating the metadata into the search process so that users' queries can yield relevant results even if the query keywords are not in 100% agreement with authors' terminology.

Also, considerable efforts were invested in 2006 into defining and implementing new relevance metrics for math search, and into designing methods for distilling hit target documents into meaningful and relevant summaries to accompany hits. These foundations will be the basis for fulfilling objectives 3 and 4 in the coming year.

The techniques and software resulting from this project will be put to use in the search engine of DLMF, and is expected to benefit thousands of digital math/science libraries worldwide. Furthermore, the knowledge generated in the project is already being used and will continue to be used by other math search engine designers and developers.

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

Digital Library of Mathematical Functions

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Nico Temme (CWI, Amsterdam)

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 by use of *metadata*, providing for much richness in Web interconnections, Web annotation, Web search, 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.

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 handbook will consist of 33 chapters devoted to individual classes of special functions plus 4 chapters on algebraic and analytical methods, asymptotic approximations, numerical methods, and computer algebra. 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 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, (v) proof-of-concept integration of software tool prototypes into the DLMF Web site, (vi) research into the frontiers of technical search methodology to enable effective queries involving fragments of technical mathematics, and (vii) integration of a prototype 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.

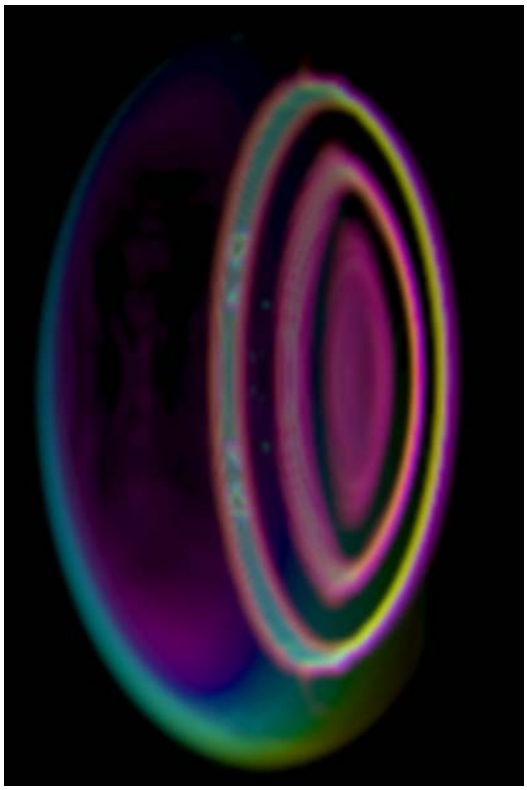

Figure 45. *Many nonlinear ordinary and partial differential equations have solutions that may be expressed in terms of Jacobian elliptic functions. These include the Schrödinger equation. This equation can be used to model the formation of vortex rings in Bose Einstein condensates. Results of such a simulation done at NIST are pictured here.*

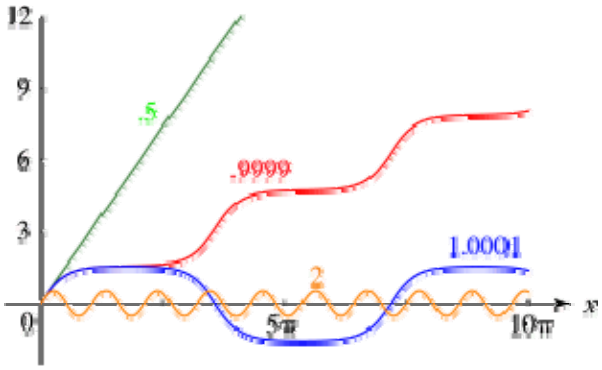

Figure 46. *The Jacobian* am*(x,k) function for four values of the parameter k. These functions arise in the classical analysis of the dynamics of pendulums.*

By the end of calendar year 2006, 30 chapters had been validated, prepared for placement on the Web, and placed on http://orion.cam.nist.gov/dlmf/ (accessible only from inside NIST). Validation confirmed the mathematical correctness of these chapters. Preparation for placement on the Web included inser-

tion of metadata that does not affect the print version in any way but that provides some of the rich interconnections we envision for initial and subsequent releases of the public Web site. For example, every symbol is linked to its definition. As an illustration, consider the equation

$$sn(x,k) = \sin(am(x,k)).$$

A Web user is able to "call up" the definitions of sn (a Jacobian elliptic function), x and k (real variables), sin (the trigonometric function), and am (the Jacobian amplitude function), whereas a book user would have to search back in the text for the definitions. Incidentally, this equation can be located using the search tool with the query "sn am". It is the second equation on the hit list.

Also in 2006, an in-depth external usability review of the Web site by Dalhousie University was completed. This review led to spirited discussions with the Dalhousie reviewers of what is the "right way" to search for and present mathematics on the screen. Of course there is not just one way, but several substantial improvements were made to the Web site as a result of these discussions.

Our targets for the remaining work are as follows: March 31 for validating the remaining 7 chapters and integrating them into the Web site, June 30 for submittal of the computer files to the publisher, and the final quarter of 2007 for publication of the book and release of the public Web site.

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

Mathematical Software Reference Databases

Ronald Boisvert
Marjorie McClain
Bruce Miller
Roldan Pozo

http://math.nist.gov/
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 calendar year 2006, the virtual server math.nist.gov satisfied nearly seven million requests for pages, or more than 19,000 per day. More than 1.7 Gbytes of data were shipped each day, and more than 539,000 distinct hosts were served. The virtual server gams.nist.gov, delivered 930,000 pages, or more than 2,500 per day. There have been nearly 115 million "hits" on MCSD Web servers since they went online as NIST's first web servers in 1994.

Among the individual software packages that we have developed and continue to distribute via our website, those with the highest number of source code downloads for 2006 were the following.

- Template Numerical Toolkit (linear algebra using C++ templates): 15,310 downloads
- Jama (linear algebra in Java): 13,656 downloads
- SparseLib++ (elementary sparse matrix manipulation in C++): 4,284 downloads

Part IV

Activity Data

Publications

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Refereed Journals

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1. D. M. Anderson, P. Cermelli, E. Fried, M. E. Gurtin, and G. B. McFadden, "General dynamical sharp-interface conditions for phase transformations in viscous heat-conducting fluids," *Journal of Fluid Mechanics*.
2. D. Cotrell and A. Kearsley, Flow Control Through the Use of Topography, *Journal of Research of NIST*.
3. J. T. Fong, J. J. Filliben, and R. J. Fields, "Uncertainty Quantification of Material Properties of Two Types of Steels at Elevated Temperatures for Stochastic Modeling of Structures on Fire," *Proceedings of a Three Metals Society (TMS) Symposium on Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World,* Feb. 25-Mar. 1, 2007, Orlando, FL.
4. J. T. Fong, J. J. Filliben, W. F. Ranson, and P. V. Marcal, "A Real-Time Non-Contact and Direct-Measurement-based Fatigue Life Prediction Methodology with Uncertainty & Risk Analyses," *Proceedings of the National Nuclear Security Administration (NNSA) Future Technologies Conference II, Track Four (Future Trends in Analysis and Characterization)*, Oct. 11-12, 2006, Washington, DC.
5. J. T. Fong, J. J. Filliben, R. J. and R. J. Fields, "An Uncertainty & Risk-based Approach toward a Cost-Effective High-Temperature Material Property Database," *Proceedings of the National Nuclear Security Administration (NNSA) Future Technologies Conference II, Track Three (Materials Technology Trends for Defense & National Security)*, Oct. 11-12, 2006, Washington, DC.
6. D. E. Gilsinn, F. A. Potra, "Integral Operators and Delay Differential Equations," *Journal of Integral Equations and Applications*.
7. D. E. Gilsinn, "Computable Error Bounds for Approximate Periodic Solutions of Autonomous Delay Differential Equations," *Nonlinear Dynamics*.
8. J. Hagedorn, S. Satterfield, J. Kelso, W. Austin, J. Terrill, and A. Peskin, "Correction of Location and Orientation Errors in Electromagnetic Motion Tracking," *Presence*.
9. Z. Levine, A. Kearsley, and J. Hagedorn, "Bayesian Tomography for Projections with an Arbitrary Transmission Function with an Application to Electron Tomography," *Journal of Research of NIST*.
10. L. Melara, A. Kearsley, and R. Tapia, "Augmented Lagrangian Homotopy Method for the Regularization of Total Variation Denoising Problems," *Journal of Optimization Theory and Applications.*
11. J. Miltat and M. Donahue, "Numerical Micromagnetics: Finite Difference Methods," in *Handbook of Magnetism and Advanced Magnetic Materials*, Wiley.
12. W. F. Mitchell, "A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids," *Journal of Parallel and Distributed Computing*.
13. R. Radebaugh, A. O'Gallagher, M.A. Lewis, and P.E. Bradley, "Proposed Rapid Cool Down Technique for Pulse Tube Cryocoolers," *Cryocoolers*.
14. B. Rust, "Carbon Dioxide, Global Warming, and Michael Crichton's 'State of Fear'," *Computing Science and Statistics* **37**.

Submitted

1. I. Beichl, S. Bullock, and D. Song, "A Quantum Algorithm Detecting Concentrated Maps," *Journal of Research of the NIST*.
2. D. L. Cotrell, G. B. McFadden, W. E. Alley, and B. J. Alder, "Effect of an Axially-periodic Radius of the Linear Stability of Pipe Flow," *Journal of Fluid Mechanics*.
3. T. Dennis, S. D. Dyer, and A. Dienstfrey, "Phase-Dispersion Light-Scattering for Quantitative Size-Imaging of Spherical Scatterers," *Optics Express*.

4. R. Dersimonian and R. Kacker, "Quantification of Uncertainty in Meta-analysis," *Controlled Clinical Trials*.

5. M. J. Donahue and R. D. McMichael, "Micromagnetics on curved geometries using rectangular cells: error correction and analysis," *IEEE Transactions on Magnetics*.

6. D. E. Gilsinn, "On Algorithms for Estimating Computable Error Bounds for Approximate Periodic Solutions of an Autonomous Delay Differential Equation," *Communications in Nonlinear Science and Numerical Simulation.*

7. D. E. Gilsinn, M. A. McClain, C. Witzgall, "Non-Oscillatory Splines on Irregular Data," *Proceedings of SIAM Conference on Geometric Design & Computing*, October 30 – November 3, 2005, Phoenix, AZ.

8. D. E. Gilsinn, G. S. Cheok, C. Witzgall, A. M. Lytle, "Construction Object Identification from LADAR Scans: An Experimental Study Using I-Beams," *Automation in Construction*.

9. D. E. Gilsinn, "Approximating Periodic Solutions of Autonomous Delay Differential Equations," *NISTIR*.

10. J. Hagedorn, J. Dunkers, S. Satterfield, A. Peskin, J. Kelso, and J. Terrill, "Measurement Tools for the Immersive Visualization Environment: Steps Toward the Virtual Laboratory," *Virtual Reality*.

11. F. Y. Hunt, A. K. Gaigalas, and L. Wang, "Mathematical Foundation of the Frequency Domain Technique for Measuring Photodegradation," *Journal of Physical Chemistry A*.

12. R. N. Kacker, and J. F. Lawrence, "Trapezoidal and Triangular Distributions for Type B Evaluations of Standard Uncertainty," *Metrologia*.

13. E. Knill, "On Protected Realizations of Quantum Information," *Physical Review A*.

14. E. Knill, G. Ortiz, R. Somma, "Optimal Quantum Measurements of Expectation Values of Observables," *Physical Review A*.

15. Y. Lei, R. Carver, R. Kacker, and D. Kung, A Combinatorial Testing Strategy for Concurrent Programs, *Software Testing, Verification, and Reliability*.

16. Y. Lei, R. Kacker, R. Kuhn, V. Okum, and J. Lawrence, IPOG: A General Strategy for t-way Software Testing, *IEEE Conference on Engineering of Computer-Based Systems.*

17. Y. Lei, R. Carver, R. Kacker, and D. Kung, "Combinatorial testing for concurrent programs," *Software Testing, Verification, and Reliability.*

18. Z. H. Levine, A. Volkovitsky, and H. K. Hung, "Alignment of Fiducial Marks in a Tomographic Tilt Series with an Unknown Rotation Axis", *Computer Physics Communications*.

19. N. Mastronardi and D. P. O'Leary, "Robust Regression and Approximations for Toeplitz Problems," *Computational Statistics and Data Analysis*.

20. P. Naidon, E. Tiesinga, W. F. Mitchell and P. S. Julienne, "Effective-range Description of a Bose Gas under Strong Confinement," *New Journal of Physics*.

21. D. P. O'Leary, Z. Strakovs, P. Tichy, "On Sensitivity of Gauss-Christoffel Quadrature," *Numerische Mathematik*.

22. R. Somma, G. Ortiz, H. Barnum and E. Knill, "Efficient Solvability of Hamiltonians and Limits on the Power of Some Quantum Computational Models," *Physical Review Letters*.

23. B.J. Thijsse and B.W. Rust, "Freestyle Data Fitting and Global Temperatures," *Computing in Science & Engineering*.

24. W. E. Wallace, C. M. Guttman, K. M. Flynn, and A. J. Kearsley Numerical Optimization of Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry: Application to Synthetic Polymer Molecular Mass Distribution Measurement, *Analytical Chemistry*.

Presentations

Invited Talks

1. I. Beichl, "Graphs and Matchings," National Security Agency, Fort Meade, MD, Sept., 19, 2006.

2. T. Burns, "Steel Flow Stress Sensitivity to Temperature and Heating Rate: Recent Results from the NIST Pulse Heated Kolsky Bar," International Symposium on Plasticity, Halifax, Nova Scotia, Canada, July 17-22, 2006.

3. A. Carasso, "APEX Blind Deconvolution of Hubble Telescope Imagery and the Use of Levy Stable Laws," University of Minnesota School of Statistics Colloquium, October 20, 2005.

4. A. Carasso, "APEX Blind Deconvolution of Hubble Space Telescope Imagery and Other Astronomical Data," Second International Conference on Scientific Computing and Partial Differential

Equations and First East Asia SIAM Symposium, Hong Kong, China, December 12-16, 2005.

5. A. Carasso, "Blind Deconvolution of Hubble Space Telescope Imagery," SIAM 2006 Image Science Meeting, Minisymposium on Variational and PDE Methods in Image Decomposition, Minneapolis, MN, May 17, 2006.
6. M. J. Donahue, "Micromagnetics on Curved Geometries Using Rectangular Cells: Error Correction and Analysis," Micromagnetics: Experiments, Modeling, and Mathematical Theory Workshop, Bonn, Germany, Sept. 5, 2006.
7. J. Fong, "NAS/NRC Postdoctoral Research Opportunities in Engineering and Mathematical Sciences at National Institute of Standards and Technology," Drexel University, Philadelphia, PA, Oct. 21, 2005.
8. J. Fong, "Stochastic Modeling of Complex Structural System Failures and a Metrology-based Approach to V&V of Computer Simulations," Drexel University, Philadelphia, PA, Oct. 21 2005.
9. J. T. Fong, "Scientific and Engineering Software (S&ES) Verification for Metrology and High-Consequence Engineering Applications," Computational & Statistical Science Seminar, Savannah River National Laboratory, Aiken, SC, April 27, 2006.
10. J. Fong, "A Real-Time Non-Contact Direct-Measurement-based Reserve Capacity Modeling of an Earthquake Monitoring System," University of British Columbia**,** Vancouver, B.C., Canada, July 21, 2006.
11. J. Fong, "A Reference-Benchmark Approach to Verification and Validation of High-Consequence Engineering System Simulations," University of British Columbia**,** Vancouver, B.C., Canada, July 28, 2006.
12. J. Fong, "Scientific and Engineering Software Verification for Metrology and High-Consequence Engineering Applications," Louisiana State University, Baton Rouge, LA., Sept. 29, 2006.
13. J. Fong, "Stochastic Finite Element Method and Design of Experiments for Pressure Vessels & Piping Decision Making," ASME Pressure Vessels & Piping Conference, Vancouver, B.C., Canada, July 26, 2006.
14. J. Fong, "Construction of a Helmholz Free Energy Function for an Isotropic Elastic-Viscoplastic Material," 2006 Meeting of the Society of Engineering Science, Penn State University, State College, PA, Aug. 14, 2006**.**
15. F. Hunt, "Visualizing the Frequency Patterns of DNA," New York University Faculty Resource Network Summer Program, New York, NY, June 16, 2006.
16. S. Glancy, "Error Analysis For Encoding A Qubit In An Oscillator," Linear Optical Quantum Information Processing Workshop, Baton Rouge, Louisiana, April 9 - 12, 2006.
17. E. Knill, "Quantum Computing With Very Noisy Gates," Workshop on Trapped Ion Quantum Computing, NIST Boulder, February 21-24, 2006.
18. E. Knill, "Fault-tolerant Architecture for Very Noisy Gates," University of Calgary, June 7, 2006.
19. D. W. Lozier, "The DLMF Project: Lessons Learned and Future Directions," AMS Eastern Section Meeting, Bard College, Annandale-on-Hudson, NY, October 8, 2005.
20. D. W. Lozier, "Math on the Web and the Digital Library of Mathematical Functions Project," SIAM Washington-Baltimore Section Meeting, Johns Hopkins University, Baltimore, MD, November 9, 2005.
21. D. W. Lozier, "The Role of Computer Algebra in the DLMF Project," East Coast Computer Algebra Day, Drexel University, Philadelphia, PA, May 6, 2006.
22. G. McFadden, "Steady States and Oscillations in the p53/Mdm2 Network," NIH Laboratory of Molecular Pharmacology in the National Cancer Institute, Modeling Journal Club, October 18, 2005.
23. B. Miller, DLMF, "LaTeXML and Some Lessons Learned", Hot Topic Workshop on The Evolution of Mathematical Communication in the Age of Digital Libraries, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, December 8-9, 2006.
24. D. P. O'Leary, "Matrix Factorizations for Information Retrieval," Stanford/Yahoo! Workshop on Modern Massive Datasets, Stanford, CA, June 2006.
25. D. Porter, Tcl Core Team Town Meeting, panel member, Portland, OR, October 26, 2005.
26. B. Saunders, "Dynamic 3D Visualizations for the NIST Digital Library of Mathematical Functions," Twenty-first Willie Bee Rajanna Lecture, Department of Mathematics, Morgan State University, April 20, 2006.
27. A. Youssef, "Relevance Ranking and Hit packaging in Math Search," Hot Topic Workshop on The Evolution of Mathematical Communication in the Age of Digital Libraries, Institute for Mathematics

and Its Applications, University of Minnesota, Minneapolis, December 8-9, 2006.

28. A. Youssef, "Roles of Math Search in Mathematics", 5th International Conference on Mathematical Knowledge Management, Wokingham, UK, August 11-12, 2006.

Conference Presentations

1. D. M. Anderson, "Sharp-interface conditions for fluid-fluid systems undergoing phase transformation," American Physical Society, Division of Fluid Dynamics Annual Meeting, Tampa, FL, November 19-21, 2006.
2. H. Bennett, A. Dienstfrey, L. Hudson, T. Oreskovic, T. Fuerst, and J. Sheppard, "Bone Mineral Density as a Biomarker for Assessing Bone Health: Bone Imaging," U.S.M.S. Workshop: Imaging as a Biomarker, NIST, Gaithersburg, Sept. 14-15, 2006.
3. T. Burns, "Effect of Rapid Heating on the Flow Stress in a Carbon Steel of Interest in Manufacturing," 6th European Solid Mechanics Conference, Budapest, Hungary, August 28 - September 1, 2006.
4. M. J. Donahue and D. G. Porter, "Magnetization Normalization Methods for Landau-Lifshitz-Gilbert," MMM 2005, San Jose, California, Nov. 1, 2005.
5. J. Dunkers, J. Hagedorn, A. Peskin, J. Kelso, J. Terrill, and L. Henderson, "Interactive, Quantitative Analysis of Scaffold Structure Using Immersive Visualization," poster presentation at 2006 Summer Bioengineering Conference, Amelia Island Plantation, Amelia Island, FL, June 21 - 25, 2006
6. W. George, J. Lancien, J. Terrill, "MPMD Program Model for Scientific Computing," Scatter/Gather Session II, Supercomputing 2005, Seattle, WA, Nov. 12-18, 2005.
7. D. E. Gilsinn, M. A. McClain, and C. Witzgall, "Non-Oscillatory Splines on Irregular Data," SIAM Conference on Geometric Design and Computing, Phoenix, AZ, October 30-November 3, 2005.
8. S. Glancy, H. Vasconcelos, and E. Knill, "Production of Optical Coherent State Superpositions Using the Kerr Effect," Southwest Quantum Information and Technology, Albuquerque, NM, Feb. 16-19, 2006.
9. J. Hagedorn, J. Terrill, J. Kelso, and J. Dunkers, "Measurement of Tissue Engineering Scaffold Material," (video) DIVERSE Birds of a Feather session at the SIGGRAPH 2006 Conference, Boston, MA, August 2, 2006.
10. R. Kacker, "Uncertainty Associated with Virtual Measurements from Computational Quantum Chemistry Models," National Conference of Standards Laboratories International (NCSLI) (www.ncsli.org), Nashville, TN, August 7-10, 2006.
11. A. Kearsley, "Recovery of Spheres from LADAR Data," IEEE Applied Imagery Pattern Recognition Workshop, Washington DC October 10, 2006
12. J. Kelso, "DIVERSE," DIVERSE Birds of a Feather (BOF) session; IEEE Visualization 2005 Conference, Seattle, WA, Nov. 12-18, 2005.
13. J. Lancien, W. George, and N. Martys, "Quaternion Dissipative Particle Dynamics," VCCTL Annual Meeting, NIST, Gaithersburg, MD, Nov. 29, 2005.
14. W .F. Mitchell, "The Addition of hp-Adaptivity to a Parallel Adaptive Finite Element Program," Twelfth SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, February 23, 2006.
15. W .F. Mitchell, "PHAML: A Parallel hp-Adaptive Multigrid Program for 2D Elliptic Problems," Fifth International Conference on Scientific Computing and Applications, Banff, Alberta, Canada, May 18-21, 2006.
16. S. Satterfield, "Shell Script VR," DIVERSE Birds of a Feather (BOF) session; IEEE Visualization 2005 Conference, Seattle, WA, Nov. 12-18, 2005.
17. B. Saunders, "From B-Spline Mesh Generation to Effective Visualizations for the NIST Digital Library of Mathematical Functions" Sixth International Conference on Curves and Surfaces, Avignon, France, June 29 - July 5, 2006.
18. J. Sims, G. Bryant, and H. Hung, "Excitons in Negative Band Gap Nanocrystals," American Physics Society March Meeting, Baltimore, MD, March 14, 2006.
19. W. E. Wallace, C. M. Guttman, K. M. Flynn, and A. J. Kearsley, "Development of NIST SRM 2881, an Absolute Molecular Mass Distribution Polymer Standard," American Society for Mass Spectrometry Annual Meeting, Seattle, WA, May 28, 2006.

Software Released

1. J. Lancien, W. George, and N. Martys, Parallel QDPD code, Virtual Cement and Concrete Testing Laboratory.
2. S. Langer, OOF2, Version 2.0 beta 8, Version 2.0.0, Version 2.0.1, http://www.ctcms.nist.gov/oof/oof2
3. B. Miller, LaTeXML, Versions 0.4.1, 0.5.0, 0.5.1. http://dlmf.nist.gov/LaTeXML/
4. W. F. Mitchell, PHAML, Version 0.9.22, Version 0.9.23, Version 0.9.24, Version 0.9.25. http://math.nist.gov/tphaml
5. W. F. Mitchell, f90gl, Version 1.2.11, Version 1.2.12. http://math.nist.gov/tf90gl
6. W. F. Mitchell (co-developer), Zoltan, Version 2.0, Version 2.1. http://www.cs.sandia.gov/Zoltan/
7. D. Porter (release manager), Tcl/Tk, Version 8.4.12, Version 8.4.13, Version 8.5a4. http://www.tcl.tk/
8. R. Pozo, Sparse Basic Linear Algebra Subprograms (Sparse BLAS), ANSI C++ reference implementation. http://math.nist.gov/spblas/
9. R. Pozo, Template Numerical Toolkit (TNT), Version 3.0, Version 3.0.1, Version 3.0.2, Version 3.0.3. http://math.nist.gov/tnt
10. R. Pozo, SciMark 2, Version 1.c (C version). http://math.nist.gov/scimark/
11. S. Satterfield, SAVG Visualization demos, http://math.nist.gov/mcsd/savg/demos/index.html

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. G.W. Stewart (MCSD), "Sparse Low-Rank Approximations to Sparse Matrices," October 12, 2005.
2. J. Benedetto (University of Maryland), "Sigma-Delta Quantization and Finite Frames," November 2, 2005.
3. B. Layton (Drexel University), "Nanometrology and Micrometrology in Biological Systems," November 29, 2005.
4. D. Tolani (Intelligent Automation, Inc.), "Symbolic Time Series Analysis (STSA) for Anomaly Detection," December 6, 2005.
5. J. Boyar (University of Southern Denmark), "Scheduling Jobs on Grid Processors," Jan. 10, 2006.
6. S. Hagstrom (Indiana University), "Hylleraas-CI Calculations on the Beryllium Atom: A Progress Report," Jan. 24, 2006.
7. C. Shakarji (MEL), "A Look at Mathematical and Computational Issues in Manufacturing Inspection Using Coordinate Measuring Machines," Jan. 31, 2006.
8. S. Dey (Naval Research Laboratory), "Recent Advances in Finite Element Methods for Structural Acoustics," Mar. 28, 2006.
9. A. Varshney (University of Maryland), "Visual Computing: At the Crossroads of Realism, Modeling, and Perception," Apr. 12, 2006.
10. C. Witzgall (ITL), G. Cheok (BFRL), A. Kearsley (ITL), "Recovery of Spheres from LADAR Data," May 23, 2006.
11. J. Teresco (Williams College), "Parallel Adaptive Scientific Computation in Heterogeneous, Hierarchical, and Non-Dedicated Computing Environments," June 15, 2006.
12. B. Sneiderman (University of Maryland), "The Thrill of Discovery: Information Visualization for High Dimensional Spaces," Oct. 3, 2006.
13. M. Mascagni (Florida State University), "Using Simple Stochastic Differential Equations to Solve Complicated Partial Differential Equations," Oct. 18, 2006.
14. S. Bullock (IDA Center for Computing Sciences), "Projecting onto Qubit Irreps of Young Diagrams," Nov. 21, 2006.
15. B. Alpert (MCSD), "Sparse Representations and High Dimensional Geometry: What's the Excitement?" Dec. 5, 2006.

Local Events Organized

1. S. Langer, Organizer, OOF2 Workshop, August 2006.
2. A. Peskin, Member, Planning Board, Metrology for the Magnetic Data Storage Industry, USMS Workshop, October 20-21, 2005.
3. J. Terrill, Member, Planning Board, Developing New Standards for Antibody Measurement: Bring-

ing Metrology to Serology, USMS Workshop, February 21-22, 2006.

External Events Organization

1. 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.
2. R. Boisvert, Co-organizer, Minisymposium on "Recent Advances in Software Tools for Scientific Computing", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
3. J. Fong, Co-developer, Panel Session, ASME Pressure Vessels and Piping Division Conference, July 23-27, 2006, Vancouver, Canada.
4. D. W. Lozier, Co-organizer, Minisymposium on "Computation and Application of Special Functions in Scientific Computing," SIAM Annual Meeting, Boston, MA, July 10-14, 2006.
5. D.W. Lozier, Program Committee, Fifth International Conference on Mathematical Knowledge Management, Reading, UK, August 10-12, 2006.
6. D. W. Lozier, Co-organizer, Minisymposium on "Mathematical Knowledge Management", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
7. W. Mitchell, Scientific Committee, International Conference of Numerical Analysis and Applied Mathematics, Crete, Greece, September 2006.
8. W. Mitchell, Program Committee, International Conference on High Performance Computing, Networking and Communication Systems, Orlando, FL, July 2007.
9. F. Potra, Co-organizer, Minisymposium on "Interior Point Methods for Linear Programming", International Congress on Industrial and Applied Mathematics (ICIAM), Zurich, July 2007.
10. S. Satterfield and J. Kelso, Co-organizers, Birds of a Feather Session on "DIVERSE", IEEE Visualization 2005 Conference, Minneapolis, MN, Oct. 23-28, 2005.
11. S. Satterfield and J. Kelso, Organizers, Birds of a Feather Session on "DIVERSE", SIGGRAPH 2006 Conference, Boston, MA, Aug. 2, 2006.

Other Professional Activities

Internal

1. R. Boisvert and Abbie O'Gallagher, ITL Diversity Committee.
2. R. Boisvert, ITL representative, NIST Nanotechnology Strategic Working Group.
3. R. Boisvert, ITL representative, NIST Scientific Computing Steering Group.
4. D. Porter, MCSD representative, ITL Awards Committee.
5. Staff members regularly review manuscripts for the Washington Editorial Review Board (WERB) and the Boulder Editorial Review Board (BERB), as well as proposals for the NIST ATP and SBIR programs.

External

Editorial

1. B. Alpert, Associate Editor, *SIAM Journal on Scientific Computing*.
2. I. Beichl, Column Editor, *Computing in Science & Engineering*.
3. R. Boisvert, Associate Editor, *ACM Transactions on Mathematical Software*.
4. R. Boisvert, Area Editor (Numerical Analysis, Mathematical Software, and Computational Engineering, Finance, and Science), Computing Research Repository (CoRR), www.arXiv.org.
5. D. Gilsinn, special issue editor, *Journal of Research of the NIST,* Vol. 111, no. 2, March-April, 2006.
6. D. Gilsinn, Associate Editor, *ASME Journal of Computational and Nonlinear Dynamics*.
7. R. N. Kacker, Member, Editorial Board, *Journal of Applied Statistics.*
8. R. N. Kacker, Member, Editorial Board, *Total Quality Management and Business Excellence*.
9. D. Lozier, Associate Editor, *Mathematics of Computation*.
10. G. McFadden, Associate Editor, *Journal of Crystal Growth.*
11. G. McFadden, Associate Editor, *Interfaces and Free Boundaries*.
12. G. McFadden, Associate Editor, *SIAM Journal on Applied Mathematics*.

13. W. Mitchell, Associate Editor, *Applied Numerical Analysis and Computational Mathematics*.
14. W. Mitchell, Associate Editor, *Journal of Numerical Analysis, Industrial and Applied Mathematics*
15. W. Mitchell, Associate Editor, *International Journal of Applied Mathematics and Computational Science*.
16. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*.
17. J. Terrill, Special Issue Co-Editor (with Yang Cai of Carnegie Mellon University), *Journal of Information Visualization* (on Visual Analysis of Human Dynamics).

Boards and Committees

1. R. Boisvert, Co-chair, Publication Board, Association for Computing Machinery (ACM).
2. R. Boisvert, Ex-Officio Member, ACM Council.
3. R. Boisvert, Member, ACM Awards Committee.
4. R. Boisvert, Chair, International Federation for Information Processing's Working Group 2.5 (Numerical Software).
5. R. Boisvert, Member, External Review Panel, Institute for Defense Analysis' Center for Computing Sciences.
6. F. Hunt, Member, Executive Committee, Association for Women in Mathematics.
7. F. Hunt, Organizer, Joint Association for Women in Mathematics and European Women in Mathematics Olga Taussky Todd Prize Committee.
8. D. Lozier, Vice Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
9. B. Miller, Member, Math Working Group, W3C (the World Wide Web Consortium).
10. D. Porter, Member, Tcl Core Team.
11. J. Terrill, OpenFPGA Working Group.
12. J. Terrill, Federal High End Computing Implementation Task Force.
13. J. Terrill, Federal High End Computing Research and Development, and Infrastructure Interagency Working Groups, Networking and Information Technology Research and Development Program.

Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including *ACM Transactions on Mathematical Software, Applied Mathematics Letters, ASME Journal of Computational and Nonlinear Dynamics, ASME Journal of Manufacturing Science and Engineering, Computing in Science and Engineering,* IEEE Society for Signal Processing, *IEEE Transactions on Magnetics, IEEE Transactions on Microwave Theory and Techniques, International Journal of Plasticity, International Journal of Information Visualization, International Journal of Plasticity, Journal of Computational and Nonlinear Dynamics, Journal for Computer-Aided Engineering and Software, Journal of Information Visualization, Journal of Magnetism and Magnetic Materials*, *Journal of Mass Spectroscopy, Journal of Mathematical Analysis and Applications*, *Journal of the Mechanics and Physics of Solids, Journal of Physics D: Applied Physics, Journal of Vibration and Control*, *Nonlinear Dynamics*, *Physical Review A, Physical Review B, Physical Review Letters, Physics Letters A*, *SIAM Journal on Optimization, SIAM Journal of Scientific Computing, Software - Practice and Experience, The International Journal for Human Computer Studies*.
2. Staff members review proposals for the following research programs: Department of Energy, Department of Homeland Security, Engineering and Physical Sciences Research Council (EPSRC), and the 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 Labs

3M
3Motion Project (UK)
American Concrete Assoc.
American Hydro Corp.
Apple Computer
Bank of America
Borg Warner Transmission Systems
Chesapeake Cryogenics
Cisco Systems
DrecWay
Dupont
Electro Science Technologies
Elligno Inc.
Fakespace
Ford Research Labs
GE Corporate R&D
GeoCap
IBM Research

Industrial Light and Magic
Intelligent Automation, Inc.
Invensys
JAMSTEC
JP Engineering
KTH Solid Mechanics
Landacorp
Mac.com
Medical Media Lab
Merck Pharmaceutical
Northwest Numerics, Inc.
O'Donnell Consulting Engineers
Proctor & Gamble
Pulsic
Quovadx
Rationelle Software-Entwicklung
Raytheon Corp.
RedOlive, Inc.
Roche Molecular Systems, Inc.
Schweitzer Engineering Laboratories, Inc.
Setterholm, Inc.
SGI
Siemens
Siemans Westinghouse Power Corporation
Simplified Logic, Inc.
The MathWorks, Inc.
Timken Company
Torrent Corp. (Spain)
UGS Corp.
United Technologies Research Center
Verari Systems
Xerox
Xilinx

Government/Non-profit Organizations

Air Force Research Lab
Army Research Lab
Catania Astrophysical Observatory
Hanscom Air Force Base
Institute for Defense Analysis
J. Stefan Institute
N. Inst. Adv. Industrial Sci. Tech. (AIST, Japan)
Kirtland Air Force Base
Lawrence Livermore national Laboratory
Los Alamos National Laboratory
Medical Res. Council Lab. of Molecular Biology (UK)
NASA
National Institutes of Health
Naval Research Laboratory
National Security Agency
National Science Foundation
Oak Ridge National Laboratory
Ohio Supercomputer Center
Sandia National Laboratories
Savannah River National Laboratory
U.S. Department of Defense

Universities

A&T State University
Arizona State University
Bard College
Beloit College
Carnegie Mellon University
California Institute of Technology
Columbia University
Dalhousie University (Canada)
Delft University of Technology (The Netherlands)
Dresden University (Germany)
Drexel University
Federal University of Parana (Brazil)
Florida State University
Georg August Universität Göttingen (Germany)
George Mason University
Georgetown University
George Washington University
Hong Kong University (China)
Howard University
Indiana University
Indiana University - Purdue University Indianapolis
International University of Bremen (Germany)
Jackson State University
Johns Hopkins University
Louisiana State University
Macalester College
Massachusetts Institute of Technology
Monash University (Australia)
Moscow State Technical University (Russia)
Penn State University
Polish Academy of Sciences (Poland)
Purdue University
Rudjer Boskovic Institute (Croatia)
Russian Academy of Sciences (Russia)
San Diego State University
Siena College
Southern Methodist University
Stanford University
State University of New York
Technische Universität Berlin (Germany)
Technische Universität Darmstadt (Germany)
Technische Universität Munchen (Germany)
Tel Aviv University
Trinity University
Tufts University
Tulane University
U. Catolica de Valparaiso
University College London
Universidade Federal de Pernambuco (Brazil)
Universidade Federal do Rio de Janeiro (Brazil)
Universitat GHS Essen
University of Abertay Dundee (UK)
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University of California Los Angeles
University of Colorado

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University of Erlangen (Germany)
University of Ferrara
University of Florida
University of Kent at Canterbury (UK)
University of Houston
University of Illinois-Urbana/Champaign
University of Indiana
University of Leeds
University of Liverpool
University of Maryland
University of Massachusetts Amherst
University of New Mexico
University of Maryland College Park
University of Maryland Baltimore Country
University of Michigan
University of Minnesota
University of Modena (Italy)
University of Pittsburgh
University of Sherbrooke (Canada)
University of South Carolina
University of Southern Denmark
University of Strathclyde (Scotland)
University of Tech. Belfort-Montbeliard (France)
University of Tennessee
University of Texas at Arlington
Univ. of Texas, MD Anderson Cancer Ctr.
University of Tokyo (Japan)
University of Torino (Italy)
University of Toronto (Canada)
University of Warwick (United Kingdom)
University of Washington
University of Waterloo (Canada)
University of Western Australia
University of Windsor (Canada)
University of Wisconsin - Madison
University of Wisconsin - Milwaukee
Virginia Polytechnic Institute and State Univ.
Wake Forest University
Washington University (St. Louis)
Wentworth Institute of Technology
Williams College

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 all appointments held during FY 2006.

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

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Marc Olano, F

Glossary of Acronyms

ACL	Association for Computational Linguistics
ACM	Association for Computing Machinery
ACS	Advanced Camera for Surveys
ADI	alternating direction implicit
AFM	atomic force microscope
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
BMC	BioMed Central
BO	Born-Oppenheimer
CEM	computational electromagnetics
CIO	NIST Chief Information Officer
CODATA	Committee on Data for Science and technology
COLING	International Committee on Computational Linguistics
CPU	central processing unit
CSS	Calderbank-Shor-Steane
CSTL	NIST Chemical Science and Technology Laboratory
CWI	Centrum voor Wiskunde en Informatica (Amsterdam)
DARPA	DOD Defense Advanced Research Projects Agency
DIVERSE	Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (visualization software)
DLMF	Digital Library of Mathematical Functions (MCSD project)
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOJ	U.S. Department of Justice
DPD	dissipative particle dynamics
DSO	distributed shared object
EEEL	NIST Electronics and Electrical Engineering Laboratory
FEM	finite element method
FFT	fast Fourier transform
FY	fiscal year
GAMS	Guide to Available Mathematical Software
GPU	Graphics processing unit
IDA	Institute for Defense Analysis
IEEE	Institute of Electronics and Electrical Engineers
IML++	Iterative Methods Library
IMPI	Interoperable Message Passing Interface
IT	information technology
ITL	NIST Information Technology Laboratory
IV	immersive visualization
IVE	immersive visualization environment
IFIP	International Federation for Information Processing
JAMA	Java Matrix package
LADAR	laser detection and ranging
MALDI-TOF	matrix-assisted laser desorption/ionization time-of-flight
MCSD	ITL Mathematical and Computational Sciences Division
MEL	NIST Manufacturing Engineering Laboratory
MIT	Massachusetts Institute of Technology
MKM	mathematical knowledge management
MPI	Message Passing Interface
MRI	magnetic resonance imaging

MSEL	NIST Materials Science and Engineering Laboratory
MV++	Matrix/Vector Library
μCT	x-ray micro-computed tomography
μmag	Micromagnetics Activity Group
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NISTIR	NIST Internal Report
NITRD	Networking and Information Technology Research and Development
NASA	National Aeronautics and Space Administration
NOAA	National Oceanographic and Atmospheric Administration
NNSA	National Nuclear Security Administration
NRC	National Research Council
NSA	National Security Agency
NSF	National Science Foundation
OCT	optical coherence tomography
ODE	ordinary differential equation
OLES	NIST Office of Law Enforcement Standards
OOF	Object-Oriented Finite Elements (software package)
OOMMF	Object-Oriented Micromagnetic Modeling Framework (software package)
PDE	partial differential equation
PET	positron emission tomography
PHAML	Parallel Hierarchical Adaptive Multi Level (software)
PITAC	President's Information Technology Advisory Committee
PL	NIST Physics Laboratory
PSF	point spread function
QDPD	quarternion-based dissipative particle dynamics
RAVE	Reconfigurable Automatic Virtual Environment
S&E	science and engineering
SAVG	MCSD Scientific Applications and Visualization Group
SECB	slow evolution from the continuation boundary
SED	NIST/ITL Statistical Engineering Division
SEM	scanning electron microscope
SIAM	Society for Industrial and Applied Mathematics
SIGGRAPH	ACM Special Interest Group on Graphics
SIMA	NIAT Systems Integration for Manufacturing Applications Program
SOR	successive overrelaxation
SPIE	International Society for Optical Engineering
SRM	standard reference material
SSS	Screen Saver Science
SURF	Student Undergraduate Research Fellowship
TNT	Template Numerical Toolkit
UMCP	University of Maryland College Park
VCCTL	Virtual Cement and Concrete Testing Laboratory
VRML	virtual reality modeling language
W3C	World Wide Web Consortium
XML	Extensible Markup Language